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Hadron physics and chiral symmetry under extreme conditions

Física hadrónica y simetría quiral en condiciones extremas

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Publications

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- A. Gómez Nicola, J. Ruiz de Elvira, and A. Vioque-Rodríguez. "The QCD topological charge and its thermal dependence: the role of the η' ." *Journal of High Energy Physics* **11** (2019), 086.
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- A. Gómez Nicola and A. Vioque-Rodríguez. "Effective Lagrangian at nonzero isospin chemical potential." *Physical Review D* **106** (2022) no.11, 114017.
- A. Gómez Nicola, J. Ruiz de Elvira and A. Vioque-Rodríguez. "The pion-kaon scattering amplitude and the $K^0(700)$ and $K^*(892)$ resonances at finite temperature." *Journal of High Energy Physics* **08** (2023), 148.
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- A. Gómez Nicola, J. Ruiz de Elvira, S. Ferreres-Solé and A. Vioque-Rodríguez. "Recent advances on chiral partners and patterns and the thermal $f_0(500)$ in chiral restoration." PoS Hadron2017 (2018), 204.
- A. Gómez Nicola, J. Ruiz de Elvira, A. Vioque-Rodríguez and S. Ferreres-Solé. "Chiral and $U(1)_A$ restoration: Ward Identities and effective theories." PoS Confinement2018 (2019), 153.
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- A. Gómez Nicola, J. Ruiz de Elvira and A. Vioque-Rodríguez. "Patterns and Partners Within the QCD Phase Diagram Including Strangeness." Springer Proc.Phys. 250 (2020), 389-394.
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Abstract

In this thesis, we will study several problems related to the Physics of Hadrons in extreme conditions of temperature and chemical potentials, with direct applications to relevant aspects of the phase diagram of QCD such as the interplay between chiral and $U(1)_A$ symmetries and its relation with the nature of the quiral transition, chiral partners, the scalar susceptibility peak, which is closely related to the role of thermal resonances, the topological susceptibility, etc. The analysis will be carried out by investigating several theoretical approaches based on effective theories which will allow us to describe the physics below the transition. We will be particularly interested in observables related to chiral symmetry restoration for which the lightest degrees of freedom provide the dominant effect.

The aim of chapter 1 is to provide the essential techniques required to understand the research presented in the following chapters. First, we will present the main features of the spectrum of light hadrons, along with the classification tools that are used in particle physics, as well as the pattern of chiral symmetry breaking in QCD. Subsequently, I will outline the theoretical foundations on which Chiral Perturbation Theory (ChPT) is based, and then I will introduce two fundamental topics that comprise this thesis, namely the Thermal Field Theory and the meson scattering amplitude.

In chapter 2 we show that the thermal $\sigma/f_0(500)$ state, plays an essential role for the description of the scalar susceptibility χ_S , signaling chiral symmetry restoration. First, we use the $O(4)$ Linear Sigma Model as a testbed to derive the connection between χ_S and the σ propagator and to check the validity and reliability of the approach where χ_S is saturated by the $\sigma/f_0(500)$ inverse self-energy, which we calculate at finite T to one loop. A more accurate phenomenological description is achieved by considering

the saturation approach as given by the thermal $f_0(500)$ state generated in Unitarized Chiral Perturbation Theory (UChPT). Such approach allows to describe fairly well recent lattice data. Finally, we compare the saturated description with one based on the Hadron Resonance Gas. Several fits to lattice data are performed, which confirm the validity of the thermal $f_0(500)$ saturated approach and hence the importance of that thermal state for chiral symmetry restoration.

In chapter 3 we show that the scalar susceptibility χ_S^κ develops a maximum above the QCD chiral transition, after which it degenerates with χ_P^K . This result provides an alternative sign for $O(4) \times U(1)_A$ restoration that can be explored in lattice simulations and highlights the role of strangeness, which regulated by the strange-quark condensate helps to reconcile the current tension among lattice results regarding $U(1)_A$ restoration. We show that the peak structure of χ_S^κ can be described when it is saturated with the $K_0^*(700)$ (or κ) meson, the dominant lowest-energy state in the isospin 1/2 scalar channel, which in turn can be computed in UChPT at finite temperature. This reveals the importance of thermal interactions and makes it possible to examine the χ_S^κ dependence on the light- and strange-quark masses. A consistent picture emerges controlled by the m_l/m_s ratio that allows studying the behavior of the $O(4) \times U(1)_A$ transition in the chiral and $SU(3)$ limits.

In chapter 4 we analyze the finite temperature pion-kaon scattering amplitude in ChPT, paying particular attention to the analytic structure of the amplitude and the main differences with respect to the zero temperature case. We also extend the Inverse Amplitude Method at finite temperature for unequal-mass scattering processes, which allows us to unitarize the amplitude and obtain the thermal evolution of the $K_0^*(700)$ and $K^*(892)$ pole parameters. As a direct application of our analysis, we show that the thermal evolution of the $K_0^*(700)$ resonance is crucial to explain the behavior of the scalar susceptibility for isospin $I = 1/2$.

In chapter 5 we will discuss some recent results within the chiral lagrangian framework related to the topological susceptibility and the fourth-order cumulant of the vacuum energy density. We perform our study within $U(3)$ ChPT up to next-to-next-to-leading order in the combined chiral and large- N_c expansion. We also describe the temperature dependence of these two quantities and compare them with previous analyses in the literature. In particular, we discuss the validity of the thermal scaling of the topological susceptibility with the quark condensate, which is intimately connected with a Ward Identity relating both quantities. We also consider isospin breaking corrections

from the vacuum misalignment at leading order in the $U(3)$ framework.

Finally, in chapter 6 we construct the most general low-energy effective lagrangian within ChPT at nonzero chemical potential. For that purpose, we work following the external source method, up to $\mathcal{O}(p^4)$ order in the chiral expansion for two light flavours. First, in section 6.2, we include local parity violating terms parametrized by an axial chemical potential μ_5 and we analyze the corrections to the pion dispersion relation and observables related to the vacuum energy density. In particular, we explore the dependence of the chiral restoration temperature T_c with μ_5 . An increasing $T_c(\mu_5)$ is consistent with our fits to lattice data of the ChPT-based expressions. Although lattice uncertainties are still large and translate into the new LEC determination, a consistent physical description of the those observables emerges from our present work, providing a theoretically robust model-independent framework for further study of physical systems where parity-breaking effects may be relevant, such as heavy-ion collisions. The same procedure is followed to incorporate isospin chemical potential μ_I (section 6.3). In addition to the contributions already considered in the literature, we discuss the effects of new terms allowed by the symmetries, as well as linear-field corrections relevant to fourth order. We study the influence of those new contributions to the energy density at zero temperature and observables derived from it, such as the pion and quark condensates and the isospin density. Corrections are shown to be compatible with lattice results, which favor nonzero values for the low-energy constants multiplying the new $\mathcal{O}(p^2)$ and $\mathcal{O}(p^4)$ field operators in the lagrangian.

Resumen

En esta tesis estudiaremos varios problemas relacionados con la Física de Hadrones en condiciones extremas de temperatura y potenciales químicos, con aplicaciones directas a aspectos relevantes del diagrama de fases de la QCD tales como la interacción entre las simetrías quirales y $U(1)_A$, los compañeros quirales, el pico de la susceptibilidad escalar, estrechamente relacionado con el papel de las resonancias térmicas, la susceptibilidad topológica, etc. El análisis se llevará a cabo investigando varios enfoques teóricos basados en teorías efectivas las cuales nos permitirán describir la física por debajo de la transición. Nos interesarán especialmente los observables relacionados con la restauración de la simetría quiral, para la que los grados de libertad más ligeros proporcionan el efecto dominante.

El capítulo 1 proporcionamos las técnicas esenciales para comprender la investigación posterior, abordando el espectro de hadrones ligeros, la clasificación de partículas, el patrón de ruptura de la simetría quiral en QCD, la Teoría de Perturbaciones Quiral (ChPT), la Teoría Cuántica de Campos a temperatura finita y la amplitud de dispersión de mesones.

En el capítulo 2 mostramos que el estado térmico $\sigma/f_0(500)$ juega un papel esencial para la descripción de la susceptibilidad escalar χ_S , señalando la restauración de la simetría quiral. En primer lugar, utilizamos el Modelo Sigma Lineal como test para derivar la conexión entre χ_S y el propagador de la σ y así comprobar la validez y fiabilidad de la aproximación en la que χ_S está saturada por la inversa de la autoenergía de la $\sigma/f_0(500)$, que calculamos a temperatura finita a un loop. Se consigue una descripción fenomenológica más precisa considerando la aproximación en la que la susceptibilidad es saturada por el estado térmico $f_0(500)$ generado en la Teoría de Per-

turbaciones Quiral Unitarizada (UChPT). Este enfoque permite describir bastante bien los datos obtenidos recientemente a partir de cálculos en el retículo. Finalmente, hemos comparado la descripción saturada con una basada en un Gas de Resonancias Hadrónicas y se han realizado varios ajustes a datos del retículo, que confirman la validez de la aproximación basada en la saturación de la susceptibilidad y la importancia de ese estado en la restauración de la simetría quiral.

En el capítulo 3 mostramos que la susceptibilidad escalar χ_S^κ presenta un máximo por encima de la transición quiral, tras lo cual degenera con χ_P^K . Este resultado proporciona una señal alternativa de la restauración $O(4) \times U(1)_A$ que puede explorarse en simulaciones del retículo y destaca el papel de la extrañeza, que regulada por el condensado de quarks extraños ayuda a reconciliar la tensión actual entre los resultados del retículo respecto a la restauración $U(1)_A$. El pico de χ_S^κ puede describirse saturando la susceptibilidad con la masa térmica del mesón $K_0^*(700)$ que a su vez puede calcularse en UChPT a temperatura finita. Esto revela la importancia de las interacciones térmicas y permite examinar la dependencia de χ_S^κ con respecto a las masas de los quarks ligeros y extraños.

En el capítulo 4 analizamos la amplitud del proceso de dispersión pión-kaón a temperatura finita haciendo uso de ChPT, prestando especial atención a la estructura analítica de la amplitud y a las principales diferencias con respecto al caso de temperatura cero. También extendemos el Método de Amplitud Inversa a temperatura finita para procesos de dispersión con masas diferentes, lo que nos permite unitarizar la amplitud y obtener la evolución térmica de los parámetros de la $K_0^*(700)$ y la $K^*(892)$. Como aplicación directa de nuestro análisis, mostramos que la evolución térmica de la resonancia $K_0^*(700)$ es crucial para explicar el comportamiento de la susceptibilidad escalar para isospin $I = 1/2$.

En el capítulo 5 discutiremos algunos resultados recientes relacionados con la susceptibilidad topológica y el cumulante de cuarto orden de la densidad de energía del vacío. Llevamos a cabo nuestro estudio dentro de $U(3)$ ChPT hasta NNLO combinando la expansión quiral y de gran- N_c . También describimos la dependencia de la temperatura de estas dos magnitudes y las comparamos con análisis previos en la literatura. En particular, discutimos la validez de la dependencia térmica de la susceptibilidad topológica con el condensado de quarks. Estas cantidades están íntimamente relacionadas a través de una identidad de Ward. También consideramos correcciones de ruptura de isospín a LO en el marco $U(3)$.

Finalmente, en el capítulo 6 construimos el lagrangiano efectivo de baja energía más general dentro de ChPT a potencial químico distinto de cero. Para ello, trabajamos haciendo uso del método de las fuentes externas, hasta el orden $\mathcal{O}(p^4)$ en la expansión quiral para dos sabores ligeros. Primero, en la sección 6.2, incluimos términos que violan localmente la paridad parametrizados por un potencial químico axial μ_5 . Analizamos las correcciones de μ_5 a varios observables. En particular, exploramos la dependencia con μ_5 de la temperatura a la que se produce la restauración quiral. Nuestros ajustes a los datos del retículo de las expresiones basadas en ChPT son compatibles con un aumento de $T_c(\mu_5)$. Aunque debido a que las incertidumbres del retículo siguen siendo grandes y se han obtenido unos errores bastante grandes para las nuevas LECs se proporciona un marco robusto e independiente teóricamente para estudios posteriores de sistemas físicos en los que los efectos de ruptura de paridad pueden ser relevantes, como las colisiones de iones pesados. Se sigue el mismo procedimiento para incorporar el potencial químico de isospín μ_I (sección 6.3). Además de las contribuciones ya consideradas en la literatura, discutimos los efectos de nuevos términos permitidos por las simetrías, así como correcciones de lineales en el campo relevantes hasta el cuarto orden. Estudiamos la influencia de esas nuevas contribuciones en la densidad de energía a temperatura cero y en los observables derivados de ella, como los condensados de piones y quarks y la densidad de isospín. Se demuestra que las correcciones son compatibles con los resultados del retículo, los cuales favorecen valores distintos de cero para las constantes de baja energía que multiplican los nuevos operadores $\mathcal{O}(p^2)$ y $\mathcal{O}(p^4)$ del lagrangiano.

General formalism

1.1 QCD and chiral symmetry

The Standard Model of Particle Physics is a theory that explains the fundamental interactions among particles in the universe. It describes three of the four known fundamental forces of nature: electromagnetic, weak, and strong interactions. Particles are classified into two types based on their spin: fermions, which have half-integer spin, and bosons, which have whole-integer spin. The elementary blocks of the three interactions mentioned consist of two types of fermions: quarks and leptons. They are distinguished by their interaction with the strong force. Quarks feel the strong interaction, while leptons do not. The strong interaction is described by Quantum Chromodynamics (QCD).

1.1.1 QCD phase diagram

In the study of the thermodynamic properties of a classical system, a phase is defined as a state of matter where the macroscopic physical properties of a substance are uniform on a macroscopic scale. It is characterized by a thermodynamic function that depends on macroscopic parameters such as temperature and pressure. A phase transition corresponds to a drastic change (i.e., non-smooth behavior) in the properties of a system when one of its parameters, such as temperature, is varied.

Phase transitions frequently involve the emergence of a symmetry breaking. To describe the evolution of a phase transition, an order parameter is used, which describes the broken symmetry. The order parameter undergoes a significant change or exhibits a non-zero value as the system goes through a phase transition. One of the best-known

examples of a phase transition is that of a ferromagnet. For ferromagnetic materials, the order parameter is the magnetization, which is obtained by averaging all the magnetic moments of the atoms. There is a temperature, the Curie temperature, at which a ferromagnetic material transitions to a paramagnetic state. Above this temperature, there is no spontaneous magnetization, which means that the magnetic moments become disordered. For temperatures below this critical value, the magnetic moments of the atoms are aligned, and the system is invariant under a rotation around an axis aligned with the magnetization. However, as the temperature increases above this critical value, the system becomes invariant under any rotation, thus recovering the symmetry.

The order of a phase transition is one of the basic thermodynamic classifications. Paul Ehrenfest classified phase transitions based on the behavior of the thermodynamic free energy as a function of other thermodynamic variables [1]. Phase transitions were labeled by the lowest derivative of the free energy that is discontinuous at the transition. There are two principal types of phase transitions. First order transitions are characterized by a jump in the first derivative of the free energy. A second order transition shows a divergence in the second derivative of the free energy, although all thermodynamic functions are continuous. Another important type of transition that will be significant throughout this thesis is the analytic crossover transition. In this case, free energy and all its derivative are continuous at critical temperature and system changes smoothly from one phase to other.

The QCD phase diagram represents the different states of QCD matter as a function of temperature and baryon chemical potential. Under normal conditions, strongly interacting matter exists in the hadronic phase. However, under certain extreme conditions of temperature and density, the transition to other phases can occur.

These characteristics of QCD allow for the distinction of two phases: a hadronic phase with confined quarks and gluons, with broken chiral symmetry, and another phase, deconfined and with restored chiral symmetry, generally referred to as quark-gluon plasma (QGP) [2,3]. Examples of QGP could be found in the matter that makes up the interior of compact objects such as neutron stars (region of high densities and low temperatures) [4], or during the early moments of the Universe's expansion. Moreover, according to theoretical calculations performed in the regime of asymptotically high densities, there might be a family of phases called color superconductors [5]. In Figure 1.1, a schematic view of the QCD phase diagram can be observed.

The QGP phase could be reached at high temperatures and densities, conditions

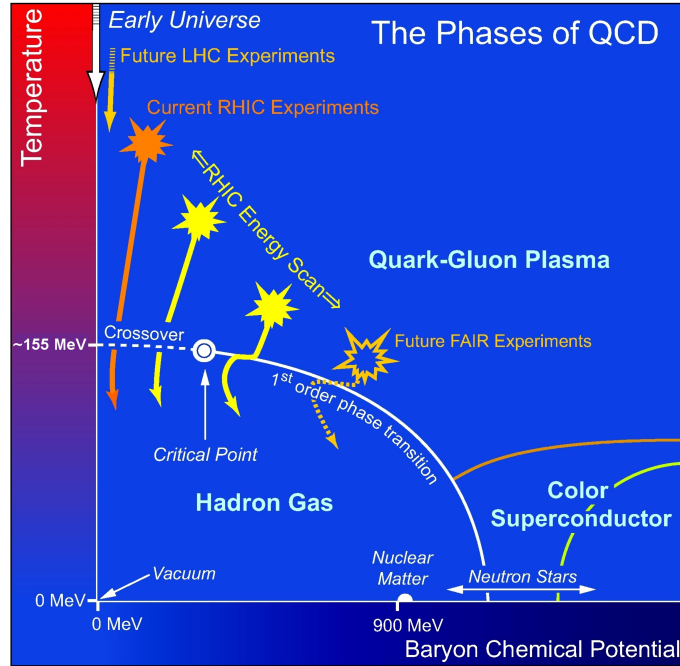


Figure 1.1: QCD phase diagram [6].

that are reachable in heavy-ion collisions (HICs). When conducting a heavy ion collision experiment, heavy nuclei are accelerated to ultra-relativistic speeds before their collision. Upon impact, the highly accelerated nuclei give rise to a strongly interacting medium characterized by extremely high temperatures of the order of several hundreds of MeV. In recent years, the construction of several heavy-ion accelerators has been carried out, where experiments are conducted to reach high temperatures in order to study the corresponding phases of the QCD phase diagram. Among these are the Nuclotron-based Ion Collider Facility (NICA), the Facility for Antiproton and Ion Research (FAIR) and the Relativistic Heavy Ion Collider (RHIC). In particular, the Beam Energy Scan (BES) is a program at the RHIC where very useful information is extracted from the experimental analysis of the evolution of particle yields and their ratios as the energy of the collision is varied [7, 8].

To study the phase structure of QCD and the deconfinement phenomenon, it is necessary to consider the low-energy range. Moreover, as we will see, a non-perturbative method is needed to understand QCD in that regime. The most systematic computational approach to calculate the strong interactions of QCD is known as Lattice QCD [9]. It is a numerical tool, in which the space-time is discretized, used to calculate non-perturbative hadronic processes in particle physics. An alternative to this technique is to use effective models that incorporate the symmetries of the theory. The formalism

of effective theories is also systematic and is the one that will be used primarily in this thesis.

1.1.2 The Quark Model

In 1932 Werner Heisenberg introduced the isotopic spin or isospin to explain the similarity between proton and neutron particles [10]. Because proton and neutron masses are almost identical, the difference between them lies in their charges. The proton has a positive charge, while the neutron is neutral. Due to this, Heisenberg proposed that the proton and neutron might really be two states of the same particle, now called the nucleon. As a consequence, there is an approximate $SU(2)$ symmetry and the proton and neutron form a doublet of $SU(2)$. In analogy with the two possible spin states of a spin $1/2$ particle, the new quantum number associated with the $SU(2)$ symmetry mentioned was called isospin (I). Later, Gell-Mann extended the concept of the isospin multiplets introduced by W. Heisenberg. In this way, the pions form an isospin triplet (π^- , π^0 , π^+) with $I = 1$.

During the 50's and 60's hundreds of strongly interacting particles were discovered. It was observed that some of these particles, such as the Lambda (Λ), Sigma (Σ) and Kaons (K), decayed rather slowly. Moreover, these particles seemed to be always produced in pairs. Murray Gell-Mann and K.Nishijima explained this associate production by introducing a new quantum number called strangeness (S), which is conserved during strong interactions. The idea is that the total strangeness of the interacting particles (summing the strangeness of all of them) must be the same before and after the reaction. An important result is given by the Gell-Mann-Nishijima formula $Q = I_3 + (B + S)/2$, which says that the strangeness of the strongly interacting hadrons is connected with the electric charge (Q), the baryon number (B) and the third component of the $SU(2)$ isospin (I_3).

In the early sixties, Gell-Mann and Yuval Ne'eman described a particle classification scheme analogous to the periodic table of elements for hadronic physics. It was called the Eightfold Way [11–13]. They realized that many of the known particle could be fitted into a series of families based on the $SU(3)$ group. In this way, the known hadrons (mesons and baryons) were classified as a function of their quantum numbers: the isospin and the strangeness or hypercharge ($Y = S + B$).

In 1964 Gell-Mann and Zweig [14, 15] independently suggested that hadrons are not really elementary particles and proposed the existence of three types of elemen-

	Light (MeV)			Heavy (GeV)		
Flavour (q)	u (up)	d (down)	s (strange)	c (charm)	b (bottom)	t (top)
Mass (m_q)	$2.16^{+0.49}_{-0.26}$	$4.67^{+0.48}_{-0.17}$	$93.4^{+8.6}_{-3.4}$	1.27 ± 0.02	$4.18^{+0.03}_{-0.02}$	172.69 ± 0.30

Table 1.1: Values for the quark masses taken from the Particle Data Group (PDG) [17] with the mass definitions provided there.

tary fermions, which Gell-Mann named quarks, in terms of which all hadrons could be constructed. To explain the electric charges and quantum numbers of hadrons, these quarks now commonly designated as up, down, and strange, are characterized by fractional electric charges ($+2/3e$ for the up quark and $-1/3e$ for down and strange quarks). Later on, three more kinds of quarks were discovered, which were called charm, bottom and top (observed between 1974 and 1995). The last three are considered heavy and do not play a relevant role in the energy range that will be studied throughout this thesis. Their contributions can be decoupled [16] when examining the low-energy mesonic sector. As shown in Table 1.1, the mass difference between light and heavy flavours is large ($> 1 \text{ GeV}$). Hence, an approximate symmetry is expected only in the space of the three light flavors. This symmetry will be more exact in the case of the two lightest flavors since the strange quark is considerably heavier than quarks u and d .

The only way to obtain representations of $SU(3)$ from more fundamental representations is to build tensor products of smaller representations. Thus, quarks are transformed as members of the fundamental representation 3 of $SU(3)$, while antiquarks are in the conjugate representation $\bar{3}$ (see Figure 1.2).

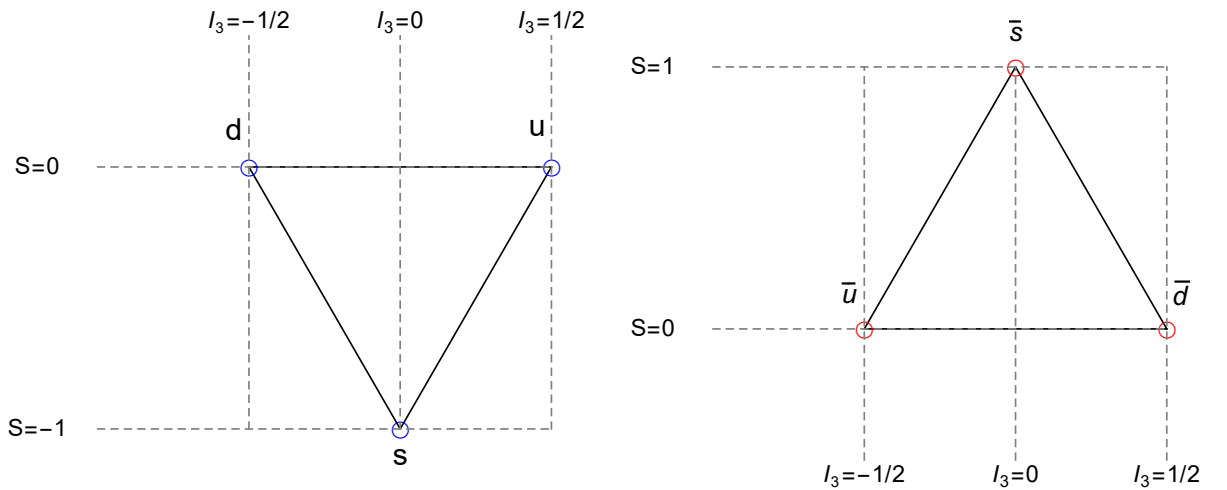


Figure 1.2: The 3 and $\bar{3}$ representation of $SU(3)$ corresponding to quarks and anti-quarks.

Therefore, different $SU(3)$ representations can be used to order hadrons. Gell-

Mann's model offered a simple picture where all mesons are shown as consisting of a quark and an antiquark, while all baryons are composed of three quarks. Thus, mesons and baryons correspond to irreducible representations coming from the products

$$3 \otimes \bar{3} = 1 \oplus 8 \qquad 3 \otimes 3 \otimes 3 = 1 \oplus 8 \oplus 8 \oplus 10 \qquad (1.1)$$

In other words, the combination of a quark and an anti-quark results in an octet and a singlet (meson nonet) and the three quarks construction then involves a singlet, a decuplet and two octets.

According to the Pauli Exclusion Principle, it is impossible for one particle to contain all quarks with the same quantum numbers. However, there exist baryons composed of three strange quarks (Ω) and three up quarks (Δ^{++}), which seemed to violate it. Because of this contradiction, Han and Nambu, Greenberg, and Gell-Mann proposed that quarks must have an additional quantum number: the colour. Each quark appears in three different colours, which are known as red, green and blue. This gave rise to the $SU(3)$ colour gauge symmetry. In this way, QCD emerges as the gauge field theory that describes the strong interactions of colored quarks mediated by gluons.

QCD implements two fundamental properties: confinement and asymptotic freedom. Because of the asymptotic freedom, quark interactions become weaker when the energy scale increases (or equivalently, at short distances). Hence the strong interactions can be perturbatively studied in a systematic way at high energies and short distances. On the contrary, at low energies, quark and gluons interact strongly and are confined in hadrons. This explains that they have not been observed in nature as free particles. Both of these phenomena are related to the nonabelian structure of QCD.

In 1973 Gross, Wilczek and Politzer [18–21] demonstrated that Yang–Mills theories are indeed asymptotically free. For this, they derived the expression of the QCD coupling constant perturbatively to one loop

$$\alpha_s(\mu) = \frac{g^2(\mu)}{4\pi} = \frac{12\pi}{(11N_c - 2N_f) \log\left(\frac{\mu^2}{\Lambda_{QCD}^2}\right)} \qquad (1.2)$$

where μ corresponds to the energy at which the theory is applied, and Λ_{QCD} is the scale of QCD. From the above equation, it is clear that, for $N_c = 3$ and $N_f \leq 16$, α_s tends to zero at the energies much above Λ_{QCD} (asymptotic freedom) and increases with decreasing energy (confinement). In this way, perturbation is not possible when $\mu \sim \Lambda_{QCD}$.

At low energies, Effective field theories are the appropriate theoretical tool to describe the low energy regime. In section 1.2, we briefly review some aspects of an Effective Field Theory called Chiral Perturbation Theory, where the pseudoscalar mesons are assumed to be the fundamental degrees of freedom in the Lagrangian.

1.1.3 Hadrons

As we have already seen, mesons are constituted by a quark-antiquark state ($q\bar{q}$). They are classified into J^{PC} multiplets. Let us start with parity, P . The parity operator, $\hat{P}$, performs spatial inversion through the origin and if the wave functions are eigenstates of the parity operator, then P represents intrinsic parity of a particle/antiparticle

$$\hat{P}\phi(\vec{r}, t) = \phi(-\vec{r}, t) = P\phi(\vec{r}, t) \quad (1.3)$$

The original state is restored by applying parity twice, so $P = \pm 1$. For a multiparticle state ϕ_{a+b} with an orbital angular momentum l , the result of a parity transformation is

$$\hat{P}\phi_{a+b} = P_a P_b (-1)^l \phi_{a+b} \quad (1.4)$$

where P_a and P_b are the intrinsic parities of the individual particles a and b . In our case, because fermions and antifermions have opposite intrinsic parity, the parity of the $q\bar{q}$ composite system is $P(q\bar{q}) = (-1)^{l+1}$.

On the other hand, q and $\bar{q}$ both have spin $\frac{1}{2}$. These can combine to give a total spin s for the $q\bar{q}$ pair of 0 (pseudoscalar mesons) or 1 (vector mesons). The possible spin states are

$$s = 0 : \frac{1}{\sqrt{2}} (|\frac{1}{2}, \frac{1}{2}\rangle |\frac{1}{2}, -\frac{1}{2}\rangle - |\frac{1}{2}, -\frac{1}{2}\rangle |\frac{1}{2}, \frac{1}{2}\rangle), \quad s = 1 : \begin{aligned} & |\frac{1}{2}, \frac{1}{2}\rangle |\frac{1}{2}, \frac{1}{2}\rangle \\ & \frac{1}{\sqrt{2}} (|\frac{1}{2}, \frac{1}{2}\rangle |\frac{1}{2}, -\frac{1}{2}\rangle + |\frac{1}{2}, -\frac{1}{2}\rangle |\frac{1}{2}, \frac{1}{2}\rangle) \\ & |\frac{1}{2}, -\frac{1}{2}\rangle |\frac{1}{2}, -\frac{1}{2}\rangle \end{aligned} \quad (1.5)$$

Note that the $s = 0$ state is antisymmetric with respect to the exchange of the two particles while the $s = 1$ states are symmetric. A state with a definite value of l and s is formed from the product $q\bar{q}$. Then, l and s can be combined to get the total angular momentum $J = l \oplus s$, where J is given by the relation $|l - s| \leq J \leq l + s$.

The charge conjugation represents a transformation of the particle into its antiparticle. It reverses the sign of the electric charge, colour charge and magnetic moment of a particle. The effect of the charge conjugation operator $\hat{C}$ upon a state ϕ_a is

$$\hat{C}\phi_a = C\phi_{\bar{a}}, \quad C = \pm 1 \quad (1.6)$$

where we have denoted a particle by the letter a and its corresponding antiparticle by $\bar{a}$. Unlike parity, only particles that are their own antiparticles (neutral states) are $\hat{C}$ eigenstates. For a state of definite l , the interchange between a particle and its antiparticle reverses their relative position vector and therefore it leads to a factor $(-1)^{l+1}$ for the charge conjugation of the system. In addition to this, $\hat{C}$ also flips the spin wave functions which introduces a factor $(-1)^{s+1}$. The combination of both effects leads to $C(q\bar{q}) = (-1)^{l+s}$.

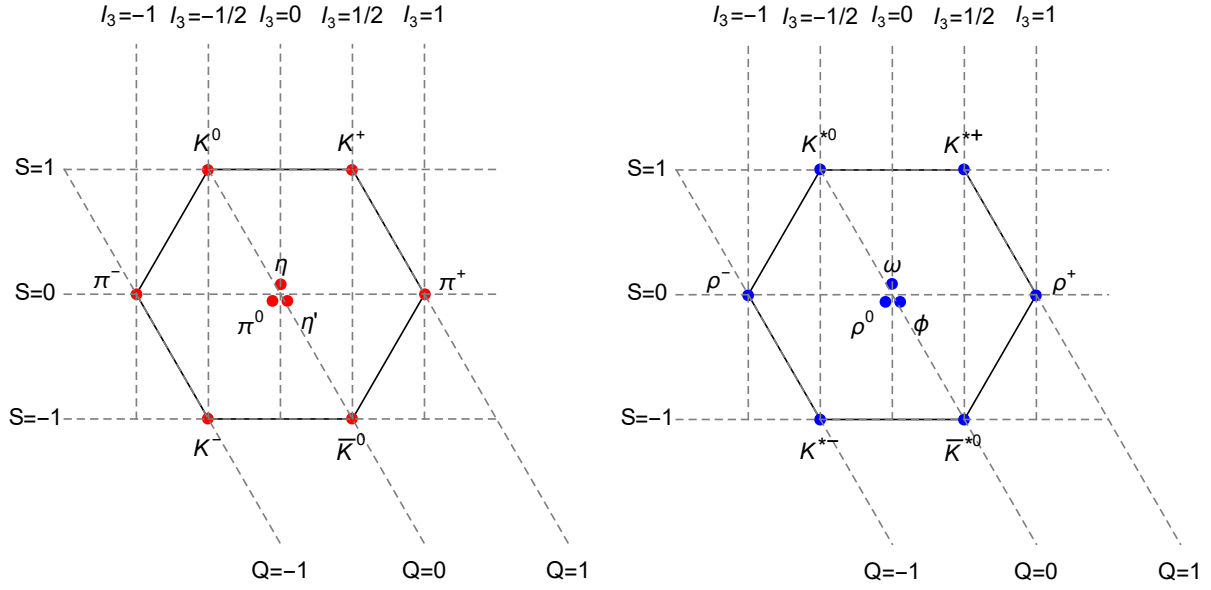


Figure 1.3: Nonet of pseudoscalar (left) and vector (right) mesons.

There exist nine possible $q\bar{q}$ combinations with the same J^{PC} . The multiplet classification provides a reasonable description of the pseudoscalar (0^{-+}) and vector (1^{--}) mesons, which are depicted in fig. 1.3.

Time reversal, denoted T , is a transformation $T\phi(\vec{r}, t) = \phi(\vec{r}, -t)$, which corresponds to changing the sign of time $t \rightarrow -t$. The idea is that if a system is invariant under T , we would not be able to discern the chronological direction of a physical event. In other words, given the reaction $1 + 2 \rightarrow 3 + 4$, the inverse process $3 + 4 \rightarrow 1 + 2$ occurs at the same rate.

P , C and T are symmetries of strong interactions and the combination of these, known as CPT , is a symmetry observed in all known interactions. In addition, the strong interaction of hadrons is governed by another symmetry: chiral symmetry. It plays a fundamental role in low-energy hadronic processes.

1.1.4 The QCD Lagrangian and Chiral symmetry

In this thesis we are interested in the study of QCD low energy dynamics, so we restrict the QCD Lagrangian to the lightest $N_f = 3$ flavours. Then, the fermionic part of the QCD Lagrangian is

$$\mathcal{L}_{QCD} = \bar{q} (i\not{D} - \mathcal{M}) q, \quad D_\mu = \partial_\mu - i g G_\mu^a \frac{\lambda^a}{2}, \quad q = \begin{pmatrix} u \\ d \\ s \end{pmatrix}, \quad (1.7)$$

where u , d and s are color triplets, $\mathcal{M}$ is the quark mass matrix given by $\mathcal{M} = \text{diag}(m_u, m_d, m_s)$ with m_q the masses of the up, down and strange quarks and D_μ is the covariant derivative which includes the Gell-Mann matrices (λ^a) , the gluon fields (G_μ^a) and the strong interaction coupling constant (g) .

In order to simplify the analysis, the left- and right- handed projections of the quark fields are introduced. These are given by

$$q_R = P_R q = \frac{1}{2} (1 + \gamma_5) q, \quad q_L = P_L q = \frac{1}{2} (1 - \gamma_5) q, \quad (1.8)$$

being $P_{R,L}$ projection operators, so they satisfy

$$P_L + P_R = 1; \quad P_L P_L = P_L; \quad P_R P_R = P_R; \quad P_L P_R = P_R P_L = 0 \quad (1.9)$$

Because of $\{\gamma_\mu, \gamma_5\} = 0$, the QCD Lagrangian in the chiral limit can be decoupled into the following sum

$$\mathcal{L}_{QCD}^{\mathcal{M}=0} = \bar{q}_R (i\not{D}) q_R + \bar{q}_L (i\not{D}) q_L. \quad (1.10)$$

In this limit, due to the left- and right-handed fields are not mixed, the Lagrangian is invariant under chiral transformations

$$q_R \rightarrow \underbrace{e^{-i\alpha_R^a \lambda^a / 2}}_{g_R} q_R, \quad q_L \rightarrow \underbrace{e^{-i\alpha_L^a \lambda^a / 2}}_{g_L} q_L, \quad (1.11)$$

where $\alpha_{R,L}^a$ are the angles characterizing the transformations. Thus, the Lagrangian is also invariant under the chiral group $SU(3)_R \times SU(3)_L$. Using the Noether theorem, one obtains the conserved currents associated with the chiral group:

$$(J_R)_\mu^a = \bar{q}_R \gamma_\mu \frac{\lambda^a}{2} q_R, \quad (J_L)_\mu^a = \bar{q}_L \gamma_\mu \frac{\lambda^a}{2} q_L, \quad \partial_\mu (J_{R,L})_\mu^a = 0. \quad (1.12)$$

From chiral transformations (1.11), it is possible to define axial and vector transformations

$$\begin{aligned} \alpha_V = \alpha_R = \alpha_L : \quad q &\rightarrow e^{-i\alpha_V^a \lambda^a} q, \\ \alpha_A = -\alpha_R = \alpha_L : \quad q &\rightarrow e^{-i\alpha_A^a \lambda^a \gamma_5} q, \end{aligned} \quad (1.13)$$

whose currents are given by

$$(J_V)_\mu^a = \bar{q}\gamma_\mu \frac{\lambda^a}{2} q, \quad (J_A)_\mu^a = \bar{q}\gamma_\mu \gamma_5 \frac{\lambda^a}{2} q. \quad (1.14)$$

Then, chiral symmetry is equivalent to the invariance under $SU(3)_V \times SU(3)_A$. The Noether charges associated to (1.14) read:

$$Q_V^a = \int d^3x (J_V)_0^a, \quad Q_A^a = \int d^3x (J_A)_0^a. \quad (1.15)$$

Furthermore, the massless Lagrangian is invariant under the global chiral phase transformations $q \rightarrow e^{-i\beta_V} q$ and $q \rightarrow e^{-i\beta_A \gamma_5} q$, so it is also invariant under the global $U(1)_V \times U(1)_A$ group. In this case, the corresponding Noether currents are: $(J_V)_\mu = \bar{q}\gamma_\mu q$ and $(J_A)_\mu = \bar{q}\gamma_\mu \gamma_5 q$. Under parity, the above mentioned currents are transformed as vector and axial quantities, namely

$$\begin{aligned} P: \quad (J_V)_\mu^a(\vec{x}, t) &\rightarrow (J_V)_\mu^a(-\vec{x}, t), \quad (J_V)_\mu(\vec{x}, t) \rightarrow (J_V)_\mu(-\vec{x}, t) \\ P: \quad (J_A)_\mu^a(\vec{x}, t) &\rightarrow -(J_A)_\mu^a(-\vec{x}, t), \quad (J_A)_\mu(\vec{x}, t) \rightarrow -(J_A)_\mu(-\vec{x}, t) \end{aligned} \quad (1.16)$$

Summarizing, the classical Lagrangian in the chiral limit is said to have the following symmetry

$$U(3)_R \times U(3)_L = U(3)_V \times U(3)_A = U(1)_V \times SU(3)_V \times U(1)_A \times SU(3)_A \quad (1.17)$$

Of course, quarks are not massless and it is easy to check that only the invariance under the $U(1)_V$ group survives when the mass term is taken into account for a general quark mass matrix. It is said that quark mass term introduces an explicit chiral symmetry breaking. The vector and axial current divergences have the form:

$$\begin{aligned} \partial^\mu (J_V)_\mu^a &= \frac{i}{2} \bar{q} [\mathcal{M}, \lambda^a] q, & \partial^\mu (J_A)_\mu^a &= \frac{i}{2} \bar{q} \gamma_5 \{ \lambda^a, \mathcal{M} \} q, \\ \partial^\mu (J_V)_\mu &= 0, & \partial^\mu (J_A)_\mu &= 2i \bar{q} \gamma_5 \mathcal{M} q, \end{aligned} \quad (1.18)$$

For equal quark masses, the introduction of the mass term reduces the symmetry as follows

$$U(3)_V \times U(3)_A \rightarrow SU(3)_V \times U(1)_V \quad (1.19)$$

As it is known, the quark strange is much heavier than the quarks up and down and, hence, the $SU(3)_V$ symmetry is explicitly broken. This means that the $SU(2)_V$ group (isospin symmetry) is a better symmetry of Nature, since $m_u \approx m_d$.

1.1.5 Spontaneous Symmetry Breaking

We can notice that the vector transformations mentioned in the previous subsection connect states in the same multiplet without changing parity. However, the axial transformations allow to relate multiplets of opposite parity. When examining the hadron spectrum, we observe that particles appear in isospin multiplets with very similar masses. This similarity in mass can be explained by explicit symmetry breaking, so the vector or isospin transformations are a symmetry of the vacuum state. However, we do not find degenerate isospin multiplets with similar mass and opposite parity (chiral partners). The mass difference between these two multiplets can not be explained by explicit symmetry breaking alone, and therefore, another mechanism is needed. A consistent explanation is that chiral symmetry is spontaneously broken down to the isospin symmetry, meaning that the QCD vacuum state is not invariant under axial transformations. This mechanism is implemented through the Nambu-Goldstone theorem [22–25].

The Nambu-Goldstone theorem notes that if the Lagrangian is invariant under a continuous symmetry group G but the Noether charges associated to this symmetry do not annihilate the ground state (only a subgroup H of G is symmetry of the vacuum), then a massless (and spinless) particle appears in the theory's spectrum for each broken generator. These particles are called Nambu-Goldstone bosons (NGB). From the point of view of the Noether charges, it means that there exists an operator X such as: $\langle 0 | [Q, X] | 0 \rangle \neq 0$ where Q is the charge associated to the conserved current J_0 and $|0\rangle$ is a vacuum state.

In order to demonstrate that, let us assume that there is an operator X that satisfies: $\langle 0 | [Q, X] | 0 \rangle = B \neq 0$, which is only true if $Q|0\rangle \neq 0$. Inserting a complete set of states:

$$\langle 0 | [Q, X] | 0 \rangle = \int d^3x \sum_n [\langle 0 | J_0 | n \rangle \langle n | X | 0 \rangle - \langle 0 | X | n \rangle \langle n | J_0 | 0 \rangle] \quad (1.20)$$

Now, if J_0 and $|0\rangle$ are translationally invariants, which implies $J_0(x) = \mathfrak{T}^{-1}(x) J_0(0) \mathfrak{T}(x)$ and $\mathfrak{T}(x)|0\rangle = |0\rangle$, with $\mathfrak{T}(x) = e^{i\Pi x}$ the translation operator and Π the four-momentum operator

$$B = \sum_n (2\pi)^3 \delta(\vec{p}_n) [\langle 0 | J_0(0) | n \rangle \langle n | X | 0 \rangle e^{-iE_n t} - \langle 0 | X | n \rangle \langle n | J_0(0) | 0 \rangle e^{iE_n t}] \neq 0 \quad (1.21)$$

In addition to this, since the conserved charges are independent of the time coordinate

$$\frac{dB}{dt} = - \sum_n i(2\pi)^3 \delta(\vec{p}_n) E_n [\langle 0 | J_0(0) | n \rangle \langle n | X | 0 \rangle e^{-iE_n t} - \langle 0 | X | n \rangle \langle n | J_0(0) | 0 \rangle e^{iE_n t}] = 0 \quad (1.22)$$

To satisfy (1.22), we need that $\langle 0|X|n\rangle\langle n|J_0(0)|0\rangle$ vanishes except for the states with $\delta(\vec{p}_n)E_n = 0$. However, according to (1.21): $\langle 0|X|n\rangle\langle n|J_0(0)|0\rangle \neq 0$ and, hence, there must exist those massless states ($E_n|_{\vec{p}_n \rightarrow 0} = 0$) so that both conditions can be true at the same time.

The spontaneously symmetry breaking of $G = SU(3)_V \times SU(3)_A$ in $H = SU(3)_V$ produces then eight NGB, one for each broken generator of $SU(3)_A$. Each Q_A^a charge that do not annihilate the ground state, $Q_A^a|0\rangle \neq 0$, corresponds to a Goldstone boson. Under parity, these states act as pseudoscalars because they have the same symmetry properties as the broken generators. The masses of the pseudoscalar mesons ($J^P = 0^-$) are considerably smaller than those of the scalar mesons (0^+). We can identify the light pseudoscalar octet (π , K and η) with the Nambu–Goldstone states. On the other hand, since the quarks are not massless, NGB acquire mass, although their masses are very light compared to the rest of hadron masses. Because of that, they are called pseudo-Nambu-Goldstone bosons.

As it has been mentioned above, $Q_A^a|0\rangle \neq 0$ and therefore $\langle 0|[Q_A^a, X]|0\rangle \neq 0$. The simplest pseudoscalar operator for X is the pseudoscalar density, for which we have

$$\langle 0|[Q_A^a, \bar{q}\gamma_5\lambda^b q]|0\rangle = -\frac{1}{2}\langle 0|\bar{q}\{\lambda^a, \lambda^b\}q|0\rangle = -\frac{2}{3}\delta^{ab}\langle 0|\bar{q}q|0\rangle \neq 0 \quad (1.23)$$

From this result, it can be seen that the spontaneous symmetry breaking can be characterized by an order parameter, it is the the so-called quark condensate $\langle 0|\bar{q}q|0\rangle$. Note that this quantity is invariant under the isospin group. However, we have shown that the Nambu-Goldstone theorem tells us that there is a massless state $|n\rangle$ that satisfies

$$\langle 0|(J_A)_\mu^a|n\rangle \neq 0 \quad (1.24)$$

which is a more strong condition than that given by $\langle 0|\bar{q}q|0\rangle \neq 0$. This means that (1.24) is a necessary condition for a spontaneous symmetry breaking, while (1.23) is a sufficient condition. As a consequence of this, the matrix element connecting the NGB states with the ground state reads

$$\langle 0|(J_A)_\mu^a|\phi^b(p)\rangle = ip_\mu e^{-ip \cdot x} F_b \delta^{ab} \quad (1.25)$$

where F_b is the decay constant associated to each NGB ϕ^b . In other words, a non-zero value of F_b in the chiral limit is a necessary criterion for spontaneous chiral symmetry breaking. Moreover, the equation (1.25) implies the partial conservation of the axial current (PCAC) [26, 27]

$$\langle 0 | \partial^\mu (J_A)_\mu^a | \phi^b(p) \rangle = i e^{-ip \cdot x} F_b M_b^2 \delta^{ab} \quad (1.26)$$

with M_b the NGB masses.

1.1.6 The $U(1)_A$ anomaly and the η'

The invariance under $U(1)_V$ is conserved at the quantum level, giving rise to the conservation of the baryon number and it allows to classify hadrons in mesons and baryons. However, the classical conservation of the axial current $(J_A)_\mu^0$ is not preserved in the quantization process and it is said that the $U(1)_A$ symmetry is anomalous.

The non-vanishing divergence of the axial current can be demonstrated in various ways. Adler, Bell and Jackiw [28–30] considered the coupling of the $U(1)_A$ current to two gluons and used diagrammatic techniques to obtain the Ward Identities (WI) containing the axial current. However, Fujikawa [31] showed it by using functional integral methods. Here, to calculate the divergence of the axial current in the quantum theory, we consider the generating functional:

$$Z_{QCD} = \int [dG] [d\bar{q}] [dq] e^{S_{QCD}} \quad (1.27)$$

where $S_{QCD} = i \int d^4x (\mathcal{L}_G + \mathcal{L}_{QCD})$ and $\mathcal{L}_G = \frac{1}{4} G_{\mu\nu}^a G^{a\mu\nu}$ is the gluon contribution. Performing the change of variable $q' \rightarrow e^{-i\beta_A(x)\gamma_5} q$ we see that the Lagrangian can be written in terms of q'

$$\mathcal{L}_{QCD}(\bar{q}', q') = \mathcal{L}_{QCD}(\bar{q}, q) + (J_A)_\mu \partial^\mu \beta_A \quad (1.28)$$

In addition to the variation of the Lagrangian under $U(1)_A$ transformations, the variation of the measure $[d\bar{q}] [dq]$ should be taken into account. For this, we have to consider the Jacobian

$$\int [d\bar{q}] [dq] = \int [d\bar{q}'] [dq'] \mathcal{J} \quad (1.29)$$

This jacobian diverges, and we need a regularization method to make this factor finite. When it is properly regularized, it can be shown that the jacobian has the form [32]

$$\mathcal{J} = \exp \left[-i \int d^4x \beta_A(x) A(x) \right], \quad A(x) = \frac{N_f g^2}{32\pi^2} G_{\mu\nu}^a \tilde{G}^{a\mu\nu} \quad (1.30)$$

where $G_{\mu\nu}^a = \partial_\mu G_\nu^a - \partial_\nu G_\mu^a + g f^{abc} G_\mu^b G_\nu^c$, $\tilde{G}^{a\mu\nu} = \epsilon^{\mu\nu\alpha\beta} G_{\alpha\beta}^a$, f^{abc} denotes the structure constants of $SU(3)$ and $\epsilon^{\mu\nu\alpha\beta}$ denotes the totally antisymmetric Levi-Civita tensor. Note

that if this Jacobian factor was equal to one, the theory would not be anomalous and the axial current would be conserved in the chiral limit.

Taking into account the axial anomaly, the divergence of the axial current including quark masses reads:

$$\partial^\mu (J_A)_\mu = 2i\bar{q}\mathcal{M}\gamma_5 q + A(x) \quad (1.31)$$

According to the quark model, it should be observed an isospin singlet with the same parity and spin quantum numbers than those of the pseudoscalar octet. The candidate to be the ninth pseudoscalar is the $\eta'(960)$. However, due to the axial anomaly, the η' mass is higher than the masses of the pseudo-NGB. In fact, it is approximately twice the kaon mass.

If the anomaly was not present, there would exist an almost conserved current for the $U(1)_A$ symmetry. Furthermore, the symmetry breaking pattern would be similar to the spontaneous chiral symmetry breaking and the singlet pseudoscalar η' would be a NGB. However, the $U(1)_A$ current is not conserved, because of the gluonic corrections, and even in the chiral limit the PCAC relation (1.26) remains nonzero.

1.1.7 The QCD vacuum

The quantity $G_{\mu\nu}^a \tilde{G}^{a\mu\nu}$ can be expressed as a total derivative of the Chern-Simons (CS) topological current,

$$A(x) = \partial^\mu J_\mu^{SC}, \quad J_\mu^{SC} = \frac{g^2}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \text{Tr}_c \left(G^\nu \partial^\rho G^\sigma - i\frac{2}{3} G^\nu G^\rho G^\sigma \right) \quad (1.32)$$

One can assign a topological (invariant) charge, known as the winding number, to a given configuration of the gauge field

$$\nu = \int d^4x \omega(x) \quad (1.33)$$

where

$$\omega(x) = \frac{1}{2N_f} A(x) \quad (1.34)$$

is the winding number topological charge density, which is a topological quantity. It must be an integer for any pure gauge field. The different gluonic configurations can be classified based on their respective topological sectors by assigning them a winding number.

By considering a suitable basis consisting of N_R right-handed eigenstates and N_L left-handed eigenstates, we can establish a relationship between the winding number

and the right and left zero modes of the Dirac operator, namely $\nu = N_R - N_L$. This is the well-known Atiyah-Singer index theorem [33] which is actually a consequence of the axial anomaly discussed in the previous section.

The vacuum of QCD is characterized by an infinite set of classical vacua, enumerated by their winding number. Tunneling effects can connect the different vacuum states $|\nu\rangle$. Instantons provide a descriptive framework to understand jumps between topological sectors. The physical vacuum must be invariant under both trivial and non-trivial gauge transformations. A gauge transformation with winding number ν transforms the states $|\nu\rangle$ into $|\nu+1\rangle$. Thus, a gauge invariant vacuum state $|\theta\rangle$ is formed by the combination of all the topological classes:

$$|\theta\rangle = \sum_{\nu=-\infty}^{\infty} e^{-i\nu\theta} |\nu\rangle \quad (1.35)$$

Let's consider an operator O which acts in the Hilbert space of the theory. The vacuum-to-vacuum transition amplitude reads:

$$\langle\theta|O|\theta\rangle = \sum_{\nu,\nu'} e^{i(\nu-\nu')\theta} \langle\nu|O|\nu'\rangle = \int [dG] [d\bar{q}] [dq] O e^{S_{QCD} - i \int d^4x \theta \omega} \quad (1.36)$$

The partition function therefore involves a sum over ν and explicitly depends on θ :

$$Z = \sum_{\nu} e^{i\theta\nu} Z_{\nu} \quad (1.37)$$

which means that the QCD generating functional can be decomposed into the sum of the contributions from each different topological sector.

There is a quantity that is intimately connected with the vacuum structure of QCD. This is the topological susceptibility, which is a measure of the topological charge fluctuations of the QCD vacuum since it is given by the mean square winding number per unit volume, i.e. $\chi_{top} = \langle\nu^2\rangle/V$ and

$$\langle\nu^2\rangle = \sum_{\nu} \frac{Z_{\nu}}{Z} \nu^2 \quad (1.38)$$

By applying two derivatives with respect to the vacuum angle θ , the mean square of the winding number can be derived from the generating functional of QCD

$$\chi_{top} = \int dx \langle \mathcal{T} \omega(x) \omega(0) \rangle ,$$

Thus, the non-trivial structure of the QCD vacuum implies the existence of an additional term in the QCD Lagrangian:

$$\mathcal{L}_{\theta} = -\frac{1}{2N_f} \theta A(x) \quad (1.39)$$

which violates P and CP for θ values different from $\theta = 0$. This new term will play a vital role since we are going to be interested in P -breaking local configurations, which can be parameterized through external sources.

1.1.8 QCD in the Presence of External Fields

An important technique that we will use the rest of the thesis is the external source method. Gasser and Leutwyler [34, 35] introduced into the Lagrangian of QCD the couplings of some external fields:

$$\text{vector: } v_\mu(x), \quad \text{axial-vector: } a_\mu(x), \quad \text{scalar: } s(x), \quad \text{pseudoscalar: } p(x).$$

In addition to this sources we can take into account the anomalous $\theta(x)$ field. The QCD Lagrangian gauged with these external fields then reads

$$\mathcal{L}_{QCD}^{ext}[\bar{q}, q, v, a, s, p, \theta] = \bar{q} [\gamma_\mu (iD^\mu + v^\mu + \gamma_5 a^\mu) - (s - ip\gamma_5)] q - \frac{1}{2N_f} \theta A \quad (1.40)$$

where the external v, a, s, p sources are matrix functions in flavor space. These fields will allow us to obtain different quark current Green functions, which are vacuum expectation values of time-ordered products, through a functional derivative of the generating functional.

In terms of the left- and right-handed quark fields, the quark part of the equation (1.40) reads

$$\mathcal{L}_{QCD}^{ext,q} = \mathcal{L}_{QCD}^{\mathcal{M}=0} + \bar{q}_R \gamma^\mu r_\mu q_R + \bar{q}_L \gamma^\mu l_\mu q_L - \bar{q}_R (s + ip) q_L - \bar{q}_L (s - ip) q_R \quad (1.41)$$

where $\mathcal{L}_{QCD}^{\mathcal{M}=0}$ was defined in (1.10) and

$$v_\mu = \frac{1}{2} (r_\mu + l_\mu), \quad a_\mu = \frac{1}{2} (r_\mu - l_\mu) \quad (1.42)$$

The fundamental idea on which the external source method is based is: the construction of a Lagrangian with coupling to external currents consistent with chiral group invariance is equivalent to demanding the invariance of the associated action when considering local chiral rotations.

In order for the extended QCD Lagrangian (1.40) to be invariant under local chiral transformations, the following transformation laws for the external fields should be

satisfied

$$\begin{aligned}
r_\mu &\rightarrow g_R(x)r_\mu g_R^\dagger(x) + ig_R(x)\partial_\mu g_R^\dagger(x) \\
l_\mu &\rightarrow g_L(x)l_\mu g_L^\dagger(x) + ig_L(x)\partial_\mu g_L^\dagger(x) \\
s + ip &\rightarrow g_R(x)(s + ip)g_L^\dagger(x) \\
s - ip &\rightarrow g_L(x)(s - ip)g_R^\dagger(x)
\end{aligned} \tag{1.43}$$

In addition, to preserve local symmetry, the covariant derivative must be

$$D_\mu q = \partial_\mu q - ir_\mu q + iql_\mu \tag{1.44}$$

Thus, l_μ and r_μ enter in the same way as gauge fields.

On the other hand, requiring the total Lagrangian of eq. (1.41) to be invariant under parity and charge conjugation leads to constraints on the transformation behavior of the external fields

$$\begin{aligned}
v^\mu &\xrightarrow{P} v_\mu, & a^\mu &\xrightarrow{P} -a_\mu, & s &\xrightarrow{P} s, & p &\xrightarrow{P} -p, \\
v_\mu &\xrightarrow{C} -v_\mu^T, & a_\mu &\xrightarrow{C} a_\mu^T, & s &\xrightarrow{C} s^T, & p &\xrightarrow{C} p^T
\end{aligned} \tag{1.45}$$

where the transposition refers to the flavor space.

If the theory contains anomalies, the transformation properties of the anomaly must be considered. For example, for a non-zero vacuum angle, in order for the $U(1)_A$ anomaly to disappear, θ should change under a $U(1)_A$ rotation $q \rightarrow e^{-i\beta_A \gamma_5} q$ as

$$\theta \rightarrow \theta - 2N_f \beta_A \tag{1.46}$$

Thus, in the case of massless quarks, the symmetry of the QCD Lagrangian is extended to $U(3)_R \times U(3)_L$. The θ shift must be taken into account in the construction of the $U(3)$ Chiral Perturbation Theory which we will present in subsection 1.2.4.

The external sources can be used to parametrize the different breakings of chiral symmetry. For example, electromagnetic processes where only external photon fields A_μ are present can be treated within this framework. In this case, the photon field must be included as an additional dynamical degree of freedom. In order to construct the effective Lagrangian in presence of external fields, the so called "spurion" fields $Q_{L,R}(x)$ are introduced [36], so we can add to the QCD Lagrangian coupled to external fields the following term

$$\mathcal{L}_Q = A_\mu \bar{q} \gamma^\mu [Q_L(x)P_L + Q_R(x)P_R] q \tag{1.47}$$

The electromagnetic interaction is then fully included by setting $v_\mu + \frac{1}{2}(Q_R + Q_L)A_\mu = QA_\mu$ with Q the quark charge matrix

$$Q = \frac{e}{3} \text{diag}(2, -1, -1) \tag{1.48}$$

Note that these spurions fields are also transformed locally in a generic way to guarantee local chiral invariance and it is only when we choose certain $Q_{L,R}$ that symmetry breaking terms are generated.

As we can see in (1.41), the vector nature of the electromagnetic interactions makes that the new term does not mix left- and right-handed fields. Because of that, if the quark charges were identical, the symmetry under the chiral group would remain unchanged. However, in the physical case the charges of the up and down quarks are quite different. Thus, chiral symmetry is broken explicitly by the quark charges.

1.2 Effective Lagrangians and Chiral Perturbation Theory

The technique of effective Lagrangians has been successfully applied in various fields of particle physics. Starting from a theory that involves certain light degrees of freedom, the basic idea is to integrate out the remaining degrees of freedom of the system in a suitable manner. The resulting theory describes the low-energy dynamics of these light particles.

The study of the hadronic processes requires an appropriate treatment of the strong interactions at low energies. Effective Lagrangians and effective field theories are particularly useful when a full calculation is not yet possible, as is the case with QCD at low energies. In this case, it is possible to build an effective Lagrangian for hadrons based on some basic properties. For example, in the chiral limit, we want the effective Lagrangian to be invariant under $SU(N_f)_L \times SU(N_f)_R \times U(1)_V$, with N_f the number of flavours. In addition, the theory should be written in terms of the relevant degrees of freedom at low energies. For energies below 1 GeV the fundamental degrees of freedom are the NGB. Therefore, the Effective Lagrangian should contain $N_f^2 - 1$ pseudoscalar degrees of freedom. The effective field theory built on this basis is called Chiral Perturbation Theory (ChPT), which was introduced by Weinberg in 1979 [37]. In this section, we will study one of the most instructive of all effective Lagrangians, the Linear Sigma Model (LSM). In addition, we are going to review some aspects of ChPT.

1.2.1 Linear Sigma Model

Let us consider a meson field theory realization of low-energy QCD where there is an explicit realization of the scalar σ as a fundamental field in the Lagrangian. A

particular example is the LSM or $O(4)$ vector model [38], which exhibits chiral symmetry restoration properties [39, 40]. We consider the light meson sector Lagrangian of this model in terms of the sigma meson σ and pions π^a :

$$\mathcal{L}_{LSM}^0 = \frac{1}{2} \partial_\mu \Phi^T \partial^\mu \Phi - V(\Phi) \quad (1.49)$$

with $\Phi^T = (\sigma, \vec{\pi})$. The associated potential is given by $V(\Phi) = \frac{\lambda}{4} [\Phi^T \Phi - v_0^2]^2$, which is invariant under the transformation belonging to $O(4)$ group. As it is shown in Fig. 1.4, for $v_0^2 > 0$, $V(\Phi)$ has minima along the circle

$$\Phi_{min}^2 = |\vec{\pi}|^2 + \sigma^2 = v_0^2 \quad (1.50)$$

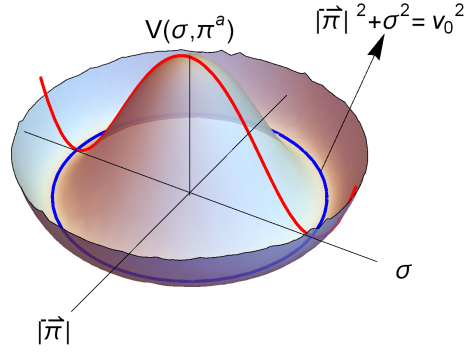


Figure 1.4: The symmetric “Mexican hat” potential $V(\Phi)$ with minima along the chiral circle.

This result shows that there exist many possible vacuum states, which are related by $O(4)$ transformations. In addition, since the pions are massive, we can make the potential asymmetric to break explicitly the $O(4)$ symmetry. It is usual to choose the σ direction to break the symmetry $O(4) \rightarrow O(3)$ adding the following term

$$\mathcal{L}_{ESB} = h\sigma \quad (1.51)$$

To define our quantum theory we have to choose a vacuum, we will take $\langle \vec{\pi} \rangle = 0$ and $\langle \sigma \rangle = v$. Therefore, because this minimum is only invariant under $O(3)$ symmetry, the model exhibits the phenomenon of spontaneous symmetry breaking.

The h term breaks explicitly the chiral symmetry, as it can be seen in Fig. 1.5, with h proportional to the pion mass squared, whereas the potential minima at $\Phi^2 = v^2 \neq 0$ implement spontaneous chiral symmetry breaking. For $h = 0$, $v = v_0$ (chiral limit)

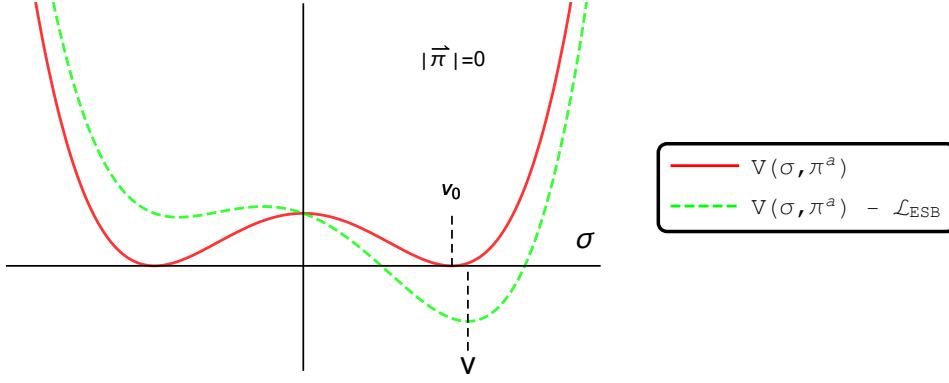


Figure 1.5: Comparison between the LSM potential with and without the explicit symmetry-breaking term of equation (1.51).

whereas for $h \neq 0$, the value of v is determined by the minimum of the potential $V(\sigma)$ as

$$h = \lambda v(v^2 - v_0^2). \quad (1.52)$$

The standard procedure is to shift the field as $\tilde{\sigma} = \sigma - v$, so that $\langle \tilde{\sigma} \rangle = 0$ to leading order. With this prescription, the Lagrangian $\mathcal{L}_{LSM} = \mathcal{L}_{LSM}^0 + \mathcal{L}_{ESB}$ becomes, in terms of the shifted $\tilde{\sigma}$ field,

$$\begin{aligned} \mathcal{L}_{LSM} = & \frac{1}{2} (\partial_\mu \tilde{\sigma} \partial^\mu \tilde{\sigma} + \partial_\mu \pi^a \partial^\mu \pi^a - M_{0\sigma}^2 \tilde{\sigma}^2 - M_{0\pi}^2 \pi_a \pi^a) - \frac{\lambda}{4} (\tilde{\sigma}^2 + \pi_a \pi^a)^2 \\ & - \lambda v \tilde{\sigma} (\tilde{\sigma}^2 + \pi_a \pi^a) - \frac{1}{4\lambda} M_{0\pi}^4 + v^2 M_{0\pi}^2, \end{aligned} \quad (1.53)$$

where $M_{0\pi}$ and $M_{0\sigma}$ are the tree-level pion and sigma masses

$$M_{0\pi}^2 = \frac{h}{v} = \lambda(v^2 - v_0^2) \quad , \quad M_{0\sigma}^2 = M_{0\pi}^2 + 2\lambda v^2, \quad (1.54)$$

An useful way of writing the LSM Lagrangian is to rewrite the pions and the sigma in terms of a matrix field

$$\Sigma = \sigma \mathbb{1} + i\pi^a \tau_a \quad (1.55)$$

and without taking into account the explicit symmetry breaking term, the *LSM* Lagrangian reads

$$\mathcal{L}_{LSM}^0 = \frac{1}{4} \text{tr} (\partial_\mu \Sigma \partial^\mu \Sigma^\dagger) - \frac{\lambda}{16} \text{tr}^2 (\Sigma \Sigma^\dagger) + \frac{\lambda}{4} v_0^2 \text{tr} (\Sigma \Sigma^\dagger) - \frac{\lambda}{4} v_0^4 \quad (1.56)$$

As we can see, this Lagrangian is invariant under chiral transformations $\Sigma \rightarrow g_L \Sigma g_R^\dagger$, with g_R and g_L given in (1.11). Furthermore, the vacuum choice $\langle \Sigma \rangle = v_0 \mathbb{1}$ is only

invariant under $g_L = g_R$ transformations, that is the isospin group. Thus, the change of variable (1.55) makes manifest the equivalences of the groups $O(4)$ with $SU(2)_R \times SU(2)_L$ and $O(3)$ with $SU(2)_V$. In other words, the $O(4) \rightarrow O(3)$ spontaneous symmetry breaking pattern is isomorphic to $SU(2)_R \times SU(2)_L \rightarrow SU(2)_V$.

Nevertheless, the Linear Sigma Model is not adequate to describe the phenomenology, because a free sigma state is not observed in the spectrum. In addition, the perturbation theory is not well defined, since to reproduce the scattering results we need $\lambda \gg 1$. For those reasons, the Non Linear Sigma Model and Chiral Perturbation Theory are introduced.

1.2.2 Non Linear Sigma Model

When $\lambda \rightarrow \infty$ the condition given by (1.50) is satisfied. Expressing σ as a power series of $\vec{\pi}$ in (1.49) using the vacuum constrain ($\sigma = \sqrt{v_0^2 - \vec{\pi}^2}$) we get the Lagrangian of the Non Linear Sigma Model (NLSM)

$$\mathcal{L}_{NLSM} = \frac{1}{2} \partial_\mu \vec{\pi} \partial^\mu \vec{\pi} + \frac{1}{2v_0^2} (\vec{\pi} \partial_\mu \vec{\pi})^2 \left(1 + \frac{\vec{\pi}^2}{v_0^2} + \dots \right) \quad (1.57)$$

In this way, σ decouples completely from the pions and we are left with a pure theory of NGB. We can now make an exponential parameterization of the NGB fields

$$U(x) = \exp(i\tau_a \pi^a(x)/v_0) \quad (1.58)$$

where, in order to comply with low-energy theorems, or ChPT to leading order [34] we have $v_0 = F$, the pion decay constant in the chiral limit, so that $v = v_0(1 + \mathcal{O}(M_\pi^2/M_\sigma^2)) = F(1 + \mathcal{O}(M_\pi^2/M_\sigma^2)) = F_\pi(1 + \mathcal{O}(M_\pi^2/M_\sigma^2))$ with $F_\pi \simeq 92.3$ MeV. With the parameterization in (1.58), the NLSM Lagrangian is given by

$$\mathcal{L}_{NLSM} = \frac{F^2}{4} \left\{ \text{tr} (\partial_\mu U \partial^\mu U^\dagger) + M_{0\pi}^2 \text{tr} (U + U^\dagger) \right\} \quad (1.59)$$

We can generalize the NLSM Lagrangian (1.59) to $SU(3)$ by simply using the following unitary matrix $U(x) = \exp(i\sqrt{2}\phi(x)/F)$ with:

$$\phi(x) = \begin{pmatrix} \frac{1}{\sqrt{2}}\pi_0 + \frac{1}{6}\eta_8 & \pi^+ & K^+ \\ \pi^- & -\frac{1}{\sqrt{2}}\pi_0 + \frac{1}{6}\eta_8 & K^0 \\ K^- & \bar{K}^0 & -\frac{2}{\sqrt{6}}\eta_8 \end{pmatrix} \quad (1.60)$$

and introducing the quark mass matrix $\mathcal{M}$ and a constant B_0 related to the chiral quark condensate:

$$\mathcal{L}_{NLSM} = \frac{F^2}{4} \left\{ \text{tr} (\partial_\mu U \partial^\mu U^\dagger) + 2B_0 \text{tr} [\mathcal{M} (U + U^\dagger)] \right\} \quad (1.61)$$

The $SU(N_f)$ matrix U inherits the chiral transformation of Σ :

$$U \rightarrow g_L U g_R^\dagger, \quad g_{R,L} \in SU(N_f = 2, 3) \quad (1.62)$$

Note that the U field transforms linearly under the chiral group, but the induced transformation on the NGB fields is nonlinear.

1.2.3 Chiral Perturbation theory

The U parameterization could have been used to get the NLSM Lagrangian combining the U fields with its derivatives following the chiral symmetry breaking pattern. In this way, the low-energy effective Lagrangian can be written as a derivative expansion. As we will explain, the leading order term has two derivatives, so there exist tree different candidates:

$$\text{tr}^2(U^\dagger \partial_\mu U), \quad \text{tr}(\partial_\mu U \partial^\mu U^\dagger), \quad \text{tr}(U^\dagger \partial_\mu U)^2, \quad (1.63)$$

The first term vanishes because $\text{tr}(U^\dagger \partial_\mu U) = 0$ for $U \in SU(N)$, and the third term can be written in terms of the second one due to $U^\dagger \partial_\mu U = -\partial_\mu U^\dagger U$.

If we wanted to write the most general effective Lagrangian consistent with the chiral symmetry, we would have an infinite number of possible terms. Therefore, in order to control the low energy description, we must establish a well-defined power counting for the fields, derivatives and external sources. For this reason, we introduce Chiral Perturbation Theory and the Weinberg's power counting.

Chiral Perturbation Theory is based on an expansion in powers of momenta. The effective Lagrangian is organized as a string of terms with an increasing number of derivatives and quark masses (n)

$$\mathcal{L}_{ChPT} = \sum_n \mathcal{L}_n = \mathcal{L}_2 + \mathcal{L}_4 + \mathcal{L}_6 + \dots \quad (1.64)$$

The chiral dimension is always a multiple of two because parity conservation requires an even number of derivatives. In the absence of other sources, the first term in the above expansion $\mathcal{L}_2$ corresponds to the NLSM Lagrangian. The higher order Lagrangian terms are multiplied by constants called Low Energy Constants (LECs). These LECs absorb the divergences coming from the loops given rise to a order by order renormalised theory.

It is necessary a systematic method of assessing the importance of the diagrams contributing to a certain process. Considering a Feynman diagram with N_L loops and

N_n vertices with n derivatives (or masses), the overall energy dimension D is given by the relation

$$D = 2 + \sum_n N_n(n - 2) + 2N_L \quad (1.65)$$

We note that a diagram containing N_L loops contributes at a power $\mathcal{O}(p^{2N_L})$ higher than the tree level. In fact, the tree-level diagrams are of order $\mathcal{O}(p^2)$ while the divergences coming from one-loop diagrams are of order $\mathcal{O}(p^4)$. The leading $D = 2$ contributions are obtained with $N_L = 0$ and $n = 2$. At NLO, we have tree-level contributions from $\mathcal{L}_4$ ($N_L = 0$, $n = 4$, $N_4 = 1$) and one-loop graphs with the lowest-order Lagrangian ($N_L = 1$, $n = 2$).

In the presence of external sources, we can build a generalized effective Lagrangian for the NGB. According to the invariance theorem, derivatives should be replaced by covariant derivatives

$$d_\mu U = \partial_\mu U - ir_\mu U + iU l_\mu \quad (1.66)$$

$$d_\mu U^\dagger = \partial_\mu U^\dagger + ir_\mu U^\dagger - iU^\dagger l_\mu \quad (1.67)$$

In the chiral counting scheme of chiral perturbation theory, one has to keep a consistent power counting for derivatives of the meson field and for the external sources in a generic momentum scale p . Thus, $U = \mathcal{O}(1)$, $d_\mu U, r_\mu, l_\mu = \mathcal{O}(p)$, $s, p = \mathcal{O}(p^2)$. In addition to this, the most general Lagrangian at a given order is built in a way that respects the invariance under P , C , Lorentz and local chiral transformations

$$\begin{aligned} U, \chi &\xleftrightarrow{P} U^\dagger, \chi^\dagger, & U, \chi &\xleftrightarrow{C} U^T, \chi^T \\ d_\mu U &\xleftrightarrow{P} d^\mu U^\dagger, & d_\mu U &\xleftrightarrow{C} (d_\mu U)^T \end{aligned} \quad (1.68)$$

In this way, the lowest order Lagrangian in the chiral expansion for an arbitrary number N_f of light quark flavours is

$$\mathcal{L}_2 = \frac{F^2}{4} \{ \text{tr} (d_\mu U d^\mu U^\dagger) + \text{tr} (\chi^\dagger U + \chi U^\dagger) \} \quad (1.69)$$

where $\chi = 2B_0(s + ip)$ and which is the NLSM Lagrangian when we take $r_\mu = l_\mu = p = 0$ and $s = 2B_0\mathcal{M}$. Thus, to leading order in the chiral low-energy expansion, the Gell-Mann-Oakes-Renner relation $\langle \bar{q}q \rangle_l = -2B_0 F^2(1 + \mathcal{O}(\mathcal{M}))$ holds.

Evaluating the trace in the quadratic mass term one can find the expression that relates the meson masses with the quark masses. In the limit $m_u = m_d = m_l$, this is

$M_{0\pi}^2 = 2B_0 m_l$ in $SU(2)$ and in $SU(3)$:

$$M_{0\pi}^2 = 2m_l B_0 \quad (1.70)$$

$$M_{0K}^2 = (m_l + m_s) B_0 \quad (1.71)$$

$$M_{0\eta}^2 = \frac{2}{3} (m_l + 2m_s) B_0 \quad (1.72)$$

Taking out the common B_0 factor, the above mass equations imply the Gell-Mann-Okubo mass relation

$$4M_{0K}^2 - M_{0\pi}^2 - 3M_{0\eta}^2 = 0 \quad (1.73)$$

Imposing the usual variational constraint $\frac{\delta \mathcal{L}_2}{\delta \Delta_a} = 0$ when we consider small variations of the U field $U'(x) = \left(1 + i \sum_a^{N_f-1} T_a \Delta_a\right) U(x)$ we get the equations of motion (EOMs) at $\mathcal{O}(p^2)$

$$(d_\mu d^\mu U^\dagger)U - U^\dagger d_\mu d^\mu U = \chi^\dagger U - U^\dagger \chi + \frac{1}{N_f} \text{tr} [U^\dagger \chi - \chi^\dagger U] \quad (1.74)$$

We can make use of the equations of motion at $\mathcal{O}(p^2)$ in order to eliminate some of the $\mathcal{O}(p^4)$ terms. Moreover, due to the $SU(N_f)$ trace identities the number of possible operators also decreases.

By implementing the previously mentioned concepts, it becomes possible to formulate the most general $SU(3)$ effective Lagrangian at $\mathcal{O}(p^4)$. For traceless r_μ and l_μ external sources and without spurions fields, it takes the form [35]:

$$\begin{aligned} \mathcal{L}_{4,SU(3)}^0 &= L_1 \text{tr}^2 [d_\mu U^\dagger d^\mu U] + L_2 \text{tr} [d^\mu U^\dagger d^\nu U] \text{tr} [d_\mu U^\dagger d_\nu U] \\ &+ L_3 \text{tr} [d_\mu U^\dagger d^\mu U d_\nu U^\dagger d^\nu U] + L_4 \text{tr} [d_\mu U^\dagger d^\mu U] \text{tr} (\chi U^\dagger + U \chi^\dagger) \\ &+ L_5 \text{tr} [d_\mu U^\dagger d^\mu U (\chi U^\dagger + U \chi^\dagger)] + L_6 \text{tr}^2 (\chi U^\dagger + U \chi^\dagger) \\ &+ L_7 \text{tr}^2 (\chi U^\dagger - U \chi^\dagger) + L_8 \text{tr} (\chi^\dagger U \chi^\dagger U + U^\dagger \chi U^\dagger \chi) \\ &- iL_9 \text{tr} (G_{\mu\nu}^R d^\mu U d^\nu U^\dagger + G_{\mu\nu}^L d^\mu U^\dagger d^\nu U) + L_{10} \text{tr} (G_{\mu\nu}^R U G^{L\mu\nu} U^\dagger) \\ &+ H_1 \text{tr} (G_{\mu\nu}^R G^{R\mu\nu} + G_{\mu\nu}^L G^{L\mu\nu}) + H_2 \text{tr} (\chi^\dagger \chi) \end{aligned} \quad (1.75)$$

where the strength tensors are

$$G_{\mu\nu}^L = \partial_\mu l_\nu - \partial_\nu l_\mu - i [l_\mu, l_\nu], \quad G_{\mu\nu}^R = \partial_\mu r_\nu - \partial_\nu r_\mu - i [r_\mu, r_\nu]. \quad (1.76)$$

i	1	2	3	4	5	6	7	8	9	10	i	1	2	3
Γ_i	$\frac{3}{32}$	$\frac{3}{16}$	0	$\frac{1}{8}$	$\frac{3}{8}$	$\frac{11}{144}$	0	$\frac{5}{48}$	$\frac{1}{4}$	$-\frac{1}{4}$	Δ_i	$-\frac{1}{8}$	$\frac{5}{24}$	-
γ_i	$\frac{1}{3}$	$\frac{2}{3}$	$-\frac{1}{2}$	2	$-\frac{1}{6}$	$-\frac{1}{3}$	0	-	-	-	δ_i	2	$\frac{1}{12}$	0

Table 1.2: Values of the renormalization coefficients for $N_f = 2$ and 3.

For $N_f = 2$, the chiral effective Lagrangian at $O(p^4)$ reads [34, 35, 41]:

$$\begin{aligned}
\mathcal{L}_{4,SU(2)}^0 = & \frac{l_1}{4} \text{tr}^2 [d_\mu U^\dagger d^\mu U] + \frac{l_2}{4} \text{tr} [d^\mu U^\dagger d^\nu U] \text{tr} [d_\mu U^\dagger d_\nu U] + \frac{l_3}{16} \text{tr}^2 (\chi U^\dagger + U \chi^\dagger) \\
& + \frac{l_4}{4} \text{tr} [d^\mu U^\dagger d_\mu \chi + d^\mu \chi^\dagger d_\mu U] + l_5 \text{tr} (G_{\mu\nu}^R U G^{L\mu\nu} U^\dagger) \\
& + i \frac{l_6}{2} \text{tr} (G_{\mu\nu}^R d^\mu U d^\nu U^\dagger + G_{\mu\nu}^L d^\mu U^\dagger d^\nu U) - \frac{l_7}{16} \text{tr}^2 (\chi U^\dagger - U \chi^\dagger) \\
& + \frac{h_1 + h_3}{4} \text{tr} (\chi^\dagger \chi) + \frac{h_1 - h_3}{2} \text{Re} (\det \chi) - h_2 \text{tr} (G_{\mu\nu}^R G^{R\mu\nu} + G_{\mu\nu}^L G^{L\mu\nu}) \quad (1.77)
\end{aligned}$$

Upon comparison with the $SU(3)$ version, it is evident that equation (1.77) exhibits a reduction in the number of independent terms, a direct outcome of employing the trace relations for 2×2 matrices.

Apart from the h_i (H_i) constants, there are seven (ten) LECs, denoted l_i (L_i), in the $SU(2)$ ($SU(3)$) Lagrangian. It is thus possible to absorb the one-loop divergences by an appropriate renormalization of the coefficients l_i , L_i , h_i and H_i

$$\begin{aligned}
L_i^r &= L_i - \Gamma_i R, & l_i^r &= l_i - \gamma_i R, \\
H_i^r &= H_i - \Delta_i R, & h_i^r &= h_i - \delta_i R,
\end{aligned} \quad (1.78)$$

where R is defined as

$$R = -\frac{\mu^{-\epsilon}}{32\pi^2} (2/\epsilon - \gamma + \log 4\pi + 1) \quad (1.79)$$

with μ the renormalization scale in the modified minimal subtraction scheme with $D = 4 - \epsilon$. The Γ_i , γ_i , Δ_i and δ_i renormalization coefficients are depicted in Table 1.2.

For the two flavour case, we will also find useful to define scale-independent LECs $\bar{l}_i$ and $\bar{h}_i$ by

$$\begin{aligned}
l_i^r &= \frac{\gamma_i}{32\pi^2} \left(\bar{l}_i + \log \frac{M_\pi^2}{\mu^2} \right) \\
h_i^r &= \frac{\delta_i}{32\pi^2} \left(\bar{h}_i + \log \frac{M_\pi^2}{\mu^2} \right)
\end{aligned} \quad (1.80)$$

which are the running couplings evaluated at the scale $\mu = M_\pi$. These values $\bar{l}_i$ and $\bar{h}_i$ are independent of the subtraction scale but depend explicitly on the pion mass.

Note that to NLO the pion mass and the decay constant must be renormalized and are given in terms of the tree level ones. The low-energy constant l_4 governs the chiral expansion of the pion decay constant, while l_3 determines the analogous contribution in the chiral expansion of the pion mass:

$$M_\pi^2 = M_{0\pi}^2 \left(1 - \frac{M_{0\pi}^2}{32\pi^2 F^2} \bar{l}_3 \right) \quad (1.81)$$

$$F_\pi^2 = F^2 \left(1 + \frac{M_{0\pi}^2}{8\pi^2 F^2} \bar{l}_4 \right) \quad (1.82)$$

1.2.4 $U(3)$ Chiral Perturbation Theory

The $1/N_c$ expansion of QCD was proposed in 1974 by Gerard 't Hooft. He was the first to note that many aspects of QCD can be understood by generalizing QCD to a $SU(N_c)$ gauge group in the limit $N_c \rightarrow \infty$. The $SU(N_c)$ gauge theory simplifies considerably at $N_c \rightarrow \infty$, while keeping the most essential properties of QCD. According to equation (1.2), $g \sim 1/\sqrt{N_c}$, this means that the running coupling constant approaches zero when N_c is larger. Therefore, the winding number charge density ω defined in (1.34), responsible for the anomalous contribution of the η' mass, is suppressed within the large- N_c counting [42–46]. In this way, the axial anomaly disappears when the limits $N_c \rightarrow \infty$ and $m_q \rightarrow 0$ (chiral) are combined and the η' appears as the ninth NGB.

Within $U(3)$ ChPT one follows a similar approach as in standard ChPT [35]. Nevertheless, in the $U(3)$ formalism, the effective Lagrangian must be modified to include the singlet η_0 , which is the main component of the physical η' state. As we have seen, given the large η' mass value, this can be done consistently only in the large- N_c framework.

In $U(3)$ ChPT, the dependence on the number of colors is carried by the chiral parameters. Thus, the expansion is performed in terms of a small parameter

$$M^2, p^2, T^2, m_l, m_s, 1/N_c = \mathcal{O}(\delta) \quad (1.83)$$

where M and p denote typical meson masses and momenta. In this counting, the tree-level pion decay constant $F^2 = \mathcal{O}(1/\delta)$ [46], which hence suppresses loop diagrams.

In the effective Lagrangian, $\theta(x)$ appears through the operator

$$X(x) = \log [\det \mathcal{U}(x)] + i\theta(x), \quad (1.84)$$

with $\mathcal{U} = \exp(i\Phi_3/F) = \exp(i\lambda^a\phi_a/F)$ the NGB matrix field including the singlet contribution (i.e., $\det\mathcal{U} \neq 1$), ϕ_i the Goldstone fields, $\lambda^{a=1,\dots,8}$ the Gell-Mann matrix and $\lambda^0 = \sqrt{2/3} \mathbf{1}$ [45],

$$\Phi_3 = \eta_0\lambda^0 + \sqrt{2}\phi = \begin{pmatrix} \pi^0 + \frac{1}{\sqrt{3}}\eta_8 + \sqrt{\frac{2}{3}}\eta_0 & \sqrt{2}\pi^+ & \sqrt{2}K^+ \\ \sqrt{2}\pi^- & -\pi^0 + \frac{1}{\sqrt{3}}\eta_8 + \sqrt{\frac{2}{3}}\eta_0 & \sqrt{2}K^0 \\ \sqrt{2}K^- & \sqrt{2}\bar{K}^0 & \frac{-2}{\sqrt{3}}\eta_8 + \sqrt{\frac{2}{3}}\eta_0 \end{pmatrix}. \quad (1.85)$$

Nevertheless, due to the $\eta - \eta'$ mixing the flavor eigenstates η_8 and η_0 are not mass eigenstates even at LO in the chiral Lagrangian. Thus, we use the angle $\hat{\theta}$ to describe their mixing at LO

$$\eta_8 = c_\theta \eta + s_\theta \eta', \quad \eta_0 = -s_\theta \eta + c_\theta \eta', \quad (1.86)$$

where

$$c_\theta = \cos \hat{\theta}, \quad s_\theta = \sin \hat{\theta}, \quad (1.87)$$

Under $U(3)_R \times U(3)_L$ the field $\mathcal{U}$ undergoes the same transformation as U in $SU(2)$ and $SU(3)$ ChPT with $g_{R,L} \in U(3)_{R,L}$ instead of $g_{R,L} \in SU(N_f = 2, 3)_{R,L}$, i.e. $\mathcal{U} \rightarrow g_R \mathcal{U} g_L^\dagger$, while θ changes as $\theta \rightarrow \theta + i \ln \det g_R - i \ln \det g_L$. By this way, the combination (1.84) ensures that any invariant operator multiplied by any function of X will be invariant under local $U(3)_L \times U(3)_R$ transformations.

The effective Lagrangian can be expressed as the sum of the contributions of order 1, δ , δ^2 , and so on. The explicit expression for the lowest order $U(3)$ Effective Lagrangian $\mathcal{L}_0^{U(3)} = \mathcal{O}(\delta^0)$ reads

$$\mathcal{L}_0^{U(3)} = \frac{F^2}{4} \text{tr} (d_\mu \mathcal{U} \partial^\mu \mathcal{U}) + \frac{F^2}{4} \text{tr} (\chi^\dagger \mathcal{U} + \chi \mathcal{U}^\dagger) + \frac{F^2}{12} M_0^2 X^2 \quad (1.88)$$

where M_0^2 is the contribution to the tree-level mass of the singlet η_0 in the chiral limit. We can see that the first and second operators in the above expression are $\mathcal{O}(N_c p^2)$, while the last one is $\mathcal{O}(p^0)$.

The process of assigning Large N_c counting rules involves a comparison between the Green functions calculated from the effective Lagrangian and those derived from Large N_c QCD. Large N_c claims that terms that contain two flavor traces are suppressed in comparison to those that only contain one single trace by a factor of $1/N_c$. On the other hand, the scattering amplitudes are $\mathcal{O}(1/N_c)$ and the contributions to the amplitude of terms that multiply the $SU(3)$ LECs are of order L_i/F^4 . We conclude from this that L_1, L_2, L_4, L_6, L_7 should be $\mathcal{O}(1)$, while $L_3, L_5, L_8, L_9, L_{10}, H_1$ and H_2 are $\mathcal{O}(N_c)$.

Moreover, it must be noted that some single trace operators can be expressed as a linear combination of terms with more flavor traces using trace identities. For example, the trace operator given by $\text{tr}(d_\mu U d_\nu U d^\mu U^\dagger d^\nu U)$ can be expressed as a linear combination of the terms multiplied by $L_{1,2,3}$ in the following way

$$\begin{aligned} \text{tr}(d_\mu U d_\nu U^\dagger d^\mu U d^\nu U^\dagger) &= -2\text{tr}(d_\mu U d^\mu U^\dagger d_\nu U d^\nu U^\dagger) + \text{tr}(d_\mu U d_\nu U^\dagger) \text{tr}(d^\mu U d^\nu U^\dagger) \\ &\quad + \frac{1}{2}\text{tr}(d_\mu U d^\mu U^\dagger)^2. \end{aligned} \quad (1.89)$$

This term is not normally included in the NLO $SU(3)$ Lagrangian since we can make use of equation (1.89) in such a way that the contribution of this term is included in $L_{1,2,3}$. In addition, it is also possible because all the LECs involved are of the same order. However, as we have shown, it does not happen in the $N_c \rightarrow \infty$ limit. To properly study the implications of that we add this term to the Lagrangian, multiplied by a constant $\hat{L}$. We can see that the trace operators multiplied by L_1 , L_2 and L_3 receive a contribution from $\hat{L}$

$$\begin{aligned} \mathcal{L}_{4,SU(3)}^0 + \hat{L} \text{tr}(d_\mu U d_\nu U^\dagger d^\mu U d^\nu U^\dagger) &= \\ \left(L_1 + \frac{1}{2}\hat{L}\right) \text{tr}(d_\mu U d^\mu U^\dagger)^2 + \left(L_2 + \hat{L}\right) \text{tr}(d_\mu U d_\nu U^\dagger) \text{tr}(d^\mu U d^\nu U^\dagger) & \quad (1.90) \\ + \left(L_3 - 2\hat{L}\right) \text{tr}(d_\mu U d^\mu U^\dagger d_\nu U d^\nu U^\dagger) + \dots \end{aligned}$$

$\hat{L}$ is $\mathcal{O}(N_c)$ due to the single trace of $\text{tr}(d_\mu U d_\nu U d^\mu U^\dagger d^\nu U)$, so the LECs $L_1 \rightarrow L_1 + \hat{L}/2$ and $L_2 \rightarrow L_2 + \hat{L}$ appearing in the $SU(3)$ Lagrangian are truly of order $\mathcal{O}(N_c)$. Nevertheless, the combination $2L_1 + L_2$ remains of order $\mathcal{O}(1)$, since the contribution from $\hat{L}$ disappears.

The term $\mathcal{L}_1^{U(3)} = \mathcal{O}(\delta)$ was constructed in [46, 47]

$$\begin{aligned} \mathcal{L}_1^{U(3)} &= L_2 \text{tr}(d_\mu \mathcal{U} d_\nu \mathcal{U}^\dagger d^\mu \mathcal{U} d^\nu \mathcal{U}^\dagger) + (2L_2 + L_3) \text{tr}(d_\mu \mathcal{U} d^\mu \mathcal{U}^\dagger d_\nu \mathcal{U} d^\nu \mathcal{U}^\dagger) \\ &\quad + L_5 \text{tr}[d_\mu \mathcal{U}^\dagger d^\mu \mathcal{U} (\mathcal{U}^\dagger \chi + \chi^\dagger \mathcal{U})] + L_8 \text{tr}(\mathcal{U}^\dagger \chi \mathcal{U}^\dagger \chi + \chi^\dagger \mathcal{U} \chi^\dagger \mathcal{U}) \\ &\quad - iL_9 \text{tr}(R_{\mu\nu} d^\mu \mathcal{U} d^\nu \mathcal{U}^\dagger + L_{\mu\nu} d^\mu \mathcal{U}^\dagger d^\nu \mathcal{U}) + L_{10} \text{tr}(R_{\mu\nu} \mathcal{U} L^{\mu\nu} \mathcal{U}^\dagger) \\ &\quad + \frac{1}{2}\Lambda_1 d_\mu \eta_0 d^\mu \eta_0 - \frac{F^2}{12}\Lambda_2 X \text{tr}(\mathcal{U}^\dagger \chi - \chi^\dagger \mathcal{U}) + \frac{1}{12}H_0 d_\mu \theta d^\mu \theta \\ &\quad + H_1 \text{tr}(R_{\mu\nu} R^{\mu\nu} + L_{\mu\nu} L^{\mu\nu}) + H_2 \text{tr}(\chi^\dagger \chi) \end{aligned} \quad (1.91)$$

and contains the contributions of order $\mathcal{O}(N_c p^4)$, $\mathcal{O}(p^2)$ and $\mathcal{O}(1/N_c)$. The first is obtained from the $\mathcal{O}(p^4)$ $SU(3)$ Lagrangian.

At $\mathcal{O}(\delta^2)$, one then has $\mathcal{O}(N_c p^6)$, $\mathcal{O}(p^4)$, $\mathcal{O}(p^2/N_c)$ and $\mathcal{O}(1/N_c^2)$ operators. The relevant ones in this thesis are the associated to the $\eta - \eta'$ mixing:

$$\mathcal{L}_2^{U(3)} = \frac{F^2}{4} \left[v_4^{(0)} X^4 + v_2^{(2)} X^2 \text{tr} (\mathcal{U}^\dagger \chi + \chi^\dagger \mathcal{U}) \right] + L_{25} X \text{tr} (\mathcal{U}^\dagger \chi \mathcal{U}^\dagger \chi - \chi^\dagger \mathcal{U} \chi^\dagger \mathcal{U}) \quad (1.92)$$

The constants carry the scalings $\Lambda_2 = \mathcal{O}(\delta)$, $v_2^{(2)} = \mathcal{O}(\delta^2)$, $v_4^{(0)} = \mathcal{O}(\delta^3)$ and $L_{25} = \mathcal{O}(\delta^0)$. As in the standard SU(3) formalism, the LECs are renormalized to absorb divergences coming from the loops.

1.3 Finite temperature

Quantum field theory at finite temperature is the relativistic field theory generalization of non-relativistic quantum statistical mechanics.

In equilibrium statistical mechanics, three common ensemble types are encountered: microcanonical, canonical, and grand canonical. In relativistic quantum systems, where particles can be created and destroyed, observables are calculated within the grand canonical ensemble.

Let us consider a dynamical system characterized by a Hamiltonian H and a set of conserved charge operators Q_i . In the context of a grand canonical ensemble, the description of the system in thermal equilibrium can be carried out by means of the partition function

$$Z(T, \mu_i) = \text{Tr} \exp \left[-\beta (H - \sum_i \mu_i Q_i) \right] \quad (1.93)$$

where $\beta = 1/T$, with T the system temperature, and μ_i are the chemical potentials associated to the conservation of the Q_i charges. The trace is taken over the full Hilbert space, that is all possible states of the system. In the grand canonical ensembles, β and μ_i may be thought of as Lagrange multipliers that determine the mean energy and the mean charges in the system respectively. Using (1.93) one defines the grand canonical average of an arbitrary operator O , as

$$\langle O \rangle = \frac{1}{Z(T, \mu_i)} \text{Tr} \left(O \exp \left[-\beta (H - \sum_i \mu_i Q_i) \right] \right) \quad (1.94)$$

All thermodynamic quantities can be generated from the partition function. Some of the observables we will analyze in the following sections are the free energy density,

the particle density, the pressure, the entropy density, the specific heat and the speed of sound

$$\epsilon = -\frac{1}{\beta V} \log Z \quad (1.95)$$

$$n = \frac{\partial \epsilon}{\partial \mu_i} \quad (1.96)$$

$$P = \epsilon_0 - \epsilon \quad (1.97)$$

$$s = \frac{\partial P}{\partial T} \quad (1.98)$$

$$c_v = T \frac{\partial s}{\partial T} \quad (1.99)$$

$$c_s^2 = \frac{\partial P}{\partial \epsilon} = \frac{s}{T} \left(\frac{\partial s}{\partial T} \right)^{-1} \quad (1.100)$$

1.3.1 Imaginary time formalism

The imaginary time formalism allow us to calculate thermal Green functions making use of the analogy of expression (1.93) with the quantum-mechanical time evolution operator.

For simplicity, we consider the case of a real scalar field $\hat{\phi}(\vec{x}, t)$ whose dynamics is governed by the Hamiltonian H . The eigenstates of the field operator satisfy $\hat{\phi}(\vec{x}, t)|\phi\rangle = \phi(\vec{x}, t)|\phi\rangle$ and the time evolution of these eigenvalues is given by

$$|\phi(\vec{x}, t)\rangle = e^{iH(t-t_0)}|\phi(\vec{x}, t_0)\rangle \quad (1.101)$$

Now, we introduce the conjugate momentum field operator $\hat{\pi}(\vec{x}, t) \equiv \partial \mathcal{L} / \partial (\partial \phi / \partial t)$, which satisfies $\hat{\pi}(\vec{x}, t)|\pi\rangle = \pi(\vec{x}, t)|\pi\rangle$, and the usual completeness and orthogonality conditions for ϕ and π

$$\begin{aligned} \int d\phi |\phi\rangle \langle \phi| &= 1, \quad \langle \phi(\vec{x}, t_1) | \phi(\vec{x}, t_2) \rangle = \delta(\phi(\vec{x}, t_1) - \phi(\vec{x}, t_2)), \\ \int \frac{d\pi}{2\pi} |\pi\rangle \langle \pi| &= 1, \quad \langle \pi(\vec{x}, t_1) | \pi(\vec{x}, t_2) \rangle = \delta(\pi(\vec{x}, t_1) - \pi(\vec{x}, t_2)), \\ \langle \phi(\vec{x}, t_1) | \pi(\vec{x}, t_2) \rangle &= \exp \left(i \int d^3x \pi(\vec{x}, t) \phi(\vec{x}, t) \right) \end{aligned} \quad (1.102)$$

Let us note that the grand canonical partition function can be written as

$$Z = \int d\phi \langle \phi(\vec{x}, t_0) | e^{-\beta H} | \phi(\vec{x}, t_0) \rangle \quad (1.103)$$

so, according to (1.101), the partition function is related with the transition amplitude for going from a state $|\phi(\vec{x}, t_0)\rangle$ to a state $|\phi(\vec{x}, t)\rangle$ after a time $t = t_0 - i\beta$. This amplitude can be calculated dividing the time interval (t_0, t) into $N = (t - t_0)/\Delta t$ equal steps for infinitesimally small times Δt , i.e $N \rightarrow \infty$, so

$$e^{-iH(t-t_0)} = \lim_{N \rightarrow \infty} (e^{-iH\Delta t})^N \quad (1.104)$$

Let us now insert a complete set of states using the completeness conditions given in (1.102):

$$\begin{aligned} \langle \phi(\vec{x}, t_0 - i\beta) | \phi(\vec{x}, t_0) \rangle &= \langle \phi(\vec{x}, t_0) | e^{-\beta H} | \phi(\vec{x}, t_0) \rangle = \lim_{N \rightarrow \infty} \int \left(\prod_{i=1}^N d\phi(\vec{x}, t_i) \frac{d\pi(\vec{x}, t_i)}{2\pi} \right) \\ &\langle \phi(\vec{x}, t_0) | \pi(\vec{x}, t_N) \rangle \langle \pi(\vec{x}, t_N) | e^{-iH\Delta t} | \phi(\vec{x}, t_N) \rangle \langle \phi(\vec{x}, t_N) | \pi(\vec{x}, t_{N-1}) \rangle \\ &\cdots \langle \phi(\vec{x}, t_2) | \pi(\vec{x}, t_1) \rangle \langle \pi(\vec{x}, t_1) | e^{-iH\Delta t} | \phi(\vec{x}, t_1) \rangle \langle \phi(\vec{x}, t_1) | \phi(\vec{x}, t_0) \rangle \end{aligned} \quad (1.105)$$

If Δt is much smaller than the eigenvalues of the Hamiltonian in the regime of physical interest, the exponents can be treated perturbatively. In this way, we can evaluate the matrix element $\langle \pi(\vec{x}, t_i) | e^{-iH\Delta t} | \phi(\vec{x}, t_i) \rangle$ as follows

$$\langle \pi(\vec{x}, t_i) | e^{-iH\Delta t} | \phi(\vec{x}, t_i) \rangle = (1 - iH_i\Delta t) \exp \left(-i \int d^3x \pi(\vec{x}, t_i) \phi(\vec{x}, t_i) \right) \quad (1.106)$$

and within the same level of approximation we can also write

$$\langle \pi(\vec{x}, t_i) | e^{-iH\Delta t} | \phi(\vec{x}, t_i) \rangle = \exp \left(-i \int d^3x [\mathcal{H}(\phi(\vec{x}, t_i), \pi(\vec{x}, t_i))\Delta t + \pi(\vec{x}, t_i)\phi(\vec{x}, t_i)] \right) \quad (1.107)$$

with $\mathcal{H}(\phi(\vec{x}, t), \pi(\vec{x}, t))$ the hamiltonian density defined by

$$H = \int d^3x \mathcal{H}(\phi(\vec{x}, t), \pi(\vec{x}, t)) \quad (1.108)$$

Putting everything together we find that the amplitude becomes

$$\begin{aligned} \langle \phi(\vec{x}, t_0) | e^{-\beta H} | \phi(\vec{x}, t_0) \rangle &= \lim_{N \rightarrow \infty} \int \left(\prod_{i=1}^N d\phi(\vec{x}, t_i) \frac{d\pi(\vec{x}, t_i)}{2\pi} \right) \delta(\phi(\vec{x}, t_1) - \phi(\vec{x}, t_0)) \\ &\exp \left\{ -i\Delta t \sum_{j=1}^N \int d^3x \left[\mathcal{H}(\phi(\vec{x}, t_j), \pi(\vec{x}, t_j)) - \pi(\vec{x}, t_j) \frac{(\phi(\vec{x}, t_{j+1}) - \phi(\vec{x}, t_j))}{\Delta t} \right] \right\} \end{aligned} \quad (1.109)$$

and taking the continuum limit we obtain

$$Z = \int_{\text{periodic}} [d\phi] \int [d\pi] \exp \left\{ i \int_{t_0}^{t_0-i\beta} dt \int d^3x \mathcal{L}(\phi, \pi) \right\} \quad (1.110)$$

with $\mathcal{L} = \pi \frac{\partial \phi}{\partial t} - \mathcal{H}$ the corresponding Lagrangian density. The term “periodic” means that the integration over the field is constrained in such a way that $\phi(\vec{x}, t_0) = \phi(\vec{x}, t_0 - i\beta)$.

Let us analytically extend the time parameter into the complex plane. Without loss of generality we can take $t_0 = 0$ in the above equations. So let time have no real component, and identify $t = -i\tau$ with a real parameter τ called imaginary time. This is the usual Wick rotation, which is used at $T = 0$ to make the path integral well-defined. Thus, we can obtain the partition function at finite temperature from the zero temperature generating functional performing an analytic continuation $it \rightarrow \tau$. We also need to restrict τ to the finite interval $0 \leq \tau \leq \beta$ and prescribe periodic boundary conditions for the fields $\phi(\vec{x}, \tau = 0) = \phi(\vec{x}, \tau = \beta)$. We observe that inverse temperature plays the role of an imaginary time variable.

1.3.2 Thermal functions

Evaluating the momentum integrals in (1.110), we obtain

$$Z = N \int_{\text{periodic}} [d\phi] \exp(S_E) \quad (1.111)$$

where S_E is the euclidean action defined as $S_E = \int_0^\beta d\tau \int d^3x \mathcal{L}$ and N is a normalization constant which depends on the temperature.

As in the $T = 0$ case, we can separate the action into two components: a free part (S_0), which is quadratic in the field, and an interacting part (S_I). We can expand it in powers of the interaction in such a way that the logarithm of the partition function of interest is

$$\begin{aligned} \log Z &= \log \left(N \int [d\phi] \exp(S_0 + S_I) \right) \\ &= \underbrace{\log \left(N \int [d\phi] \exp(S_0) \right)}_{\log Z_0} + \sum_{l=1}^{\infty} \frac{(-1)^l}{l!} \frac{\int [d\phi] \exp(S_0) S_I^l}{\int [d\phi] \exp(S_0)} \end{aligned} \quad (1.112)$$

This also breaks into two parts: the first one is the non interacting or ideal gas contribution while the second one is given by the corrections, which consist of the sum of all loop diagrams without external legs.

Free energy density of a non interacting field

The periodicity condition discretises the frequency spectrum of the wave-functions. In such a way that Fourier expansion of thermal bosonic fields contained in a box of size $V \times \beta$ is given by

$$\phi(\vec{x}, \tau) = \sqrt{\frac{\beta}{V}} \sum_{n=-\infty}^{\infty} \sum_{\vec{p}} e^{i(\vec{p} \cdot \vec{x} + \omega_n \tau)} \phi_n(\vec{p}) \quad (1.113)$$

with $\omega_n = 2\pi n/\beta$ the Matsubara frequencies and $n \in \mathbb{Z}$. By replacing the Fourier expansion (1.113) into the partition function, we obtain

$$\begin{aligned} Z_0(T) &= N(\beta) \int [d\phi] \exp \left\{ -\frac{\beta^2}{2} \sum_n \sum_{\vec{p}} (\omega_n^2 + E_i^2(p)) |\phi_n(\vec{p})|^2 \right\} \\ &= N(\beta) \prod_n \prod_{\vec{p}} [\beta^2 (\omega_n^2 + E_i^2(p))]^{-1/2} \end{aligned} \quad (1.114)$$

where $E_i(p) = \sqrt{|\vec{p}|^2 + M_i^2}$ and M_i is the mass of the field. Using the following identity,

$$\log [(2\pi n)^2 + \beta^2 x^2] = \int_1^{\beta^2 x^2} \frac{dy^2}{y^2 + (2\pi n)^2} + \log [1 + (2\pi n)^2] \quad (1.115)$$

and the result of the frequency sum given by equation (A.7) we get

$$\log Z_0(T) = \log N' - \frac{1}{2} \sum_{\vec{p}} \int_1^{\beta x} dx \left(1 + \frac{2}{e^x - 1} \right) \quad (1.116)$$

It can be demonstrated that the term coming from the log in equation (1.115) is both temperature dependent and infinite and its temperature dependent contribution to $\log Z_0$ is canceled by the presence of $\log N(\beta)$, resulting in a constant N' that is independent of the temperature.

Taking the continuum limit of $\vec{p}$ and calculating the above integral leads to

$$\log Z_0(T) = \log N' - V \int \frac{d^3 \vec{p}}{(2\pi)^3} \left[\frac{\beta E_i(p)}{2} + \log(1 - e^{-\beta E_i(p)}) \right] \quad (1.117)$$

Thus, the temperature dependent part of the free energy density of a scalar field i is given by

$$\epsilon_i^S(T) = T \int \frac{d^3 \vec{p}}{(2\pi)^3} \log [1 - e^{-\beta E_i(p)}] \quad (1.118)$$

Integrating by parts, we get

$$\epsilon_i^S(T) = -\frac{1}{2} g_0(M_i, T) \quad (1.119)$$

with

$$g_0(M, T) = \frac{T^4}{3\pi^2} \int_{M/T}^{\infty} dx \frac{[x^2 - (M/T)^2]^{3/2}}{e^x - 1} \quad (1.120)$$

For fermions, however, instead of periodic boundary conditions one has anti-periodic conditions (see [48] for more details). The temperature dependence of the free energy of a fermion field is very similar to the analogous formula (1.118) for scalar particles. A change of sign emerges due to the disparity between the fermion and boson properties. The integration involving anti-commuting variables leads to an overall minus sign, and the difference in periodicity conditions brings about an additional sign change for the logarithmic term in (1.118). In this way, we get

$$\epsilon_i^F(T) = -T \int \frac{d^3\vec{p}}{(2\pi)^3} \log [1 + e^{-\beta E_i(p)}] \quad (1.121)$$

Thermal propagator and tadpole diagram of a scalar field

We are now in a position to write down the 2-point Green function for a free bosonic field of mass M_i . By definition

$$G(M_i; \vec{x}, \tau) = \langle \mathcal{T} \{ \phi(\vec{x}, \tau) \phi(\vec{0}, 0) \} \rangle = \frac{1}{Z} \int [d\phi] \phi(\vec{x}, \tau) \phi(\vec{0}, 0) e^{S_E} \quad (1.122)$$

where $\mathcal{T}$ prescribes the time ordering

$$\mathcal{T} \{ \phi(\vec{x}, \tau) \phi(\vec{x}', \tau') \} = \begin{cases} \phi(\vec{x}, \tau) \phi(\vec{x}', \tau') & \tau > \tau' \\ \phi(\vec{x}', \tau') \phi(\vec{x}, \tau) & \tau' > \tau \end{cases} \quad (1.123)$$

An important result is obtained from the Heisenberg equation for the field operator $\phi(\vec{x}, \tau) = e^{H\tau} \phi(\vec{x}, 0) e^{-H\tau}$. Using the cyclic permutation property of a trace we get the following result

$$\langle \phi(\vec{x}, \tau) \phi(\vec{x}', 0) \rangle = \langle \phi(\vec{x}', \beta) \phi(\vec{x}, \tau) \rangle \quad (1.124)$$

which implies periodic boundary condition for the thermal propagators. This is called the Kubo-Martin-Schwinger relation (KMS).

Within the imaginary-time formalism of Thermal Field Theory, Feynman rules in momentum space are the same in euclidean space at $T = 0$ and at finite T except for the replacements $p_0 = i\omega_n$ (the zero components of four vectors contain the Matsubara frequencies) and

$$\int \frac{d^4p}{(2\pi)^4} \rightarrow T \sum_{n=-\infty}^{\infty} \int \frac{d^3\vec{p}}{(2\pi)^3} \equiv \oint_p \quad (1.125)$$

so the thermal free-propagator in position space becomes

$$G(M_i; \vec{x}, \tau) = T \sum_{n=-\infty}^{\infty} \int \frac{d^3 \vec{p}}{(2\pi)^3} e^{-i\omega_n \tau} e^{i\vec{p} \cdot \vec{x}} \frac{1}{\omega_n^2 + E_i^2(p)} \quad (1.126)$$

This sum can be easily carried out by using the contour integral method showed in appendix A. The result is

$$G(M_i; \vec{x}, \tau) = \int \frac{d^3 \vec{p}}{(2\pi)^3} e^{i\vec{p} \cdot \vec{x}} \frac{1}{2 E_i(p)} [(1 + n_B[E_i(p)])e^{-E_i(p)\tau} + n_B[E_i(p)]e^{E_i(p)\tau}] \quad (1.127)$$

An important result coming from this equation, which we will use in the following sections is the finite temperature integral of the tadpole diagram 1.6. This is given by

$$G(M, T) \equiv G(M_i; \vec{0}, 0) = G(M, T=0) + g_1(M, T) \quad (1.128)$$

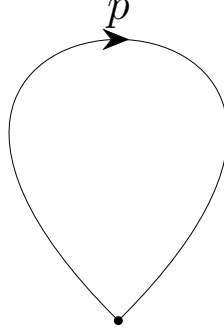


Figure 1.6: Tadpole diagram.

The divergent parts of the above loop integral will be parameterized in dimensional regularization (DR). Their explicit expressions including finite parts can be found in [34] at $T = 0$

$$G(M, 0) = -2M^2 R - \frac{M^2}{16\pi^2} \log \frac{M^2}{\mu^2} \quad (1.129)$$

with μ the renormalization scale and R defined in equation (1.79).

The g_1 function defined in [49] is

$$g_1(M, T) = \frac{T^2}{2\pi^2} \int_{M/T}^{\infty} dx \frac{[x^2 - (M/T)^2]^{1/2}}{e^x - 1} \quad (1.130)$$

Bubble loop diagram

Another thermal function we will use in this thesis is the one-loop bubble integral J_0 :

$$J_0(M_a, M_b; k_0, \vec{k}, T) = T \sum_{n=-\infty}^{\infty} \int \frac{d^3 \vec{p}}{(2\pi)^3} \frac{1}{[p^2 - M_a^2] [(p-k)^2 - M_b^2]}, \quad (1.131)$$

where $p = (i\omega_n, \vec{p})$, $k = (i\omega_m, \vec{k})$ and $i\omega_m \rightarrow z$ by analytic continuation which can be performed after the Matsubara sums are carried out (see Appendix A).

The J_0 function for unequal masses is given by [50]

$$J_0(M_a, M_b; z, \vec{k}, T) = - \int \frac{d^3\vec{p}}{(2\pi)^3} \frac{1}{4E_1E_2} \left[(1 + n_B(E_1) + n_B(E_2)) \left(\frac{1}{z - E_1 - E_2} - \frac{1}{z + E_1 + E_2} \right) + (n_B(E_2) - n_B(E_1)) \left(\frac{1}{z - E_1 + E_2} - \frac{1}{z + E_1 - E_2} \right) \right] \quad (1.132)$$

where we denote $E_1 \equiv E_1(p) = \sqrt{|\vec{p}|^2 + M_a^2}$ and $E_2 \equiv E_2(p - k) = \sqrt{|\vec{p} - \vec{k}|^2 + M_b^2}$.

Following the original analysis in [51], one can use (1.132) to obtain the cuts in the real k_0 axis for which the imaginary part of the J_0 integral is nonzero. The discontinuity along the cuts can be calculated from the above result setting $z = k_0 + i\epsilon$ ($\epsilon \rightarrow 0$) with $k_0 \in \mathbb{R}$ and using

$$\text{Im} \left(\frac{1}{k_0 \pm (E_1 \pm E_2) + i\epsilon} \right) = \mp \pi \delta[k_0 \pm (E_1 \pm E_2)] \quad (1.133)$$

In this way, the imaginary part of the J_0 function is given by

$$\begin{aligned} \text{Im } J_0(M_a, M_b; k_0 + i\epsilon, \vec{k}, T) = & \pi \int \frac{d^3\vec{p}}{(2\pi)^3} \frac{1}{4E_1E_2} \{ (1 + n_B(E_1) + n_B(E_2)) (\delta(k_0 - E_1 - E_2) - \delta(k_0 + E_1 + E_2)) \\ & + (n_B(E_1) - n_B(E_2)) (\delta(k_0 + E_1 - E_2) - \delta(k_0 - E_1 + E_2)) \} \end{aligned} \quad (1.134)$$

On the one hand, we have the standard unitary cut, which corresponds to the region of the integrand where $E_1 + E_2 = |k_0|$ (first term in (1.134)) requiring the condition $k^2 \geq (M_a + M_b)^2$ with $k^2 = k_0^2 - |\vec{k}|^2$. This cut is the one giving rise to unitarity already at $T = 0$. On the other hand, the second term in (1.134) gives rise to the so-called Landau cut, for $E_1 - E_2 = |k_0|$, which requires $-|\vec{k}|^2 \leq k^2 \leq (M_a - M_b)^2$ [52, 53]. This cut is purely thermal, i.e., it vanishes at $T = 0$. The analytic structure of the J_0 integral is represented in Fig. 1.7.

According to the optical theorem the imaginary part of the self energy of a particle can be obtained using the square of the amplitude of the decay process associated to it. The integral J_0 usually appears in the thermal self-energy, so it is possible to provide a physical interpretation for it in terms of decay and recombination processes. The Bose-Einstein function n_B and $1 + n_B$ weight the probability for absorption and production of particles, respectively. Consider, for example, a thermal bath with Ψ_0 , Ψ_1 and Ψ_2

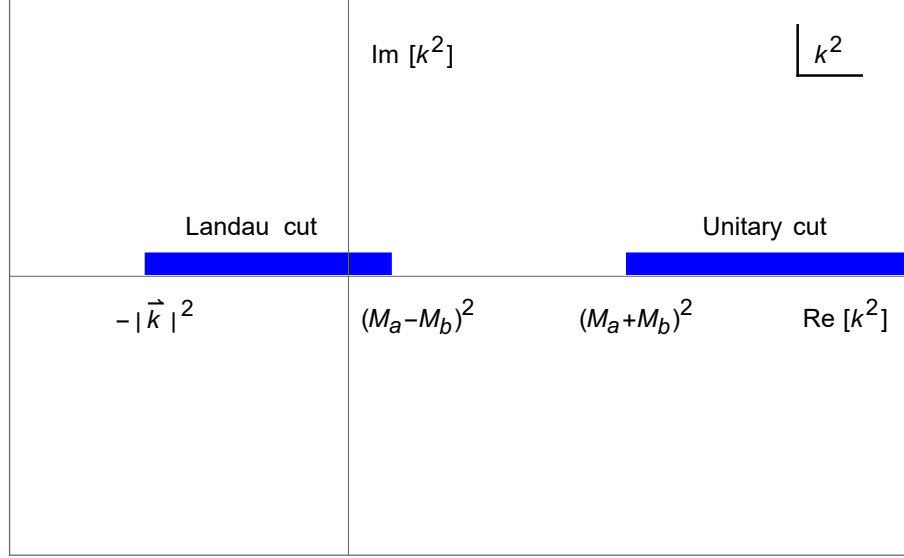


Figure 1.7: Cuts of the $J_0(M_a, M_b; k_0, \vec{k}, T)$ integral in (1.132) in the k^2 complex plane.

particles. For the decay $\Psi_0 \rightarrow \Psi_1 \Psi_2$, the in-medium Ψ_1 and Ψ_2 particles increase the available phase space by a statistical weight $[1 + n_B(E_1)][1 + n_B(E_2)]$. In addition to this, in the heat bath, it is also conceivable that Ψ_0 particles could spontaneously arise through inverse decay, i.e. $\Psi_1 \Psi_2 \rightarrow \Psi_0$, with weight $n_B(E_1) n_B(E_2)$ for absorption. Then writing $1 + n_B(E_1) + n_B(E_2) = [1 + n_B(E_1)][1 + n_B(E_2)] - n_B(E_1) n_B(E_2)$, we can see the correspondence between the distribution function present in the first term of (1.134) and the difference of these two rates. The term proportional to $n_B(E_1) - n_B(E_2)$ comes from processes like $\Psi_1 \rightarrow \Psi_0 \Psi_2$ and $\Psi_2 \rightarrow \Psi_0 \Psi_1$. This gives rise to the Landau cuts mentioned above, which we will explain in more detail in chapter 4.

A particularly interesting limit is the static one $\vec{k} = 0$. For $M_a = M_b = M$, the finite temperature part of $J_0(M; k_0, \vec{k} = \vec{0}, T)$ can be found for instance in [54, 55]. For $k_0 = 0$ satisfies

$$J_0(M; k_0 = 0, \vec{k} = \vec{0}, T) \equiv G_2(M, T) = -dG(M, T)/dM^2 = G_2(M, T = 0) + g_2(M, T) \quad (1.135)$$

with

$$g_2(M, T) = -\frac{dg_1(M, T)}{dM^2} = \frac{1}{4\pi^2} \int_{M/T}^{\infty} dx \frac{[x^2 - (M/T)^2]^{-1/2}}{e^x - 1} \quad (1.136)$$

The above functions g_0 , g_1 and g_2 are positive, vanish for $T = 0$ and increase with T for any mass M . In the chiral limit $g_0(0, T) = \pi^2 T^4/45$, $g_1(0, T) = T^2/12$ and $g_2(M \rightarrow 0^+, T) \rightarrow T/(8\pi M) + \mathcal{O}(\log M^2)$.

1.3.3 Chiral symmetry restoration at finite temperature

Chiral symmetry restoration and its nature are surely among the key problems for our present understanding of the QCD phase diagram. As depicted in Fig. 1.1, we expect a transition curve $\{T_c, (\mu_B)_c\}$ indicating the restoration of chiral symmetry and deconfinement. It is well established that in the physical case of $N_f = 2+1$ flavours with $m_l \ll m_s$ quark masses, the chiral transition is a crossover at a transition temperature of about $T_c \sim 155 - 160$ MeV for vanishing baryon density ($\mu_B = 0$) [56–59]. The ideal chiral restoration phase transition is reached only for $N_f = 2$ and $m_l = 0$, while in the physical case it is approached in the light chiral limit $m_l \rightarrow 0^+$ [60].

The main features of chiral symmetry restoration can be read from the quark condensate and the scalar susceptibility, derived from the vacuum energy density as

$$\langle \bar{q}q \rangle_l = \langle \bar{u}u + \bar{d}d \rangle = \frac{\partial \epsilon}{\partial m_l} = 2B_0 \frac{\partial \epsilon}{\partial M_{0\pi}^2} \quad (1.137)$$

$$\chi_S = -\frac{\partial \langle \bar{q}q \rangle_l}{\partial m_l} = -2B_0 \frac{\partial \langle \bar{q}q \rangle_l}{\partial M_{0\pi}^2} \quad (1.138)$$

Quark condensates at finite temperature in the lattice are affected by $T = 0$ finite-size divergences. Therefore, one needs to consider condensate combinations for which lattice analysis yield definite predictions, being free of finite-size divergences. One of the condensate combinations that bears this property is the subtracted quark condensate

$$\Delta_{l,s}(T) = m_s \langle \bar{q}q \rangle_l(T) - 2m_l \langle \bar{s}s \rangle(T), \quad (1.139)$$

although its normalized form $\bar{\Delta}_{l,s}(T) = \Delta_{l,s}(T)/\Delta_{l,s}(0)$ is also commonly used.

The chiral crossover transition would be characterized by the quark condensate developing a sharp inflection point at the transition temperature T_c and the scalar susceptibility developing a peak at T_c , as confirmed by lattice analyses [61, 62]. The inflection point around T_c is clearly seen in the Fig. 1.8. We also plot in Fig. 1.9 the subtracted scalar susceptibility $\Delta\chi_S = \chi_S(T) - \chi_S(0)$, showing the expected peak around T_c .

The ChPT expansion is adequate to provide the low and intermediate temperature behaviour for those quantities, i.e., in the T region where the hadron gas is dominated by the lightest states. As the temperature rises, hadron states with higher masses become more important due to their distinctive Boltzmann weight. This behaviour can be seen in Fig. 1.10 where we plot the particle density (defined in equation (1.96)) of the pion and kaon component of the hadron gas, compared with the rest of hadron states quoted by the Particle Data Group with masses below 2 GeV.

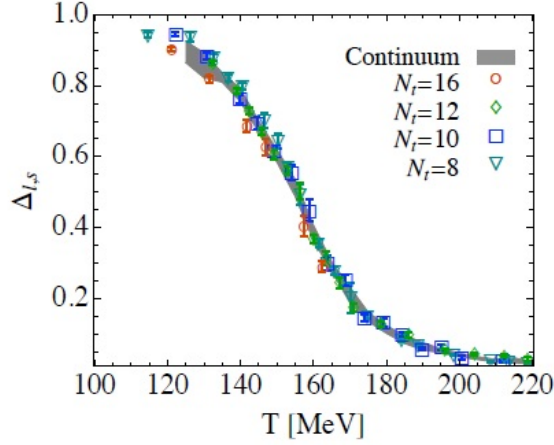


Figure 1.8: Subtracted chiral condensate $\Delta_{l,s}$ normalized to its value at zero temperature [63].

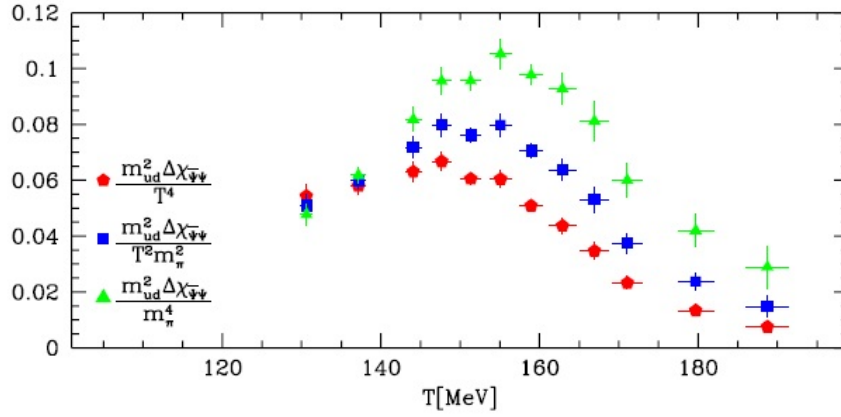


Figure 1.9: Temperature dependence of the renormalized chiral susceptibility [56].

More accurate predictions need the inclusion of higher mass states, as in the Hadron Resonance Gas approximation described below or the approach provided in this thesis and explained in section 2.3. However, the pion gas may still provide a valid qualitative picture of chiral restoration close to the chiral (or infrared) limit $M_{0\pi} \rightarrow 0^+$ which can be formally understood as $T \gg M_{0\pi}$, and where the pions are meant to be the main component responsible for the melting of the quark condensate [49, 64]. In addition, near the chiral limit, the transition temperature determined in ChPT as the vanishing of the quark condensate coincides with other determinations such as the degeneration temperature of the scalar and pseudoscalar susceptibilities [65].

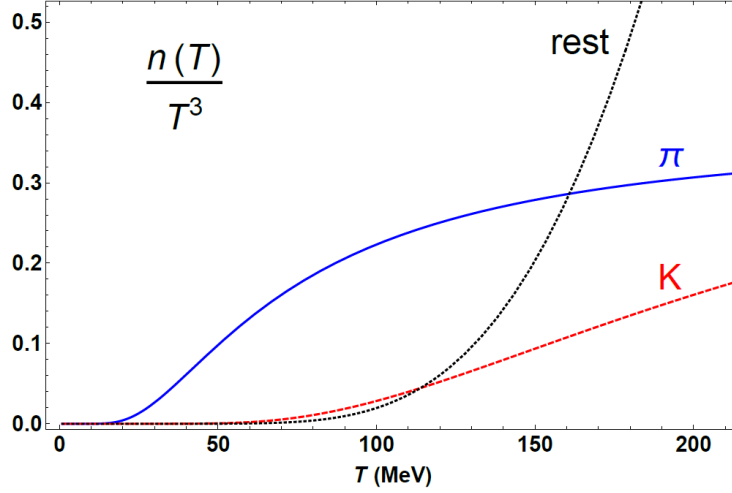


Figure 1.10: Particle density calculated within the free particle density for pions, kaons and the rest of states in the Particle Data Group with masses below 2 GeV.

1.3.4 Hadron Resonance Gas

From the theoretical side, it is important to provide reliable approximations which could describe the expected behaviour for the quark condensate and the scalar susceptibility and eventually be used to fit lattice data. The most widely used approach in this context has been the Hadron Resonance Gas (HRG) approximation [66–73]. This approximation works quite well below T_c , where it is meant to be valid, although qualitatively it does not reproduce the inflection point expected for the quark condensate, nor the peak of the scalar susceptibility in the crossover regime.

The HRG is a statistical model of QCD which considers a non-interacting gas of hadrons and resonances, including in principle all hadron states quoted in the PDG [74] up to a given energy above which Boltzmann suppression is effective. The interactions between hadrons can be neglected in a sufficiently dilute gas. In such cases, the QCD partition function can be factorized into one-particle partition functions

$$\log Z = \sum_i \log Z_i \quad (1.140)$$

The free energy density in the simplest HRG approximation, i.e., considering only free resonant states without including their width nor their interactions, is given by

$$\epsilon(T) = \epsilon_M(T) + \epsilon_B(T), \quad (1.141)$$

$$\epsilon_M(T) = \sum_M d_i \epsilon_i^S(T), \quad (1.142)$$

$$\epsilon_B(T) = \sum_B d_i \epsilon_i^F(T) \quad (1.143)$$

where M and B stand for the meson and baryon contributions and ϵ_i^S and ϵ_i^F are the energy density of scalar and fermionic fields respectively, which are given in eqs. (1.118) and (1.121). The sum extends to hadron states with degeneracy d_i and mass M_i quoted in the PDG [74]. Here, we will consider only hadron states up to $M = 2$ GeV, following [73].

From the pressure or the free energy density one can in principle derive straightforwardly the light quark condensate according to (1.137)

$$\langle \bar{q}q \rangle_l(T) = \langle \bar{q}q \rangle_{l,M}(T) + \langle \bar{q}q \rangle_{l,B}(T) \quad (1.144)$$

$$\langle \bar{q}q \rangle_{l,M}(T) - \langle \bar{q}q \rangle_{l,M}(0) = \frac{1}{2} \sum_M d_i \frac{\partial M_i^2}{\partial m_l} g_1(M_i, T) \quad (1.145)$$

$$\langle \bar{q}q \rangle_{l,B}(T) - \langle \bar{q}q \rangle_{l,B}(0) = \frac{1}{2} \sum_B d_i \frac{\partial M_i^2}{\partial m_l} g_1^F(M_i, T) \quad (1.146)$$

and the scalar susceptibility (1.138),

$$\chi_S(T) = \chi_{S,M}(T) + \chi_{S,B}(T) \quad (1.147)$$

$$\chi_{S,M}(T) - \chi_{S,M}(0) = \frac{1}{2} \sum_M d_i \left[\left(\frac{\partial M_i^2}{\partial m_l} \right)^2 g_2(M_i, T) - \frac{\partial^2 M_i^2}{\partial m_l^2} g_1(M_i, T) \right] \quad (1.148)$$

$$\chi_{S,B}(T) - \chi_{S,B}(0) = \frac{1}{2} \sum_B d_i \left[\left(\frac{\partial M_i^2}{\partial m_l} \right)^2 g_2^F(M_i, T) - \frac{\partial^2 M_i^2}{\partial m_l^2} g_1^F(M_i, T) \right] \quad (1.149)$$

where

$$g_1^F(M_i, T) = 2 \frac{\partial \epsilon_i^F(T)}{\partial M_i^2}, \quad g_2^F(M_i, T) = - \frac{\partial g_1^F}{\partial M_i^2}. \quad (1.150)$$

As we have seen, the HRG formulation is parametrized in terms of hadron masses, so that any calculation involving quark mass derivatives requires modeling the hadron mass dependence on quark masses. Several approximations for such dependence have been followed in the literature within the HRG context, starting from a simple linear dependence of the form $\frac{\partial M_h}{\partial M_\pi^2} = 2C$ with constant C [67, 69] to more elaborated ones [68, 70, 71, 73].

As a toy model, we can calculate the quark condensate and the scalar susceptibility (Fig. 1.11) using only the LO masses given in (1.72) for the pseudo-NGB:

$$\frac{\langle \bar{q}q \rangle_l(T)}{\langle \bar{q}q \rangle_l(0)} = 1 - \frac{3}{4F_\pi^2} g_1(M_\pi, T) - \frac{1}{4F_\pi^2} g_1(M_K, T) - \frac{1}{6F_\pi^2} g_1(M_\eta, T) \quad (1.151)$$

$$\frac{\chi_S(T) - \chi_S(0)}{4B_0^2} = \frac{3}{2} g_2(M_\pi, T) + \frac{1}{2} g_2(M_K, T) + \frac{9}{32} g_2(M_\eta, T) \quad (1.152)$$

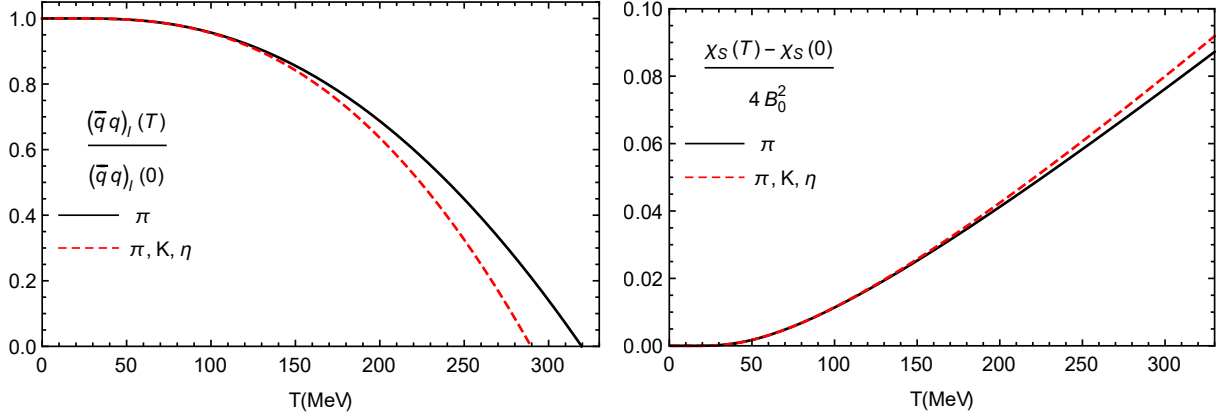


Figure 1.11: Quark condensate and scalar susceptibility considering interactions between pions (black line) and pion, kaon and eta mesons (red dashed line).

In Fig. 1.11 we note that the transition temperature increases with the number of resonances we consider in the study. Two opposing effects appear when we introduce more hadrons into the calculation. On the one hand, entropy increases, resulting in a decrease in the temperature at which the transition occurs. On the other hand, there is a greater symmetry breaking, which leads to an increase in the transition temperature. As the hadrons become heavier, their contribution to the condensate diminishes, so the effect that has the most impact is the increase in entropy. That is, the introduction of massive states, which is a ferromagnetic-like effect, is overshadowed by the paramagnetic-like disorder introduced by adding degrees of freedom to the system. The scalar susceptibility increases without reaching a maximum at the critical temperature. Moreover, the introduction of additional hadrons leads to an accelerated growth rate, consistently with the previously mentioned idea of the decreasing critical temperature.

1.4 Scattering and Unitarity

1.4.1 The scattering amplitude

The unitary operator that connects asymptotic in $|i\rangle$ and out $|f\rangle$ states is called the S -matrix. In other words, after the collision we have a state $|f\rangle = S|i\rangle$ and the amplitude to go from $|i\rangle$ to $|f\rangle$ is

$$\langle f|S|i\rangle \quad (1.153)$$

The physical importance of the S -matrix is that the largest part of the experimental data of quantum field theory are about scattering experiments.

The scattering matrix S is related to the transition matrix $\mathcal{T}$ by

$$S = \mathbb{1} + i\mathcal{T} \quad (1.154)$$

where trivial identity corresponds to the case when no interaction occurs at all and $\mathcal{T}$ encodes all the information on the interactions.

To begin our study of the analyticity of relativistic amplitudes, we will discuss the kinematics that relate two-body crossed reactions. It is desirable to express the invariant amplitude as a function of variables invariant under Lorentz transformations. We will consider scattering of particles with definite momentum p_μ . The momentum of a particle satisfies the on-shell condition

$$p_i^2 = (p_i^0)^2 - |\vec{p}_i|^2 = m_i^2 \quad (1.155)$$

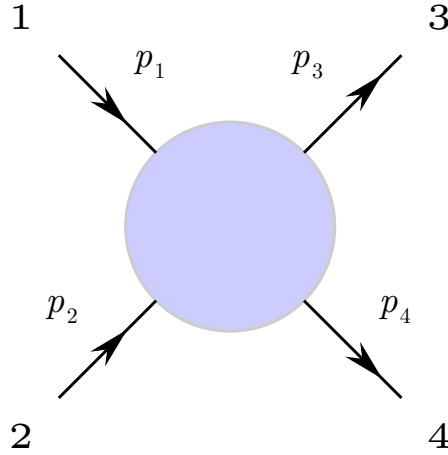


Figure 1.12: Two-body scattering process $1 + 2 \rightarrow 3 + 4$.

For a reaction $1 + 2 \rightarrow 3 + 4$ (Fig. 1.12), where the particles have masses m_i and four-momentum $p_i = (p_i^0, \vec{p}_i)$, the Lorentz invariant Mandelstam variables, s , t and u are defined by:

$$s = (p_1 + p_2)^2 = (p_3 + p_4)^2 \quad (1.156)$$

$$t = (p_1 - p_3)^2 = (p_2 - p_4)^2 \quad (1.157)$$

$$u = (p_1 - p_4)^2 = (p_2 - p_3)^2 \quad (1.158)$$

These quantities can take on all real values consistent with

$$s + t + u = \sum_i m_i^2 \quad (1.159)$$

Equation (1.159) means that the dynamic of the process depends not only on s , but also on the variable t (or u).

By reversing the signs of some of the four-momenta, Fig. 1.12 can also represent the t -channel process $1 + \bar{3} \rightarrow \bar{2} + 4$ and the u -channel process $1 + \bar{4} \rightarrow 3 + \bar{2}$, where the bar denotes the antiparticle. The s -channel center of mass (CM) frame is defined by $\vec{p}_1 + \vec{p}_2 = \vec{p}_3 + \vec{p}_4 = \vec{0}$ and the four momenta can be taken to be

$$\begin{aligned} p_1 &= (p_1^0, \vec{p}), & p_3 &= (p_3^0, \vec{k}), \\ p_2 &= (p_2^0, -\vec{p}), & p_4 &= (p_4^0, -\vec{k}) \end{aligned} \quad (1.160)$$

where $\vec{p}$ is the three-momentum of particle 1 and $\vec{k}$ the three-momentum of particle 3 in this frame. The energies p_i^0 are expressed in term of the invariant s and the masses

$$\begin{aligned} p_1^0 &= \frac{(s + m_1^2 - m_2^2)}{2\sqrt{s}}, & p_3^0 &= \frac{(s + m_3^2 - m_4^2)}{2\sqrt{s}} \\ p_2^0 &= \frac{(s + m_2^2 - m_1^2)}{2\sqrt{s}}, & p_4^0 &= \frac{(s + m_4^2 - m_3^2)}{2\sqrt{s}} \end{aligned} \quad (1.161)$$

and the momenta are defined as

$$|\vec{p}|^2 = p_1^0 - m_1^2 = \frac{1}{4s} (s - (m_1 + m_2)^2) (s - (m_1 - m_2)^2) \quad (1.162)$$

$$|\vec{k}|^2 = p_3^0 - m_3^2 = \frac{1}{4s} (s - (m_3 + m_4)^2) (s - (m_3 - m_4)^2) \quad (1.163)$$

The variables given in (1.158) can be expressed in terms of the modulus of the particle momenta $|\vec{p}|$ and $|\vec{k}|$ in addition to the scattering angle θ

$$\begin{aligned} s &= (p_1^0 + p_2^0)^2 \\ t &= m_1^2 + m_3^2 - 2(p_1^0 p_3^0 - |\vec{p}| |\vec{k}| \cos \theta) \\ u &= m_1^2 + m_4^2 - 2(p_1^0 p_4^0 + |\vec{p}| |\vec{k}| \cos \theta) \end{aligned} \quad (1.164)$$

In the elastic scattering of unequal mass particles $m_1 = m_3 = M_a$, $m_2 = m_4 = M_b$, with $M_a > M_b$, equation (1.164) simplifies to

$$\begin{aligned} s &= (p_1^0 + p_2^0)^2 \\ t &= -2p_{\text{CM}}^2 (1 - \cos \theta) \\ u &= \frac{(M_a^2 - M_b^2)^2}{s} - 2p_{\text{CM}}^2 (1 + \cos \theta) \end{aligned} \quad (1.165)$$

Note that, in this case, the momentum in the CM frame satisfies $p_{\text{CM}} = |\vec{p}| = |\vec{k}|$, i.e.

$$p_{\text{CM}}^2(s; M_a, M_b) = \frac{1}{4s} (s - (M_a + M_b)^2) (s - (M_a - M_b)^2) \quad (1.166)$$

All values of s , t and u for which $p_{\text{CM}} \geq 0$ and $|\cos \theta| \leq 1$ compose the physical region in the s-channel. The limits on t and u are obtained in terms of $\cos \theta = \pm 1$. Thus, using equation (1.165) we get the physical region for the s-channel

$$\text{s-channel: } s \geq (M_a + M_b)^2, \quad t \leq 0, \quad u \leq \frac{(M_a^2 - M_b^2)^2}{s} \quad (1.167)$$

For the t-channel process $1 + \bar{3} \rightarrow \bar{2} + 4$ we have

$$\begin{aligned} (p_1 + p_3)^2 &= (p_1 - p_3)^2 = t \\ (p_1 - p_2)^2 &= (p_1 - p_2)^2 = s \end{aligned} \quad (1.168)$$

and the physical region is

$$\text{t-channel: } t \geq 4M_a^2, \quad s \leq 0, \quad u \leq \frac{(M_a^2 - M_b^2)^2}{s} \quad (1.169)$$

In the same way, for the u-channel we have

$$\text{u-channel: } u \geq (M_a + M_b)^2, \quad t \leq 0, \quad s \leq \frac{(M_a^2 - M_b^2)^2}{u} \quad (1.170)$$

where we can see that the u-channel process is kinetically the same as that the s-channel exchanging $s \leftrightarrow u$.

To display the symmetry between channels the physical regions can be depicted on a two dimensional plot, the so-called Mandelstam diagram (Fig. 1.13). From (1.167), (1.169), and (1.170) we can see that the scattering angle condition forces the physical region to be delimited by the hyperbola $u = (M_a^2 - M_b^2)^2/s$. For equal mass elastic scattering, the geometry of the boundaries of the physical regions immediately becomes easier, which can be seen in Fig. 1.14.

The crossing relations concept assumes that there exists a single analytic function $\mathcal{T}(s, t, u)$ with the following properties:

$$\mathcal{T}(s, t, u) = \begin{cases} \mathcal{T}_{12 \rightarrow 34}(s, t, u) & s \geq (M_a + M_b)^2, \quad t \leq 0, \quad u \leq (M_a^2 - M_b^2)^2/s, \\ \mathcal{T}_{1\bar{3} \rightarrow \bar{2}4}(t, s, u) & t \geq 4M_a^2, \quad s \leq 0, \quad u \leq (M_a^2 - M_b^2)^2/s, \\ \mathcal{T}_{1\bar{4} \rightarrow 3\bar{2}}(u, t, s) & u \geq (M_a + M_b)^2, \quad t \leq 0, \quad s \leq (M_a^2 - M_b^2)^2/u. \end{cases}$$

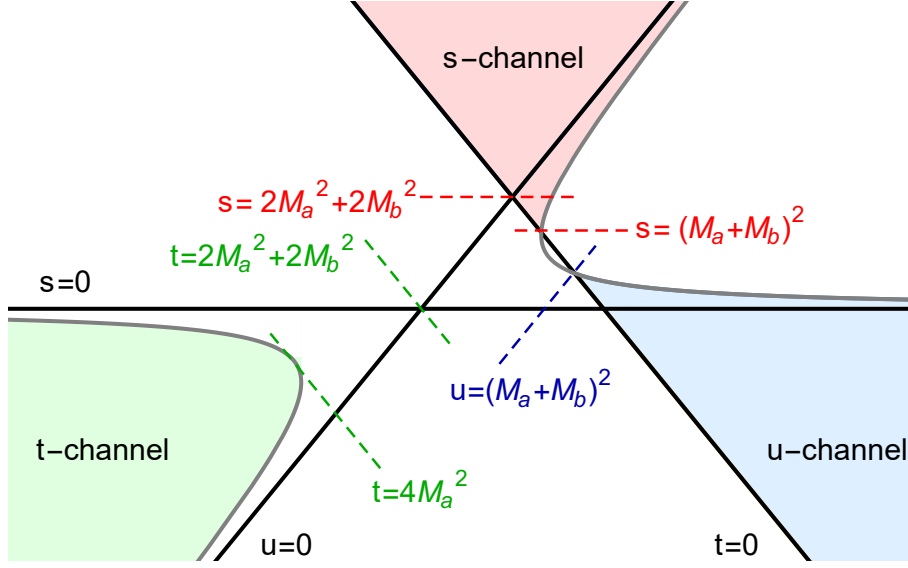


Figure 1.13: Mandelstam diagram for elastic scattering of unequal mass particles.

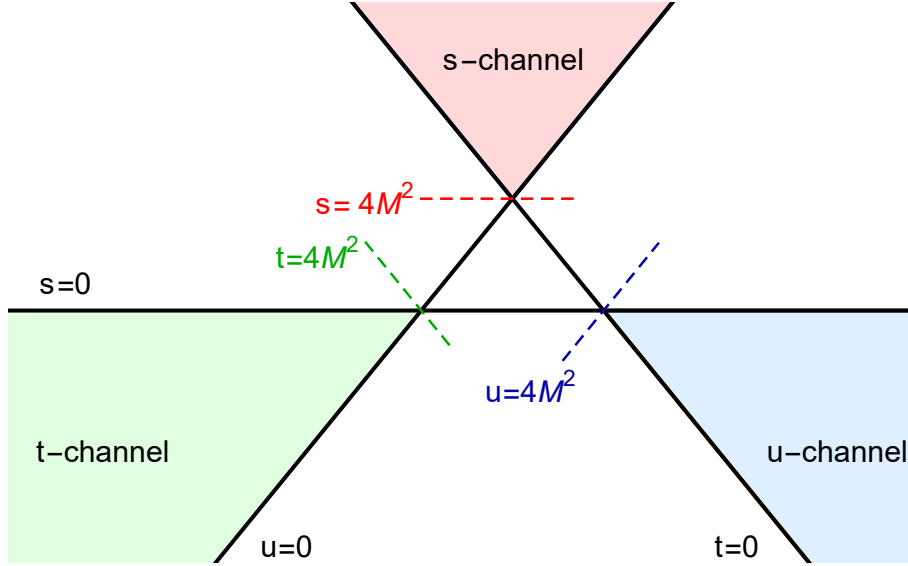


Figure 1.14: Mandelstam diagram for elastic scattering of equal mass particles ($M = M_a = M_b$).

Once the isospin amplitudes are calculated, it is also very useful to work with partial waves of well defined isospin I and angular momentum J . Let us denote by t^{IJ} the partial wave of the scattering amplitude and $\mathcal{T}_I$ the projection of the isospin amplitude,

$$t^{IJ}(s) = \frac{1}{32\pi N} \int_{-1}^1 dx P_J(x) \mathcal{T}_I(s, t(s, x), u(s, x)) \quad (1.171)$$

where $x = \cos \theta$ is the cosine of the scattering angle in the CM frame and $P_J(x)$ is the Legendre Polynomial of the first kind, of order J . Note that we have introduced an overall factor of N , which is equal to one except in the case of the scattering of identical

particles where $N = 2$.

Partial wave amplitude can be parameterized with a real phase δ_{IJ} , called phase shift, as

$$t^{IJ} = \frac{\sqrt{s}}{2p_{\text{CM}}} e^{i\delta_{IJ}} \sin(\delta_{IJ}) \quad (1.172)$$

At low energies, it is also characterized by two expansion parameters, namely the scattering length a_J^I and the slope b_J^I

$$\text{Re } t^{IJ} = \frac{\sqrt{s}}{2} p_{\text{CM}}^{2J} [a_J^I + p_{\text{CM}}^2 b_J^I + \mathcal{O}(p_{\text{CM}}^4)] \quad (1.173)$$

Besides the right cut, the projection amplitudes in partial waves will produce an additional source of singularities one has to take into account, which involves the angular integration over the Legendre polynomials P_J in (1.171). This is due to the singularities that are produced inside the amplitude for t or u values. The easiest way to analyze these singularities is through the so-called Froissart-Gribov representation of scattering partial waves, which, in turn, is expressed in terms of the Legendre functions of second kind $Q_J(x)$. The functions $Q_J(x)$ are analytic in the x plane but for two discontinuities with branch points at $x = \pm 1$. Thus, in the CM frame, partial waves will be singular at those values of s satisfying

$$1 + \frac{t}{2p_{\text{CM}}^2} = \pm 1, \quad 1 + \frac{1}{2p_{\text{CM}}^2} \left(u - \frac{(M_a^2 - M_b^2)^2}{s} \right) = \pm 1. \quad (1.174)$$

for values of t and u in the ranges

$$4M_b^2 \leq t, \quad (M_a + M_b)^2 \leq u, \quad (1.175)$$

The solutions of (1.174) and (1.175) involve two additional discontinuities. Namely, around the circle $|s| \leq M_a^2 - M_b^2$ and along the negative real axis from $s \in (-\infty, 0]$, arising from the t channel; along the real axis from $(M_a - M_b)^2$ to $-\infty$, arising from the u channel. Therefore, we can conclude that the partial wave possesses the analytic structure depicted in Fig. 1.15.

1.4.2 Unitarity

In quantum mechanics and in quantum field theory, unitarity is understood as the restriction on the system dynamics such that starting from the initial state, the probability of ending up in some final state is unity.

$$1 = \sum_f |\langle f|S|i \rangle|^2 = \sum_f \langle i|S^\dagger|f \rangle \langle f|S|i \rangle = \langle i|S^\dagger S|i \rangle \quad (1.176)$$

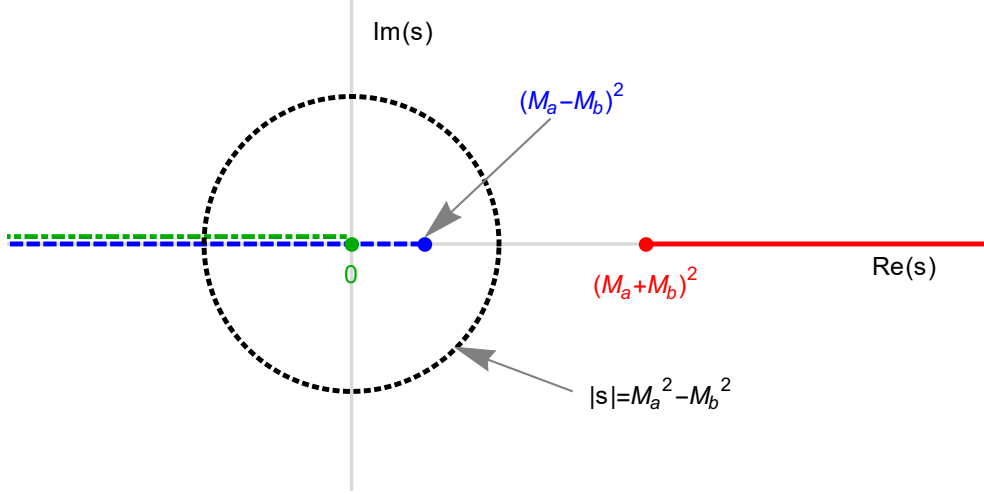


Figure 1.15: General cut structure of the partial waves of the scattering of two particles with different masses M_a and M_b .

From the unitarity of the S -matrix it follows that

$$SS^\dagger = \mathbb{1} + i(\mathcal{T} - \mathcal{T}^\dagger) + |\mathcal{T}|^2 = \mathbb{1} \quad (1.177)$$

Let us consider again the process of Fig. 1.12 where $|i\rangle = |p_1, p_2\rangle$ and $|f\rangle = |p_3, p_4\rangle$. For the partial waves, above the physical threshold $s \geq (M_a + M_b)^2$ and below other possible thresholds for the IJ channel, unitarity imposes the following constraint

$$\text{Im } t_{IJ} = \sigma_{ab}(s) |t_{IJ}|^2 \quad (1.178)$$

where $\sigma_{ab}(s)$ is the two particle phase space. Explicitly:

$$\sigma_{ab}(s) = \frac{2}{\sqrt{s}} p_{\text{CM}}(s; M_a, M_b) = \sqrt{\left(1 - \frac{(M_a + M_b)^2}{s}\right) \left(1 - \frac{(M_a - M_b)^2}{s}\right)} \quad (1.179)$$

The phase space can be extended at finite temperature replacing it by the thermal phase space $\sigma_{ab}^T(s)$ defined as

$$\sigma_{ab}^T(s) = \sigma_{ab}(s) \left[1 + n_B \left(\frac{s + \Delta_{ab}}{2\sqrt{s}} \right) + n_B \left(\frac{s - \Delta_{ab}}{2\sqrt{s}} \right) \right]. \quad (1.180)$$

1.4.3 Scattering amplitude at finite temperature in ChPT

In the following discussion, we will begin by briefly examining the concept of thermal scattering amplitude. For the scope of our objectives, we will assume that the system is in thermal equilibrium.

In Thermal Field Theory, the term "amplitude" commonly refers to a thermal Green function, instead of an S-matrix element. As in previous analyses at finite temperature [54, 75–77], the scattering amplitude is defined by connecting the four-point Green function with the $\mathcal{T}$ -matrix element through the Lehman-Symanzik-Zimmerman (LSZ) reduction formula with respect to the asymptotic external legs [78]. In doing so, one has to take into account the modification of the free particle dispersion relation due to self-interactions. Thus, the LSZ formula extracts the residue of the Green function at the poles given by the dispersion relation of the external legs.

As we have already explained, in the framework of imaginary-time formalism we can calculate the time-ordered product at $T \neq 0$. For the definition of the scattering amplitude at finite temperature, we follow the standard prescription and assume that the temperature dependence arises in the loops from the Thermal Field Theory Feynman rules.

At $T = 0$ energy-momentum conservation and the on-shell condition for external legs leave only three Lorentz-invariant quantities for a generic scattering process $p_1 p_2 \rightarrow p_3 p_4$, e.g., $p_1 \cdot p_2$, $p_1 \cdot p_3$, $p_2 \cdot p_3$ or s, t, u . However, at $T \neq 0$, an important aspect to consider is the need to explicitly distinguish between the time and space-like components of any four-vector due to the loss of Lorentz covariance resulting from the choice of the thermal bath rest frame. In this way, one has six independent rotation invariants, e.g., $\vec{p}_1 \cdot \vec{p}_2$, $\vec{p}_1 \cdot \vec{p}_3$, $\vec{p}_2 \cdot \vec{p}_3$, p_1^0 , p_2^0 , p_3^0 . If we define $\mathbf{S} = p_1 + p_2$, $\mathbf{T} = p_1 - p_3$ and $\mathbf{U} = p_1 - p_4$ the amplitude will depend on $\mathbf{S}$, $\mathbf{T}$, $\mathbf{U}$, S^0 , T^0 , U^0 . In this case, the on-shell condition (1.159) reduces the number of independent variables to five.

In the following, we are going to be interested in the elastic $\pi\pi \rightarrow \pi\pi$ and $K\pi \rightarrow K\pi$ scattering amplitudes. The relevant type of Feynman diagrams are shown in Fig. 1.16 up to $\mathcal{O}(p^4)$ in the chiral power counting.

The general structure of the amplitude is as follows. First, as for $T = 0$, one has to consider the contributions from the S, T, U - channels corresponding to the different ways of pairing incoming and outgoing external momenta in the reaction $p_1 p_2 \rightarrow p_3 p_4$ as shown in Fig. 1.16. For every one of those channels and for the sum of them, crossing symmetry still holds in terms of $\mathbf{S}$, $\mathbf{T}$ and $\mathbf{U}$ (since the temperature does not modify the vertices) and the amplitude at finite temperature can be written according to the general structure

$$\mathcal{T}(\mathbf{S}, \mathbf{T}, \mathbf{U}; T) = \mathcal{T}_2(s, t, u) + \overbrace{\mathcal{T}_4^{tree}(s, t, u) + \mathcal{T}_4^G(\mathbf{S}, \mathbf{T}, \mathbf{U}; T) + \mathcal{T}_4^J(\mathbf{S}, \mathbf{T}, \mathbf{U}; T)}^{\mathcal{T}_4(\mathbf{S}, \mathbf{T}, \mathbf{U}; T)}, \quad (1.181)$$

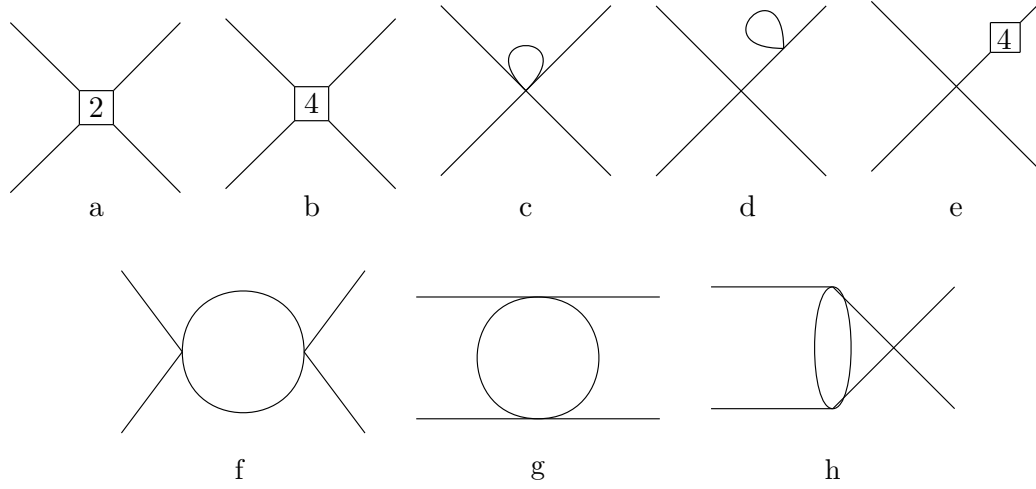


Figure 1.16: Feynman diagrams corresponding to the $\pi\pi \rightarrow \pi\pi$ and $K\pi \rightarrow K\pi$ scattering amplitude up to fourth order in ChPT.

The different contributions to the amplitude read as follows: $\mathcal{T}_2(s, t, u)$ is the tree-level $\mathcal{O}(p^2)$ contribution to the amplitude coming from the $\mathcal{L}_2$ Lagrangian (diagram a in Fig. 1.16) and $\mathcal{T}_4(\mathbf{S}, \mathbf{T}, \mathbf{U}; T)$ is the $\mathcal{O}(p^4)$ contribution. Diagram b comes from $\mathcal{L}_4$ at tree level, diagram c is the one-loop tadpole correction coming from the $\mathcal{O}(p^2)$ six-pion vertex, diagrams d and e account for the renormalization of the external legs at this order and therefore give rise to the modification of the dispersion relation, while diagrams f, g, h correspond, respectively, to the S, T, U channels of the one-loop contributions with two $\mathcal{O}(p^2)$ four-pion vertices. In this way, we can express the $\mathcal{T}_4(\mathbf{S}, \mathbf{T}, \mathbf{U}; T)$ thermal amplitude as the sum of $\mathcal{T}_4^{tree}$, which is the $\mathcal{O}(p^4)$ tree-level $\mathcal{L}_4$ contribution, plus $\mathcal{T}_4^G$ and $\mathcal{T}_4^J$, which are the one-loop contributions, from which the temperature dependence arises, standing for the tadpole-like and J -like thermal integrals in diagrams c, d, f-h in Fig. 1.16.

Since one-loop diagrams in the $\mathcal{T}_4$ contributions are obtained from the $\mathcal{L}_2$ Lagrangian and it contains only two derivatives, loop integrals with up to four moments in the numerator appear in the amplitude. These integrals can be expressed as a combination of tadpole and bubble loop integrals. In addition to the J_0 function, the thermal amplitude is also expressed in terms of J_1 and J_2 quantities, which are defined as follows

$$J_k(M_a, M_b; \mathcal{Q}_0, \vec{\mathcal{Q}}, T) = T \sum_{n=-\infty}^{\infty} \int \frac{d^3\vec{p}}{(2\pi)^3} \frac{p_0^k}{[p^2 - M_a^2] [(p - \mathcal{Q})^2 - M_b^2]}, \quad k = 0, 1, 2, \quad (1.182)$$

We will also use the notation $J_k^{ab}(\mathcal{Q}_0, \vec{\mathcal{Q}}, T)$ instead of $J_k(M_a, M_b; \mathcal{Q}_0, \vec{\mathcal{Q}}, T)$ throughout

the thesis.

For equal masses $M_a = M_b$, the relations that help to simplify the amplitude expression as a function of the G and J integrals were given in [54]. In the same paper, the J_k thermal integrals for thermal pion scattering were also analyzed. For the unequal mass case, the functions $J_{1,2}$ will be discussed in chapter 4.

Once the amplitude $\mathcal{T}(\mathbf{S}, \mathbf{T}, \mathbf{U}; T)$ has been calculated, the corresponding isospin projections are performed. One can then set the center of mass conditions to construct the projection into IJ partial waves. In the $12 \rightarrow 34$ elastic scattering with $m_1 = m_3 = M_a$, $m_2 = m_4 = M_b$, we define the partial-wave projection [79] as

$$t^{IJ}(s, T) = \frac{1}{32\pi N} \int_{-1}^1 dx P_J(x) \times \times \mathcal{T}_I \left[S_0 = \sqrt{s}, \vec{S} = \vec{0}, T_0 = 0, |\vec{T}|^2 = -t(s, x), U_0 = \frac{\Delta_{ab}}{\sqrt{s}}, |\vec{U}|^2 = 2p_{\text{CM}}^2(1+x); T \right] \quad (1.183)$$

with $\Delta_{ab} = M_a^2 - M_b^2$.

The pion-pion scattering amplitude at finite temperature was calculated in [54]. In chapter 4, we will study pion-kaon scattering.

1.4.4 Unitarization methods

Because ChPT constitutes a perturbative expansion in energy, it does not respect exact unitarity, therefore additional methods are necessary to get its unitarization.

A well-established framework used to describe resonances, without having to appeal to an explicit field Lagrangian realization, is Unitarized Chiral Perturbation Theory (UChPT). One starts from the ChPT series for the scattering amplitude in a given channel, projected into partial waves, namely

$$t^{IJ}(s, T) \simeq t_2^{IJ}(s) + t_4^{IJ}(s, T) + \dots \quad (1.184)$$

where $t_n^{IJ} = \mathcal{O}(p^n)$. The t_4 contribution contains one-loop diagrams from the second-order ChPT Lagrangian as well as tree level terms from the fourth order one proportional to the LECs. The temperature corrections arise in loops and are therefore included from the t_4 contribution onwards. The ChPT series ensures the model-independent low-energy behaviour and is unitary only perturbatively, i.e. for one open channel with $s \geq (M_1 + M_2)^2$ we have:

$$\text{Im } t_2 = 0 \quad (1.185)$$

$$\text{Im } t_4 = \sigma_{ab}^T |t_2|^2 \quad (1.186)$$

and so on for higher orders. In that way, it is possible to obtain the term t_n^{IJ} from the previous ones. According to that, chiral expansion grows arbitrarily with energy and, for these reason, partial waves cannot reproduce resonances.

For an elastic process, unitarity implies that

$$\text{Im } t = \sigma_{ab}^T(s) |t|^2 \Rightarrow \text{Im } \frac{1}{t} = \frac{\text{Im } t}{|t|^2} = -\sigma_{ab}^T \quad (1.187)$$

which means that the imaginary part of the inverse of the amplitude for $s \geq (M_a + M_b)^2$ is known at any orders. Therefore, this means that

$$\frac{1}{t} = \text{Re } \frac{1}{t} - \sigma_{ab}^T \Rightarrow t = \frac{1}{\text{Re } \frac{1}{t} - \sigma_{ab}^T} \quad (1.188)$$

An exactly unitary amplitude can be constructed by several methods. The so-called K-matrix method is one of the most popular unitarization procedures. See, for instance, refs. [80,81]. The K-matrix amplitude satisfies unitarity for partial waves and reproduces the first term of the ChPT series at low energies, i.e. to obtain it from (1.188) we approximate $\text{Re } 1/t \simeq 1/t_2$ to find

$$t_K(s, T) = \frac{t_2(s)}{1 - \sigma_{ab}^T(s) t_2(s)}. \quad (1.189)$$

Although the above amplitude is unitary, it is not analytic due to the phase space factor, so it cannot be properly extended to the complex s-plane, in particular to define properly the Second Riemann Sheet (2RS). The requirement of analyticity is then crucial. With some modifications, we can construct two different methods consistent within unitarity and analyticity requirements for the thermal amplitude:

$$t_{U,i}(s, T) = \frac{t_2^2(s)}{t_2(s) - t_{4,i}(s, T)}. \quad (1.190)$$

with

$$\text{Method 1 : } t_{4,1}(s, T) = 16\pi t_2(s)^2 \tilde{J}_0^{ab}(\sqrt{s}, \vec{0}, T), \quad (1.191)$$

$$\text{Method 2 : } t_{4,2}(s, T) = t_4(s, 0) + 16\pi t_2(s)^2 \left[J_0^{ab}(\sqrt{s}, \vec{0}, T) - J_0^{ab}(\sqrt{s}, \vec{0}, 0) \right], \quad (1.192)$$

and J the loop thermal integral defined in (1.182), which comes from the s -channel scattering amplitude in the center of momentum frame, responsible for the unitarity contribution [54]. Method 1 is essentially the finite temperature extension of the "Chiral Unitary approach" developed at $T = 0$ in [82,83]. $\tilde{J}_0^{ab}$ denotes the finite part of J_0^{ab} , renormalized by a subtraction constant fitted to scattering data at $T = 0$ [84,85]. The

unitarized amplitude (1.190) can be understood as obtained from (1.189) by replacing the $\sigma_{ab}^T(s)$ contribution in the denominator by an analytic function in s satisfying unitarity, since $\text{Im } J_0^{ab}(\sqrt{s}, \vec{0}, T) = \sigma_{ab}^T(s)/(16\pi)$ for $s \geq (M_a + M_b)^2$. The main advantage of Method 2 is that is consistent with the perturbative chiral expansion at $\mathcal{O}(p^4)$ at $T = 0$; hence, providing better control over the quark mass dependence of the amplitude.

One of the most extensively used unitarization techniques is the $\mathcal{O}(p^4)$ Inverse Amplitude Method (IAM). An introduction to this method can be found in refs. [86, 87]. In that approach, exact unitarity and matching to the low-energy ChPT expansion are demanded. The unitarized IAM partial waves read

$$t_{IAM}(s, T) = \frac{t_2(s)^2}{t_2(s) - t_4(s, T)}. \quad (1.193)$$

The above amplitude is analytic off the real axis and satisfies the exact unitarity relation. In addition, the IAM amplitude reproduces the ChPT series up to $\mathcal{O}(p^4)$ when expanded at low energies and is analytical in the complex s plane [88], which ultimately allows to search for resonances as poles in the 2RS.

1.4.5 Analytic continuation to the 2RS and resonances

Let us recall the theorem known as the Schwarz reflection principle, which tells us that a function $f(z)$ must satisfy the equation

$$f(z^*) = f(z)^* \quad (1.194)$$

if $f(z)$ satisfies that is analytic in a domain C in the complex plane and is real in a segment in C .

As we commented before, the amplitude is analytical on the complex plane off the real axis, it has a right unitarity cut starting at the threshold $s = (M_a + M_b)^2$. This analytical properties allow us to define the unitarized amplitude in the second Riemann sheet which requires continuity over the threshold

$$\text{Im } t^{II}(s - i\epsilon) = \text{Im } t^I(s + i\epsilon) \quad \text{for } s \geq (M_a + M_b)^2 \quad (1.195)$$

and because there is a region below threshold where $\text{Im } t^I(s) = 0$

$$t^{II}(s + i\epsilon) = [t^{II}(s - i\epsilon)]^* = [t^I(s + i\epsilon)]^* \quad (1.196)$$

From the Schwarz reflection and taking into account the unitarity condition we can see that imaginary parts produce discontinuities between the $s + i\epsilon$ and $s - i\epsilon$ values of the

amplitude

$$\begin{aligned} t^I(s+i\epsilon) - t^I(s-i\epsilon) &= t^I(s+i\epsilon) - [t^I(s+i\epsilon)]^* \\ &= 2i \operatorname{Im} t^I(s+i\epsilon) = 2i \sigma_{ab}^T [t^I(s+i\epsilon)] [t^I(s+i\epsilon)]^* \end{aligned} \quad (1.197)$$

This result, together with (1.196), allows us to write the amplitude in the 2RS in terms of the one in the first Riemann sheet

$$t^{II}(s, T) = \frac{t^I(s, T)}{1 + 2i \sigma_{ab}^T(s) t^I(s, T)} \quad (1.198)$$

In addition, to ensure the Schwartz reflection symmetry of above the amplitude, i.e. $t^{II}(s^*, T) = [t^{II}(s, T)]^*$, we have to chose the determination of the σ_{ab}^T such that on the lower half s plane $\sigma_{ab}^T(s^*) = -\sigma_{ab}^T(s)^*$.

Extending unitarized amplitudes to the complex plane, we can look for poles which will help us to determine some properties of the corresponding resonances. These poles can be parameterized as customary as

$$s_p = \left(M_p - i \frac{\Gamma_p}{2} \right)^2 \quad (1.199)$$

where M_p and Γ_p would approximately correspond to the mass and width of a resonance in the Breit-Wigner limit $\Gamma_p \ll M_p$.

In Fig. 1.17 we show the surface and the contour plots of the imaginary part of the $\pi\pi$ elastic scattering amplitude in the 2RS calculated up to NLO in ChPT, unitarized within the IAM for the $IJ = 00$ channel. The pole of the amplitude in this channel

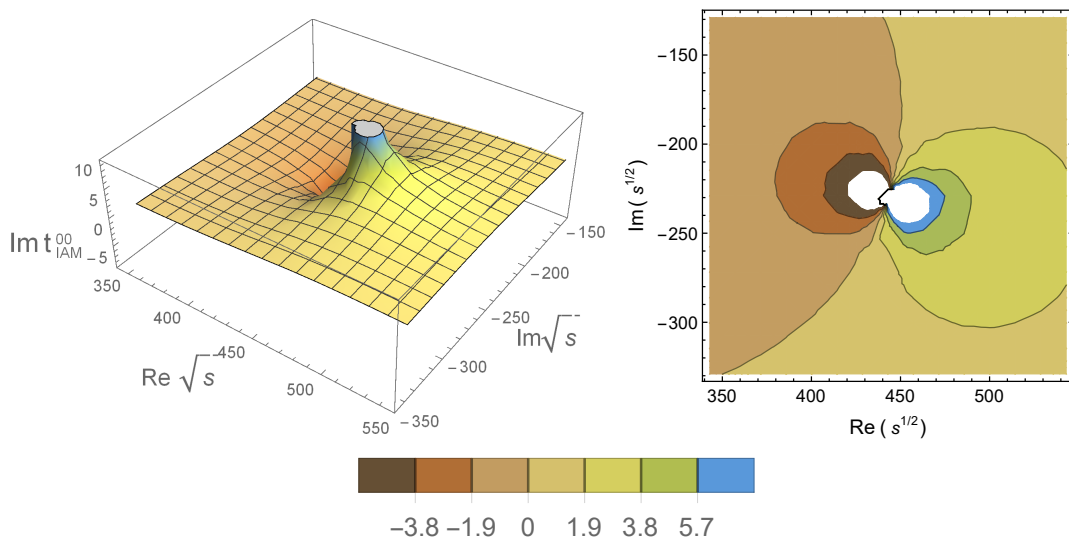


Figure 1.17: Surface (left) and contour (right) plots showing the imaginary part of the $\pi\pi$ scattering scalar partial wave amplitude in the 2RS calculated within the IAM.

corresponds to the pole position of the $f_0(500)$. Similarly, the $\rho(770)$ pole is found in the $IJ = 11$ channel. On the other hand, the poles associated with the $K_0^*(700)$ and $K^*(892)$ particles can be generated with the elastic $K\pi$ scattering.

The role of the $f_0(500)$ in chiral symmetry restoration

The lightest meson resonances play a crucial role in the low energy description of the strong interaction in different phenomena related to hot and dense medium created both in Relativistic Heavy Ion Collisions.

Calculations of the thermodynamics including interactions among hadrons encompass the ChPT description of the light meson gas [49], which provides a model-independent and consistent treatment. Although restricted to low temperatures, it captures well the contribution of the lightest states. An alternative is the virial approach, where interactions are incorporated within a small fugacity expansion [89]. Both ChPT and the virial approach predict similar results consistent with chiral symmetry restoration [90], although higher order states are needed, as provided by the HRG, to obtain results compatible with the lattice.

An important issue, not often considered, is the importance of the interactions among the thermal bath components, which ultimately give rise to a temperature dependence of the hadron spectral parameters (mass and width, generally speaking). As a particular example, the ChPT analysis of pion scattering at finite temperature combined with unitarity arguments [54, 88] allows to obtain the temperature dependence of the $\rho(770)$ and $f_0(500)$ poles in the 2RS. In the ρ case, the results are compatible with the observed widening in dilepton spectrum, parametrized through the pion form factor [91], but the more important consequence for our present study concerns the $f_0(500)$ channel, since the analysis in [92] shows that the scalar susceptibility saturated by such thermal $f_0(500)$ state has a maximum very close to the expected transition point, which is quite

remarkable given the approximations used.

In this chapter we will explore in detail some phenomenological and theoretical aspects related to the scalar susceptibility description through the $f_0(500)$ thermal state. Our aim and motivation are to investigate to what extent the thermal $f_0(500)$ must be taken into account when describing observables regarding the chiral transition. The scalar susceptibility is the candidate for which the influence of such state is meant to be dominant, since, as we will explain below in detail, it should scale roughly as the inverse thermal mass squared of the scalar propagator, for which the $f_0(500)$ gives the lightest contribution.

We will discuss the connection of the scalar susceptibility with the lightest scalar meson state, the σ or $f_0(500)$. This connection will be studied first within the framework of the LSM as a testbed which will allow to check the different approximations used. Secondly, within UChPT we will consider a saturated approach in terms of the thermal $f_0(500)$ generated as a pole in $\pi\pi$ scattering.

2.1 Linear Sigma Model description

On the one hand, we have focussed the analysis on the LSM, because it implements the chiral symmetry restoration pattern, including explicitly the σ degree of freedom. We consider the meson sector lagrangian of the LSM.

In chapter 1, we have presented a summary of the standard procedure to be followed in the study of the LSM at zero temperature. At $T \neq 0$, one can allow the vacuum expectation value of the σ to be temperature dependent, i.e. $\langle \sigma \rangle (T) \equiv v(T)$. However, note that $v(T)$ is not equal to the vacuum expectation value at zero temperature v defined in subsection 1.2.1. Consequently, if one decides to use the shifted field $\tilde{\sigma} = \sigma - v$, as done for instance in [40], it should be taken into account that $\langle \tilde{\sigma} \rangle (T) = v(T) - v \neq 0$, which in particular implies that one-particle reducible (1PR) diagrams enter in the calculation of correlators, as in the case of the $\tilde{\sigma}$ propagator. An alternative, followed in [39], is to use instead the shifted field $\hat{\sigma} = \sigma - v(T)$, so that $\langle \hat{\sigma} \rangle = 0$. The temperature dependence of $v(T)$ can be determined within the LSM, for instance from the mean field approach to leading order in λ [39].

With the first prescription, the LSM lagrangian in terms of $\tilde{\sigma}$ is given by (1.53). Thus, the quark condensate (1.137) and the scalar susceptibility (1.138) of the LSM can be written as follows:

$$\langle \bar{q}q \rangle_l(T) = -\frac{dh}{dm_l} v(T), \quad (2.1)$$

$$\chi_S(T) = \left(\frac{d^2 h}{dm_l^2} \right) v(T) + \left(\frac{dh}{dm_l} \right)^2 \int_T dx \{ \langle \mathcal{T} \tilde{\sigma}(x) \tilde{\sigma}(0) \rangle - \langle \tilde{\sigma} \rangle^2(T) \}. \quad (2.2)$$

with h in (1.52).

The subtraction of $\langle \tilde{\sigma} \rangle^2$ in χ_S above ensures that the self-energy can be written in terms of standard connected Feynman diagrams (including 1PR contributions) and is free of contact divergences proportional to $\delta^{(4)}(k=0)$. Nevertheless, we will work in the Dimensional Regularization scheme, so that $\delta^{(D)}(0)$ terms formally vanish [93]. Thus, we can write:

$$\chi_S(T) = \left(\frac{d^2 h}{dm_l^2} \right) v(T) + \left(\frac{dh}{dm_l} \right)^2 \Delta_\sigma(k=0; T), \quad (2.3)$$

where

$$\Delta_\sigma(k; T) = \frac{1}{k^2 + M_{0\sigma}^2 + \Sigma(k_0, \vec{k}; T)} \quad (2.4)$$

is the Euclidean propagator of the $\tilde{\sigma}$ field and $\Sigma(k_0, \vec{k}; T)$ is the self-energy, which in the thermal field theory framework, as we have seen, may depend separately on the space and time components of the four-momentum k [48].

The coefficients of $v(T)$ and $\Delta_\sigma(k=0; T)$ in (2.3) can be written in terms of v , $M_{0\sigma}$ and $M_{0\pi}$, using (1.54), as

$$\begin{aligned} \frac{dh}{dm_l} &= 2B_0 v \left(\frac{M_{0\sigma}^2}{M_{0\sigma}^2 - M_{0\pi}^2} \right), \\ \frac{d^2 h}{dm_l^2} &= 4B_0^2 v \frac{2M_{0\sigma}^2 - 3M_{0\pi}^2}{(M_{0\sigma}^2 - M_{0\pi}^2)^2}. \end{aligned} \quad (2.5)$$

The result (2.3) allows to relate the scalar susceptibility with the propagator of the scalar field. Note that the first term of that equation is meant to be negligible near chiral restoration since it vanishes proportionally to the light quark condensate. Another argument that leads to the same conclusion is the following: around the transition region, χ_S tends to become degenerate with the pseudoscalar pion susceptibility χ_P^π defined in (B.11), confirmed in lattice simulations [59]. On the other hand, the Ward Identity given by (B.23) allows to write $\chi_P^\pi = -\langle \bar{q}q \rangle_l / m_l$ at any temperature. Therefore, near the transition, replacing $v(T) = -(dh/dm_l)^{-1} \langle \bar{q}q \rangle_l(T) = -m_l (dh/dm_l)^{-1} \chi_P^\pi(T) \simeq$

$-m_l(dh/dm_l)^{-1}\chi_S(T)$ in the first term in the r.h.s. of (2.3), that term is $\mathcal{O}(M_{0\pi}^2/M_{0\sigma}^2)$ suppressed with respect to $\chi_S(T)$ in the l.h.s. of (2.3).

Therefore, near the transition, the scalar susceptibility is proportional to the $s = 0$ euclidean scalar propagator, and its temperature behaviour in that region is therefore dominated by the inverse self-energy of the lightest state, which in this case is the σ of the LSM:

$$\chi_S(T) \simeq 4B_0^2 v^2 \left(\frac{M_{0\sigma}^2}{M_{0\sigma}^2 - M_{0\pi}^2} \right)^2 \Delta_\sigma(k=0; T) \Rightarrow \frac{\chi_S(T)}{\chi_S(0)} \simeq \frac{M_{0\sigma}^2 + \Sigma(k=0; T=0)}{M_{0\sigma}^2 + \Sigma(k=0; T)}. \quad (2.6)$$

We will refer to the above result as the saturated LSM approach, where the scalar susceptibility is approximately described as the inverse of the self-energy of the lightest scalar state. A similar approach will be carried out and studied extensively in next sections for the UChPT framework. In the latter approach, the self-energy contribution is taken as the real part of the pole position in the 2RS of the complex $s = k^2$ plane for the pion scattering amplitude (in the center of momentum frame $\vec{k} = \vec{0}$). We will then use the present LSM analysis to study the above saturation approach, in particular to compare it with a strictly perturbative result for χ_S (see details below) so that we can use it as a testbed for the UChPT description, more realistic concerning the $f_0(500)$ pole determination.

The first step would be then to provide a well-defined calculation of the σ self-energy in the LSM including finite-temperature corrections. For clarity, we will stick to the perturbative approach in λ . Although, as we are about to check, the real values of λ needed to achieve reasonable phenomenological results are quite large [80], the one-loop corrections to the self-energy lie around a 15% at $T = 0$ [80]. Besides, as commented above, our main goal within the LSM is not to provide a reliable phenomenological description, but to provide a better understanding of the different approximations for χ_S performed in this work, at least parametrically in λ .

The one-loop diagrams contributing to the sigma self-energy are given in Fig. 2.1. It is important to remark that a consistent perturbative expansion requires that $M_{0\sigma}^2, M_{0\pi}^2$ remain of $\mathcal{O}(1)$ in the λ expansion so that $k^2 + M_\sigma^2$ remains the leading order of the inverse propagator. Hence, using (1.54), all the one-loop self-energy contributions remain of $\mathcal{O}(\lambda)$. Namely, the contributions of every diagram in Fig. 2.1 read [40]:

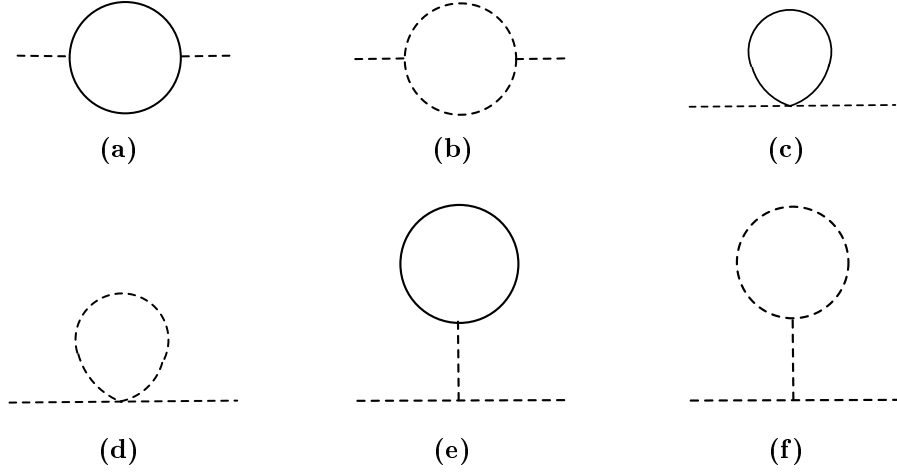


Figure 2.1: One-loop contributions to the σ self-energy in the LSM. The solid lines represent the pion fields and the dashed lines the sigma one.

$$\begin{aligned}
\Sigma_a(k_0, \vec{k}; T) &= -3\lambda (M_{0\sigma}^2 - M_{0\pi}^2) J(M_{0\pi}; k_0, \vec{k}, T), \\
\Sigma_b(k_0, \vec{k}; T) &= -9\lambda (M_{0\sigma}^2 - M_{0\pi}^2) J(M_{0\sigma}; k_0, \vec{k}, T), \\
\Sigma_c(T) &= 3\lambda G(M_{0\pi}, T), \\
\Sigma_d(T) &= 3\lambda G(M_{0\sigma}, T), \\
\Sigma_e(T) &= -9\lambda \frac{M_{0\sigma}^2 - M_{0\pi}^2}{M_{0\sigma}^2} G(M_{0\pi}, T), \\
\Sigma_f(T) &= -9\lambda \frac{M_{0\sigma}^2 - M_{0\pi}^2}{M_{0\sigma}^2} G(M_{0\sigma}, T).
\end{aligned} \tag{2.7}$$

where G and J are the finite- T integrals of the bubble and tadpole diagrams defined in (1.128) and (1.182) respectively.

As we are about to see, a standard LSM renormalization will allow us to express the self-energy as a finite quantity. Before that, we will provide a check of our result (2.3). From the lagrangian (1.53) we have, within the perturbative λ expansion,

$$\begin{aligned}
v(T) &= \frac{d}{dh} \log Z \\
&= -\frac{1}{2} \frac{dM_{0\sigma}^2}{dh} G(M_{0\sigma}, T) - \frac{3}{2} \frac{dM_{0\pi}^2}{dh} G(M_{0\pi}, T) - \frac{1}{4\lambda} \frac{dM_{0\pi}^4}{dh} + \frac{dv^2}{dh} M_{0\pi}^2 \\
&+ v^2 \frac{dM_{0\pi}^2}{dh} + \mathcal{O}(\lambda^2) = v \left[1 - \frac{3\lambda}{M_{0\sigma}^2} (G(M_{0\sigma}, T) + G(M_{0\pi}, T)) + \mathcal{O}(\lambda^2) \right]
\end{aligned} \tag{2.8}$$

Thus, the light quark condensate is

$$\langle \bar{q}q \rangle_l(T) = -2B_0 v^2 \frac{M_{0\sigma}^2}{M_{0\sigma}^2 - M_{0\pi}^2} \left[1 - \frac{3\lambda}{M_{0\sigma}^2} (G(M_{0\sigma}, T) + G(M_{0\pi}, T)) + \mathcal{O}(\lambda^2) \right]. \tag{2.9}$$

The above result is actually compatible with the mean field approximation, where interactions and fluctuations are considered small (see [39] in the chiral limit). Taking one more mass derivative, we obtain then the purely perturbative expression for the scalar susceptibility:

$$\chi_S(T) = \frac{6B_0^2}{\lambda} \left[1 + \lambda (3G_2(M_{0\sigma}, T) + G_2(M_{0\pi}, T)) + \mathcal{O}(\lambda^2) \right]. \quad (2.10)$$

with G_2 defined in equation (1.135).

One can now check that we arrive exactly to the same result by expanding (2.3) in powers of λ and using (2.8) and (2.7).

Our next step will be to provide a finite and scale-independent result for the self-energy at finite temperature. The DR pole can be absorbed in the $T = 0$ renormalization of the pion and sigma masses:

$$M_{0\sigma}^2 - M_{0\pi}^2 = (M_\sigma^2 - M_\pi^2) \left[1 + \frac{6\lambda}{16\pi^2} \left(\frac{2}{\epsilon} - \gamma + \log 4\pi + 1 - \log \frac{M_\sigma^2}{\mu^2} - \frac{1}{6} \right) \right] + \mathcal{O}(\lambda^2), \quad (2.11)$$

$$M_{0\pi}^2 = M_\pi^2 \left\{ 1 - \frac{3\lambda}{16\pi^2} \left[\left(\frac{2}{\epsilon} - \gamma + \log 4\pi + 1 \right) \left(1 - \frac{3M_\pi^2}{M_\sigma^2} \right) + \left(\frac{3M_\pi^2}{M_\sigma^2} - 2 \right) \log \frac{M_\pi^2}{\mu^2} + \log \frac{M_\sigma^2}{\mu^2} \right] \right\} + \mathcal{O}(\lambda^2), \quad (2.12)$$

with μ the DR renormalization scale. The above renormalization coincides with that in the chiral limit provided by [34]. See also the $T = 0$ calculation of the σ propagator in [94]. With the above renormalization, we get the LSM one-loop self-energy finite and scale-independent:

$$\begin{aligned} \Delta_\sigma^{-1} &= M_\sigma^2 + \Sigma(k_0, \vec{k}; T), \\ \Sigma(s, T=0) &= \frac{3\lambda}{16\pi^2} (M_\sigma^2 - M_\pi^2) \left[\sigma_\pi(s) \log \left(\frac{\sigma_\pi(s) + 1}{\sigma_\pi(s) - 1} \right) + 3\sigma_\sigma(s) \log \left(\frac{\sigma_\sigma(s) + 1}{\sigma_\sigma(s) - 1} \right) \right. \\ &\quad \left. + \log \left(\frac{M_\pi^2}{M_\sigma^2} \right) - \frac{13}{3} \right] + \mathcal{O}(\lambda^2), \\ \Sigma(k_0, \vec{k}; T) &= \Sigma(s, T=0) + 3\lambda \left\{ \frac{3M_\pi^2 - 2M_\sigma^2}{M_\sigma^2} [g_1(M_\pi, T) + g_1(M_\sigma, T)] \right. \\ &\quad \left. - (M_\sigma^2 - M_\pi^2) \left[\delta J(M_\pi; k_0, \vec{k}, T) + 3\delta J(M_\sigma; k_0, \vec{k}, T) \right] \right\} + \mathcal{O}(\lambda^2), \end{aligned} \quad (2.13)$$

where $\sigma_i(s)$ is the phase space given in (1.179) for $M_a = M_b = M_i$ and $\delta J(M; k, T) = J(M; k, T) - J(M; k, 0)$ with J defined in (1.182).

The pole of the propagator and its evolution with temperature can now be readily calculated. Perturbatively, the pole of the propagator is at $s_p = M_\sigma^2 + \Sigma(k^2 = M_\sigma^2)$, which we will parametrize as customary as $s_p = (M_p - i\Gamma_p/2)^2$. At $T \neq 0$, it will be enough for our purposes here to consider the pole at $\vec{k} = \vec{0}$. At $T = 0$, we get, for $M_\sigma > 2M_\pi$,

$$\begin{aligned} \text{Re } s_p &= M_\sigma^2 + \frac{3\lambda(M_\sigma^2 - M_\pi^2)}{16\pi^2} \left[-\frac{13}{3} + \sqrt{3}\pi + \log\left(\frac{M_\pi^2}{M_\sigma^2}\right) \right. \\ &\quad \left. + \sigma_\pi(M_\sigma^2) \log\left|\frac{\sigma_\pi(M_\sigma^2) + 1}{\sigma_\pi(M_\sigma^2) - 1}\right| \right], \end{aligned} \quad (2.14)$$

$$\text{Im } s_p = -\frac{3\lambda(M_\sigma^2 - M_\pi^2)}{16\pi} \sigma_\pi(M_\sigma^2), \quad (2.15)$$

which agrees with the result in [95] in the chiral limit.

Following [80], we will set our reference values for the numerical parameters of the model as those for which the σ pole values lie near the experimental determination for the $f_0(500)$ in the PDG [74], namely $M_p^{PDG} \simeq (400 - 550)$ MeV, $\Gamma_p^{PDG} \simeq (400 - 700)$ MeV. As noted in [80], there is no way to accomodate the LSM parameters to get good agreement both for M_p and Γ_p . We show in Fig. 2.2 the dependence on λ of M_p and Γ_p for the physical $M_\pi = 140$ MeV, which confirms the previous statement. In our numerical results we have taken for the tree level $M_\sigma^2 = M_\pi^2 + 2\lambda F_\pi^2$ with $F_\pi \simeq 93$ MeV. In view of those results we select as a reference range for our numerical results the interval $\lambda \sim 10 - 20$ where the deviations from the PDG value are not large in either M_p or Γ_p , the lower (higher) value of λ favoring M_p (Γ_p) as showed for some sample values in Table 2.1, where we also include the chiral limit values. In turn, we note that, even though the typical λ values needed are large, the one-loop corrections remain reasonably under control, lying between 10-15 % for the corrections to M_p compared to the tree level M_σ .

M_π (MeV)	M_p (MeV)	Γ_p (MeV)	λ
0	450.0	172.5	8.4
0	775.1	550.0	20.0
140	450.0	159.2	9.6
140	750.1	550.0	21.2

Table 2.1: Pole mass and width at $T = 0$ for sample values of λ , with $M_p = \text{Re } \sqrt{s_p}$ and $\Gamma_p = -2\text{Im } \sqrt{s_p}$.

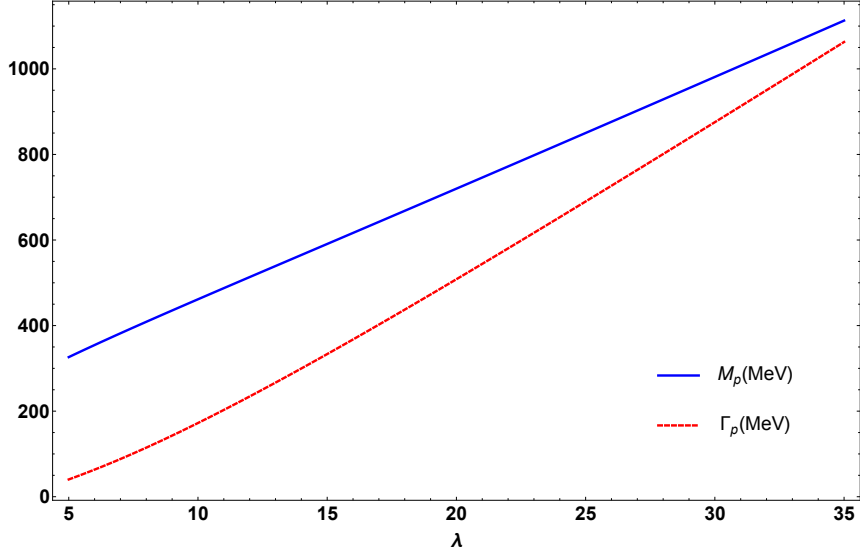


Figure 2.2: Pole parameters M_ρ and Γ_ρ in the one-loop LSM as a function of λ for the physical mass M_π .

Our next step will be to provide the results for the different approaches to the scalar susceptibility mentioned above. Taking the $k \rightarrow 0^+$ limit for the self-energy, we can get $\chi_S(T)$ from the saturated approach (2.6). From (2.13), taking into account that

$$\lim_{s \rightarrow 0} \sigma_i(s) \log \frac{\sigma_i(s) - 1}{\sigma_i(s) + 1} = -2,$$

we have:

$$\begin{aligned} \Sigma(k=0; T) &= \frac{\lambda}{16\pi^2} (M_\sigma^2 - M_\pi^2) \left[11 + 3 \log \left(\frac{M_\pi^2}{M_\sigma^2} \right) \right] \\ &+ 3\lambda \left\{ \frac{3M_\pi^2 - 2M_\sigma^2}{M_\sigma^2} [g_1(M_\pi, T) + g_1(M_\sigma, T)] \right. \\ &- \left. (M_\sigma^2 - M_\pi^2) [g_2(M_\pi, T) + 3g_2(M_\sigma, T)] \right\} + \mathcal{O}(\lambda^2). \end{aligned} \quad (2.16)$$

In Fig. 2.3 we show our results for $\chi_S(T)$ in the saturated approach, compared to the perturbative one arising from (2.10). For an easier comparison with lattice data and with our results in next sections, we are using for the saturated LSM susceptibility the following normalization:

$$\chi_S^{sat, LSM}(T) = A \frac{M_\pi^4}{4m_l^2} \frac{M_{0\sigma}^2 + \Sigma(k=0; T=0)}{M_{0\sigma}^2 + \Sigma(k=0; T)}. \quad (2.17)$$

For the results in Fig. 2.3 we have taken $A = A_{ChPT} \simeq 0.15$ (see comments below). Nevertheless, the corresponding value for the normalization constant A from the nor-

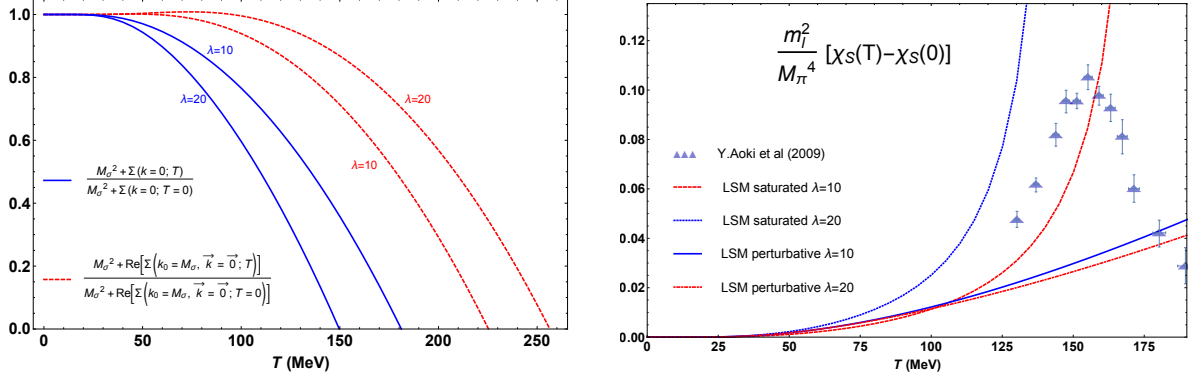


Figure 2.3: Left: LSM thermal self-energy at $k = 0$ and at $k_0 = M_\sigma$, $\vec{k} = \vec{0}$, for the range $\lambda = 10 - 20$. Right: Saturated susceptibility in the LSM compared to lattice data and to the purely perturbative one. In both figures $M_\pi = 140$ MeV. The lattice data and errors are from [56].

malization given in (2.6) would be around $A_{LSM} \approx 4F_\pi^2/M_S^2(0) \approx 0.07 - 0.17$ for the range of values showed in Table 2.1 and hence compatible with the ChPT value.

The main conclusion that we extract from the results showed in Fig. 2.3 is that the saturated approach provides a much stronger growth with temperature than the purely perturbative one, actually covering lattice data below the transition for the range of values of $\lambda \sim 10 - 20$ corresponding to the $T = 0$ poles in Table 2.1. However, the saturated susceptibility actually diverges around the transition point, even in the massive case and therefore is not able to reproduce either the crossover peak. As we will see in the following section, the UChPT approach will considerably improve this behaviour. Nevertheless, an important comment is that even within this LSM approach, which has its own limitations as we are discussing here, a saturated description of the scalar susceptibility in terms of the thermal self-energy seems to be able to describe lattice data reasonably without adding additional degrees of freedom. That feature is shared also by the UChPT approach and is one of our main conclusions. Finally, in Fig. 2.3 we have showed also a comparison of the $s = 0$ result for the self-energy temperature dependence with the same approach evaluating the real part of the self-energy at $s = s_p$, the latter being the point at which the equivalent to the self-energy is naturally evaluated within the UChPT approach. The qualitative behaviour is the same, although numerically the temperature at which the self-energy vanishes (divergent susceptibility) moves to a higher value. In both cases, the dropping behaviour can be understood as a chiral symmetry restoration tendency, since $M_\sigma^2 + \text{Re} \Sigma$ corresponds to the T -dependent scalar mass, which is meant drops below the transition approaching

the pion mass [39].

2.2 Thermal $f_0(500)$ saturation approach

According to (2.3), we expect the scalar susceptibility $\chi_S(T)$ to be proportional to the inverse of $\Sigma(k=0)$, Σ denoting generically the self-energy of the $f_0(500)$ state. However, within the UChPT approach, the $f_0(500)$ state is dynamically generated and then emerges as a 2RS pole of the scattering amplitude rather than a time-ordered product or thermal correlator, as in the case of the LSM discussed in the previous section. Thus, within UChPT, instead of Σ we have access to the pole parameters of the $f_0(500)$ state, namely, M_p , Γ_p and $g_{\sigma\pi\pi}$, the effective $\sigma\pi\pi$ effective coupling [80], so that the 2RS amplitude reads around the pole

$$t^{II} = \frac{1}{16\pi} \frac{g_{\sigma\pi\pi}^2}{s - s_p} + \dots, \quad (2.18)$$

and the dots denote subdominant terms around $s \sim s_p$. Note that if we regard (2.18) as the exchange of a scalar state f_0 , the self-energy of such state would satisfy $\Sigma_{f_0}(s_p) = s_p$, where we have included in Σ_{f_0} the equivalent of the tree-level mass. On the other hand, $\text{Im} \Sigma_{f_0}(k=0) = 0$ since at $k=0$ there are no decay channels open, so that assuming that the sensitivity of $\text{Re} \Sigma_{f_0}$ from s_p to $s=0$ lies within the typical uncertainty range of this approach which we will analyze in detail below, we are led to the following definition of the unitarized scalar susceptibility, which corresponds to the saturated thermal $f_0(500)$ state approach within UChPT:

$$\chi_S^U(T) = A \frac{M_\pi^4}{4m_l^2} \frac{M_S^2(0)}{M_S^2(T)}, \quad (2.19)$$

where we follow the same normalization as in (2.17) and where the scalar thermal pole mass (defined as the real part of self-energy at the pole) is

$$M_S^2(T) = \text{Re } s_p(T) = M_p^2(T) - \frac{1}{4} \Gamma_p^2(T). \quad (2.20)$$

and the temperature dependence of $M_p(T)$ and $\Gamma_p(T)$ is determined from the 2RS pole of the unitarized amplitude, as discussed in section 1.4. The thermal mass definition (2.20) shows a dropping behaviour compatible with the expected chiral restoring features, unlike the $I=J=1$ channel, where the mass has a much softer T dependence [88, 92]. Moreover, in [92], it has been shown that if the normalization A is chosen to match the perturbative ChPT one-loop result for χ_S at $T=0$, i.e.,

$$A_{ChPT} = \frac{4m_l^2}{M_\pi^4} \chi_S^{ChPT}(0) = \frac{\chi_S^{ChPT}(0)}{B_0^2} \simeq 0.15, \quad (2.21)$$

the resulting χ_S^U follows closely the ChPT curve for low temperatures and develops a maximum at a temperature around 157 MeV (with the LEC used in [92]), supporting strongly our previous assumptions. One of our main purposes here is to test in a more quantitative way the reliability of that saturated approach to describe lattice data, as compared with other approaches such as the HRG discussed in section 2.3, the LSM described in section 2.1 or $\chi_S(T)$ obtained perturbatively in ChPT or the virial approach [90].

The theoretical uncertainties involved in χ_S^U in (2.19) can be parametrized into three main types: the normalization factor A , the choice of the unitarization method and the numerical uncertainties of the LEC involved in $\pi\pi$ scattering for the pole determination. Here we will analyze in detail the sensibility of this approach to those three sources, focusing on its description of lattice data at finite temperature while complying with the $T = 0$ predictions for scattering data, the $f_0(500)$ pole and the ChPT low-energy approach.

Let us consider first the LEC dependence. As stated above, we will use as a reference set of LECs, those given in [96], namely

$$\begin{aligned} l_1^r &= -(3.7 \pm 0.2) \times 10^{-3}, & l_2^r &= (5.0 \pm 0.4) \times 10^{-3}, \\ l_3^r &= (0.8 \pm 3.8) \times 10^{-3}, & l_4^r &= (6.2 \pm 5.7) \times 10^{-3}, \end{aligned} \quad (2.22)$$

where l_i^r are the SU(2) renormalized LEC according to the notation in (1.77), evaluated at a DR scale $\mu = 770$ MeV. The above LEC were obtained by a fit of the IAM (1.193) to scattering data, leaving l_3^r and l_4^r fixed to their original ChPT values in [34]. We remark that the LEC appearing in the $\pi\pi$ scattering vertices are $l_{1,2}^r$, and are those to which the pole position parameters of resonances are most sensitive, while $l_{3,4}^r$ arise from the renormalization of the pion mass M_π (1.81) and the pion decay constant F_π (1.82).

We will estimate the range of variation of the saturated susceptibility by considering, for every T , the mean square error of the results obtained for the eight combinations of upper and lower values given by (2.22). The resulting uncertainty band is showed in Fig. 2.4, where the central line correspond to the average value and where we compare our prediction for χ_S based on the saturated thermal $f_0(500)$ approach, with lattice data coming from the collaboration [56], whose results can be easily translated into our present normalization. We consider also in the figure the uncertainty band generated

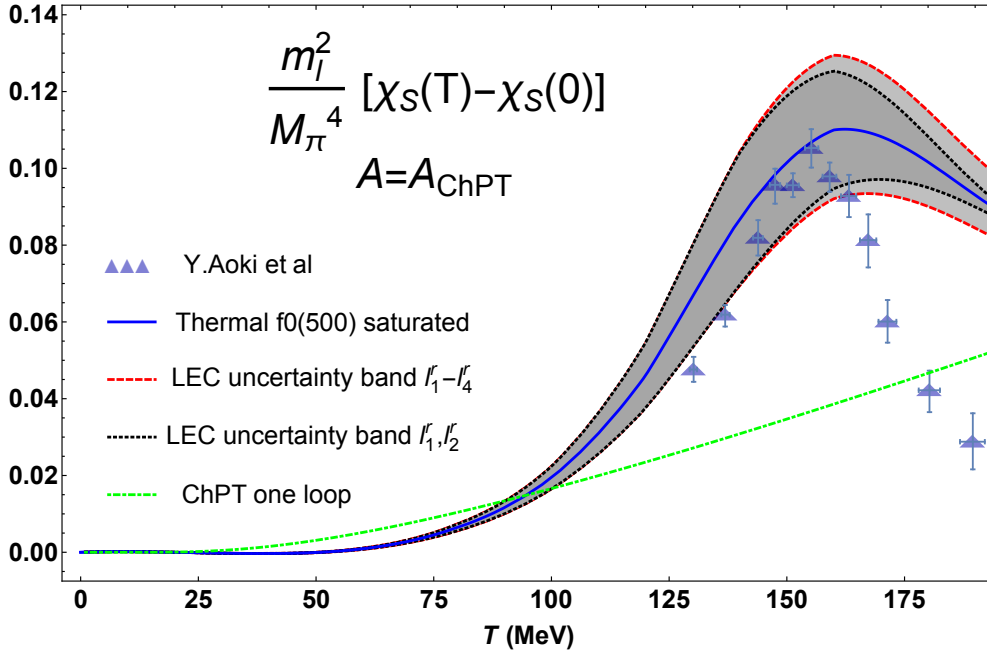


Figure 2.4: Results for the $f_0(500)$ saturated scalar susceptibility (2.19) normalized with A_{ChPT} in (2.21) including the uncertainties coming from the LEC (2.22). The lattice data and errors are from [56]. The central curves corresponding to the two uncertainty bands showed lie on top of each other.

solely by l_1^r and l_2^r , which as we see remains very close to the band of the four LEC, confirming our previous observation about the sensitivity of the pole parameters to the LEC. We also include in the figure the one-loop ChPT curve with the LECs given in [90]. Note that the ChPT result lies close to the LSM perturbative one in Fig. 2.3 since the leading behaviour in the LSM result (2.10) comes from $g_2(M_\pi, T)$ which is precisely the ChPT pion gas contribution [90].

These results lead to interesting conclusions: as we had anticipated, the saturated UChPT result reproduces the expected crossover peak around the transition and hence improves over the saturated LSM in section 2.1. We will actually see here that the adequate description of the $T = 0$ pole of the UChPT result, as well as other basic requirements such as analyticity and unitarity, produce this behaviour. Moreover, most of the lattice data fall into the uncertainty band, the approach being especially adequate near the transition region. Put in different words, one could use the LEC as fit parameters to reproduce the lattice χ_s at finite temperature and the results of the fit would be in the range allowed by the $T = 0$ determinations of those LECs based on experimental information.

On the other hand, since we are using the LECs in [96], fitted with the full IAM, to be consistent we have to ensure that the modified amplitude (1.190) reduces at $T = 0$ to the IAM one in (1.193). This guarantees also that the $T = 0$ $f_0(500)$ pole remains at the same value, compatible with the PDG, with these two different unitarization methods at finite temperature. In addition, in this way we will be able to test again the sensitivity to the LEC uncertainties in (2.22). As for the finite temperature correction in (1.190), we are taking the minimal contribution ensuring unitarity and analyticity, i.e., the T -dependent part of $J_0^{\pi\pi}(\sqrt{s}, \vec{0}, T)$. As we are about to see, keeping the three requirements of analyticity, unitarity and the $T = 0$ pole lead to a qualitative behaviour compatible with the crossover.

In Fig. 2.5 we plot the resulting $M_S^2(T)$ defined in (2.20), with two unitarization methods we have discussed in section 1.4, the IAM and the Method 2 ($t_{U,2}$) described by eqs. (1.190) and (1.192), which here we call *Umod*. We also consider the same function taking the light chiral limit ($M_\pi \rightarrow 0^+$) in our expressions (recall that the l_i^r in (2.22) are mass-independent). We observe that the qualitative behaviour around the transition is the same with both methods, i.e, they both develop a minimum around $T \simeq 150$ MeV in the massive case. However, we see that the curve of the *Umod* method reaches zero before the minimum, which would give rise to a divergent susceptibility at that point, pretty much like the LSM saturated approach except that in the LSM the thermal mass does not develop a minimum. That difference between the two methods remains when the uncertainty bands for the LECs are included. In that figure, we also show the constant M_π^2 reference value. The fact that the two methods give rise to a decreasing function approaching the pion mass squared strengthens the interpretation of $M_S^2(T)$ as a scalar mass, since $O(4)$ restoration would imply the degeneration of $\sigma - \pi$ states, while the thermal dependence of the pion mass is meant to be smooth [97].

Therefore, the requirements of thermal unitarity and analyticity, together with the $T = 0$ pole prediction, guarantee the key qualitative features of a crossover behaviour in terms of the position of the minimum as compared to the lattice prediction for T_c , reasonably maintained within the LEC uncertainty band. This is then a robust result. However, the additional requirement, only fulfilled by the IAM, of complying with the ChPT thermal scattering amplitude up to fourth order is needed to describe the scalar susceptibility accurately.

The previous difference between the two methods is washed out in the chiral limit, as Fig. 2.5 shows. There, both methods yield results compatible among them within the

LEC uncertainty band, predicting a critical temperature where the scalar mass vanishes, which is consistent with the expected reduction of the lattice T_c of around 15 – 20% in the chiral limit [58].

These results might seem somehow a striking result, since we are describing a thermodynamical observable near the transition with just one effective state, the thermal $f_0(500)$, without using the information coming from the rest of the hadronic spectrum. Qualitatively, we had observed the same feature in the LSM. Actually, this is our main motivation to compare the UChPT analysis with the HRG approximation. In this regard, one must take into account that, as stated above, $\chi_S(T)$ is precisely the observable where the lightest scalar state is meant to dominate, while this conclusion may not be extensible to other quantities such as the quark condensate. Thus, the thermal unitarization procedure seems to incorporate in a natural way the relevant information of higher order states, encoded precisely in the LECs. Our results may look at first at odds with the usual claim within the HRG approach stating that the $f_0(500)$ state can be ignored in the list of hadron states contributing to the partition function, motivated partly by a cancellation between the $IJ = 00$ and $IJ = 20$ channels in the $T = 0$ partial waves when considering the virial expansion [90,98]. However, it is important to point out that we are including here, as a key ingredient, the *thermal* corrections to the $\pi\pi$ scattering amplitude, which include higher order finite- T corrections not included in the usual virial approach, where scattering is included only at $T = 0$. Those thermal corrections, as explained above, account for the thermal unitarity processes giving rise ultimately to the main modifications of the $f_0(500)$ pole parameters, directly connected with chiral symmetry restoration as we are seeing here.

In connection with the last comment, one may wonder what would be the effect of the $f_0(500)$ state and its thermal modifications in other observables relevant in Heavy Ion Collisions, such as hadron multiplicities and yields. The latter have been successfully described within the so called thermal statistical models, very much in the same spirit as the HRG [8,99–101] (see section 2.3) where the different PDG states contribute through their free partition function, and the resonances width can be incorporated by integrating in energy with a suitable Breit-Wigner shape [99]. The decay channels of those resonances feed the hadron yields at chemical freeze-out. Following this approach, the effect of including the $f_0(500)$ was first studied in [100], resulting in a few percent increase in the pion yield from the $\pi\pi$ decay channel. That analysis showed also little dependence on variations of the $f_0(500)$ mass and width, which would lead to the con-

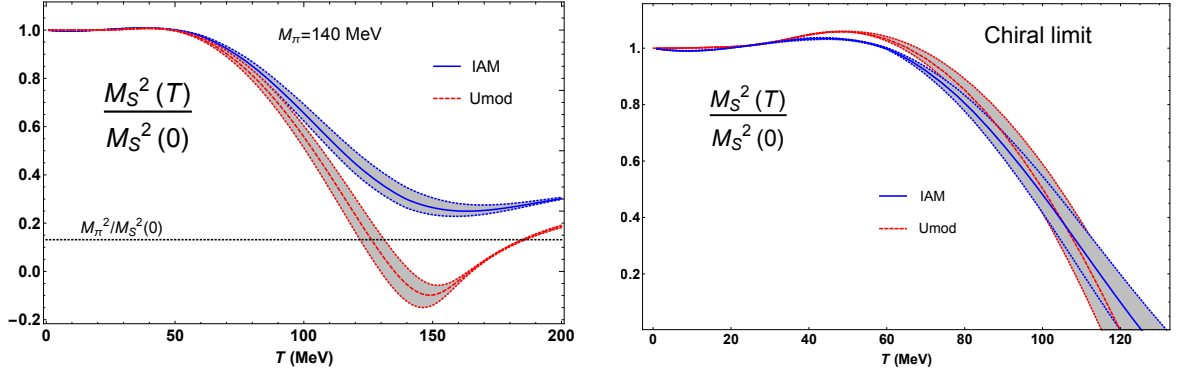


Figure 2.5: Squared scalar $f_0(500)$ thermal mass as defined by (2.20), calculated with the IAM and Umod unitarization methods in (1.193) and (1.190) respectively. Left: for the physical pion mass, where we show the pion mass squared value. Right: in the chiral limit. In both cases, the bands reflect the uncertainties in the LEC l_1^r and l_2^r given in (2.22) with l_3^r and l_4^r fixed at their central values.

clusion that the finite- T corrections we are discussing here would not have a significant effect for those observables. Regarding the connection with the QCD phase transition, hadron yields and multiplicities are correlated to hadronization rather than to chiral symmetry [8] and hence we would expect a smaller effect of the $f_0(500)$ modifications addressed in the present work.

However, as we have discussed above, the $f_0(500)$ should be treated as a broad resonance, and hence the Breit-Wigner approach is not quite adequate in that case. In addition, as we have just mentioned, the $IJ = 20$ repulsive channel would produce a cancellation of the $f_0(500)$ effect that has to be accounted for. Such an analysis has been performed in Ref. [98] within the virial approach, showing that such a cancellation takes place also for the pion yield, resulting in a much smaller effect, around a 0.3% decrease. Within that approach, the quantity controlling the particle spectra for those channels and hence the pion yield and multiplicity is

$$d_{IJ}(E) = \frac{1}{\pi} \frac{d\delta_{IJ}(E)}{dE} \quad (2.23)$$

with $E = \sqrt{s}$ and δ_{IJ} the corresponding IJ channel phase shift. Thus, to provide here a rough estimate of the possible effects of the $f_0(500)$ spectral modifications, we have calculated the $d_{00}(E)$ and $d_{20}(E)$ distributions in (2.23) with the phase shifts obtained from the IAM, both at $T = 0$ and at $T = 156$ MeV, which is the freeze-out temperature considered in Ref. [98]. The result is that the qualitative picture that we have just described with $T = 0$ phase shifts does not change much for the isospin-

weighted combination $(2I+1)(2J+1)d_{IJ}$, the modification being smaller as E increases. The modifications for the individual d_{IJ} follow a similar behavior.

The previous arguments indicate that the thermal effects on the $f_0(500)$ discussed here are not expected to produce large corrections regarding the pion multiplicity and yield, unlike the case of the scalar susceptibility. A different story, though, would be the study of correlations such as $\pi^+\pi^-$, which are not isospin averaged so that the previous cancellation does not occur [98]. In this sense, a promising line of research is the analysis of correlations and fluctuations in heavy ion collisions and their connection with the QCD phase diagram [102].

Generally speaking, it would be interesting to examine how the thermal dependence of other PDG states can affect different observables, including hadron yields and correlations. Although such an analysis is beyond the scope of this work, there are significant examples of light mesons which might be of interest. Apart from the ρ meson and its well-known influence in the photon and dilepton spectrum, already mentioned in the Introduction, other relevant states which are in the line of our present approach are the κ and a_0 mesons, which play a crucial role in understanding the pattern of chiral symmetry restoration in connection with the $U(1)_A$ symmetry [103].

2.3 Hadron Resonance Gas approach

The results in the previous sections show that one can actually describe correctly the lattice results for the scalar susceptibility, saturating it with just the contribution from the thermal $f_0(500)$ state. On the other hand, one would expect that any thermodynamical quantity should be sensitive to higher order hadron states as the transition point is approached, according to the standard framework of the HRG, as we have mentioned before. Therefore, the inclusion of the thermal effects in the $f_0(500)$ pole and the LEC dependence somehow account effectively for the effect of those states, generating novel additional features such as the crossover-like behaviour discussed in the previous section. To make this comparison more clear, we will provide in this section the result for the scalar susceptibility within the HRG approach, which has been used extensively in the literature to describe the hadron gas below the transition.

Here, we will follow the approach in [70, 73], which gives a good fit for the quark condensate to the $N_t = 12$ lattice data in [56], used here as a lattice reference set of data both for the quark condensate and for the scalar susceptibility. Within that approach,

the dependence of pseudo NGB is extracted directly from the one-loop ChPT calculation

$$\frac{\partial M_\pi^2}{\partial m_l} = -\frac{\langle \bar{q}q \rangle_l(0)}{F_\pi^2} \left(1 + 2\kappa \frac{M_\pi^2}{F_\pi^2} \right) \quad (2.24)$$

$$\frac{\partial M_K^2}{\partial m_l} = -\frac{\langle \bar{q}q \rangle_l(0) + \langle \bar{s}s \rangle(0)}{2F_K^2} \left(1 + 2\kappa \frac{M_K^2}{F_\pi^2} \right) \quad (2.25)$$

where $\langle \bar{q}q \rangle_l(0)$ and $\langle \bar{s}s \rangle(0)$ are the one-flavour light and strange condensates at $T = 0$ with $\langle \bar{q}q \rangle_l(0) = -(240\text{MeV})^3$ and $\langle \bar{s}s \rangle(0) = 0.8\langle \bar{q}q \rangle_l(0)$. The NLO corrections are included in the parameter $\kappa = 4(2L_8^r - H_2^r) = 0.021$ [104]. The above result for the quark dependence of the pion and kaon comes from the $SU(3)$ NLO chiral corrections to the Gell-Mann-Oakes-Renner relations

$$2m_l \langle \bar{q}q \rangle_l(0) = -F_\pi^2 M_\pi^2 \left(1 - \kappa \frac{M_\pi^2}{F_\pi^2} \right) \quad (2.26)$$

$$(m_s + m_l) \langle \bar{s}s \rangle(0) = -F_K^2 M_K^2 \left(1 - \kappa \frac{M_K^2}{F_\pi^2} \right) \quad (2.27)$$

The masses of the rest of hadrons are taken to scale within a constituent quark picture as

$$\begin{aligned} \frac{\partial M_B}{\partial m_{l,s}} &= (3 - N_s) \frac{\partial M_l}{\partial m_{l,s}} + N_s \frac{\partial M_s}{\partial m_{l,s}}, \\ \frac{\partial M_M}{\partial m_{l,s}} &= (2 - N_s) \frac{\partial M_l}{\partial m_{l,s}} + N_s \frac{\partial M_s}{\partial m_{l,s}}, \end{aligned} \quad (2.28)$$

where the constituent masses M_l , M_s for light and strange quarks are extracted from the NJL model calculation in [105]. We follow [73] for the assignments of the hadron strangeness content for open and hidden strange mesons, as well as for singlet and octet members.

We show in Fig. 2.6 the light quark condensate and the scalar susceptibility within the HRG approach. As it is known, within this approach the quark condensate drops monotonically and vanishes at a given temperature, for physical quark masses. There is a substantial reduction with respect to ChPT in the transition temperature, estimated here as the vanishing condensate point, when all the hadron degrees of freedom are included. The value obtained from the plot in Fig. 2.6 is $T_c \simeq 178.5$ MeV, while the value obtained for instance in ChPT with three-loop pion interactions [49], or in the virial approach [90], is around $T_c \simeq 250$ MeV. We will actually see that allowing some uncertainty in the normalization of the HRG expressions, to account in a simple way for the different uncertainties involved, allows for a fairly good description of lattice data.

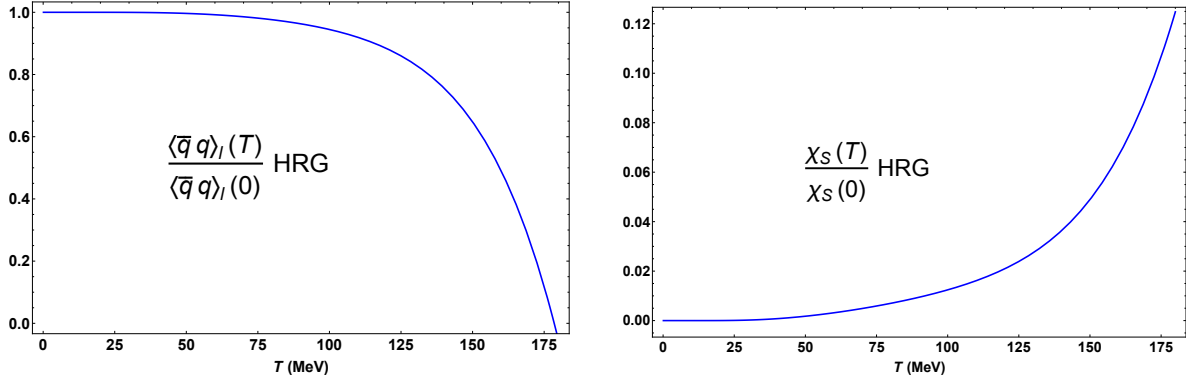


Figure 2.6: Light quark condensate and scalar susceptibility in the Hadron Resonance gas approach described in the main text.

As for the scalar susceptibility, the HRG approach showed here gives rise to a monotonically increased function, just as ChPT or virial approaches [49, 90], i.e, not reproducing the transition crossover peak. Also in the next section, we will carefully explore to what extent the HRG approach can describe simultaneously the quark condensate and susceptibility lattice results.

2.4 Fits to lattice data

In this section we will perform a more detailed analysis of the description of lattice data within the theoretical framework developed in this work. We will concentrate mostly in the scalar susceptibility, since, as explained before, this is the thermodynamic observable for which the role of the thermal $f_0(500)$ is expected to be more important. In particular, we will compare the description provided by thermal $f_0(500)$ saturation approach with that of the HRG, in a more quantitative way.

As an effective way to parametrize the uncertainties in both approaches, we will allow for a normalization constant which we will consider as our fit parameter. Thus, in the thermal $f_0(500)$ saturation definition (2.19), we fit the A parameter instead of fixing it to its ChPT value, which accounts at least partially for the uncertainties inherent of this method and discussed in section 2.2. The results we have obtained in section 2.2 show that we could alternatively fit the LEC within their $T = 0$ uncertainties to get a good description of lattice points, especially around the transition peak. As for the HRG approach, we normalize $\epsilon \rightarrow B\epsilon$ in (1.141) as a simple way to parametrize the uncertainties in this approach such as the quark mass dependence of hadron masses, the upper limit of the resonances included or the absence of interactions and decay channels.

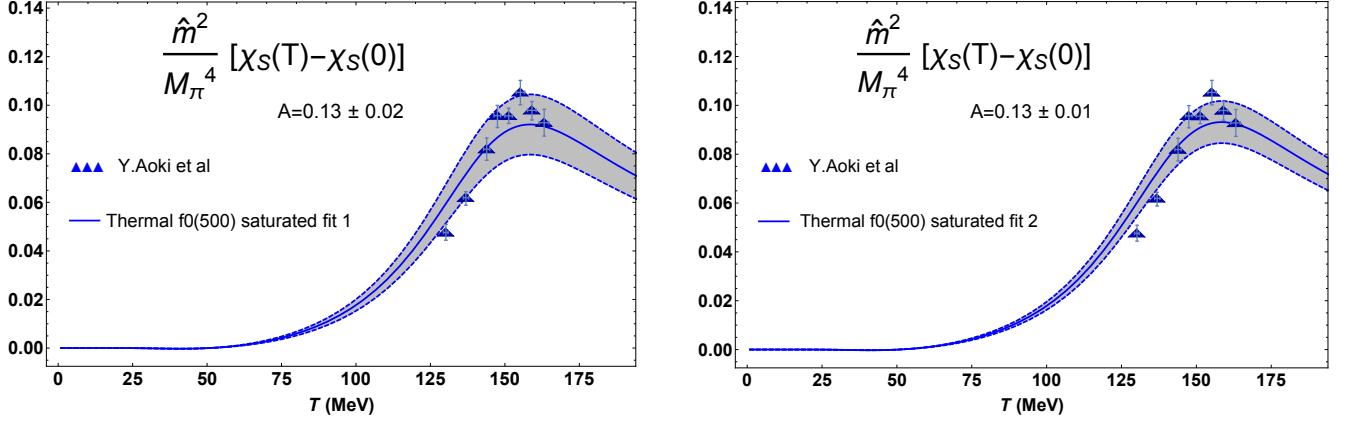


Figure 2.7: Fits of the thermal $f_0(500)$ saturated scalar susceptibility with the normalization constant as fit parameter and with the central values of the LEC given in (2.22). Fit 1 corresponds to fitting data up to $T \leq T_c = 155$ MeV while in fit 2 we include two more lattice points, up to $T = 163$ MeV. The quoted uncertainties in the A parameter and the bands correspond to the 95% confidence level of the fit. The lattice data and errors are from [56].

We show in Fig. 2.7 the results of two different fits of the thermal $f_0(500)$ saturated approach. The difference between those two fits is just the number of points included. Thus, in fit 2 we include two more points around the transition point. The result for the A parameter is shown in the figure, together with the uncertainty band corresponding to the 95% confidence level of the fit. The different fit parameters, as well as the goodness of fit indicators are collected in Table 2.2 for all the fits performed in this section. Note that the values of A quoted in the table are compatible with the ChPT value in (2.21), and therefore the predictions of the fitted curve for lattice data do not spoil the expected $T = 0$ value for the scalar susceptibility, as given by the ChPT result.

Fit	A	B	χ^2/dof	R^2	T_{max} (MeV)
Thermal $f_0(500)$ fit 1	0.13 ± 0.02	—	6.25	0.986	155
Thermal $f_0(500)$ fit 2	0.13 ± 0.01	—	4.93	0.989	165
HRG fit 1	—	1.90 ± 0.02	1.33	0.997	155
HRG fit 2	—	1.71 ± 0.23	10.30	0.978	165
HRG fit 3	—	1.06 ± 0.12	3.77	0.998	155

Table 2.2: Parameters for the different fits as explained in the main text.

On the other hand, in Fig. 2.8 we show the results of two fits with the HRG approach (HRG fits 1 and 2), corresponding to fit only the susceptibility lattice points, with the same sets of data used for fits 1 and 2 with the thermal $f_0(500)$ approach. We see that, as long as we keep the data points below T_c , the HRG gives a slightly better fit than the

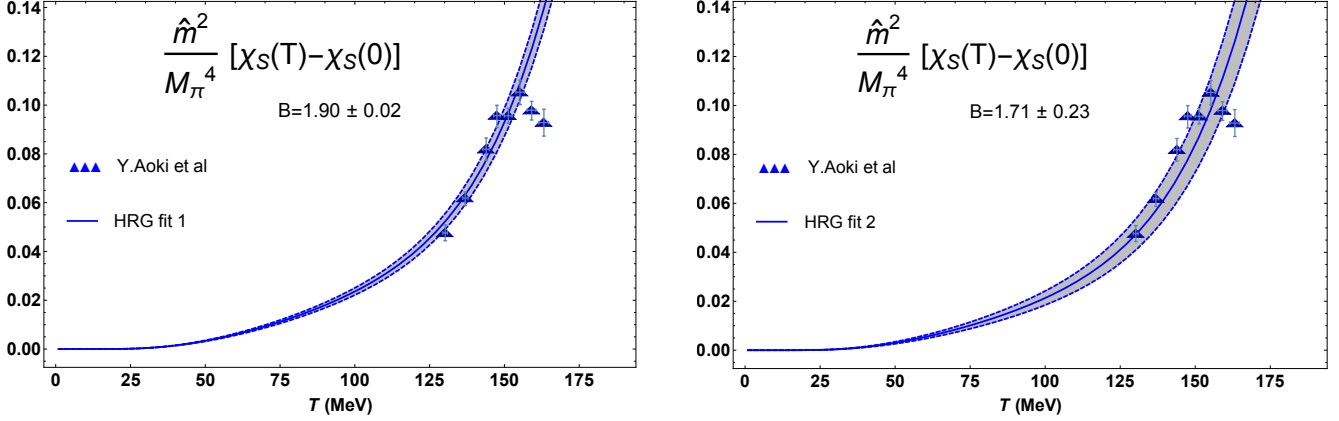


Figure 2.8: Fits of the HRG scalar susceptibility with the normalization constant as fit parameter. Fit 1 corresponds to fitting data up to $T \leq T_c = 155$ MeV while in fit 2 we include two more lattice points, up to $T = 163$ MeV. The quoted uncertainties in the B parameter and the bands correspond to the 95% confidence level of the fit. The lattice data and errors are from [56].

thermal $f_0(500)$ one, as it would be naturally expected from a HRG approach. However, including only two more points around T_c worsens the HRG in favor of the $f_0(500)$ one, which is consistent with the different qualitative behaviour of both curves around the maximum and confirms our previous comments about the role of the thermal $f_0(500)$.

Regarding the HRG description, an important observation must be taken into account: the values of B needed to fit the susceptibility are in conflict with those needed to fit the quark condensate. Let us justify this conclusion in detail. For that purpose, we consider the HRG result for the reduced quark condensate (equation (1.139)), which is one of the condensate combinations for which lattice analysis yield definite predictions, being free of finite-size divergences [56–59]. We include the fitting B parameter as explained before (recall that B multiplies only the finite temperature correction of quark condensates, not their $T = 0$ part). The result of such fit (HRG fit 3) is provided in Fig.2.9, the fit parameters being given in Table 2.2, and shows a very good description of the reduced condensate, with a value of B compatible with unity and therefore in agreement with the analysis in [73]. However, that value is incompatible with that in fit 2, i.e., the HRG scalar susceptibility fit in the same temperature range. Such incompatibility is clearly seen in the prediction for χ_S showed in the right panel of that figure. Recall that those lattice data for both quantities come exactly from the same collaboration and lattice setup. The previous claim is confirmed if we try to fit jointly the reduced condensate and scalar susceptibility lattice points. In that case, we

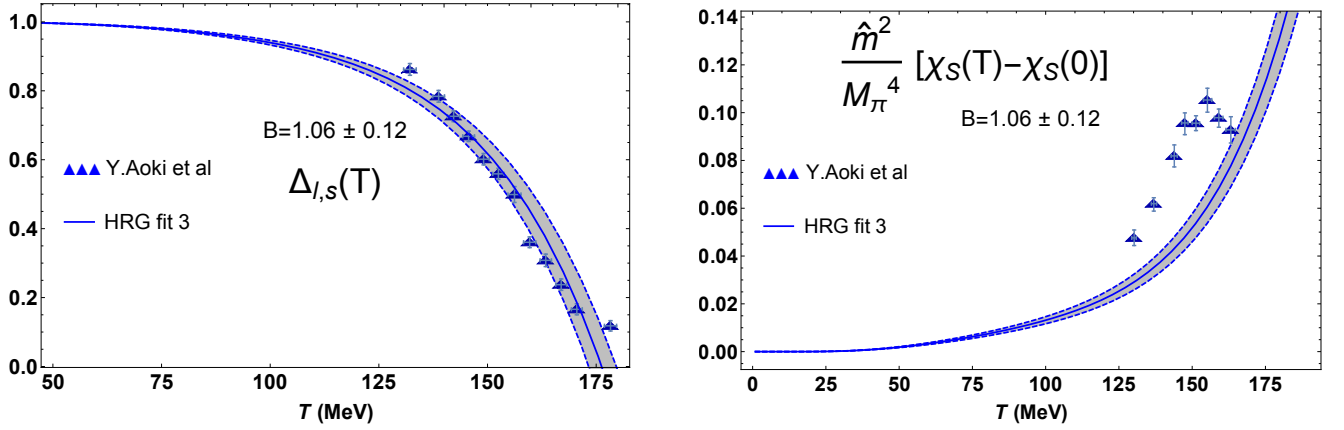


Figure 2.9: Left: Fit of the HRG reduced condensate with the normalization constant as fit parameter, fitting data up to $T \leq T_c = 155$ MeV. The quoted uncertainties in the B parameter and the bands correspond to the 95% confidence level of the fit. The lattice data and errors are from [56]. Right: prediction for the scalar susceptibility with the same B central value and uncertainty.

obtain a $\chi^2/\text{dof} \simeq 71$ indicating clearly that such a joint description of both quantities within the HRG approach is not feasible.

We could of course perform more elaborated fits, such as considering the LEC in the thermal $f_0(500)$ or the hadron masses and their quark mass dependence in the HRG as additional fit parameters. However, the main objective of our present analysis is to compare both approaches and show that actually the thermal $f_0(500)$ one is competitive with respect to the HRG around the transition, and a simple one-parameter fit is enough for such purposes.

2.5 Conclusions

In this chapter we have performed a detailed analysis of the importance of the thermal corrections to the $f_0(500)$ resonance spectral parameters, regarding the description of the scalar susceptibility χ_s around the region of chiral symmetry restoration. Such analysis has been carried out for different realizations of the thermal $f_0(500)$ state within effective theories. First, using the LSM as a testbed, we have showed that a direct relation can be established between the scalar susceptibility and the propagator of the lightest scalar state at zero momentum. Through the analysis of the LSM one-loop σ self-energy at finite temperature, we have shown that the susceptibility saturated by the σ propagator has a much larger growth than the purely perturbative one, approaching

better lattice data, although with a divergent behaviour in the massive case. The LSM analysis provides additional support for the formulation of χ_S through the UChPT saturated approach, where the $f_0(500)$ arises as a resonance in $\pi\pi$ scattering, including thermal corrections. The UChPT approach provides a much more reliable description of the $T = 0$ $f_0(500)$ pole and of $\chi_S(T)$ as long as the basic requirements of unitarity and analyticity are maintained. Within the IAM formulation, such approach actually reproduces correctly the crossover peak and lattice data within the sensitivity of the ChPT low-energy constants. The requirements of unitarity, analyticity and a good determination of the $T = 0$ pole are crucial to achieve the expected qualitative behaviour for the thermal scalar mass, although a correct description of the saturated susceptibility is achieved when the full $\mathcal{O}(p^4)$ corrections to the thermal amplitude are taken into account.

A conclusion shared by the LSM and UChPT approaches is that a saturated approach for $\chi_S(T)$ where only this thermal state is included, can account for most of lattice data below and even around the transition. For that reason, we have performed several fits of the UChPT saturated approach, with a single parameter fit (normalization factor) comparing it with a description based on the Hadron Resonance Gas where all hadron states below 2 GeV have been included. The HRG result for $\chi_S(T)$, which had not been analyzed before, provides a better fit than UChPT for temperatures below the transition. However, as values closer to T_c are included, the UChPT improves over the HRG, since it can describe the susceptibility peak. In addition, the HRG fits for the scalar susceptibility are in conflict with those of the quark condensate, using a single-parameter fit.

Through the various approaches analyzed, we conclude that the thermal $f_0(500)$ state is crucial to describe correctly the scalar susceptibility and hence to understand correctly the chiral restoration transition. We believe that our results can be useful in that sense and we leave for future work related problems such as the possibility to include thermal interactions for the scalar channel within the HRG which could help to understand previous studies regarding the role of the $f_0(500)$ in that approach.

The role of the κ and strangeness in chiral and $U(1)_A$ restoration

The nature of the chiral transition is intimately connected to the anomalous $U(1)_A$ symmetry, which is restored only asymptotically [106]. However, there is currently no agreement as to whether this symmetry is effectively restored close to the critical temperature. While several phenomenological [65, 103, 107–109] and lattice [110–114] analyses for $N_f = 2$ light flavors support the idea that the $U(1)_A$ symmetry can be effectively restored at the chiral transition in the chiral limit, lattice results for $N_f = 2+1$ suggest that the anomalous $U(1)_A$ symmetry is still broken in the chiral crossover region [59, 115–117]. This phenomenon has also implications for the hadron spectrum [108, 118, 119] as well as phenomenological effects driven by the associated reduction of the anomalous η' mass and the topological susceptibility in a thermal environment [120–123].

As we have seen, the main observables commonly employed to study chiral symmetry restoration, both in the lattice and in phenomenological analyses, are the light-quark condensate $\langle \bar{q}q \rangle_l$ and the scalar susceptibility χ_S . Nevertheless, since the axial anomaly is consequence of a short-distance quantum effect there is no corresponding order parameter to study $U(1)_A$ restoration.

The manifestation and restoration of global symmetries such as the chiral $SU(2)_V \times SU(2)_A \approx O(4)$ and the $U(1)_A$ ones can be studied through the particle spectrum. For instance, states of opposite parity related under axial $SU(2)_A$ rotations (the so-called chiral partners) are expected to degenerate at the chiral transition. Correlation functions of chiral partners and properties derived from them such as susceptibilities ($p = 0$ correlator in Fourier space) or spatial screening masses ($p_0 = 0$, $|\vec{p}| \rightarrow 0^+$)

should also degenerate as the transition is reached. In the same way, an effective $U(1)_A$ restoration should be indicated by the degeneracy of correlation functions belonging to a $U(2) \times U(2)$ universality class.

The study of the degeneration of relevant partners under chiral and $U(1)_A$ symmetries provides a valuable method to analyze the interplay between chiral and $U(1)_A$ restoration. Consider for instance the quark bilinears for the isospin channels $I = 0, 1$ and total angular momentum $J = 0$ corresponding to the pseudoscalar and scalar meson nonets

$$\sigma_l = \bar{q}_l q_l \quad \eta_l = i\bar{q}_l \gamma_5 q_l \quad \sigma_s = \bar{s} s \quad \eta_s = i\bar{s} \gamma_5 s \quad (3.1)$$

$$\pi^a = i\bar{q}_l \gamma_5 \tau^a q_l, \quad \delta^a = \bar{q}_l \tau^a q_l, \quad (a = 1, 2, 3) \quad (3.2)$$

with q_l the light quark doublet in flavour space. Chiral symmetry restoration implies $\pi^a - \sigma_l$ and $\delta^a - \eta_l$ degeneration, where the π^a , σ_l , δ^a and η_l quark bilinears correspond to the pion, $f_0(500)$ (or σ) and the light components of the $a_0(980)$ and η [124], respectively. Likewise, $\pi^a - \delta^a$ and $\sigma - \eta_l$ are expected to degenerate once the $U(1)_A$ symmetry is effectively restored. Summarizing

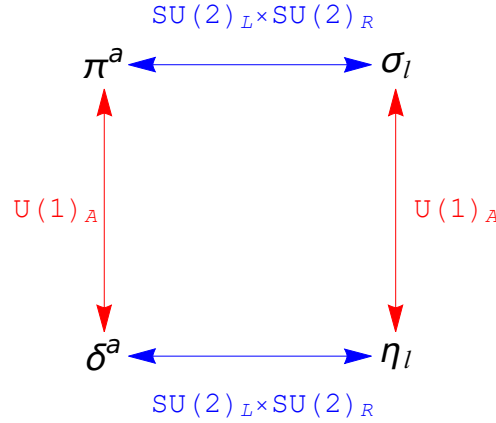


Figure 3.1: Scalar and pseudo-scalar mesons connected by chiral and axial symmetry transformations.

Whereas chiral degeneration above T_c has been clearly observed in the lattice both using screening masses [113, 125] and susceptibilities [59], hence confirming theoretical predictions at finite temperature and/or density [65, 92, 126–131], lattice results concerning $U(1)_A$ restoration are not conclusive; while $N_f = 2$ simulations suggest $\pi - \delta$ degeneration close to the chiral limit [110–112] and for physical quark masses [113, 114],

$N_f = 2 + 1$ lattice results report sizable differences between the π and δ susceptibilities in the region where $\pi - \sigma$ degeneration occurs [59, 115].

3.1 K - κ degeneration

For the $I = 1/2$ channel we consider the pseudoscalar and scalar bilinears

$$K^b = i\bar{q}\gamma_5\lambda^b q \quad \kappa^b = \bar{q}\lambda^b q, \quad (b = 4, 5, 6, 7) \quad (3.3)$$

whose lightest states are the kaon and $K_0^*(700)$ mesons, respectively, and q is the quark triplet. The K and κ bilinears can be related by both a chiral $O(4)$ and a $U(1)_A$ transformation [103]. Namely, a general $SU(2)_A \times U(1)_A$ rotation of the up and down quark fields

$$\begin{array}{c} q' \rightarrow e^{i\gamma_5(\alpha_0 \mathbb{1}_2 + \alpha_b \tilde{\tau}^b)} q, \\ \swarrow \quad \searrow \\ \boxed{\begin{array}{c} SU(2)_A \\ q' \rightarrow e^{i\gamma_5 \alpha_b \tilde{\tau}^b} q \end{array}} \quad \boxed{\begin{array}{c} U(1)_A \\ q' \rightarrow e^{i\gamma_5 \alpha_0 \mathbb{1}_2} q \end{array}} \end{array}$$

with $\mathbb{1}_2 = \text{diag}(1, 1, 0)$, $\tilde{\tau}^b = \begin{pmatrix} \tau^b & \\ & 0 \end{pmatrix}$, and $b = 1, 2, 3$, acting on the K^a bilinear

$$K^a(x)' \rightarrow \cos \alpha_0 \cos \alpha_b K^a(x) - \sin \alpha_0 \cos \alpha_b \kappa^a(x) - 2d_{abc} \sin \alpha_b \kappa^c(x), \quad (3.4)$$

with $d_{abc} = \pm 1/2$ and $a, c = 4, \dots, 7$, connects it with κ^a field. This connection has some important consequences:

1. Both $O(4)$ and $U(1)_A$ exact restoration imply $K - \kappa$ degeneration.
2. The opposite is not necessarily true; there might be a region where $\chi_P^K \sim \chi_S^\kappa$ but the $O(4)$ or $U(1)_A$ symmetries are still significantly broken, i.e., $K - \kappa$ degeneration is a necessary but not sufficient condition for $O(4) \times U(1)_A$ restoration. Nevertheless, throughout this work we will provide evidences supporting the actual connection between $K - \kappa$ degeneration and $O(4) \times U(1)_A$ restoration.
3. Exact $O(4)$ restoration at T_c takes place only for $N_f = 2$ in the light chiral limit $m_l \rightarrow 0$. Note that in this case, WIs for pure $U(1)_A$ observables, like the topological susceptibility or the difference between the π and η_l susceptibilities, imply $O(4) \times U(1)_A$ restoration at the exact $O(4)$ transition [65, 103]. Thus, in this limit $K - \kappa$ should also degenerate at T_c .

4. In the physical case with $N_f = 2 + 1$ and nonzero quark masses, $\langle \bar{q}q \rangle_l$ vanishes only asymptotically and the $O(4)$ symmetric phase is reached only approximately. In addition, the $U(1)_A$ symmetry vanishes also asymptotically above T_c . Thus, in this case $\chi_P^K - \chi_S^\kappa$ might be still different to zero above the crossover chiral transition.
5. In the $SU(3)$ limit, i.e., for $m_s = m_l$, the K and $K_0(700)/\kappa$ are expected to degenerate with the π and $f_0(500)/\sigma$, respectively [132,133] and hence, one should expect $K - \kappa$ degeneration at the chiral transition, understood as the region where π and σ degenerate.

Furthermore, recent theoretical analyses from the Nambu–Jona-Lasinio model [131] and ChPT [65] have shown that in the physical case $K - \kappa$ degeneration occurs above the crossover region, but around the same temperature where the isoscalar and isovector $O(4) \times U(1)_A$ partners degenerate. Actually, within ChPT, the temperature at which χ_P^K matches χ_S^κ is practically the same at which the $U(1)_A$ partners π and δ degenerate. Consistent results pointing in the same direction are obtained from lattice analyses of K and κ screening masses [125,134], which only degenerate at temperatures above 200 MeV, again in the same region of $O(4) \times U(1)_A$ partner degeneration.

In that context, the advantage of the WIs in the $I = 1/2$ sector (B.25)-(B.26) is that χ_P^K and χ_S^κ are expressed in terms of well-measured quark condensates, as discussed below, whose thermal behavior provide a model independent tool to study their degeneration. Before discussing in more detail the consequences of $K - \kappa$ degeneration for $O(4) \times U(1)_A$ restoration, we will first analyze in the next section what can be learned about χ_P^K and χ_S^κ using the WIs (B.25)-(B.26).

3.2 Properties of χ_P^K and χ_S^κ

The light-quark condensate $\langle \bar{q}q \rangle_l$, as the order parameter of the chiral transition, is expected to drop abruptly at the transition temperature, with an inflection point at T_c for physical quark masses. However, $\langle \bar{s}s \rangle$ is supposed to decrease much softly due to the explicit chiral symmetry breaking of the heavier strange quark [58], being m_l/m_s the parameter regulating the relative drop of these two condensates. These trends can be clearly observed in lattice analyses. For illustrative purposes we show in Fig. 3.2 the light (Δ_l^R) and strange (Δ_s^R) subtracted condensates reported in [58]; while Δ_l^R drops abruptly close to the chiral transition and asymptotically above T_c , Δ_s^R remains large at

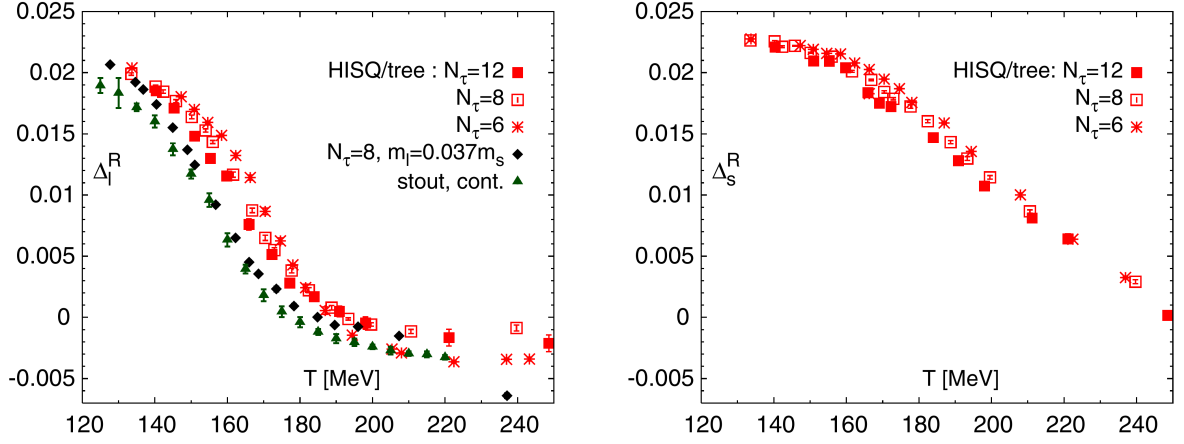


Figure 3.2: Light- (left panel) and strange-quark (right panel) subtracted condensates around $T_c \sim 155$ MeV computed in [57,58]. They are defined as $\Delta_{l,s}^R = d + 2m_s r_1^4 (\langle \bar{\psi}\psi \rangle_T - \langle \bar{\psi}\psi \rangle_0)$, with $\psi = q, s$ and d, r_1 lattice parameters defined in [58]. Figure taken from [58].

the critical temperature, showing only a smooth decrease. Note that, as we mentioned in subsection 1.3.3, lattice quark condensates usually have to be subtracted to remove UV divergences $\langle \bar{q}_i q_i \rangle \sim m_i/a$, with a the lattice spacing and m_i the quark mass as defined in [58].

On the one hand, since both the light- and strange-quark condensates are negative quantities, (B.25) indicates that χ_P^K should decrease continuously at all temperatures, with an abrupt drop off around T_c coming from the light-quark condensate. On the other hand, (B.26) implies that below and around the chiral transition $\chi_S^\kappa(T)$ should grow following the $\langle \bar{q}q \rangle_l$ decrease and the roughly constant behavior of $\langle \bar{s}s \rangle$. Nevertheless, above the $O(4)$ transition the light-quark condensate starts decreasing only asymptotically, while at some temperature the $\langle \bar{s}s \rangle$ reduction takes over, hence changing the trend of $\chi_S^\kappa(T)$ to a slowly decreasing behavior towards degeneration with $\chi_P^K(T)$.

The previous argument implies that in the physical case, χ_S^κ should have a maximum at a temperature $T > T_c$ and that the behavior of the curve above the maximum is driven by the $\langle \bar{s}s \rangle$ drop. In addition, near the chiral $m_l/m_s \rightarrow 0$ limit one should expect a steepest growth below the maximum, dictated by $\langle \bar{q}q \rangle_l$, but a flattening above it, from $\langle \bar{s}s \rangle$, pointing out for $K - \kappa$ degeneration at lower temperatures. On the contrary, in the $SU(3)$ $m_l/m_s \rightarrow 1$ limit, the peak should be more pronounced from both sides, consistently with κ and σ degeneration.

The existence and properties of the $\chi_S^\kappa(T)$ peak, coming from WIs and confirmed with our lattice and theoretical UChPT analysis below, are key results of the present work.

3.3 Results from lattice data

Without direct $\chi_S^\kappa(T)$ and $\chi_P^K(T)$ lattice data available, the above hypotheses can be tested using lattice results for the combinations of light- and strange-quark condensates appearing in (B.25) and (B.26), which we denote as reconstructed susceptibilities. In Fig. 3.3 we show the results of the reconstructed susceptibilities using the unsubtracted condensate data in [58, 135] for two different quark-mass configurations: $m_s = 20 m_l$, which is close to the physical point, and $m_s = 40 m_l$, closer to the chiral limit.

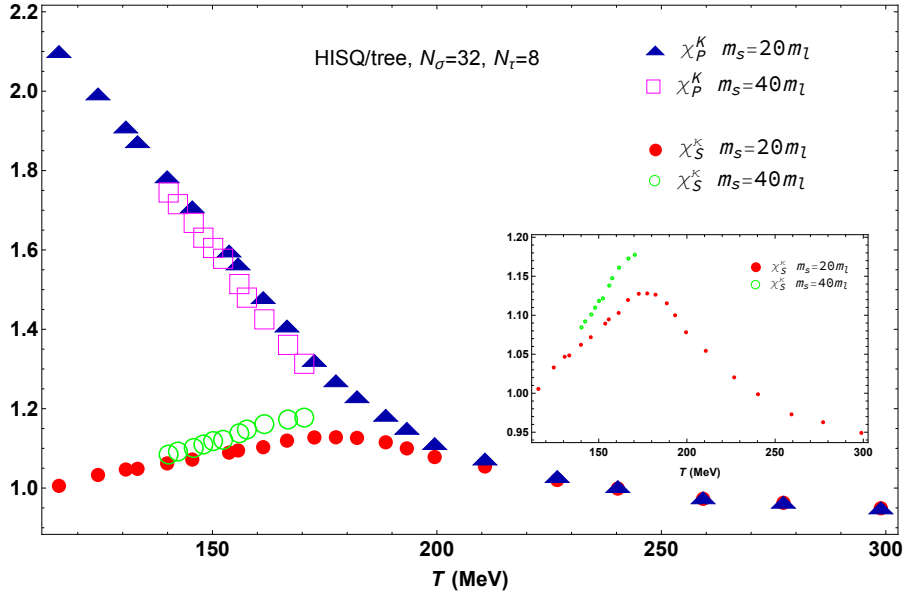


Figure 3.3: Reconstructed pseudoscalar and scalar susceptibilities (in lattice units) in the $I = 1/2$ channel from (B.25) and (B.26), respectively, with light- and strange-quark condensate data from [58, 135]. In the inset panel we show $\chi_S^\kappa(T)$ separately in order to emphasize the peak behavior. For such lattice setup, the continuum extrapolation to the physical mass case $m_s = 27 m_l$ gives $T_c = 154 \pm 9$ MeV.

The results in Fig. 3.3 are fully consistent with the theoretical expectations. First, χ_P^K decreases at all temperatures, with a smooth asymptotic behavior above T_c . Second, the scalar susceptibility χ_S^κ develops a maximum around T_c , after which it shows a smooth temperature dependence, degenerating with χ_P^K at temperatures $T \gtrsim 180$ MeV. Such degeneration is ultimately driven by strangeness through $\langle \bar{s}s \rangle$. In fact, the data for $m_s = 40 m_l$ reflect the expected behavior below T_c and seem to indicate $\chi_S^\kappa - \chi_P^K$ degeneration at lower temperatures, as expected from the softer $\langle \bar{s}s \rangle$ T -dependence. Unfortunately, available lattice results for condensates closer to the chiral limit [58, 136] do not reach the temperatures of interest for our purposes here.

The results in Fig. 3.3 are also supported by lattice analyses of screening masses [125, 134]. Although screening masses and susceptibilities measure different limits of meson correlators at vanishing four momenta (the susceptibility behaves as the inverse pole mass squared while the screening mass measures the exponential falloff of the correlator at large spatial separation), these two quantities follow a similar temperature scaling [65, 131, 137]. Lattice results show a minimum around the transition for the κ screening mass, hence playing the counterpart of the χ_S^κ maximum in Fig. 3.3. Moreover, all scalar channels analyzed in [125, 134] show a similar minimum driven by its degeneration with their corresponding pseudoscalar partner, which might constitute a global meson pattern.

3.4 Theoretical analysis from Effective Theories

In order to analyze the behavior of χ_S^κ from the theoretical side at and beyond the physical point, we consider a UChPT approach where $\chi_S^\kappa(T)$ is saturated by its lowest pole, the $K_0^*(700)/\kappa$ meson, generated in πK scattering at finite temperature. Namely,

$$\chi_S^{\kappa,U}(T) = A_\kappa \frac{M_\kappa^2(0)}{M_\kappa^2(T)} \quad (3.5)$$

where we fix A_κ to reproduce the perturbative ChPT result at $T = 0$, i.e., $A_\kappa = \chi_S^{\kappa,\text{ChPT}}(0)$ calculated in [65], and $M_\kappa^2(T) = M_p^2(T) - \Gamma_p^2(T)/4$, with $s_p = (M_p - i\Gamma_p/2)^2$ the resonance pole position in the second Riemann sheet of the complex s -plane for the unitarized πK $I = 1/2$ scalar partial wave. Thus, $M_\kappa^2(T)$ is the real part of the $K_0^*(700)$ self-energy at the pole, which is expected to provide the dominant temperature dependence of χ_S^κ . Since susceptibilities are $p = 0$ correlators, the sensibility to the p -dependence of the self-energy and the T -dependence of its residue in (3.5) are assumed to lie within the uncertainty bands. That is actually the case when the scalar susceptibility $\chi_S(T)$ is saturated by the thermal $f_0(500)/\sigma$, as we saw in the previous chapter. Namely, this approach has been proven to reproduce the $\chi_S(T)$ transition peak and to describe lattice data around it.

For the unitarized πK scattering amplitude we rely on the UChPT techniques described in subsection 1.4.4. For the $\mathcal{O}(p^4)$ contribution to the amplitude we consider two different methods consistent within unitarity and analyticity requirements for the thermal amplitude.

As a test of the capability of Methods 1 and 2 to describe the $K_0^*(700)$, we get at $T = 0$ $\sqrt{s_p^{(1)}} = (731 \pm 7) - i(280 \pm 9)$ MeV and $\sqrt{s_p^{(2)}} = (679 \pm 6) - i(289 \pm 8)$ MeV,

for method 1 and 2, respectively, where we have used the subtraction constant value and error in [138] for method 1 and the LECs of the global fit in [139] for method 2. For the latter, the uncertainties are computed from the propagation in quadrature of the LEC errors. These results are perfectly consistent with the most precise dispersive calculations [140–142].

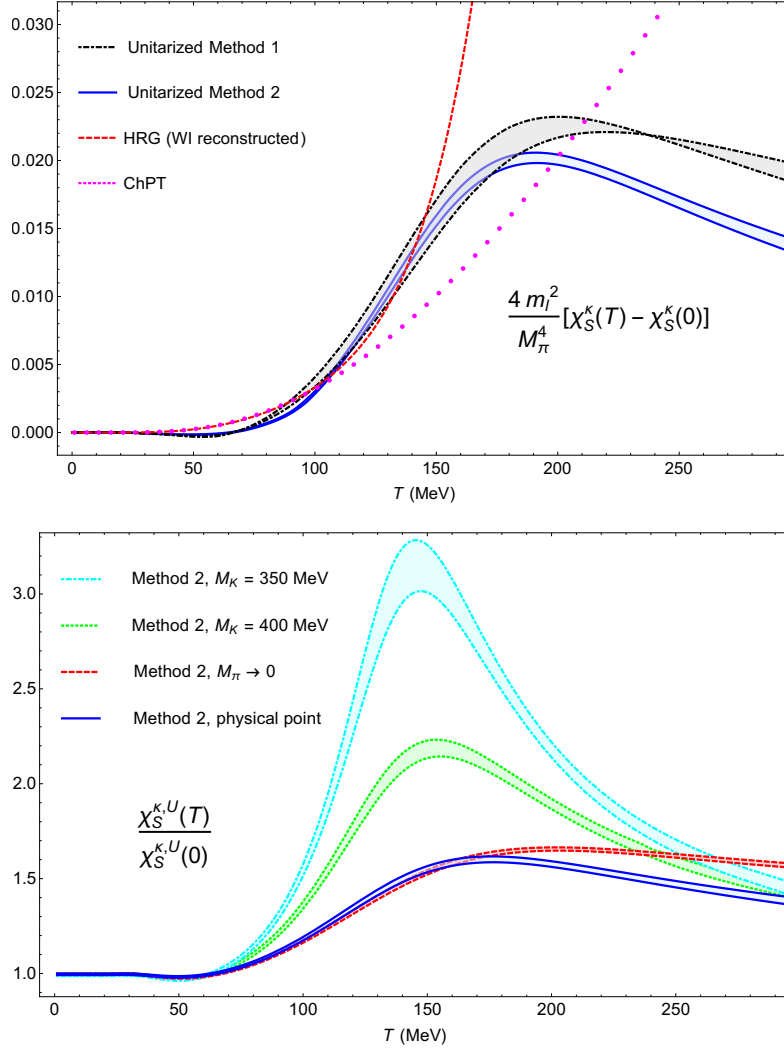


Figure 3.4: Upper panel: κ susceptibility from UChPT with the two methods explained in the main text, including their theoretical uncertainty bands, the perturbative ChPT result and the HRG one extracted from the quark condensate combination in (B.26). Lower panel: Unitarized κ susceptibility for physical masses, the light chiral limit and for M_K closer to the $SU(3)$ limit.

The $\chi_S^{\kappa,U}$ results for both unitarization methods, including their uncertainties, are plotted in Fig. 3.4 together with the reconstructed scalar susceptibility from the WI in (B.26) using for the light- and strange-quark condensates the HRG results in [73]. As

we saw in the previous chapter, the HRG includes hadron resonances of masses below 2 GeV and is meant to capture the relevant thermodynamics below the transition, hence providing a check of consistency for our unitarized results and a way to estimate the importance of such higher states for this observable. In addition, we also include the perturbative ChPT prediction calculated in [65]. The two thermal unitarized methods remain fairly consistent between them and compatible with the perturbative ChPT and HRG results below the transition, indicating the robustness of the approach. In addition, both reproduce the expected $\chi_S^{\kappa,U}$ peak behavior, unlike the ChPT or HRG, which are monotonically increasing. This reveals the importance of considering thermal interactions in order to describe these non-perturbative phenomena around the transition.

Finally, we study the chiral and $SU(3)$ limits using method 2, which at $T = 0$ reproduces the light- and strange-quark mass dependence of the πK amplitude predicted in ChPT. The behavior of $\chi_S^{\kappa,U}$ in the two limits is plotted in Fig. 3.4, showing the expected results. On the one hand, when approaching the chiral limit we find a steepest growth below the maximum and a flatter curve above it. On the other hand, the reduction of the kaon mass enhances the size of the peak and moves it to lower temperatures closer to T_c , so that $\chi_S^{\kappa,U}$ tends to resemble the behavior of χ_S consistently with $SU(3)$ symmetry.

3.5 Consequences for $O(4) \times U(1)_A$ restoration

The results described in section 3.2 show that χ_S^κ develops a maximum, after which it degenerates with χ_P^K . This prediction is obtained from rigorously derived WIs and hence, it can be considered as a model independent result. In that context, some comments are in order to relate this sector with $O(4) \times U(1)_A$ restoration:

(i)- Close to the physical point, i.e., using the $m_s = 20 m_l$ lattice data for the light- and strange-quark condensates in [58, 135], one observes that the position of the χ_S^κ peak lies well above the $O(4)$ crossover region—the temperature at which χ_S develops a maximum and $\pi - \sigma$ degenerate. There is no contradiction since $K - \kappa$ degeneration should happen at T_c only if $O(4)$ restoration is exact i.e., for $N_f = 2$ and $m_l \rightarrow 0$.

Conversely, the temperature at which the reconstructed χ_S^κ and χ_P^K degenerate lies close to region where current $N_f = 2 + 1$ lattice data [59, 115] find $\pi - \delta$ degeneration; even when $K - \kappa$ degeneration only imposes a lower bound for $U(1)_A$ restoration, this result shows that, for physical quark masses, such degeneration lies around the point

where $U(1)_A$ symmetry is assumed to be asymptotically restored in $N_f = 2 + 1$ lattice simulations. Thus, $K - \kappa$ degeneration might be considered as an additional sign to study asymptotic $O(4) \times U(1)_A$ restoration. Additional arguments supporting this proposal are the degeneration of $K - \kappa$ lattice screening masses in the $T \sim 200$ MeV region of $O(4) \times U(1)_A$ restoration [134], and results in ChPT and NJL models showing coincidence of the $K - \kappa$ degeneration temperature with that of the $U(1)_A$ partners, like $\pi - \delta$ [65, 131].

Further information can be obtained by taking the difference between (B.25) and (B.26),

$$\chi_S^\kappa(T) - \chi_P^K(T) = \frac{2}{m_s^2 - m_l^2} \Delta_{l,s}(T), \quad (3.6)$$

where $\Delta_{l,s}(T)$ is the subtracted condensate defined in (1.139). Eq. (3.6) provides information on $K - \kappa$ degeneration in terms of a well-determined lattice quantity. In Fig. 3.5 we plot the normalized $\bar{\Delta}_{l,s}(T) = \Delta_{l,s}(T)/\Delta_{l,s}(0)$ results given in [58], where one can see that at T_c this difference has reduced its value by half, and only at much larger temperatures $T > 200$ MeV $\Delta_{l,s}$ shows an asymptotic vanishing behavior compatible with effective $O(4) \times U(1)_A$ restoration. Thus, even when $\Delta_{l,s}$ is usually considered equivalent to $\langle \bar{q}q \rangle_l$, i.e., as an order parameter for $O(4)$ restoration, this is only true in the light chiral limit. In the physical case, Eq. (3.6) indicates that its vanishing actually provides a sign of $O(4) \times U(1)_A$ restoration. Note, however, that its inflection point practically coincides with that of $\langle \bar{q}q \rangle_l$ since the variation of $\langle \bar{s}s \rangle$ with T is almost negligible at that temperatures and hence, the $\Delta_{l,s}$ subtracted condensate works perfectly well to estimate the crossover temperature. This is not in conflict with the $\Delta_{l,s}$ vanishing signaling $O(4) \times U(1)_A$ restoration, being $\langle \bar{s}s \rangle$ ultimately responsible for the $\Delta_{l,s}$ tail behavior.

(ii)- Let us consider now the $m_s \gg m_l$ expansion. On the one hand, the right-hand side in (3.6) reads

$$\chi_S^\kappa(T) - \chi_P^K(T) \Big|_{m_s \gg m_l} = \frac{2}{m_s} \langle \bar{q}q \rangle_l(T) \Big|_{\text{SU}(2)} + \mathcal{O}(1/m_s^2). \quad (3.7)$$

On the other hand, the left-hand side of (3.6) in this limit can be studied in ChPT, where at leading order in this expansion one finds $\chi_S^\kappa(T) - \chi_P^K(T) \Big|_{m_s \gg m_l} \propto 1/m_s$ [65]. Thus, at leading order, this regime is nothing but the $N_f = 2$ limit, where the strange quark is fully decoupled for $m_s \rightarrow \infty$. Even though the K and κ susceptibilities are pure $SU(3)$ quantities and, in the physical case, the strange quark should be taken as a dynamical degree of freedom, its difference has a well-defined $N_f = 2$ limit.

Furthermore, Eq. (3.7) implies $K - \kappa$ degeneration at T_c in the $m_l \rightarrow 0$ limit, since in this case the light-quark condensate vanishes exactly. This is consistent with the

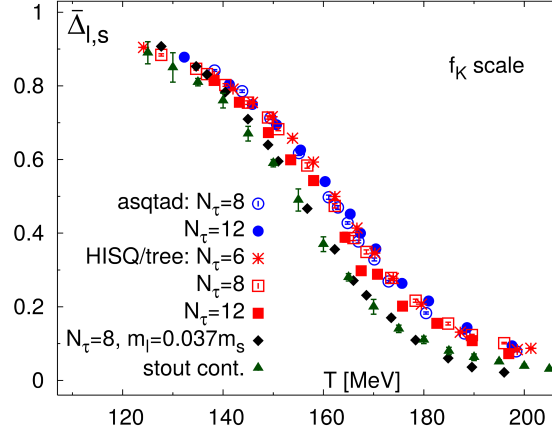


Figure 3.5: Subtracted quark condensate normalized to its value at zero temperature as given in [58]. At T_c , $\bar{\Delta}_{l,s}$ has reduced its value by half and only at higher temperatures it shows an asymptotic vanishing behavior compatible with $O(4) \times U(1)_A$ restoration. Figure taken from [58].

analysis in [65, 103] and two-flavor lattice results [110–114], which suggest $O(4) \times U(1)_A$ restoration at the $O(4)$ transition for $N_f = 2$ in the light chiral limit. Thus, our analysis helps then to reconcile lattice results in these two different regimes.

(iii)- It is also relevant to discuss the light chiral limit for $N_f = 2 + 1$. As can check in ChPT, both χ_S^κ and χ_P^K are well behaved quantities in this case [65], and hence, Eq. (3.6) simplifies to

$$\chi_S^\kappa(T) - \chi_P^K(T)|_{m_l=0} = \frac{2}{m_s} \langle \bar{q}q \rangle_l(T)|_{m_l=0}. \quad (3.8)$$

Note that the difference between (3.7) and (3.8) is that for the latter, the light-quark condensate appearing in the right-hand side is the $SU(3)$ result in the light chiral limit, which does not vanish at T_c and hence, the $K - \kappa$ susceptibility difference does not vanish either. Even though the susceptibility difference in this case is expressed in terms of the chiral condensate¹, Eq. (3.8) does not imply any consequence regarding $O(4) \times U(1)_A$ restoration since both symmetries are explicitly broken. Clearly, $m_l \rightarrow 0$ accelerates chiral $O(4)$ restoration with respect to the physical case, but it also does so with $U(1)_A$ restoration, since we are closer to the regime where exact $O(4)$ restoration implies an exact $O(4) \times U(1)_A$ symmetric phase. This is actually reflected in the behavior of the χ_S^κ peak in the light chiral limit analyzed in section 3.2 both for the reconstructed lattice data and the UChPT. Only when the $m_l/m_s \rightarrow 0$ limit is taken, Eqs. (3.8) and (3.7)

¹This comes as no surprise since exact $O(4)$ implies $K - \kappa$ degeneration.

coincide, the strange quark decouples and the previous conclusion about $O(4) \times U(1)_A$ restoration at T_c follows.

(iv)- The $SU(3)$ $m_l/m_s \rightarrow 1$ limit in (3.6) is also well behaved and illustrative. Evaluating it once again in ChPT, we get

$$\chi_S^\kappa(T) - \chi_P^K(T)|_{m_s \rightarrow m_l} = \chi_S + \frac{\langle \bar{q}q \rangle_l}{m_l} = \chi_S - \chi_P^\pi, \quad (3.9)$$

where χ_P^π stands for the pion pseudoscalar susceptibility. This confirms our previous statement about this limit, where the κ and the $I = 0$ scalar susceptibilities degenerate one into another. Thus, if this limit is obtained by reducing the strange-quark mass but keeping the light-quark mass fixed, one expects χ_S^κ to resemble the χ_S crossover peak, as we do observe in our UChPT analysis. Finally, it is worth noting that even when the $K - \kappa$ susceptibility difference is expressed once more in terms of two $O(4)$ quantities, they are nonzero at T_c in $N_f = 2 + 1$. Thus, $O(4) \times U(1)_A$ would not be restored near T_c in this limit because one is far away from the strange-quark decoupling regime.

Our arguments in this section justify then that m_l/m_s is the relevant parameter regarding the behavior of the $K - \kappa$ susceptibility difference and its connection with $O(4) \times U(1)_A$ restoration.

3.6 Conclusions

We have performed a detailed analysis of the scalar and pseudoscalar susceptibilities in the $I = 1/2$ channel based on Ward Identities, lattice data and Unitarized Chiral Perturbation Theory, which provides an alternative way to study the interplay between chiral and $O(4) \times U(1)_A$ restoration and the role of strangeness in that context. This joint analysis gives rise to the following consistent results:

1. The κ scalar susceptibility develops a peak, which in the physical limit and for $N_f = 2 + 1$ lies above the chiral crossover. Below this peak, the rise of the susceptibility is controlled by the light-quark condensate and then it is mostly related to chiral restoration. Above the peak, the susceptibility drop is driven by the strange-quark condensate and the κ susceptibility tends to degenerate with the K one.
2. Although there are no direct lattice results for the $I = 1/2$ susceptibilities available, we reconstruct them from WIs and condensate data. The results confirm

the existence of the χ_S^κ peak and the $\chi_S^\kappa - \chi_P^K$ degeneration. In the physical case, the position of the peak lies within the region of $O(4) \times U(1)_A$ restoration, i.e., the temperature where lattice analyses suggest the vanishing of the topological susceptibility or $\pi - \delta$ degeneration.

3. Within a UChPT approach, we have studied the κ scalar susceptibility by saturating it with the thermal pole of the $K_0^*(700)/\kappa$, the lightest $I = 1/2$ scalar state, which is dynamically generated through unitarized πK scattering at finite temperature. The result confirms again the presence of the peak, which other approaches such as ChPT or the HRG are not able to provide, hence highlighting the importance of including properly thermal interactions. Our analytic UChPT approach has also the advantage of allowing us to tune the meson masses beyond the physical limit to study the behavior of the κ susceptibility in the chiral and SU(3) limits.
4. The parameter m_l/m_s controls effectively the transition from the $N_f = 2$ to the $N_f = 2 + 1$ cases for the observables analyzed here. This offers a way to reconcile lattice results in these two scenarios regarding $O(4) \times U(1)_A$ restoration and suggest that $\chi_S^\kappa - \chi_P^K$ is an alternative useful sign to study this problem. In the physical case, our work, based on lattice data, is consistent with previous ChPT and NJL analyses, as well as with results from lattice screening masses, all pointing to $\chi_S^\kappa - \chi_P^K$ degeneration in the region where $O(4) \times U(1)_A$ restoration takes place.
5. The $\chi_S^\kappa - \chi_P^K$ susceptibility difference can be related to $\Delta_{l,s}$, one of the subtracted quark condensates customarily analyzed in the lattice. For $m_l/m_s \rightarrow 0$, the strange quark decouples, the $N_f = 2$ limit is reached and our analysis suggests that the $O(4)$ and $O(4) \times U(1)_A$ transitions coincide at T_c , hence consistently with previous WIs analyses and $N_f = 2$ lattice data. In the same way, our UChPT result shows a flattening of χ_S^κ above the peak in the light chiral limit, reflecting degeneration with χ_P^K . In the opposite limit, $m_l/m_s \rightarrow 1$, the degenerate SU(3) phase is achieved, which implies χ_S^κ and χ_S degeneration. Within UChPT, we confirm this behavior by lowering the kaon mass, which makes the χ_S^κ peak grow and displace to the left towards T_c , thus resembling the behavior of χ_S at the crossover region.

We believe that our present analysis provides new insight about the $I = 1/2$ sector, which may be useful for future theoretical and lattice analyses. Furthermore, it helps

to better understand the role of strangeness in the current tension between $N_f = 2 + 1$ and $N_f = 2$ lattice results regarding $O(4) \times U(1)_A$ restoration.

The pion-kaon scattering amplitude and the $K_0^*(700)$ and $K^*(892)$ resonances at finite temperature

In the present chapter, we will compute the πK elastic scattering amplitude at finite temperature within ChPT, as well as study its unitarization and the generation of the thermal $K_0^*(700)$ and $K^*(890)$ resonances. Updated analyses and reviews about these resonances at $T = 0$ can be found, for e.g., in [141–144], where their present theoretical and experimental status, as well as precise determinations of their spectral properties, are studied.

The interest in the $K_0^*(700)$ resonance at finite temperature has increased lately. For instance, in [145], its thermal properties are studied within thermal sum rules, and in [146], using virial expansion methods. Nevertheless, these two references do not take into account the thermal modifications of the πK amplitude at finite temperature. Our analysis also has direct implications for the chiral transition and its nature since, in Chapter 3, it has been proved using WI that the $I = 1/2$ scalar susceptibility should also have a peak above T_c . This peak indicates the onset of $U_A(1)$ restoration via the degeneration of the scalar and pseudoscalar channels, whose lightest states are the $K_0^*(700)$ and the kaon, respectively. In addition it has been shown that such a peak can be reproduced by saturating the $I = 1/2$ scalar susceptibility with the $K_0^*(700)$ thermal pole, which, in turn, is generated via the unitarization of a simplified πK thermal amplitude. While at $T = 0$ such amplitude corresponds to the full ChPT prediction, at finite temperature it only includes the S -channel contribution responsible for thermal

unitarity, along the lines discussed in [138].

Therefore, the purpose of this chapter is to provide the full calculation of the πK scattering amplitude in ChPT at finite temperature and analyze its main phenomenological consequences for the topics discussed above related to the QCD phase diagram. The main advantages and novelties of our analysis are the following:

1. By construction, ChPT includes the correct thermal dependence of any GB scattering amplitude at low temperatures, not only the effects related to thermal unitarity. In particular, as we will see in detail, the analytical structure of a thermal amplitude gets much more complicated due to the loop integrals involved. We will then incorporate all effects properly, of which those weighted by Bose-Einstein distribution functions evaluated at the pion mass are expected to have a significative effect near T_c . In particular, we will include thermal tadpoles, which were neglected in [147], and only partially considered in [138] as corrections to thermal masses.
2. The pion-kaon amplitude is renormalized consistently within the standard ChPT dimensional regularization scheme, where the LECs absorb ultraviolet divergences at $T = 0$. Therefore, we will be able to use recent LECs determinations when performing our numerical analysis.
3. The pion and kaon mass dependence of the amplitude is under control within ChPT. This will be particularly useful when discussing the light chiral limit, which is of great relevance for chiral and $U(1)_A$ restoration, as well as the behavior towards the $SU(3)$ limit of pion-kaon degeneration¹.
4. The complete πK perturbative amplitude and its unitarization at finite temperature will provide a rigorous check of the consistency and robustness of previous approaches for the $I = 1/2, J = 0$ channel regarding the thermal behavior of the $K_0^*(700)$ pole, as well as its connection with chiral restoration.
5. We obtain in turn the $I = 1/2, J = 1$ vector partial wave at finite temperature. Thus, we also study the thermal properties of the $K^*(892)$ pole, which has not been studied before in this context. Note that while scalars meson can be reproduced

¹Note that studying the exact $SU(3)$ limit would require a coupled-channel analysis since, in this case, the ηK and πK thresholds coincide. Instead, we will study only the behavior towards $SU(3)$ degeneration, limiting ourselves to kaon masses for which an elastic approximation still makes sense.

reasonably well within the type of unitarization methods used in [138, 147], vector mesons require an accurate fourth-order ChPT description. The $K^*(892)$ meson can be indeed produced in heavy-ion collisions [148], and recent estimations predict small in-medium modifications (temperature and baryon chemical potential) of its spectral properties compared with the $\rho(770)$ [149], consistently with not observing a significative reduction in $K^*(892)$ production.

4.1 Analytical and cut structure of the thermal amplitude. Thermal unitarity and Landau cuts

In this section, we discuss the analytic structure in the complex- s plane of the perturbative ChPT partial waves at finite temperature and obtain a generalized thermal unitarity relation, which includes the Landau cut contribution arising from the pion-kaon mass difference $M_K - M_\pi$. Such thermal unitarity relation generalizes the results in [54] for equal-mass scattering and supports the unitarization method explained in subsection 1.4.4. In Appendix C.2, we provide a detailed description of the analytic structure of the J -loop integrals in the S , T , and U channels.

As we have already seen, at nonzero T , the generic J_k thermal functions given in (1.182) can be integrated using standard contour techniques, leading to

$$\begin{aligned} \Delta J_k^{ab}(\mathcal{Q}_0, |\vec{\mathcal{Q}}|, T) &= \frac{1}{4\pi^2} \int_0^\infty dq q^2 \int_{-1}^1 dx \frac{1}{4E_1 E_2} \times \\ &\quad \left\{ \frac{1}{E_1 + E_2 + \mathcal{Q}_0 + i\epsilon} [(-E_1)^k n_B(E_1) + (\mathcal{Q}_0 + E_2)^k n_B(E_2)] \right. \\ &\quad + \frac{1}{E_1 + E_2 - \mathcal{Q}_0 - i\epsilon} [(E_1)^k n_B(E_1) + (\mathcal{Q}_0 - E_2)^k n_B(E_2)] \\ &\quad - \frac{1}{E_1 - E_2 + \mathcal{Q}_0 + i\epsilon} [(-E_1)^k n_B(E_1) - (\mathcal{Q}_0 - E_2)^k n_B(E_2)] \\ &\quad \left. - \frac{1}{E_1 - E_2 - \mathcal{Q}_0 - i\epsilon} [(E_1)^k n_B(E_1) - (\mathcal{Q}_0 + E_2)^k n_B(E_2)] \right\} \quad (4.1) \end{aligned}$$

where we have denoted $\Delta J(T) = J(T) - J(0)$. Note that the result given in 1.132 is recovered for $k = 0$. The contribution of thermal processes becomes clearer by considering the imaginary part of these thermal integrals

$$\begin{aligned} \text{Im } J_k^{ab}(\mathcal{Q}_0, |\vec{\mathcal{Q}}|, T) &= \pi \int \frac{d^3 \vec{p}}{(2\pi)^3} \frac{E_1^k}{4E_1 E_2} \times \\ &\quad \times \left\{ [1 + n_B(E_1) + n_B(E_2)] [\delta(E_1 + E_2 - \mathcal{Q}_0) + (-1)^{k+1} \delta(E_1 + E_2 + \mathcal{Q}_0)] \right. \\ &\quad \left. - [n_B(E_1) - n_B(E_2)] [\delta(E_1 - E_2 - \mathcal{Q}_0) + (-1)^{k+1} \delta(E_1 - E_2 + \mathcal{Q}_0)] \right\}. \quad (4.2) \end{aligned}$$

so the analytical structure of J_1 and J_2 is the same as that of J_0 shown in Fig. 1.7. Remember that the modifications with respect to the $T = 0$ case are twofold: first, the unitary cut contribution for $\mathcal{Q}^2 \equiv s \geq (M_a + M_b)^2$ is weighted by the combination of Bose-Einstein functions $1 + n_1 + n_2$, where n_i is short for $n_B(E_i)$ and the unity contribution stands for the $T = 0$ part; second, a new cut, denoted as the Landau cut, appears for $-|\vec{\mathcal{Q}}|^2 \leq s \leq (M_a - M_b)^2$ and is weighted by $n_1 - n_2$.

The presence of these two cuts and their statistical Bose-Einstein weights are explained by scattering processes coming from the interactions of particles in the thermal bath with the incoming and/or outgoing asymptotic states [51, 54, 150, 151]. Namely, for a generic scattering process $12 \rightarrow 34$, one has to take into account the stimulated production of the 3 and 4 states from scattering with the thermal bath components, as well as their absorption by the thermal bath. These possible interactions with the bath fall into two categories corresponding to the unitary and the Landau cuts, namely, processes with even and odd numbers of particles in the initial and final states.

In more detail, denoting by a bar the particles in the bath, the unitary-like processes are the stimulated production process $\bar{1}\bar{2} \rightarrow 34$ (in other words, $\text{bath} \rightarrow \text{bath} + 34$) weighted by the function $(1 + n_3) \times (1 + n_4)$, and the absorption $34 \rightarrow \bar{1}\bar{2}$ ($\text{bath} + 34 \rightarrow \text{bath}$) weighted by $-n_3 \times n_4$. For negative energies E_3 and/or E_4 , one could have instead the production process $0 \rightarrow \bar{1}\bar{2}34$ weighted by $(1 + n_3) \times (1 + n_4)$, minus absorption $\bar{1}\bar{2}34 \rightarrow 0$ weighted by $n_3 \times n_4$. The net contribution in both cases is $(1 + n_3) \times (1 + n_4) - n_3 \times n_4 = 1 + n_3 + n_4$, which we readily identify as the $1 + n_1 + n_2$ factor associated to the unitary cut in (4.2). The Landau-like processes correspond to either $\bar{1}\bar{2}3 \rightarrow 4$ ($\text{bath} \rightarrow \text{bath} + 4$) weighted by $n_3 \times (1 + n_4)$, minus the inverse process $4 \rightarrow \bar{1}\bar{2}3$ ($\text{bath} + 4 \rightarrow \text{bath}$) weighted by $n_4 \times (1 + n_3)$, or the reactions $\bar{1}\bar{2}4 \rightarrow 3$ weighted by $n_4 \times (1 + n_3)$ minus $3 \rightarrow \bar{1}\bar{2}4$ weighted by $n_3 \times (1 + n_4)$. The net contribution is proportional to $n_3 - n_4$ corresponding to the $n_1 - n_2$ contribution in (4.2).

Note that not all these reactions will be allowed by the kinematics of a given scattering process (see below) and that, in the above thermal processes, an antiparticle state is understood as an incoming line changed into an outgoing one with respect to $12 \rightarrow 34$ scattering or conversely.

As the case of interest here, the possible thermal bath processes for $K\pi \rightarrow K\pi$ scattering are depicted in Fig 4.1. As we will immediately explain, the only allowed processes for which all of the particles involved are physical, i.e., with positive energies, are those labeled as U_1 and L_1 in the figure.

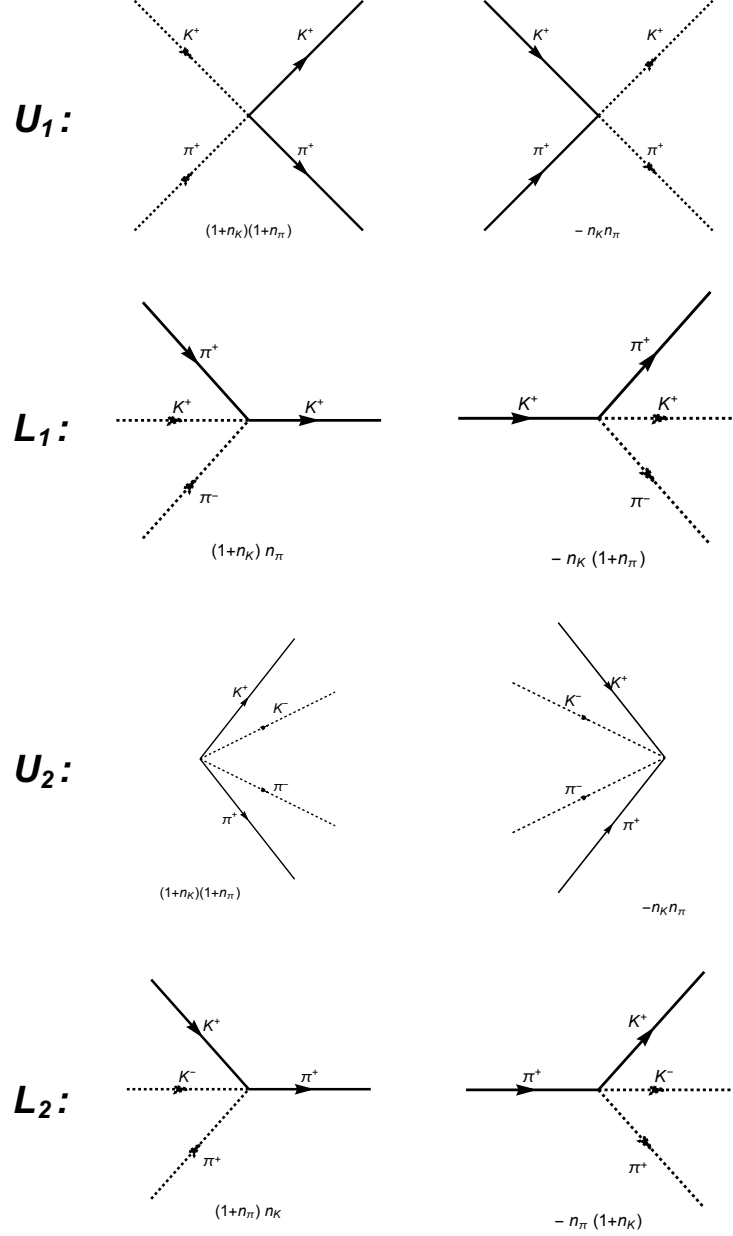


Figure 4.1: Processes contributing to $K^+\pi^+ \rightarrow K^+\pi^+$ scattering in the thermal bath. Dashed lines denote thermal bath particles, solid lines correspond to states produced or absorbed in the bath, while U and L stand for processes contributing to the Unitary or Landau cut, respectively. We also include the statistical Bose-Einstein factors associated with every process, where $n_{\pi,K}$ stand for $n_B(E_{\pi,K})$. Note that for each process of thermal production of π^+ , K^+ outgoing states, there is an absorption process carrying a relative minus sign with respect to the production one.

In the following, we will provide the explicit expressions for the imaginary part of the πK partial waves alongside the S -channel physical cuts including thermal scattering processes and the position of the unphysical T , U -channel cuts. We have summarized in Fig. 4.2 the different discontinuities contributing to the πK scattering partial waves

arising from this analysis.

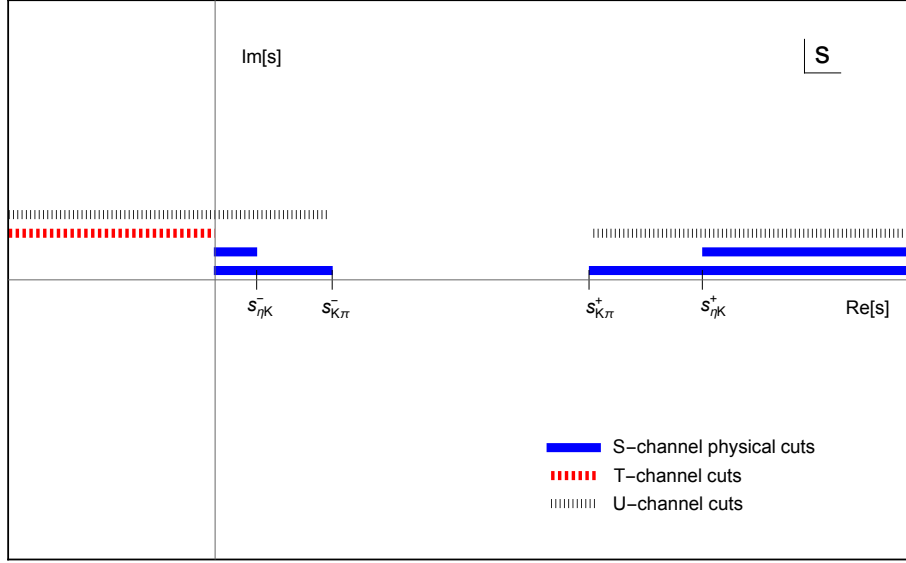


Figure 4.2: General cut structure of πK scattering partial waves at finite temperature with $s_{ab}^\pm = (M_a \pm M_b)^2$. Note that in the $I = 3/2$ channel, the physical cuts opening above $s > s_{\eta k}^+$ and $s < s_{\eta k}^-$ are not present. The circular cut discussed at the end of subsection 1.4.1 is not displayed here.

4.1.1 Physical S -channel cuts: thermal unitarity

For a given isospin channel, the $J_k(S)$ thermal integrals provide the S -channel discontinuity or physical cut, which is related to the physical processes taking place in the thermal bath and renders the thermal unitarity relation, as we are about to see.

At $T = 0$, one has only the standard unitary cuts starting from each two-particle scattering threshold. For πK scattering, the first such cut opens at $s \geq (M_K + M_\pi)^2$ coming from the $J^{K\pi}(S)$ integrals. For the $I = 1/2$ channel, a second physical cut (inelastic) starts at $s \geq (M_K + M_\eta)^2$, corresponding to the process $K\pi \rightarrow K\eta$ and coming from the $J^{\eta K}(S)$ loop function. Note that due to this inelastic contribution, the unitarization of the $I = 1/2$ channel would require a coupled-channel approach [79, 85]. However, the main properties of the $K_0^*(700)$ and $K^*(890)$ resonances can be understood by considering only the elastic region [141, 143] and we will follow the same approach here.

At nonzero T , we have, on the one hand, the thermal correction to $\text{Im } J^{K\pi}(S)$ in the unitary cut. For the $K^+\pi^+ \rightarrow K^+\pi^+$ process, i.e., the $I = 3/2$ one, the thermal bath processes contributing to such modification are those labeled as $U_{1,2}$ in Fig. 4.1. However,

it is easy to see that the U_2 -like processes require negative energies for at least one of the incoming (outgoing) states since the sum of all particle energies has to vanish. Therefore, the only physical processes contributing to the unitary cut at finite temperature are the U_1 ones. Note that in the CM frame, these processes give rise to the first contribution to the imaginary part of $J^{K\pi}(S)$ in (C.14), with $\mathcal{Q}_0 = E_K + E_\pi = \sqrt{s} > 0$, $E_K = \frac{s+\Delta_{K\pi}}{\sqrt{s}}$, $E_\pi = \frac{s-\Delta_{K\pi}}{\sqrt{s}}$, which are both positive since $s > \Delta_{K\pi} > 0$ at the unitary cut.

On the other hand, the Landau cut is generated by the processes $L_{1,2}$ in Fig. 4.1. For L_1 , we have $\bar{E}_K + \bar{E}_\pi = E_K - E_\pi = \sqrt{s}$, where the bars correspond to the thermal bath particles; i.e, we are denoting $s = (p_K - p_\pi)^2 = (\bar{p}_K + \bar{p}_\pi)^2$ so that in the CM frame, $\vec{p}_\pi - \vec{p}_K = \vec{0}$. With positive energies of the thermal bath particles, the solution to the energy conservation equation in the CM frame is $E_K = \frac{s+\Delta_{K\pi}}{\sqrt{s}}$ and $E_\pi = \frac{\Delta_{K\pi}-s}{\sqrt{s}}$ with $\mathcal{Q}_0 = E_K + E_\pi$, which satisfy $E_K > E_\pi > 0$ since $0 < s < (M_K - M_\pi)^2 < \Delta_{K\pi}$ for the Landau cut. These processes provide the second contribution to $\text{Im } J^{K\pi}(S)$ in (C.14). For the L_2 -like processes, we have $\bar{E}_K + \bar{E}_\pi = E_\pi - E_K$, which cannot be satisfied for all positive energies since $M_\pi < M_K$ and they do not contribute to the imaginary part of $J^{K\pi}(S)$.

The crucial point for obtaining the thermal unitarity relation at one-loop order in ChPT is to realize that at $T = 0$,

$$\text{Im } t^{IJ}(s) = \text{Im } t_4^{IJ}(s) = 16\pi \text{Im } J_0^{K\pi}(s) [t_2^{IJ}(s)]^2 = \sigma_{K\pi}(s) [t_2^{IJ}(s)]^2, \quad (4.3)$$

where t_2^{IJ} and t_4^{IJ} stand for the $\mathcal{O}(p^2)$ and $\mathcal{O}(p^4)$ ChPT amplitudes, respectively, and $\sigma_{K\pi}(s)$ is the two-body phase space defined in equation (1.179). It implies that, for any IJ channel, $\text{Im } J_0^{K\pi}(s)$ in the t_4 ChPT amplitude comes multiplied by $16\pi [t_2^{IJ}(s)]^2$. At finite temperature, once the relations (C.10) and (C.11) are used, the T -independent function multiplying $J_0(\sqrt{s}, \vec{0}; T)$ is the $T = 0$ one. In addition, we have to take into account those processes allowed in the thermal bath. For instance, the process $K^+\pi^+\pi^- \rightarrow K^+$ with momenta $p_K p_\pi \bar{p}'_\pi \rightarrow p'_K$, which can be obtained from the $K^+\pi^+ \rightarrow K^+\pi^+$ reaction by changing $\bar{p}'_\pi \rightarrow -p'_\pi$. This transformation leaves the t_2 amplitude invariant in terms of the variables $s = (p_K + p_\pi)^2 = (p'_K - p'_\pi)^2$, $t = (p_K - p'_K)^2 = (p_\pi + p'_\pi)^2$, and $u = (p_K + p'_\pi)^2 = (p'_K - p_\pi)^2$. The same argument applies to the thermal amplitude in terms of s, t, u, S^0, T^0 , and U^0 variables. Thus, an extended thermal perturbative unitarity relation can be obtained by including the physical Landau-type process multiplied by its corresponding thermal phase-space factor (C.14) for that cut. In the $I = 1/2$ channel, one also has to take into account the contribution from the ηK intermediate

sate, which involves $\text{Im } J_0^{\eta K}(S)$, this time multiplied by $\left[t_2^{K\pi \rightarrow K\eta}\right]^2$. Nevertheless, one arrives to the same conclusion regarding the inclusion of the thermal bath processes $\bar{K}_0\pi^0 \rightarrow \bar{K}_0\eta$ and $\bar{K}_0K_0\pi^0 \rightarrow \eta$.

Altogether, the generalized thermal unitarity relation for the perturbative $K\pi \rightarrow K\pi$ ChPT amplitude for the $I = 3/2$, $J = 0, 1$ channels reads:

$$\begin{aligned} \text{Im } t_4^{K\pi \rightarrow K\pi}(s; T) &= \\ &= \sigma_{K\pi}^T(s) \left[t_2^{K\pi \rightarrow K\pi}(s)\right]^2 \theta \left[s - (M_K + M_\pi)^2\right] \\ &+ \tilde{\sigma}_{K\pi}^T(s) \left[t_2^{K\pi\pi \rightarrow K}(s)\right]^2 \theta \left[(M_K - M_\pi)^2 - s\right] \theta(s) \\ &= \left[t_2^{K\pi \rightarrow K\pi}(s)\right]^2 \left\{ \sigma_{K\pi}^T(s) \theta \left[s - (M_K + M_\pi)^2\right] + \tilde{\sigma}_{K\pi}^T(s) \theta \left[(M_K - M_\pi)^2 - s\right] \theta(s) \right\}, \end{aligned} \quad (4.4)$$

while for $I = 1/2$, $J = 0, 1$ one has

$$\begin{aligned} \text{Im } t_4^{K\pi \rightarrow K\pi}(s; T) &= \\ &= \sigma_{K\pi}^T(s) \left[t_2^{K\pi \rightarrow K\pi}(s)\right]^2 \theta \left[s - (M_K + M_\pi)^2\right] \\ &+ \sigma_{\eta K}^T(s) \left[t_2^{K\eta \rightarrow K\pi}(s)\right]^2 \theta \left[s - (M_K + M_\eta)^2\right] \\ &+ \tilde{\sigma}_{K\pi}^T(s) \left[t_2^{K\pi\pi \rightarrow K}(s)\right]^2 \theta \left[(M_K - M_\pi)^2 - s\right] \theta(s) \\ &+ \tilde{\sigma}_{\eta K}^T(s) \left[t_2^{KK\pi \rightarrow \eta}(s)\right]^2 \theta \left[(M_\eta - M_K)^2 - s\right] \theta(s) \\ &= \left[t_2^{K\pi \rightarrow K\pi}(s)\right]^2 \left\{ \sigma_{K\pi}^T(s) \theta \left[s - (M_K + M_\pi)^2\right] + \tilde{\sigma}_{K\pi}^T(s) \theta \left[(M_K - M_\pi)^2 - s\right] \theta(s) \right\} \\ &+ \left[t_2^{K\eta \rightarrow K\pi}(s)\right]^2 \left\{ \sigma_{\eta K}^T(s) \theta \left[s - (M_K + M_\eta)^2\right] + \tilde{\sigma}_{\eta K}^T(s) \theta \left[(M_\eta - M_K)^2 - s\right] \theta(s) \right\}, \end{aligned} \quad (4.5)$$

with the thermal phase space factor $\sigma_{12}^T(s)$ defined in equation (1.180) and

$$\tilde{\sigma}_{ab}^T(s) = \sigma_{ab}(s) \left[n_B \left(\frac{\Delta_{ab} - s}{2\sqrt{s}} \right) - n_B \left(\frac{s + \Delta_{ab}}{2\sqrt{s}} \right) \right], \quad (4.6)$$

where $\Delta_{ab} = M_a^2 - M_b^2$, so that the above equations can be used to easily generalize thermal unitarity for any thermal scattering amplitude.

4.1.2 T -channel cuts

The analytic properties of the $J(0, \sqrt{-t(s, \theta)}, T)$ thermal integrals with $t(s, \theta)$ in (1.165), are collected in Appendix C.2.2, where one can see that, in the CM frame, the only imaginary part arises for $s < 0$, and the range of the scattering angle where $(M_a + M_b)^2 < t(s, \theta) < -4p_{\text{CM}}^2$. We remind that for the πK scattering amplitude, only $J^{12}(T)$ integrals with $M_a = M_b$ arise.

4.1.3 U -channel cuts

The $J(U)$ integrals contributing to the πK partial waves with $I = 1/2$ and $3/2$ come from the loop-functions $J_k^{K\pi}(U)$ and $J_k^{\eta K}(U)$. In the CM frame, taking into account (1.165), we can see that the Mandelstam variable $u(s, \theta)$ is bounded by

$$\begin{aligned} -s + 2\Sigma_{K\pi} &\leq u \leq \Delta_{K\pi}^2/s, & \text{for } p_{CM}^2(s; M_K, M_\pi) \geq 0, \\ \Delta_{K\pi}^2/s &\leq u \leq -s + 2\Sigma_{K\pi}, & \text{for } p_{CM}^2(s; M_K, M_\pi) \leq 0, \end{aligned}$$

since the cosine of the scattering angle varies between -1 and 1 , and where we have used

$$\Delta_{K\pi}^2/s - 4p_{CM}^2(s; M_K, M_\pi) = -s + 2\Sigma_{K\pi}, \quad \Sigma_{K\pi} = M_K^2 + M_\pi^2.$$

First, for $s \geq (M_K + M_\pi)^2$, and taking into account that in that region

$$p_{CM}^2(s; M_K, M_\pi) \geq 0 \quad \text{and} \quad \Delta_{K\pi}^2/s \leq (M_K - M_\pi)^2 \leq (M_K + M_\pi)^2 \leq (M_K + M_\eta)^2, \quad (4.7)$$

it can be seen that the $J^{K\pi}(U)$ and $J^{\eta K}(U)$ loop functions develop a Landau cut but not the unitary one. Note that in this region $u \geq -|\vec{U}|^2$ since $U_0^2 = \Delta_{K\pi}^2/s > 0$ and that u can take any value in the range $-|\vec{U}|^2 < u < 0$ for arbitrarily large values of s . One of the most important conclusions of this result is that this unphysical U -channel discontinuity overlaps with the physical unitary cuts corresponding to the $K\pi \rightarrow K\pi$ and $K\pi \rightarrow K\eta$ processes discussed in subsection 4.1.1, as shown in Fig. 4.2, which is a genuine thermal effect.

Second, in the interval $(M_K - M_\pi)^2 \leq s \leq (M_K + M_\pi)^2$, where $p_{CM}^2(s; M_K, M_\pi) \leq 0$, there is no Landau-cut contribution either from $J^{K\pi}(U)$ or from $J^{\eta K}(U)$ since $\Delta_{K\pi}^2/s \geq (M_K - M_\pi)^2 \geq (M_\eta - M_K)^2$. In addition, the maximum value of $-s + 2\Sigma_{K\pi}$ in this interval is $(M_K + M_\pi)^2 < (M_\eta + M_K)^2$ reached at $s = (M_K - M_\pi)^2$; hence, these values of u lie also outside the unitary cut. It implies that the amplitude remains real in that interval, which allows one to apply Schwarz's reflection principle for the analytic continuation of the different partial waves.

Third, in the interval $0 \leq s \leq (M_K - M_\pi)^2$, $p_{CM}^2(s; M_K, M_\pi) \geq 0$ and $\Delta_{K\pi}^2/s \geq (M_K + M_\pi)^2$, so that u takes arbitrarily large values near $s = 0$. It implies that the unitary cuts of both $J^{K\pi}(U)$ and $J^{\eta K}(U)$ are reached for $\cos\theta$ sufficiently close to -1 . On the contrary, the minimum value of $-s + 2\Sigma_{K\pi}$ is $(M_K + M_\pi)^2 > (M_K - M_\pi)^2 > (M_\eta - M_K)^2$, so that $J^{K\pi}(U)$ and $J^{\eta K}(U)$ do not develop Landau cuts.

Finally, for $s < 0$, $p_{CM}^2(s; M_K, M_\pi) \leq 0$ and $-s + 2\Sigma_{K\pi} > 2\Sigma_{K\pi} > (M_K + M_\pi)^2$ so that both unitary cuts of $J^{K\pi}(U)$ and $J^{\eta K}(U)$ are reached, while $U_0^2 = \Delta_{K\pi}^2/s < 0$ so that u lies off the Landau cuts for those integrals.

4.2 Results for ChPT partial waves and scattering lengths

We have calculated the πK elastic scattering amplitude at a finite temperature using ChPT according to the procedure described in subsection 1.4.3. In Appendix D we collect the finite temperature $K^+\pi^+ \rightarrow K^+\pi^+$ amplitude. We also give in Appendix C some useful relations between the G_a and J_k^{ab} loop thermal integrals, which help to simplify the expression for the amplitude.

In this section, we provide the numerical results from the perturbative ChPT calculation of the πK scattering amplitude at finite temperature.

For our calculations we have used: $M_\pi = 139.6$ MeV, $M_K = 495.8$ MeV, $M_\eta = 552.5$ MeV, $F_\pi = 92.3$ MeV, $F_K = 110.6$ MeV, $F_\eta = 119.2$ MeV and the LECs extracted from [139] given in Table 4.1. In addition, all error bands shown below are obtained through the propagation in quadrature of the LECs uncertainties.

	L_1^r	L_2^r	L_3^r	L_4^r
LECs $\times 10^3$	$0.70^{+0.01}_{-0.01}$	1.04	$-3.44^{+0.04}_{-0.04}$	$-0.08^{+0.03}_{-0.04}$

	L_5^r	L_6^r	L_7^r	L_8^r
LECs $\times 10^3$	$0.98^{+0.07}_{-0.05}$	$0.24^{+0.08}_{-0.06}$	$0.008^{+0.090}_{-0.140}$	$0.098^{+0.100}_{-0.110}$

Table 4.1: $\mathcal{O}(p^4)$ chiral parameters ($\times 10^3$) obtained in the Global Fit IV in [139].

From the ChPT πK thermal amplitude, we can obtain the thermal evolution of any low-energy observables. For instance, we show in Fig. 4.3 the results for the πK phase shifts of the S and P waves, which at low energies can be defined as $\delta_{IJ} = \sigma_{\pi K}^T \text{Re}(t_{IJ})$.²

The thermal evolution of the $I = 1/2$, $J = 0$, and $J = 1$ phase shifts follow a similar trend as the $I = J = 0$ and $I = J = 1$ waves in $\pi\pi$ scattering, respectively, obtained in [54]. Namely, the phase shifts increase with temperature at low energies, reflecting

²Note that in the elastic region a partial wave is parameterized as $t_{IJ}(s) = \sin \delta_{IJ}(s) e^{i\delta_{IJ}(s)} / \sigma_{IJ}(s)$, so that, at low energies, one has, $\sigma_{IJ}(s) \text{Re} t_{IJ}(s) = \sin 2\delta_{IJ}(s)/2 \sim \delta_{IJ}(s)$.

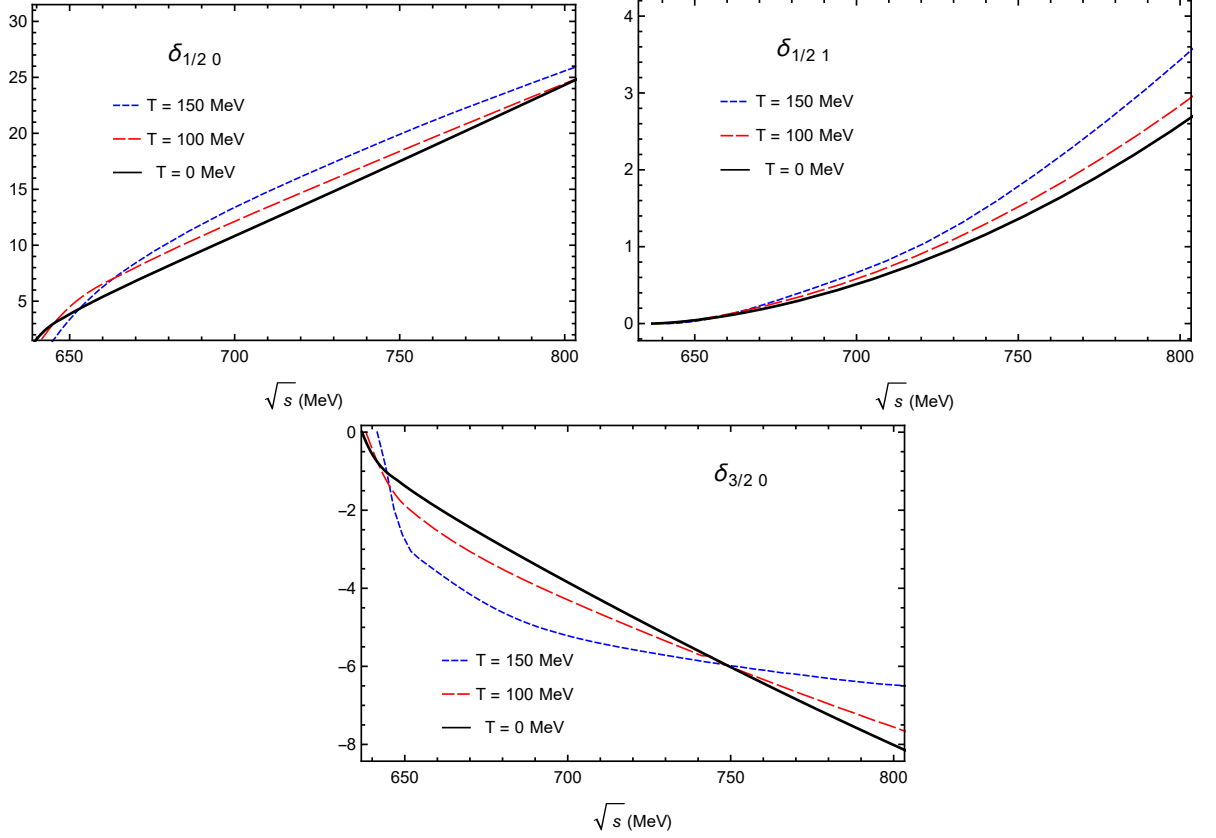


Figure 4.3: Temperature evolution of the phase shifts δ_{IJ} for $IJ = 1/2\ 0$ (left), $IJ = 1/2\ 1$ (right) and $IJ = 3/2\ 0$ (bottom).

the increase in the interaction strength due to the thermal bath. On the contrary, the $I = 3/2, J = 0$ phase shift becomes more repulsive (negative) at higher temperatures, at least at low energies where the ChPT expansion is well-behaved, hence resembling the thermal tendency of the $IJ = 20$ wave in $\pi\pi$ scattering. Note that we have considered the thermal dependence of the masses in the initial and final asymptotic states. As a consequence, there is a shift of the pion-kaon threshold at $T \neq 0$ in Fig. 4.3.

We also provide in Fig. 4.4 the temperature dependence of the corresponding scattering lengths, defined as in equation (1.173)

$$a_0^I = \frac{2}{M_\pi + M_K} \text{Re } t^{I0}((M_\pi + M_K)^2, T).$$

Their thermal evolution follows similar trends to those discussed above for the partial waves, highlighting that the strength of the interaction increases in the thermal bath as the temperature rises, for low and moderate energies where the ChPT approach is reliable.

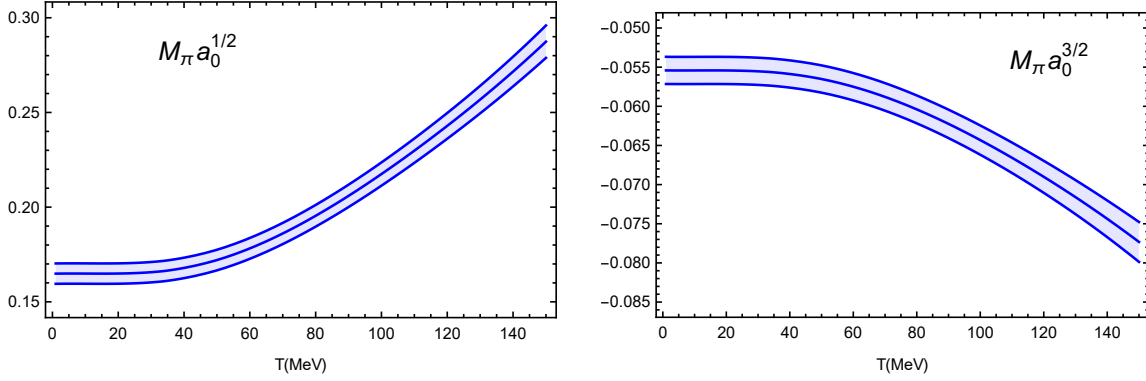


Figure 4.4: Temperature evolution of the scattering lengths a_J^I for $IJ = 1/2\ 0$ (left) and $IJ = 3/2\ 0$ (right). The bands correspond to the LECs uncertainties, as explained in the text.

4.3 Unitarization and the thermal $K_0^*(700)$ and $K^*(892)$ poles

So far we have been dealing with the perturbative ChPT πK thermal amplitude, satisfying the generalized thermal unitarity relation for partial waves derived in (4.4) and (4.5). Our purpose in this section is to construct a unitarized thermal amplitude through the IAM.

Remember that, as explained before, we are sticking to the one-channel case for the πK amplitude, i.e., we are demanding exact unitarity only below the $K\eta$ threshold, the relevant kinematic region to reproduce the behavior of the $K_0^*(700)$ and $K^*(892)$ resonances.

Note that the unitarized partial wave in (1.193) satisfies $\text{Im}(1/t_{IAM}) = -\text{Im} t_4/t_2^2$, so that, from (4.4) and (4.5), we see that the unitarized amplitude satisfied exact (single channel) thermal unitarity, as expected from our generic definition of a thermal amplitude, i.e,

$$\text{Im} t_{IAM}(s, T) = \begin{cases} \sigma_{12}^T(s) [t_{IAM}(s, T)]^2, & s \geq (M_a + M_b)^2, \\ \tilde{\sigma}_{12}^T(s) [t_{IAM}(s, T)]^2, & 0 \leq s \leq (M_a - M_b)^2, \end{cases} \quad (4.8)$$

with the thermal phase-space factors given in (1.180) and (4.6). The relations (4.8) are then inherited from the thermal ChPT perturbative relations, including the new Landau-type contributions coming from scattering in the thermal bath. Furthermore, $t_{IAM} = t_2 + t_4 + \dots$ perturbatively, as requested.

It is also important to stress that except for the possible presence of poles in $t^{-1}(s; T)$ corresponding to zeros of $t(s, T)$, the cut structure of the unitarized amplitude is the

same as that of the perturbative one depicted in Fig. 4.2, which on the S -like physical cuts turns into the thermal unitarity relation just discussed. However, although the T and U cuts remain in the same place, the imaginary part of t_{IAM} and t_4 only coincide in the left-hand cut perturbatively, as it also happens at $T = 0$ [79].

Having the correct analytic structure, the unitarized πK partial wave in the 2RS can be continued into the complex plane looking for resonance poles, which at $T = 0$ allows one to reproduce the $K_0^*(700)$ and $K^*(892)$ states in the $I = 1/2, J = 0$ and $I = 1/2, J = 1$ channels, respectively [141–144, 152]. Likewise, we can now obtain the temperature dependence of the pole position of those resonances in the 2RS.

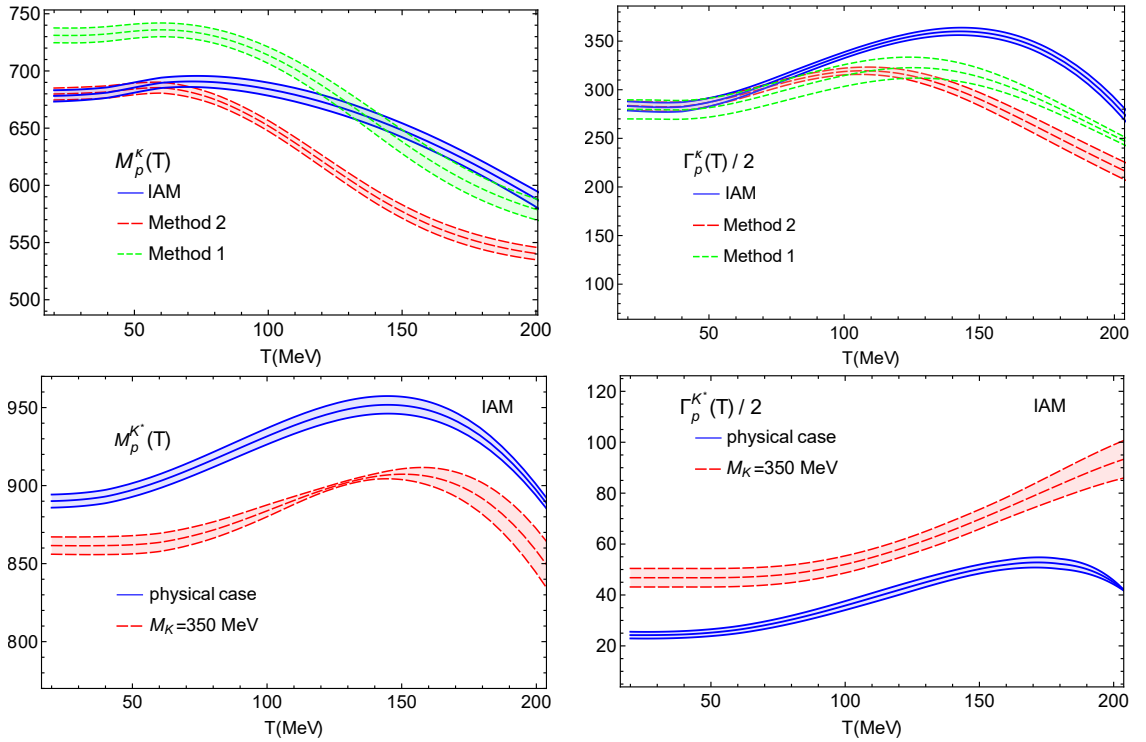


Figure 4.5: Upper panels: Pole parameters M_p (upper left panel) and Γ_p (upper right panel) of the $K_0^*(700)$ (κ) at finite temperature calculated within the three different unitarization methods explained in the main text. Lower panels: M_p (lower left panel) and Γ_p (lower right panel) parameters of the $K^*(892)$ obtained within the IAM unitarization method at finite temperature. For the $K^*(892)$ we also show the result of reducing the kaon mass from its physical value to $M_K = 350$ MeV.

In Fig. 4.5 and Fig. 4.6 we present our results for the T -dependence of the $K_0^*(700)$ and $K^*(892)$ poles. We have displayed in Fig. 4.5 the curves corresponding to the thermal dependence of the pole parameters M_p , Γ_p , while in Fig. 4.6 we show the thermal pole trajectories, that is, we plot the width as a function of the mass when increasing the temperatures from 0 to 200 MeV. In the case of the $K_0^*(700)$, we compare our analysis

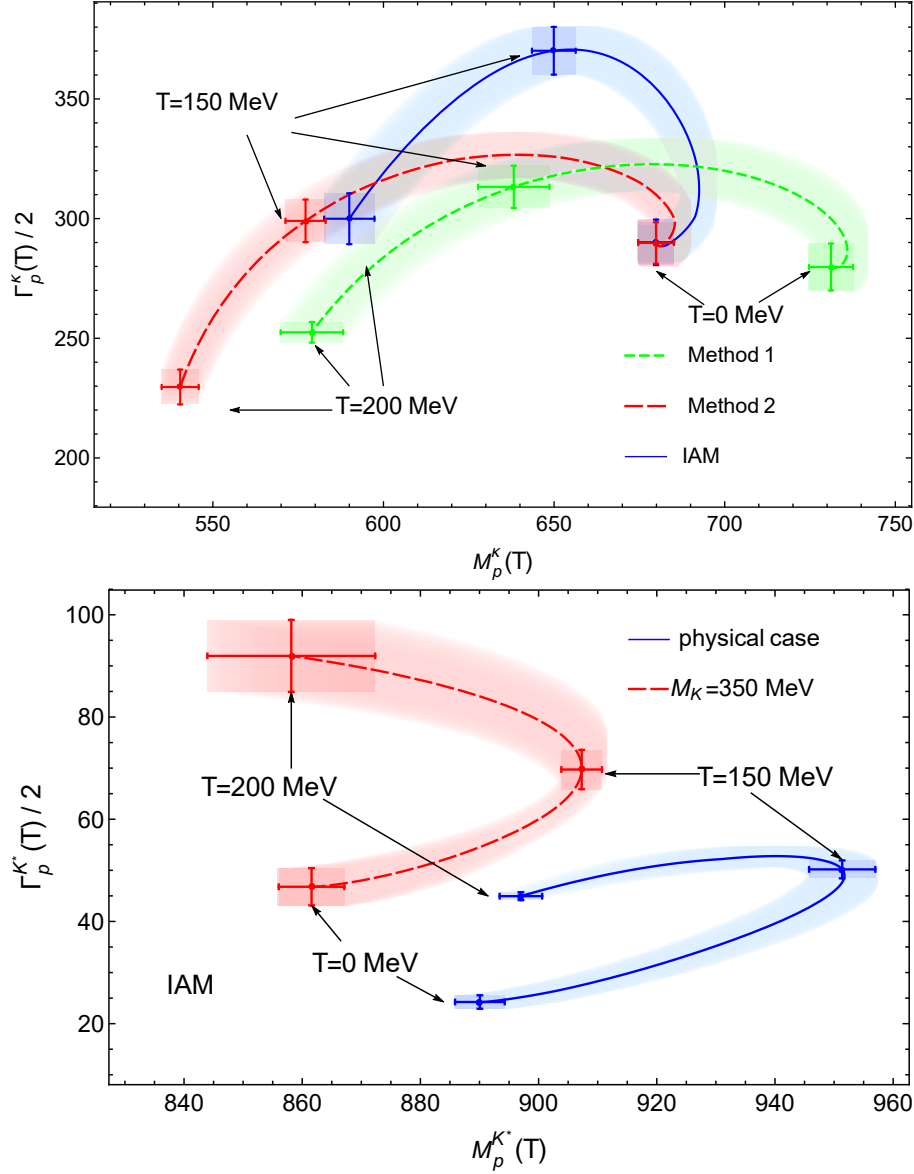


Figure 4.6: Upper (lower) panel: the temperature dependence of the pole position of the $K_0^*(700)$ ($K^*(892)$) resonance when increasing the temperature T from 0 to 200 MeV. The bands correspond to the LECs uncertainties. In both panels, we have also plotted the pole position at $T = 0, 150$, and 200 MeV with their respective uncertainties.

with the results in [138], which we call method 1. The unitarized amplitude in method 1 includes only the contribution from the $J_{K\pi}(S)$ loop function in the fourth-order partial waves, i.e., it neglects the $T - U$ channel contributions and their modification of the analytic structure discussed in section 4.1. In addition, it does not include any tadpole-like corrections. A variant of this method was considered in [147] (here method 2) by considering in the full one-loop ChPT amplitude at $T = 0$ but including only the thermal modifications for the $J^{K\pi}(S)$ part.

The results in Fig. 4.5 for the $K_0^*(700)$ confirm qualitatively the findings in the previous chapter, although we observe sizable quantitative differences for $T > 100$ MeV. On the one hand, the real part of $\sqrt{s_p}$, i.e., $M_p(T)$, stays constant up to temperatures around $T \sim 75$ MeV, from which it shows a decreasing behavior. On the other hand, $\Gamma_p(T)$ increases at low temperatures (roughly driven by the increase of thermal phase space in (1.180)) and decreases for T closer to the transition, which can be understood as the regime where the reduction of phase space driven by the mass drop dominates over the increase given by (1.180). This behavior is very similar to that of the $f_0(500)$ pole obtained in chapter 2, and in both cases is fully consistent with the expected trends for the scalar susceptibility in terms of chiral and $U(1)_A$ restoration, as we will see in detail in section 4.4.

As for the $K^*(892)$, the results in Fig. 4.5 confirm a softer temperature dependence for the pole, consistently with the analysis in [149] based on heavy-ion data, which predict a softer medium dependence than for the $\rho(770)$, i.e., its corresponding $I = 1$ partner in the vector octet. Actually, one of the main advantages of the IAM is that it encodes the correct quark-mass dependence inherited from ChPT; hence, with our present formalism, we can examine the behavior towards the $SU(3)$ degeneration limit, $m_l/m_s \rightarrow 1$, to check whether the $K^*(892)$ pole parameters become similar to those of the $\rho(770)$, for which M_p varies slowly with T , but $\Gamma_p(T)$ increases considerably instead [88]. In our case, we confirm this behavior by reducing the kaon mass. For a kaon mass of 350 MeV, we find that Γ_p increases in all the considered temperature ranges. Moreover, as we can see in Fig. 4.5, the width rises by 45 MeV from $T = 0$ to $T = 200$ MeV, roughly doubling its value, while this gap is equal to 20 MeV for the physical kaon mass. The variation of $M_p(T)$ on the contrary lies below the 10% range in both cases.

Finally, in Fig. 4.7, we plot the thermal dependence of the modulus of the $K_0^*(700)$ and $K^*(892)$ pole residues, obtained from the contour integral of the amplitudes in the second Riemann sheet around the pole position,

$$\text{Res}(T) = \frac{1}{2\pi i} \oint ds t_{IJ}(s, T)^{II}. \quad (4.9)$$

In the case of elastic resonances, well-isolated from other singularity structures, resonance residues can be related to the pole widths [153], which can be clearly observed by comparing Figs. 4.7 and 4.5.³ Finally, note that the thermal dependence of both

³In our convention, the thermal dependence of the width can be related to the product of the residue and thermal phase space for narrow resonances [154].

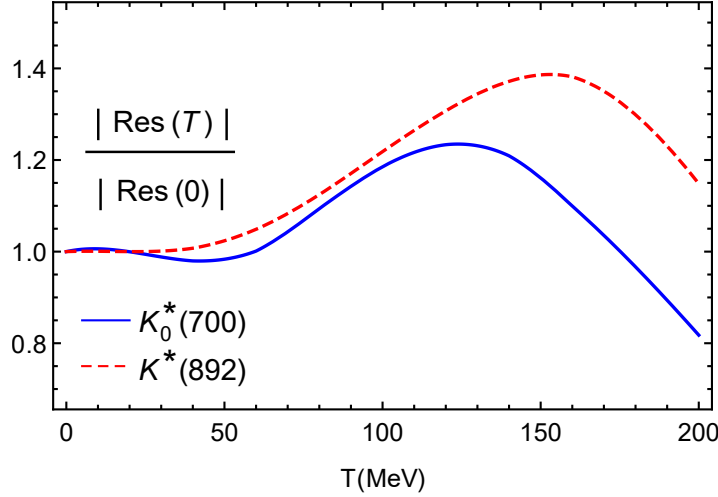


Figure 4.7: Temperature dependence of the couplings of the $K_0^*(700)$ and the $K^*(892)$ resonances to $K\pi$.

residues has a maximum in a temperature range between 120-170 MeV, with the $K^*(892)$ residue's maximum being slightly above the $K_0^*(700)$ one, confirming the correlation with the widths in Fig. 4.5.

4.4 The $I = 1/2$ scalar susceptibility and consequences for chiral and $U(1)_A$ restoration

Here, we compute χ_S^κ by saturating it with the thermal $K_0^*(700)$ pole determined with the IAM. We show our results for $\chi_S^{\kappa,U}(T)$ (defined in equation (3.5)) in Figs. 4.8 and 4.9. The peak of the κ scalar susceptibility is clearly reproduced, as well as the expected behavior as the m_l/m_s ratio is varied. In Fig. 4.8 we see that, near the light chiral limit of vanishing pion mass (with fixed m_s), the growth of the curve below the peak is more pronounced and compatible with a flattening above the peak. The evolution towards the $m_l/m_s \rightarrow 1$ limit is shown in Fig. 4.9, where we see the displacement of the peak towards T_c and its growth, consistently with its degeneracy with χ_S . We also compare our complete unitarized ChPT calculation here with the method followed in chapter 3. The results are qualitatively similar, which supports their robustness. In the chiral limit, the results in this work show more clearly the expected trend.

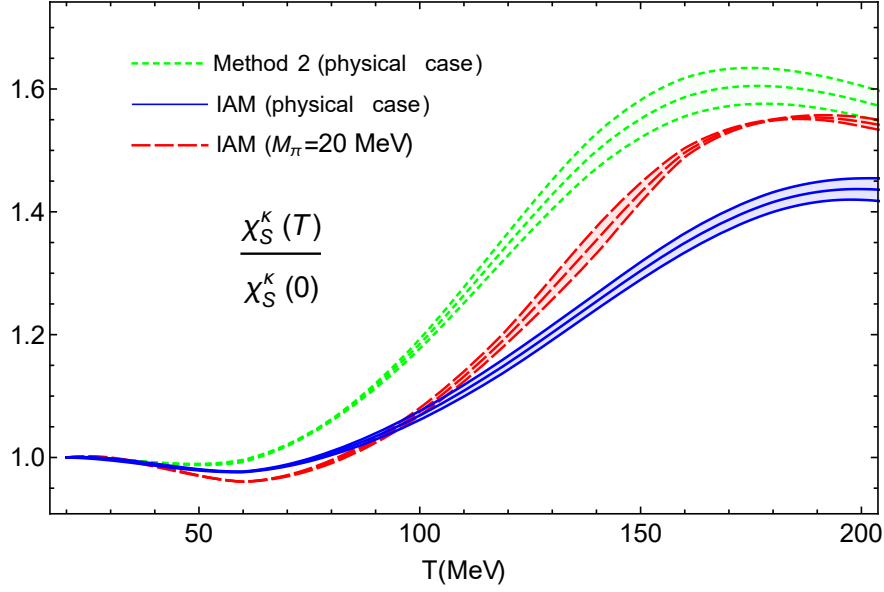


Figure 4.8: Unitarized κ susceptibility calculated using the IAM for physical masses and the light chiral limit, including the theoretical uncertainty bands of the LECs. We have also plotted the susceptibility obtained with the unitarization method 2.

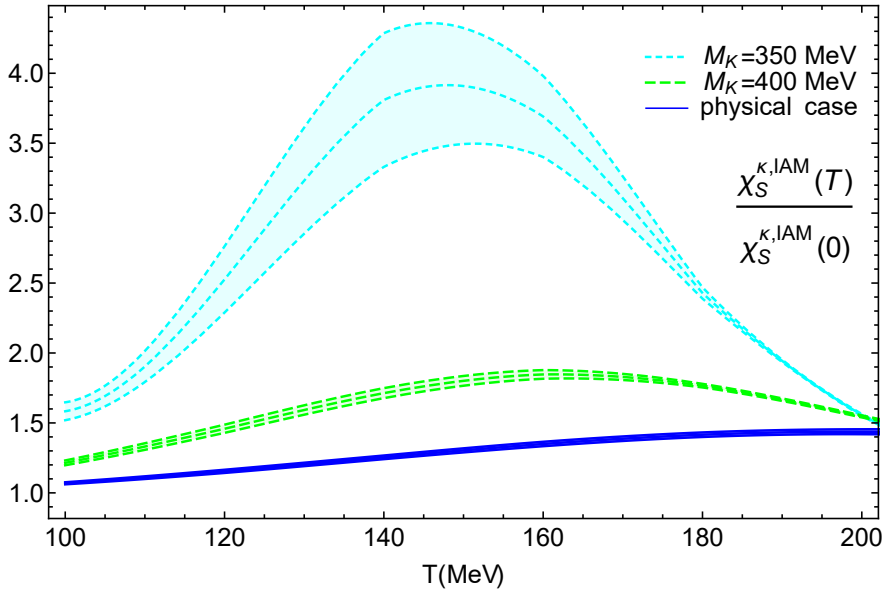


Figure 4.9: Unitarized κ susceptibility for physical masses and for M_K closer to the SU(3) limit. The bands correspond to the LECs uncertainties.

4.5 Conclusions

In this chapter, we have calculated the πK elastic scattering amplitude at finite temperature T in Chiral Perturbation Theory and we have obtained its unitarized version through the Inverse Amplitude Method, which allows one to generate the $K_0^*(700)$ and

$K^*(890)$ poles. The thermal evolution of these states has been studied and related with a relevant application for the QCD phase diagram; namely, the connection of the $K_0^*(700)$ pole with chiral and $U(1)_A$ restoration through its role in the $I = 1/2$ scalar susceptibility.

The analytical structure of the amplitude shows interesting features at $T \neq 0$; apart from the standard $T = 0$ cuts, including the unitarity cut above threshold, at $T \neq 0$ Landau cuts arise, which are related to physical processes taking place inside the thermal bath. The latter gives rise to an extended thermal unitarity relation, derived here for the first time for unequal-mass meson-meson scattering, such as the πK case. The unitarized thermal amplitude constructed here through the one-loop Inverse Amplitude Method satisfies exact unitarity, including the Landau-type processes, while matching the next-to-leading order ChPT series at low energies.

By extracting the poles of the unitarized amplitude in the second Riemann sheet, we have obtained the thermal evolution of the $K_0^*(700)$ and the $K^*(892)$ resonances in the $I = 1/2$, $J = 0$ and $I = 1/2$, $J = 1$ channels, respectively. In addition, we have analyzed their behavior in the light chiral limit $m_l/m_s \rightarrow 0$ and when approaching the $SU(3)$ $m_l/m_s \rightarrow 1$ limit, both reachable within our theoretical framework.

In the vector channel, the $K^*(892)$ pole position varies much more smoothly with temperature than its corresponding $I = 1$ state in the vector meson nonet, i.e., the $\rho(770)$. This is in accordance with recent estimates based on heavy-ion data. We have examined the behavior towards the $m_l/m_s \rightarrow 1$ limit, where the $SU(3)$ nonet members are meant to share physical properties. This analysis provides the expected results since the width of the $K^*(892)$ increases significantly with the temperature when the value of the kaon mass approaches the pion mass, thus resembling the behavior of the $\rho(770)$ at finite T in the literature.

As for the $K_0^*(700)$, we have explored in detail the connection of the pole at finite T with properties regarding the restoration of chiral and $U(1)_A$ symmetries, relevant for the QCD phase diagram. In particular, through a saturation approach, the pole of the $K_0^*(700)$ can be related to the scalar susceptibility in the $I = 1/2$ channel. The susceptibility obtained confirms that behavior and satisfies the expected trend around that peak as m_l/m_s is varied. On the one hand, as we approach the $m_l/m_s \rightarrow 1$ limit, the susceptibility tends to show the same behavior as for the $I = J = 0$ channel one, saturated by the $f_0(500)$. In that case, chiral restoration dominates, the susceptibility peak increases and its center moves towards T_c . On the other hand, in the $m_l/m_s \rightarrow$

0 light chiral limit, the susceptibility slope increases below the peak, driven by the amplification of chiral restoration effects, while it tends to flatten above the peak due to a more efficient $K - \kappa$ partner degeneration.

We have also computed the residues of both resonances and found that their thermal dependence resembles the behavior of the corresponding pole widths, and in particular, it shows a maximum in the region around 120-170 MeV.

The QCD topological charge in $U(3)$ ChPT

The rich topological structure of the QCD vacuum is encoded in the θ -angle dependence of the vacuum energy density $\epsilon_{vac}(\theta)$. The expansion of ϵ_{vac} around $\theta = 0$ can be expressed as

$$\epsilon_{vac}(\theta) = \sum_{n=1}^{\infty} \frac{c_{2n}}{(2n)!} \theta^{2n} \quad (5.1)$$

with $c_2 = \chi_{top}$ the topological susceptibility introduced in (1.39) and c_4 the fourth-order cumulant, which in Euclidean space-time read

$$\begin{aligned} \chi_{top} &= \int_T dx \langle \mathcal{T} \omega(x) \omega(0) \rangle , \\ c_4 &= - \int_T dx dy dz \left[\langle \mathcal{T} \omega(x) \omega(y) \omega(z) \omega(0) \rangle - 3 \langle \mathcal{T} \omega(x) \omega(0) \rangle^2 \right] , \end{aligned} \quad (5.2)$$

As we have already seen in chapter 1, the topological susceptibility is meant to be connected with the η' mass through the $U_A(1)$ anomaly. More specifically, in the quenched approximations where quarks loops are absent, $\chi_{top}^{quenched}$ is related to the mass of the η' (or rather its singlet part η_0) for N_f massless quarks as [42, 155]

$$\chi_{top}^{quenched} = \frac{1}{2N_f} F^2 M_0^2 = \frac{F^2 \left[M_{\eta_0}^{m_q=0} \right]^2}{2N_f}, \quad (5.3)$$

where M_0 denotes the anomalous contribution to the η' mass and F is the pion decay constant in the chiral $m_u = m_d = m_s = 0$ limit. The quenched approximation is formally valid in the $N_c \rightarrow \infty$ limit, where meson-loop contributions are suppressed and the mass of the η_0 becomes of the same order than the other members of the NGB meson octet, since the $U(1)_A$ anomaly scales with $1/N_c$.

However, even when the fluctuation of the winding number is directly linked to the $U(1)_A$ anomaly, meson-loop corrections are indeed very relevant and one of the reasons why the QCD topological charge can be analyzed using low-energy effective field theories. This can be seen by looking at the LO low-energy chiral prediction for the topological susceptibility, a well-known result in ChPT that for three light flavors $N_f = 2 + 1$ reads [35, 43, 156]

$$\chi_{top}^{SU(3),LO} = \Sigma \left[\frac{1}{m_u} + \frac{1}{m_d} + \frac{1}{m_s} \right]^{-1} \equiv \Sigma \bar{m}, \quad (5.4)$$

where $\Sigma = -\langle \bar{q}q \rangle = B_0 F^2$ is the single-flavor quark condensate in the chiral limit and $B_0 = M_{0\pi^\pm}^2 / (m_u + m_d)$, with $M_{0\pi^\pm}$ the mass of the charged pions. The result in (5.4) can be easily extended to a larger number of flavors [43, 156], while the two-flavor result can be recovered by taking the $m_s \gg m_{u,d}$ limit.

One of the main consequences of (5.4) is that the topological susceptibility is linearly proportional to the quark mass and hence, unlike the pure gluonic quenched result (5.3), it vanishes in the chiral limit. Thus, meson loop corrections generate terms that cancel the contribution in (5.3). This fact is actually crucial to understand why the QCD topological charge can be reliably described just by including the lightest degrees of freedom.

In addition, (5.4) also shows that at LO in the chiral expansion the topological susceptibility is proportional to the quark condensate. This property has been used in several lattice analyses to extract the value of $\langle \bar{q}q \rangle$ in the chiral limit from χ_{top} , both for $N_f = 2$ [157, 158] and $N_f = 2 + 1$ [159, 160]. In these analyses, χ_{top} is determined at different quark-mass values and then fitted using ChPT predictions to extract the quark condensate. This relation has been emphasized in [161] to study the strange mass paramagnetic suppression of the three-flavor condensate. Recent values of the quark condensate obtained with this method can be found in [162], while direct lattice measurements of χ_{top} are provided in [163–165] for $N_f = 2 + 1$, in [166] for $N_f = 2$ and in [167] within the framework of two fermion families. Therefore, obtaining explicit analytic expressions for χ_{top} and studying its quark mass dependence within the effective Lagrangian framework under different approximations is of the utmost importance from the point of view of lattice analyses.

Nevertheless, higher order corrections change the simple linear dependence of χ_{top} with the quark condensate given in (5.4). In this sense, an important result that hints towards more complicated dependencies is the existence of the following family of WIs

connecting quark condensates with the topological and pseudoscalar susceptibilities in the isospin limit [65, 109, 137, 168]:

$$\chi_{top} = -\frac{1}{4} [m_l \langle \bar{q}q \rangle_l + m_l^2 \chi_P^l] \quad (5.5)$$

$$= -[m_s \langle \bar{s}s \rangle + m_s^2 \chi_P^{ss}] \quad , \quad (5.6)$$

where χ_P^l , χ_P^{ss} are the pseudoscalar susceptibilities corresponding to the quark bilinear operators η_l and η_s respectively.

The identities (5.5) and (5.6) have been verified in $U(3)$ ChPT up to NNLO in [137]. Furthermore, the identity (5.5) has been used in lattice works to determine χ_{top} indirectly at finite temperature [59, 169] and in [103] to justify that $U(1)_A$ restoration approaches the $O(4)$ phase transition when the chiral symmetry is exactly restored.

Now, note that for $N_f = 2$ in the isospin limit, the first term in the r.h.s. of (5.5) corresponds to the LO ChPT expression (5.4) when $m_s \gg m_l$. Therefore, the term proportional to χ_P^l necessarily includes higher order corrections in the chiral series and/or terms suppressed as m_l/m_s for $N_f = 2+1$ flavors. An immediate conclusion is that χ_{top} is not necessarily proportional to the light quark condensate to all orders. In fact, as we will see here in detail, the dependence with temperature of the two terms in the r.h.s. of (5.5) is completely different. Namely, the condensate term drops with T signaling chiral restoration while the χ_P^l term shows a much smoother behavior.

Higher order corrections to the topological susceptibility within the chiral Lagrangian framework have been obtained in [170] to NLO (one-loop) in $SU(N_f)$ ChPT. This result has been incorporated in the lattice analysis of [158] to extract the quark condensate and in [171, 172] to provide a numerical estimate of χ_{top} in terms of the low-energy constants of the $\mathcal{O}(p^4)$ effective Lagrangian. Higher order isospin-breaking corrections as well as an analysis of χ_{top} within the so called resummed ChPT can be found in [161], whereas in the recent work [172] NNLO and electromagnetic corrections in $SU(2)$ ChPT have been computed.

Another important motivation for the study of the topological susceptibility is its relation with the Peccei-Quinn axion [173, 174] and hence with various cosmological and astrophysical implications. The axion mass is directly proportional to χ_{top} , which allows for numerical estimates based on chiral Lagrangians [171, 172, 175]. In addition, the fourth-order self-coupling of the axion field can be obtained from the fourth-order cumulant c_4 of the $\epsilon_{vac}(\theta)$ expansion in (5.1), which has been thoroughly analyzed within $SU(N_f)$ ChPT up to NLO [170, 176, 177] and computed in the lattice [160, 178–180].

In addition, the large- N_c behavior of the topological susceptibility and the fourth-order cumulant have been recently analyzed in [181] and compared with the lattice results provided at different large- N_c values in [178].

The thermal dependence of the vacuum energy density $\epsilon(\theta)$ is important for several reasons: as stated above $\chi_{top}(T)$ plays an important role in the relation between chiral and $U(1)_A$ restoration. In addition, the connection of χ_{top} with the light- and strange-quark condensate as a function of temperature is relevant for lattice analyses and for the understanding of the temperature dependence of the different contributions in the WI (5.5)-(5.6). Thermal corrections to the axion potential and its mass are also of importance in the cosmological and astrophysical context [171]. A ChPT analysis for $\chi_{top}(T)$ for $N_f = 2$ has been performed in [171]. In that paper, the fact that for $N_f = 2$ the one-loop corrections to χ_{top} can be encoded in the physical pion mass and decay constant is used to establish the scaling $\chi_{top}(T)/\chi_{top}(0) = \langle \bar{q}q \rangle_l(T)/\langle \bar{q}q \rangle_l(0)$, valid at that order. Actually, that scaling law is nothing but the first term in the r.h.s. of (5.5), which opens the question of how relevant are the additional corrections provided by the second term in that identity. As we have already mentioned, we will discuss that particular aspect in detail in the present chapter.

As for lattice results at finite temperature, direct measurements of the topological susceptibility have typically large errors. Results can be found e.g. in [163–165, 182]. As commented above, indirect measurements can be obtained precisely through (5.5). Higher order cumulants at finite temperature in the lattice have been analyzed in [163, 183].

With the above motivation in mind, in this chapter we will carry out a ChPT-based analysis of the topological susceptibility and the fourth-order cumulant, concentrating in particular in the following aspects:

- We will provide a NNLO calculation of the topological susceptibility and the fourth-order cumulant within the formalism of $U(3)$ ChPT, in which the singlet η_0 is incorporated as a ninth pseudo-Goldstone boson within the large- N_c framework [42, 45, 46]. This approach allows us to study η' meson effects and to assess its contribution. Our calculation will also allow us to estimate numerically the effect of the additional $U(3)$ corrections in terms of the LECs involved. As mentioned above, many lattice analyses of the quark condensate rely on the chiral expansion of χ_{top} . In that respect, studying the influence of an additional heavier degree of freedom is important. The η' case is especially significant due to its direct

connection with the axial anomaly and its relevant role in the Ward identities described above. In addition, our $U(3)$ analysis will provide a natural way to establish contact with recent large- N_c analysis of the topological susceptibility and the fourth-order cumulant. Our study will also have the advantage of including explicitly the dependence of those quantities on the $\eta - \eta'$ mixing angle.

- We will also calculate the leading isospin-breaking $m_u \neq m_d$ corrections within the $U(3)$ formalism, thus extending previous $SU(3)$ works. The importance of isospin breaking corrections to the topological susceptibility and the fourth-order cumulant stems from the vacuum misalignment induced by the combined $m_u \neq m_d$ and $\theta \neq 0$ effects [35, 43, 170, 172, 177]. It implies corrections proportional to $(m_u - m_d)/(m_u + m_d)$, hence much larger than the typical isospin-breaking correction in other quantities, such as quark condensates or the $\pi^0\eta$ mixing [184], which are proportional to $(m_u - m_d)/m_s$. Recent estimates within the $SU(2)$ formalism show that these isospin contributions give rise to around a 4% correction to $\chi_{top}^{1/4}$. As a natural extension to those analysis, we will include isospin breaking in the LO $U(3)$ correction to $\epsilon_{vac}(\theta)$ to estimate its numerical effect.
- We will extend our analysis to finite temperature. In this way, we will account for corrections both within the $SU(3)$ and $U(3)$ formalisms for the different contributions in the Ward identities (5.5) and (5.6). This will also allow us to test the robustness of the $N_f = 2$ scaling performed in [171] when corrections from m_q/m_s and η, η' loops are properly incorporated. As commented before, the evolution of quark condensates and susceptibilities towards chiral restoration makes it interesting to clarify their relation with the topological susceptibility as the temperature grows, within the context of chiral and $U(1)_A$ restoration. In addition, we recall that the finite temperature dependence of the η' mass has been analyzed within the $U(3)$ ChPT formalism in [185, 186], in fermion models [131] and in the lattice [187], confirming the $U(1)_A$ restoring behavior, as in the recent analysis of the $\eta - \eta'$ mixing angle [65].

5.1 The topological susceptibility

Following the same steps as in [188], the topological susceptibility can be calculated by taking functional derivatives with respect to the vacuum angle θ . Thus, taking into

account the θ -vacuum coupling in the QCD Lagrangian defined in (1.40), one can derive expectation values or thermal correlators involving the winding number density. In this way, the topological susceptibility reads

$$\begin{aligned}\chi_{top} &= \int_T dx \frac{\delta}{\delta\theta(x)} \frac{\delta}{\delta\theta(0)} \log Z(\theta) \Big|_{\theta=0} \\ &= \int_T dx \left\{ \left\langle \frac{\delta\mathcal{L}_{\text{eff}}(x)}{\delta\theta(x)} \frac{\delta\mathcal{L}_{\text{eff}}(0)}{\delta\theta(0)} \right\rangle_{\theta=0} + \left\langle \frac{\delta}{\delta\theta(x)} \frac{\delta}{\delta\theta(0)} \mathcal{L}_{\text{eff}}(x) \right\rangle_{\theta=0} \delta^4(x) \right\},\end{aligned}\quad (5.7)$$

where we have used that $\langle\omega(0)\rangle = 0$.

The first non-vanishing contribution to the topological susceptibility is $\mathcal{O}(\delta^0)$ in the counting (1.83). On the one hand, the second term in the r.h.s. of (5.7) gives rise at this order to a constant term, which is nothing but the contribution (5.3) with $[M_{\eta_0}^{m_q=0}]^2 = M_0^2$ and $N_f = 3$. On the other hand, the first term in the r.h.s of (5.7) gives rise to terms of the type $M_0^4 \int dx \langle \eta^{(\prime)}(x) \eta^{(\prime)}(0) \rangle \sim M_0^4 / M_{\eta^{(\prime)}}^2$, i.e., tree level two-point functions at $p = 0$, where $\eta^{(\prime)}$ denotes generically η or η' fields. Gathering the two types of contribution yields in the isospin limit

$$\chi_{top}^{U(3), LO, IL} = \frac{F^2 M_0^2}{6} \left[1 - \frac{M_0^2}{M_{0\eta}^2} s_\theta^2 - \frac{M_0^2}{M_{0\eta'}^2} c_\theta^2 \right], \quad (5.8)$$

where $M_{0\eta}$ and $M_{0\eta'}$ are respectively the η and η' masses at tree level and c_θ and s_θ were defined in equation (1.87). They depend on the quark (or meson) masses and on M_0 . Their explicit expressions in the isospin limit $m_u = m_d = m_l$ can be found e.g. in [189]. Thus, in terms of quark masses, (5.8) can be recast as:

$$\chi_{top}^{U(3), LO, IL} = \frac{F^2 M_0^2 B_0 m_l m_s}{(2m_s + m_l) M_0^2 + 6B_0 m_l m_s} = \frac{\Sigma M_0^2 \bar{m}_{IL}}{M_0^2 + 6B_0 \bar{m}_{IL}} = \Sigma \hat{m}_{IL}, \quad (5.9)$$

where $\bar{m}_{IL}$ denotes the isospin limit value of $\bar{m}$ in (5.4), i.e.,

$$\bar{m}_{IL} = \frac{m_l m_s}{2m_s + m_l}, \quad (5.10)$$

and

$$\hat{m}_{IL} = \frac{M_0^2 \bar{m}_{IL}}{M_0^2 + 6B_0 \bar{m}_{IL}}. \quad (5.11)$$

The result in (5.8) and (5.9) is the extension to $N_f = 2 + 1$ flavors of the result given in [156] for N_f degenerated flavors in the large- N_c limit. Note that our $U(3)$ LO result can be obtained from the $SU(3)$ one by replacing $\bar{m}$ with $\hat{m}$, which also holds when including isospin breaking corrections at LO, as we will see in section 5.4. In the $M_0 \rightarrow \infty$ limit one recovers the $SU(3)$ expression in (5.4) for $m_u = m_d = m_l$, since

$\hat{m}_{IL} \rightarrow \bar{m}_{IL}$ in this limit. Furthermore, $\chi_{top}^{U(3),LO}$ vanishes in the chiral limit, as it also does in the SU(3) case. Actually, in this limit the second and third terms in the r.h.s. of (5.8) (coming from η, η' propagators) cancel the first term, as one can check from the chiral limit behavior of $s_\theta, M_{0\eta}, M_{0\eta'}$.

Our present U(3) calculation has also the advantage that one can formally recover the quenched result in (5.3) by taking the limit $M_0 \ll \bar{m}$. This limit can also be achieved by re-expanding (5.9) in the $1/N_c$ expansion. Taking into account the $1/N_c$ scaling of the different constants involved, namely $F^2 = \mathcal{O}(N_c)$, $M_0^2 = \mathcal{O}(1/N_c)$ and so on, the $1/N_c$ LO contribution to (5.9) gives

$$\chi_{top}^{U(3),IL} = \frac{F^2 M_0^2}{6} + \mathcal{O}\left(\frac{1}{N_c}\right) = \frac{F^2}{6} (M_{0\eta'}^2 + M_{0\eta}^2 - 2M_{0K}^2) + \mathcal{O}\left(\frac{1}{N_c}\right), \quad (5.12)$$

which coincides with the result in (5.3) for $N_f = 3$. The last equality in (5.12) reproduces the result given in [155], where M_{0i} denote tree-level meson masses.

The NLO ($\mathcal{O}(\delta)$) and NNLO ($\mathcal{O}(\delta^2)$) results require including the higher-order effective Lagrangians (1.91)-(1.92) in (5.7). They involve one-loop corrections to the η - and η' -meson propagators at zero momentum, which include the LECs $L_6, L_7, L_{25}, C_{19}, C_{31}, \Lambda_2$ and $v_2^{(2)}$ [189]. The renormalization of these LECs and the constant B_0 [45, 46, 189] allows one to absorb all one-loop divergences, rendering the result finite and independent of the renormalization scale μ . In addition, the calculation of $\chi_{top}, \chi_P^l, \chi_P^{ss}$ and $\langle \bar{q}q \rangle_l$ up to NNLO in the U(3) expansion allow one to verify the Ward Identities (5.5)-(5.6). The explicit results for the topological susceptibility at NLO and NNLO in U(3) ChPT are given explicitly in Appendix E in the isospin limit. Note that the NLO and NNLO U(3) results do not correspond to simply perform the replacement $\bar{m} \rightarrow \hat{m}$ as it happened at LO.

In order to compare with the SU(3) calculation in ChPT, as given for instance in [161, 170, 171], we recall that the NLO order ChPT result is included distributed among the NLO and NNLO U(3) outcome. On the one hand, we have checked that the $M_0 \rightarrow \infty$ limit of $\chi_{top}^{U(3),NLO}$ in (E.1) yields the contribution proportional to the renormalized LEC L_8^r in [161, 170, 171] while $\chi_{top}^{U(3),NNLO}$ in (E.2) for $M_0 \rightarrow \infty$ provides the rest of the SU(3) contributions, proportional to L_6^r, L_7 and $\log(M_{\pi,K,\eta}^2/\mu^2)$. On the other hand, the surviving term proportional to $\log(M_{\eta'}^2/\mu^2)$ is absorbed in L_6^r .

Finally, we remark that our present U(3) formalism allows us to study systematically the large N_c corrections in (5.12), corresponding to the Witten-Veneziano result. Performing the $1/N_c$ expansion on the different orders in the U(3) ChPT expansion we

obtain the $\mathcal{O}(1/N_c)$ correction to (5.12), namely

$$\begin{aligned}
\chi_{top}^{U(3),IL} &= \frac{F^2 M_0^2}{6} \left\{ 1 + \frac{1}{3} M_0^2 \left(\frac{1}{M_{0\pi}^2 - 2M_{0K}^2} - \frac{2}{M_{0\pi}^2} \right) + \frac{16 M_0^2 L_8^r}{F^2} - 2\Lambda_2 \right. \\
&+ \frac{2(2M_{0K}^2 + M_{0\pi}^2)}{3F^4 M_0^2} \left[24 C_{19} F^2 M_0^4 + 16 C_{31} F^2 M_0^4 + 9 F^4 v_2^{(2)} + 16 F^2 \Lambda_2 M_0^2 L_8^r \right. \\
&+ \left. \left. 24 F^2 M_0^2 L_{25}^r - 128 M_0^4 (L_8^r)^2 \right] \right\} + \mathcal{O}\left(\frac{1}{N_c^2}\right) + \mathcal{O}(\delta^3) . \tag{5.13}
\end{aligned}$$

The above result is consistent with the large- N_c scaling analysis of the topological susceptibility provided in [181].

5.2 Fourth-order cumulant

The fourth-order cumulant is defined in (5.2) and involves the difference between the four- and two-point function square of the winding number density. Similarly to χ_{top} , it can be computed by taking functional derivatives with respect to the θ -vacuum angle. Taking into account again the θ -angle coupling in the QCD action, the fourth-order cumulant can be written as

$$\begin{aligned}
c_4 &= - \int_T dx dy dz \left[\frac{\delta}{\delta\theta(x)} \frac{\delta}{\delta\theta(y)} \frac{\delta}{\delta\theta(z)} \frac{\delta}{\delta\theta(0)} \log Z(\theta) \Big|_{\theta=0} - 3 \left(\frac{\delta}{\delta\theta(x)} \frac{\delta}{\delta\theta(0)} \log Z(\theta) \Big|_{\theta=0} \right)^2 \right] \\
&= - \left[\left\langle \frac{\delta^4 \mathcal{L}_{\text{eff}}(0)}{\delta\theta(0)^4} \right\rangle_{\theta=0} \right. \\
&+ \int_T dx \left\{ 4 \left\langle \frac{\delta^3 \mathcal{L}_{\text{eff}}(x)}{\delta\theta(x)^3} \frac{\delta \mathcal{L}_{\text{eff}}(0)}{\delta\theta(0)} \right\rangle_{\theta=0} + 3 \left\langle \frac{\delta^2 \mathcal{L}_{\text{eff}}(x)}{\delta\theta(x)^2} \frac{\delta^2 \mathcal{L}_{\text{eff}}(0)}{\delta\theta(0)^2} \right\rangle_{\theta=0} - 3 \left\langle \frac{\delta^2 \mathcal{L}_{\text{eff}}(x)}{\theta(x)^2} \right\rangle_{\theta=0}^2 \right\} \\
&+ 6 \int_T dx dy \left\{ \left\langle \frac{\delta^2 \mathcal{L}_{\text{eff}}(x)}{\delta\theta(x)^2} \frac{\delta \mathcal{L}_{\text{eff}}(y)}{\delta\theta(y)} \frac{\delta \mathcal{L}_{\text{eff}}(0)}{\delta\theta(0)} \right\rangle_{\theta=0} - \left\langle \frac{\delta^2 \mathcal{L}_{\text{eff}}(x)}{\delta\theta(x)^2} \right\rangle_{\theta=0} \left\langle \frac{\delta \mathcal{L}_{\text{eff}}(y)}{\delta\theta(y)} \frac{\delta \mathcal{L}_{\text{eff}}(0)}{\delta\theta(0)} \right\rangle_{\theta=0} \right\} \\
&+ \left. \int_T dx dy dz \left\{ \left\langle \frac{\delta \mathcal{L}_{\text{eff}}(x)}{\delta\theta(x)} \frac{\delta \mathcal{L}_{\text{eff}}(y)}{\delta\theta(y)} \frac{\delta \mathcal{L}_{\text{eff}}(z)}{\delta\theta(z)} \frac{\delta \mathcal{L}_{\text{eff}}(0)}{\delta\theta(0)} \right\rangle_{\theta=0} - 3 \left\langle \frac{\delta \mathcal{L}_{\text{eff}}(x)}{\delta\theta(x)} \frac{\delta \mathcal{L}_{\text{eff}}(0)}{\delta\theta(0)} \right\rangle_{\theta=0}^2 \right\} \right] , \tag{5.14}
\end{aligned}$$

where we have used once more that $\langle \omega(0) \rangle = 0$. The last terms in all rows are associated to the square of χ_{top} and hence they provide disconnected contributions, i.e., terms proportional to the Euclidean four-dimensional volume that should cancel out exactly with the disconnected contributions coming from the four-point function. Thus, the calculation of the fourth-order cumulant involves five connected contributions associated

to all possible combinations of a total even number of derivatives with respect to θ applied to the effective Lagrangian. The LO topologies for each of these five connected contributions are depicted in Fig. 5.1¹. Following the notation given in [176], the θ -

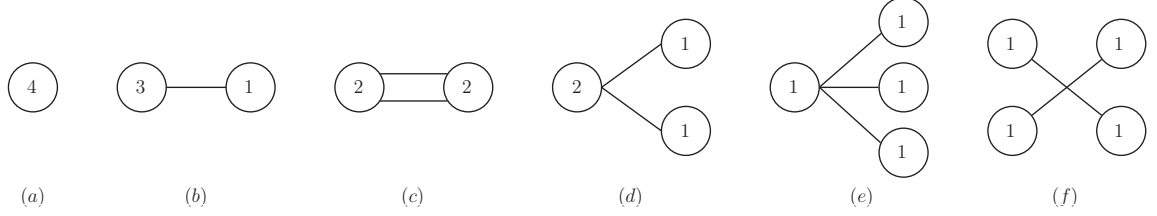


Figure 5.1: LO topologies for each of the five different connected contributions of the fourth-order cumulant in (5.14). Following the notation in [176], θ -induced vertices are denoted by its number of derivatives with respect to θ applied to the effective Lagrangian $\mathcal{L}_{\text{eff}}$. Note that we only refer to the LO for each different connected topology, irregardless of their corresponding counting in the δ expansion.

induced vertices are classified in terms of their number of derivatives with respect to the θ -vacuum angle. Meson lines are always coupled to one θ -induced source coming from a single, second or third derivative with respect to the vacuum angle², which in the isospin limit involve η and η' meson propagators at zero momentum. The four different θ -induced vertices contributing to the topologies in Fig. 5.1 read

$$\left. \frac{\delta^4 \mathcal{L}_{\text{eff}}(x)}{\delta \theta(x)^4} \right|_{\theta=0} = 6F^2 v_4^{(0)} + \mathcal{O}(\delta^3), \quad (5.15)$$

$$\left. \frac{\delta^3 \mathcal{L}_{\text{eff}}(x)}{\delta \theta(x)^3} \right|_{\theta=0} = 6\sqrt{6}F v_4^{(4)} (c_\theta \eta'(x) - s_\theta \eta(x)) + \mathcal{O}(\delta^{7/2}), \quad (5.16)$$

$$\begin{aligned} \left. \frac{\delta^2 \mathcal{L}_{\text{eff}}(x)}{\delta \theta(x)^2} \right|_{\theta=0} &= -F^2 \left[\frac{M_0^2}{6} + (2m_l + m_s) B_0 v_2^{(2)} \right] + \frac{2}{3} v_2^{(2)} B_0 \left[\left((m_l + 2m_s) c_\theta^2 \right. \right. \\ &\quad \left. \left. - 2\sqrt{2}(m_l - m_s) c_\theta s_\theta + (2m_l + m_s) s_\theta^2 \right) \eta(x)^2 + 2(m_l - m_s) \left(\sqrt{2} c_\theta^2 - c_\theta s_\theta - \sqrt{2} s_\theta^2 \right) \eta(x) \eta'(x) \right. \\ &\quad \left. + \left((2m_l + m_s) c_\theta^2 + 2\sqrt{2}(m_l - m_s) c_\theta s_\theta + (m_l + 2m_s) s_\theta^2 \right) \eta'(x)^2 \right] \\ &\quad + 18v_4^{(0)} (c_\theta \eta'(x) - s_\theta \eta(x))^2 + \dots + \mathcal{O}(\delta^4), \end{aligned} \quad (5.17)$$

¹Note that we only refer about the LO topology for each connected contribution in (5.14) independently of their corresponding counting in the U(3) expansion.

²The fourth derivative is just a contact term without any meson line up to NNLO in the δ expansion.

$$\begin{aligned}
\left. \frac{\delta \mathcal{L}_{\text{eff}}(x)}{\delta \theta(x)} \right|_{\theta=0} = & -\frac{F}{\sqrt{6}} \left[M_0^2 (c_\theta \eta'(x) - s_\theta \eta(x)) + \frac{2}{3} \Lambda_2 B_0 \left((2m_l + m_s) (c_\theta \eta'(x) - s_\theta \eta(x)) \right. \right. \\
& \left. \left. + \sqrt{2} (m_l - m_s) (c_\theta \eta'(x) + s_\theta \eta(x)) \right) + 12 B_0 v_2^{(2)} (2m_l + m_s) (c_\theta \eta'(x) - s_\theta \eta(x)) \right] \\
& + 16 \sqrt{\frac{2}{3}} \frac{B_0^2}{F} L_{25} \left[(2m_l^2 + m_s^2) (c_\theta \eta'(x) - s_\theta \eta(x)) + \sqrt{2} (m_l^2 - m_s^2) (c_\theta \eta'(x) - s_\theta \eta(x)) \right] \\
& + \frac{1}{9\sqrt{3}F} B_0 \Lambda_2 \left[\left(\sqrt{2} (m_l + 2m_s) c_\theta^3 - 3m_l c_\theta^2 s_\theta - 3\sqrt{2} m_s c_\theta s_\theta^2 + 2(m_l - m_s) s_\theta^3 \right) \eta(x)^2 \eta'(x) \right. \\
& + \left(2(m_l - m_s) c_\theta^3 + 3m_s c_\theta^2 s_\theta - 3\sqrt{2} m_l c_\theta s_\theta^2 - \sqrt{2} (m_l + 2m_s) s_\theta^3 \right) \eta(x) \eta'(x)^2 \\
& + \frac{1}{3} \left(\sqrt{2} (2m_l + m_s) c_\theta^3 + 6(m_l - m_s) c_\theta^2 s_\theta + 3\sqrt{2} (m_l + 2m_s) c_\theta s_\theta^2 + (m_l - 4m_s) s_\theta^3 \right) \eta'(x)^3 \\
& \left. + \frac{1}{3} \left((m_l - 4m_s) c_\theta^3 - 3\sqrt{2} (m_l + 2m_s) c_\theta^2 s_\theta + 6(m_l - m_s) c_\theta s_\theta^2 - \sqrt{2} (2m_l + m_s) s_\theta^3 \right) \eta(x)^3 \right] \\
& + \frac{2}{F} \sqrt{\frac{2}{3}} B_0 v_2^{(2)} (c_\theta \eta'(x) - s_\theta \eta(x)) \left[\left((m_l + 2m_s) c_\theta^2 - 2\sqrt{2} (m_l - m_s) c_\theta s_\theta \right. \right. \\
& + \left. (2m_l + m_s) s_\theta^2 \right) \eta(x)^2 + 2(m_l - m_s) \left(\sqrt{2} c_\theta^2 - c_\theta s_\theta - \sqrt{2} s_\theta^2 \right) \eta(x) \eta'(x) \\
& \left. + \left((2m_l + m_s) c_\theta^2 + 2\sqrt{2} (m_l - m_s) c_\theta s_\theta + (m_l + 2m_s) s_\theta^2 \right) \eta'(x)^2 \right] \\
& + \frac{6\sqrt{6}}{F} v_4^{(4)} (c_\theta \eta'(x) - s_\theta \eta(x))^3 + \dots + \mathcal{O}(\delta^{9/2}) \tag{5.18}
\end{aligned}$$

where the ellipses denote further terms involving π 's and K 's fields, which do not contribute to connected contributions.

The diagram displayed in Fig. 5.1 (a) is generated from the fourth-order derivative induced vertex in (5.15). It implies a contact term proportional to $F^2 v_4^{(0)}$ and hence it only contributes at $\mathcal{O}(\delta^2)$. The diagram (b) in Fig. 5.1 comes from the third-order derivative induced vertex (5.16) and the LO contribution in the δ expansion to the single-derivative vertex, i.e., first term in (5.18). It involves a single $\eta^{(\prime)}$ propagator at vanishing momentum and hence terms proportional to $F^2 M_0^2 v_4^{(0)} / M_{0\eta^{(\prime)}}^2$, where $\eta^{(\prime)}$ stands for a η or η' field, that contribute at $\mathcal{O}(\delta^2)$. Diagram (c) is coming from the product of two second-order derivative vertices at NLO in the δ expansion, hence involving two $\eta^{(\prime)}$ propagators. Nevertheless, it contributes only at $\mathcal{O}(\delta^4)$ and it will not enter in the NNLO $U(3)$ calculation for the fourth-order cumulant. The topology shown in Fig. 5.1 (d) is produced from the NLO $U(3)$ contribution of the second derivative vertex in (5.17) and two single-derivative vertices at LO in the δ expansion. It involves two $\eta^{(\prime)}$ propagators and terms proportional to $M_0^4 v_2^{(2)} / M_{0\eta^{(\prime)}}^4$ and $M_0^4 v_4^{(0)} / M_{0\eta^{(\prime)}}^4$. Thus, it

contributes at $\mathcal{O}(\delta^2)$. Finally, diagrams (e) and (f) involve four single-derivative vertices. Diagram (e) requires one of the vertices to emit three $\eta^{(\prime)}$ lines, i.e., the last three term in brackets in (5.18), and the three remaining producing only one meson line, which in total entails three $\eta^{(\prime)}$ propagators. It involves terms proportional to $M_0^6 \Lambda_2 / M_{0\eta^{(\prime)}}^6$, which are $\mathcal{O}(\delta)$, and terms multiplying $M_0^6 v_2^{(2)} / M_{0\eta^{(\prime)}}^6$, $M_0^6 v_4^{(0)} / M_{0\eta^{(\prime)}}^6$ and $M_0^4 \Lambda_2^2 / M_{0\eta^{(\prime)}}^6$, contributing at $\mathcal{O}(\delta^2)$. Finally, at LO in U(3) diagram (f) implies an interaction vertex with four internal legs, which in turn involves four $\eta^{(\prime)}$ propagators evaluated at zero momentum. It implies that only mass terms contribute to the interaction vertex, leading to a total contribution proportional to $F^2 M_0^8 m_{l,s} / M_{0\eta^{(\prime)}}^8$ at $\mathcal{O}(1)$, $F^2 M_0^6 \Lambda_2 m_{l,s}^2 / M_{0\eta^{(\prime)}}^8$ at $\mathcal{O}(\delta)$ or terms proportional $F^2 M_0^6 v_2^{(2)} m_{l,s}^2 / M_{0\eta^{(\prime)}}^8$ and $F^2 M_0^4 \Lambda_2^2 m_{l,s}^3 / M_{0\eta^{(\prime)}}^8$ at $\mathcal{O}(\delta^2)$.

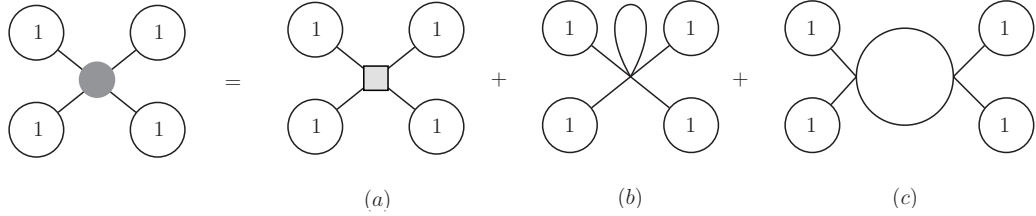


Figure 5.2: Topologies entering in c_4 from higher-order contributions to the four-point interaction vertex. Diagram (a) denotes a LECs contribution, while diagram (b) and (c) represent a tadpole or rescattering topology, respectively.

Furthermore, since diagram (f) is the only one contributing at $\mathcal{O}(1)$ and $\mathcal{O}(\delta)$, it can be also dressed at higher orders in two different ways. On the one hand, the four-point interaction vertex can be dressed by including the higher-order diagrams depicted in Fig. 5.2. Namely, the LO four-point vertex can be replaced by its NLO counterpart in the U(3) expansion, i.e., by including a LEC, Fig. 5.2 (a). Since the propagators are evaluated at $p = 0$ this diagram only involves the LECs L_6 , L_7 , L_8 from the $\mathcal{L}_4$ Lagrangian and C_{19} , C_{31} from $\mathcal{L}_6$. In addition, one might add a loop to the vertex either by including a π , K or $\eta^{(\prime)}$ tadpole, Fig. 5.2 (b), or a rescattering diagram Fig. 5.2 (c). Note that in these two cases off-shell momentum-dependent terms enter. In addition, the one-loop contribution in Fig. 5.2 (c) is evaluated at $p = 0$, which leads to the function $M_{0i}^{2n} \log M_{0i}^2 / \mu^2$, where M_{0i} denote a π , K , η or η' and $n = 0, 1, 2$ depending on the fields and derivatives running in the loop. Terms proportional to the LEC L_8 are $\mathcal{O}(\delta)$. The remaining LECs and loop topologies enter only at $\mathcal{O}(\delta^2)$. On the other hand, one or more of the $\eta^{(\prime)}$ propagators can be dressed at NLO in the U(3) expansion. The $\eta^{(\prime)}$ self energies were computed in [189] in U(3) ChPT. At zero momentum they involve the LECs Λ_2 , L_8 at $\mathcal{O}(\delta)$ and L_6 , L_7 , L_{25} , v_2^2 , L_8^2 , $L_8 \Lambda_2$, Λ_2^2 at $\mathcal{O}(\delta^2)$, Fig. 5.3 (a), as well

as further π , K or $\eta^{(\prime)}$ tadpole diagrams entering at $\mathcal{O}(\delta^2)$, Fig. 5.3 (b). Finally, the product of the topology in Fig. 5.2 (a) proportional to L_8 and in Fig. 5.3 (a) multiplying Λ_2 and L_8 also contribute at $\mathcal{O}(\delta^2)$.

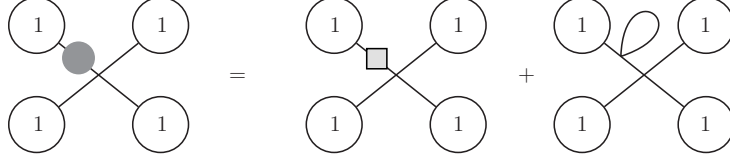


Figure 5.3: Topologies entering in c_4 from the NLO contribution to the η and η' propagators.

All together, the LO contribution in the δ expansion to the fourth-order cumulant in the isospin limit reads

$$\begin{aligned}
 c_4^{U(3), LO, IL} = F^2 M_0^8 B_0 \left[\frac{s_\theta^4}{162 M_{0\eta}^8} \left(m_l \left(c_\theta^4 - 4\sqrt{2} c_\theta^3 s_\theta + 12 c_\theta^2 s_\theta^2 - 8\sqrt{2} c_\theta s_\theta^3 + 4 s_\theta^4 \right) \right. \right. \\
 + 2m_s \left(4c_\theta^4 + 8\sqrt{2} c_\theta^3 s_\theta + 12 c_\theta^2 s_\theta^2 + 4\sqrt{2} c_\theta s_\theta^3 + s_\theta^4 \right) \Big) \\
 - \frac{2c_\theta s_\theta^3}{81 M_{0\eta}^6 M_{0\eta'}^2} \left(m_l \left(\sqrt{2} c_\theta^4 - 5c_\theta^3 s_\theta + 3\sqrt{2} c_\theta^2 s_\theta^2 + 2c_\theta s_\theta^3 - 2\sqrt{2} s_\theta^4 \right) \right. \\
 - 2m_s \left(2\sqrt{2} c_\theta^4 + 2c_\theta^3 s_\theta - 3\sqrt{2} c_\theta^2 s_\theta^2 - 5c_\theta s_\theta^3 - \sqrt{2} s_\theta^4 \right) \Big) \\
 + \frac{c_\theta^2 s_\theta^2 (m_l + 2m_s)}{27 M_{0\eta}^4 M_{0\eta'}^4} \left(2c_\theta^4 - 2\sqrt{2} c_\theta^3 s_\theta - 3c_\theta^2 s_\theta^2 + 2\sqrt{2} c_\theta s_\theta^3 + 2s_\theta^4 \right) \\
 + \frac{2c_\theta^3 s_\theta}{81 M_{0\eta}^2 M_{0\eta'}^6} \left(m_l \left(-2\sqrt{2} c_\theta^4 - 2c_\theta^3 s_\theta + 3\sqrt{2} c_\theta^2 s_\theta^2 + 5c_\theta s_\theta^3 + \sqrt{2} s_\theta^4 \right) \right. \\
 + 2m_s \left(\sqrt{2} c_\theta^4 - 5c_\theta^3 s_\theta + 3\sqrt{2} c_\theta^2 s_\theta^2 + 2c_\theta s_\theta^3 - 2\sqrt{2} s_\theta^4 \right) \Big) \\
 + \frac{c_\theta^4}{162 M_{0\eta'}^8} \left(m_l \left(4c_\theta^4 + 8\sqrt{2} c_\theta^3 s_\theta + 12 c_\theta^2 s_\theta^2 + 4\sqrt{2} c_\theta s_\theta^3 + s_\theta^4 \right) \right. \\
 \left. \left. + 2m_s \left(c_\theta^4 - 4\sqrt{2} c_\theta^3 s_\theta + 12 c_\theta^2 s_\theta^2 - 8\sqrt{2} c_\theta s_\theta^3 + 4 s_\theta^4 \right) \right) \right]. \quad (5.19)
 \end{aligned}$$

Expressing once more the tree-level η and η' masses and mixing angle in terms of M_0 , m_l and m_s , (5.19) simplifies remarkably leading to

$$c_4^{U(3), LO, IL} = - \frac{B_0 F^2 M_0^8 m_l m_s (m_l^3 + 2m_s^3)}{(M_0^2 (m_l + 2m_s) + 6B_0 m_l m_s)^4} = - \frac{\Sigma \bar{m}_{IL}^4}{\bar{m}_{IL}^{[3]} (M_0^2 + 6B_0 \bar{m}_{IL})^4} = - \frac{\Sigma \hat{m}_{IL}^4}{\bar{m}_{IL}^{[3]}}, \quad (5.20)$$

where we have expressed the tree-level η and η' masses and mixing angle in terms of M_0 , m_l and m_s and where

$$\bar{m}_{IL}^{[n]} = \left[\frac{2}{m_l^n} + \frac{1}{m_s^n} \right]^{-1}. \quad (5.21)$$

Like the topological susceptibility, c_4 vanishes in the chiral limit $m_l \rightarrow 0$ pointing out once more that it is a chiral quantity. The SU(3) result for the fourth-order cumulant at LO in the chiral expansion can be recovered by taking the limit $M_0 \rightarrow \infty$. In that case $\hat{m}_{IL} \rightarrow \bar{m}_{IL}$ and one retrieves the results in [170, 176]. In addition, one can also study the opposite limit, i.e., the quenched approximation for which $M_0 \ll \hat{m}$. In that case one obtains

$$c_4^{U(3), LO, IL} = -\frac{F^2 M_0^8}{1296 B_0^3 \bar{m}_{IL}^{[3]}} + \mathcal{O}\left(\frac{1}{N_c^4}\right). \quad (5.22)$$

The NLO $\mathcal{O}(\delta)$ results are always proportional to the $\mathcal{O}(N_c)$ LECs Λ_2 and L_8 , while NNLO $\mathcal{O}(\delta^2)$ results involve the remaining pieces. Namely, terms proportional to the LECs L_6 , L_7 , L_{25} , C_{29} , C_{31} , $v_4^{(0)}$, $v_2^{(2)}$, L_8^2 , $L_8 \Lambda_2$, Λ_2^2 and meson logarithms. The renormalization of the LECs [45, 46, 189] render a finite and scale-independent result. The explicit formulas are too long to be displayed here and they are provided as supplementary material. In addition, in the SU(3) $M_0 \rightarrow \infty$ limit we recover the NLO results in the chiral expansion given in [176].

Finally, we can also study the large- N_c expansion of the fourth-order cumulant. While the LO N_c behavior of χ_{top} was well established time ago [42, 155, 156], the large- N_c behavior of c_4 is still under debate. On the one hand, in [178, 180] it was argued from the large- N_c structure of the vacuum energy density that the fourth-order cumulant should scale as $\mathcal{O}(1/N_c^2)$. On the other hand, an explicit calculation based on $U(N_f)$ ChPT at NLO in the chiral expansion for degenerate quark masses [181] suggests that it goes as $\mathcal{O}(1/N_c^3)$. Our LO $\mathcal{O}(1)$ and NLO $\mathcal{O}(\delta)$ results do indeed reproduce the predictions in [181], since we obtain that they are $\mathcal{O}(1/N_c^3)$ and $\mathcal{O}(1/N_c^4)$, respectively. Nevertheless, at NNLO $\mathcal{O}(\delta^2)$ the fourth-derivative contribution in (5.15) involves the contact term $-6F^2 v_4^0 \sim \mathcal{O}(1/N_c^2)$. In fact, one can show that it is the only term contributing to c_4 at this large- N_c order. Namely, the leading- N_c dependence of any $U(N_f)$ chiral operator $\hat{O}(X)$ involving the field X in (1.84) is given by [45, 190]

$$\hat{O}(X) = N_c^{2-\#(Tr)-\#(X)}, \quad (5.23)$$

where $\#(Tr)$ and $\#(X)$ denote the number of chiral flavor traces and powers of the operator X in (1.84), respectively. Thus, any higher order operators in X will be suppressed both by their large- N_c counting and the pion decay constants F . It also implies that any n th-order cumulant of the topological charge distribution should scale as N_c^{2-n} .

All together, we obtain

$$c_4^{U(3), IL} = -6F^2 v_4^0 - \frac{F^2 M_0^8}{1296 B_0^3 \bar{m}_{IL}^{[3]}} - \frac{4F^2 M_0^2}{\bar{m}_{IL} B_0} \left[v_4^0 + \frac{M_0^2}{216} (v_2^{(2)} - \Lambda_2^2) + \frac{M_0^6}{27F^4} \left(3C_{19}^r + 4C_{31}^r + \frac{160}{3} L_8^{r^2} \right) \right] + \mathcal{O}\left(\frac{1}{N_c^4}\right) + \mathcal{O}(\delta^3). \quad (5.24)$$

where, as explained, the first term in the r.h.s. is $\mathcal{O}(1/N_c^2)$ and the rest of the displayed terms are $\mathcal{O}(1/N_c^3)$.

5.3 Numerical results

In Table 5.1 we provide the numerical results for $\chi_{top}^{1/4}$, $(-c_4)^{1/4}$ and $b_2 = c_4/(12\chi_{top})$ (the latter is defined following standard lattice analyses, see below) calculated in ChPT for SU(2), SU(3) and U(3) at different orders in the chiral or δ expansion. The numerical values for the parameters involved, i.e., F , M_0 , meson masses and the LECs L_6^r , L_7^r , L_8^r , Λ_1 , Λ_2 , C_{19} and C_{31} are taken from [189]. Note that the U(3) LECs do not correspond to the usual SU(3) ChPT quantities, but larger differences might be expected between them. More precisely, we consider the values of the NNLOFit-B, i.e., their best fit to lattice results for the η and η' masses. However, the constants L_{25}^r , $v_4^{(0)}$ and $v_2^{(2)}$ are not included in [189]. L_{25}^r and $v_2^{(2)}$ were estimated in [186] in an additional fit to lattice data for the η and η' parameters and they enter both in $\chi_{top}^{1/4}$ and c_4 . On the contrary, $v_4^{(0)}$ remains unknown and it only contributes to the fourth-order cumulant. In addition, while these LECs play a very small role on the topological susceptibility, $v_2^{(2)}$ and $v_4^{(0)}$ have a much more sizable effect on c_4 . In fact, taking L_{25}^r and $v_2^{(2)}$ from [186] and assuming the NNLO U(3) correction for c_4 to agree within uncertainties with the NLO estimate, one obtains for $v_4^{(0)} = 218(10)$. Nevertheless, in order to avoid any bias in the behavior of the U(3) expansion, we will set instead the value of $v_4^{(0)}$ value to zero. Thus, since there are no current estimates for $v_4^{(0)}$ and it would be inconsistent to include only $v_2^{(2)}$, we simply set the values of L_{25}^r , $v_4^{(0)}$ and $v_2^{(2)}$ to zero. Furthermore, we will neglect the NNLO U(3) corrections coming from Λ_2^2 since they are of the same order as the $v_2^{(2)}$ and $v_4^{(0)}$ effects that we are ignoring.

We also include the LECs uncertainties quoted in [189]. One can see in Table 5.1 that the uncertainties of the U(3) LECs are much larger than the standard SU(2) and SU(3) errors, the main source of error coming from F^2 . In that sense, let us remark that the SU(3) and SU(2) values quoted in Table 5.1 are obtained from the U(3) expressions by taking the $M_0 \rightarrow \infty$ limit, plus the $m_s \rightarrow \infty$ one in SU(2), but keeping the numerical

$\chi_{top}^{1/4}$ [MeV]	U(3)	SU(2)	SU(3)
LO	74(3)	75(3)	75(3)
NLO	74(3)	78(3)	83(2)
NNLO	81(2)		
Lattice	73(9) [163]		

$(-c_4)^{1/4}$ [MeV]	U(3)	SU(2)	SU(3)
LO	50(3)	53(2)	52(2)
NLO	50(3)	60(2)	61(2)
NNLO	58(2)		

$b_2 = \frac{c_4}{12\chi_{top}}$	U(3)	SU(2)	SU(3)
LO	-0.01737(4)	-0.02083	-0.01960
NLO	-0.018(2)	-0.029(2)	-0.025(1)
NNLO	-0.023(2)		
Lattice	-0.0216(15) [180]		

Table 5.1: Topological susceptibility, fourth-order cumulant and the b_2 coefficient, calculated in SU(2), SU(3) and U(3) ChPT to LO, NLO and NNLO in the isospin limit. The lattice values mentioned in the main text have been also quoted here for reference. The numerical values of the masses, decay constants and LECs involved, as well as their uncertainties, are taken from [189], except L_{25} , $v_2^{(0)}$ and $v_4^{(0)}$, which are set to zero, (see main text).

values of the U(3) LECs and their uncertainties. The reason for this is that our main purpose here is to calibrate the numerical effect of the η' as compared with the rest of the light degrees of freedom. Recall that, according to our previous discussion, the NNLO U(3) contribution includes the NLO SU(3) one in the limit where the η' is decoupled and the NLO SU(2) results when also kaons and eta decouple. This has however the drawback of losing numerical precision with respect to the corresponding purely SU(2) and SU(3) LECs. For instance, recent estimates of the pure SU(2) calculation are $\chi_{top}^{1/4} = 75.5(5)$ MeV at NLO [171] and $\chi_{top}^{1/4} = 75.44(34)$ MeV at NNLO [172] for typical LECs values of SU(2) and SU(3) [191]. Note that the NNLO calculated for SU(2) in [171] includes $\mathcal{O}(p^6) = \mathcal{O}(\delta^3, \delta^4)$ corrections, which are beyond our present analysis. In particular, we do not recover those corrections when taking the $M_0 \rightarrow \infty$ and $m_s \rightarrow \infty$ limits. For that reason, we do not include those results in Table 5.1 where, as explained, we aim to discuss the different contributions that are obtained as limiting cases of our present approach. In any case, it is pointed out in [171], despite the uncertainties in the $\mathcal{O}(p^6)$ LECs, the NNLO SU(2) numerical corrections are one order of magnitude smaller than the NLO ones. In the case of the b_2 coefficient, the LO SU(2) and SU(3) expressions are LEC independent and therefore, they are given

without theoretical uncertainty in Table 5.1. The cancellation of the F^2 dependence in the $U(3)$ LO for b_2 , e.g. from (5.9) and (5.20), explains also its smaller error compared to higher orders.

The results in Table 5.1 are obtained in the isospin limit. In the case of the topological susceptibility they have to be compared with the lattice result $[\chi_{top}^{latt}]^{1/4} = 73(9)$ MeV in that case [163]. As for lattice results on c_4 , customarily given in terms of the b_2 coefficient, they are provided only for pure gauge $SU(N)$ theories in [178–180] and for domain-wall $N_f = 2 + 1$ fermions with large light quark masses $m_l/m_s \geq 0.25$ [160]. Remarkably, the value of b_2 seems to be quite stable under those different approximations and close to the simplest $SU(2)$ ChPT value, as pointed out in [163]. We quote for reference the isospin-limit value for $N_c = 3$ gluodynamics, $b_2 = -0.0216(15)$ [180]. Nevertheless, more accurate lattice determinations for c_4 and b_2 for the physical $N_f = 2 + 1$ case would be needed to make further claims.

From the results in Table 5.1 we also observe the following features. First, in the three theoretical frameworks, the perturbative corrections remain reasonably under control. Second, although the $SU(2)$ approach already reproduces the main contribution, the η' meson and mixing angle corrections that we are including in the present work are actually comparable to the kaon and η ones introduced in the $SU(3)$ approach. For χ_{top} , those corrections lower the central value and get closer to the lattice prediction and so on for $|b_2|$. Actually, we see that the full $U(3)$ calculation for both observables remains compatible with the lattice results within the range provided by the LECs uncertainties, which in the case of χ_{top} holds also for all the different approximations collected in Table 5.1. The latter confirms that these are good chiral quantities in the sense that they can be accurately described within ChPT.

5.4 Isospin breaking corrections to χ_{top} and c_4

As mentioned in the introduction, isospin breaking corrections can become important for the topological charge distribution. The main reason is that for $\theta \neq 0$ and $m_u \neq m_d$, the constant field configuration that minimizes the vacuum energy density is not $U_0 = \mathbb{1}$, but generally $U_0 = \text{diag}(e^{\phi_1}, \dots, e^{\phi_{N_f}})$ [35, 43, 170, 177]. In the $SU(3)$ framework, the constraint $\det U_0 = 1$ leads to $\sum_j \phi_j = 0$. However, within our present $U(3)$ formalism, such constraint does not hold, since the determinant of U_0 is an additional degree of freedom [43]. The U_0 configuration should be such that the vacuum energy density

$\epsilon_{vac}(\theta)$ is minimized, which is indeed achieved for a constant value of U_0 . Therefore, to LO in the chiral expansion, we have to consider just the usual NGB mass term plus the M_0^2 term in (1.88) for the Euclidean action. Namely,

$$\begin{aligned}\epsilon_{vac}^{LO}(\theta) &= -\frac{F^2 B_0}{2} \text{tr} [U_0 \mathcal{M}^\dagger + \mathcal{M} U_0^\dagger] - \frac{F^2}{12} M_0^2 [i\theta + \log \det U_0]^2 \\ &= -F^2 B_0 \sum_{j=1}^{N_f} m_j \cos [\phi_j(\theta)] + \frac{F^2 M_0^2}{12} \left(\theta + \sum_{j=1}^{N_f} \phi_j(\theta) \right)^2, \quad (5.25)\end{aligned}$$

with $\mathcal{M} = \text{diag}(m_u, m_d, m_s)$ the quark mass matrix and $\phi_j(\theta)$ are such that they minimize $\epsilon_{vac}^{LO}(\theta)$, i.e.,

$$B_0 m_k \sin [\phi_k(\theta)] + \frac{M_0^2}{6} \left(\theta + \sum_{j=1}^{N_f} \phi_j(\theta) \right) = 0 \quad (k = 1, \dots, N_f). \quad (5.26)$$

Note that the solution to (5.26) is equivalent to encode the θ dependence in a complex quark mass matrix $\mathcal{M} \exp(-i\theta/N_f)$ as in [170, 177] with the change of variable $\phi_j \rightarrow \phi_j + \theta/N_f$.

Now, following the same procedure as in [170], in order to solve the minimization problem we expand $\cos \phi_j$ in powers of ϕ_j . The reason for this is that we are only interested in the power expansion of $\epsilon_{vac}(\theta)$ around $\theta = 0$ and hence around the solution $\phi_j = 0$ of (5.26) for $\theta = 0$. For $N_f = 2$ and $M_0 = 0$ the solution of (5.26) can be found in [170, 177]. The solution of the system (5.26) to $\mathcal{O}(\phi_j)$ for $N_f = 3$ is $\phi_j(\theta) = \phi_j^0 \theta + \mathcal{O}(\theta^3)$ with

$$\phi_j^0 = -m_j \left(\frac{6B_0}{M_0^2} + \frac{1}{\bar{m}} \right) \quad (j = u, d, s), \quad (5.27)$$

with $\bar{m}$ defined in (5.4). Replacing the above linear order in the vacuum energy density (5.25) yields

$$\epsilon_{vac}^{LO}(\theta) = \epsilon_{vac}(0) + \frac{1}{2} \chi_{top}^{U(3), LO} \theta^2 + \mathcal{O}(\theta^4), \quad (5.28)$$

with

$$\chi_{top}^{U(3), LO} = \Sigma \hat{m}, \quad (5.29)$$

and

$$\hat{m} = \frac{M_0^2 \bar{m}}{M_0^2 + 6B_0 \bar{m}},$$

The above result is the extension to $m_u \neq m_d$ of the LO $U(3)$ result in (5.9), which amounts to the replacement $\bar{m}_{IL} \rightarrow \bar{m}$ and reproduces the LO result with isospin breaking in $SU(3)$ in (5.4) by replacing $\bar{m} \rightarrow \hat{m}$.

In order to provide a numerical estimate of the isospin breaking effect, we write (5.29) as

$$\chi_{top}^{U(3),LO} = \frac{F^2 M_0^2}{6 + \frac{(1+z)^2}{z} \frac{M_0^2}{M_{0\pi^0}^2} + \frac{(1+z)M_0^2}{(1+z)M_{0K^0}^2 - M_{0\pi^0}^2}} \quad (5.30)$$

where $z = m_u/m_d$. Using the central value $z = 0.485$ of the recent lattice analysis [191], we get $[\chi_{top}^{U(3),LO}]^{1/4} = 72$ MeV, to be compared with the $U(3)$ LO value in Table 5.1, which corresponds to $z = 1$ in (5.30). Thus, the isospin correction to LO $U(3)$ is within the 5% range and lies within the theoretical LO uncertainty. It is therefore numerically safe to consider isospin breaking only for the LO $U(3)$ result in our present analysis.

Following the same approach to the next order in the θ expansion allows us to calculate the isospin breaking corrections to the fourth-order cumulant. Thus, we expand (5.26) up to $\mathcal{O}(\phi_j^3)$ and write its solution as $\phi_j(\theta) = \phi_j^0\theta + \phi_j^1\theta^3 + \mathcal{O}(\theta^5)$ and keep only up to $\mathcal{O}(\theta^3)$ in the equation, thus solving linearly for the ϕ_j^1 . Replacing then the solution in (5.25) yields:

$$\epsilon_{vac}^{LO}(\theta) = \epsilon_{vac}(0) + \frac{1}{2}\chi_{top}^{U(3),LO}\theta^2 + \frac{1}{24}c_4^{U(3),LO}\theta^4 + \mathcal{O}(\theta^6) \quad (5.31)$$

with the fourth order cumulant

$$c_4^{U(3),LO} = -\Sigma \frac{\hat{m}^4}{\bar{m}^{[3]}} \quad (5.32)$$

where, following the notation of [176], we have defined, consistently with (5.21),

$$\bar{m}^{[3]} = \left[\frac{1}{m_u^3} + \frac{1}{m_d^3} + \frac{1}{m_s^3} \right]^{-1}. \quad (5.33)$$

The result (5.32) for the fourth-order cumulant corresponds again to the $SU(3)$ one in [170, 176, 177] with the replacement $\bar{m} \rightarrow \hat{m}$. As in the previous case, we also can write in terms of measurable meson parameters:

$$c_4^{U(3),LO} = -\frac{F^2 M_0^8 (1+z)^3 \left[\frac{1}{[(1+z)M_{0K^0}^2 - M_{0\pi^0}^2]^3} + \frac{1+z^3}{z^3 M_{0\pi^0}^6} \right]}{\left[6 + \frac{(1+z)M_0^2}{(1+z)M_{0K^0}^2 - M_{0\pi^0}^2} + \frac{(1+z)^2}{z} \frac{M_0^2}{M_{0\pi^0}^2} \right]^4} \quad (5.34)$$

which yields $(-c_4^{U(3),LO})^{1/4} = 53$ MeV, so that the correction lies also within the 5% level when compared with the isospin-limit values in Table 5.1.

Finally, we recall that at the order we are considering the isospin-breaking corrections, temperature dependence is absent since it only enters through loop contributions.

5.5 Finite temperature dependence

From our present U(3) ChPT analysis, we can straightforwardly include the temperature dependence coming from meson loops. In the case of χ_{top} , loop effects only arise at NNLO in the δ expansion from tadpole contributions coming from the Euclidean tree-level propagator $G_i(\vec{0}, 0)$. Its finite part reads

$$\mu_i(T) = \frac{M_{0i}^2}{32\pi^2 F^2} \log \frac{M_{0i}^2}{\mu^2} + \frac{g_1(M_{0i}, T)}{2F^2}, \quad (5.35)$$

with g_1 defined in (1.130) and where $i = \pi, K, \eta, \eta'$, M_{0i} are the tree level masses and μ is the renormalization scale.

In the case of c_4 , in addition to tadpoles, which enter again from the Euclidean tree-level propagator $G_i(\vec{0}, 0)$ in Fig 5.3 (b) but also from the six-point interaction vertex in Fig. 5.2 (b), one has to take into account the one-loop function depicted in Fig. 5.2 (c), which finite part can be written in terms of

$$\nu_i(T) = F^2 \frac{d}{dM_{0i}^2} \mu_i(T) = \frac{1}{32\pi^2} \left[1 + \log \frac{M_{0i}^2}{\mu^2} \right] - \frac{g_2(M_{0i}, T)}{2}, \quad (5.36)$$

with g_2 the function given in equation (1.136).

That said, we want to remark that the U(3) thermal expansion is based on a perturbative calculation and hence, it is only expected to converge at very low temperatures. The fact that thermal corrections arise at NNLO in the δ expansion implies that the series breaks down as soon as thermal effects are sizable. In Fig. 5.4, we show the temperature dependence of $\chi_{top}(T)$ and $b_2(T)$ for the same parameter values and errors used for the $T = 0$ results in Table 5.1. In addition, we also plot the lattice data results for the topological susceptibility obtained in [163] and [165] and for b_2 in [163]. In the latter case, lattice errors are larger than for the susceptibility and we have actually not considered the data set for $a = 0.0824$ fm which has even larger errors than those showed in the figure.

We see that the present U(3) ChPT analysis is consistent with the lattice within uncertainties, even beyond its applicability range, which as mentioned before lies at low temperatures, well below the transition. Consequently, its extrapolation close and above T_c has to be taken with care. However, the good agreement with the lattice observed in Fig. 5.4 reveals once more that accounting properly for the lightest meson degrees of freedom is crucial for the description of the topological susceptibility and the cumulant.

This implies an important difference with other thermodynamic observables like the quark condensate, which accurate description based on effective theories requires the

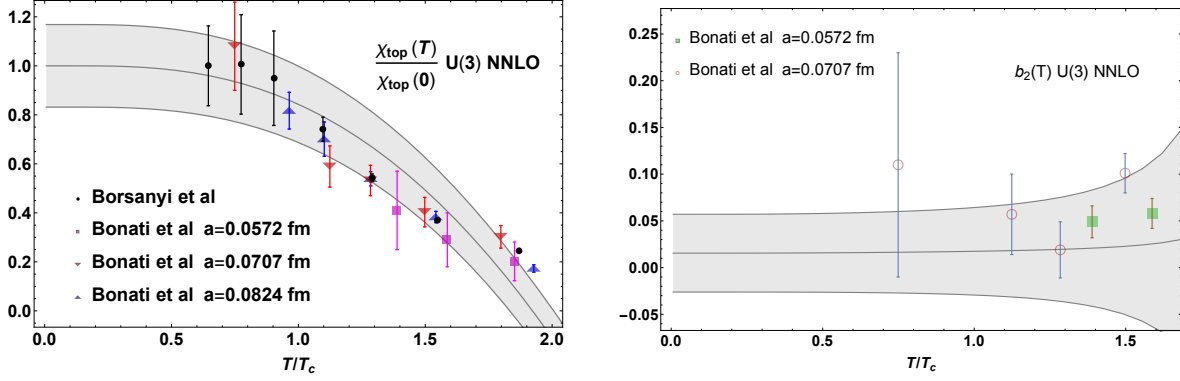


Figure 5.4: Left: Temperature dependence of the topological susceptibility calculated within the $U(3)$ formalism compared to lattice data from [163] and [165]. Here, we have taken $T_c = 155$ MeV. Right: Temperature dependence of the b_2 coefficient, with lattice data from [163].

contribution of many hadronic states, like for instance in the HRG approach. Actually, in Fig. 5.5 we compare different orders of the finite- T ChPT approach for the topological susceptibility and we see that the $SU(3)$ and $U(3)$ calculations represent rather small deviations from the $SU(2)$ one.

In the case of b_2 , our theoretical $U(3)$ result in Fig. 5.4 is quite flat with temperature, and lattice data are less accurate. This indicates that both quantities $\chi(T)$ and $c_4(T)$ decrease with T in a roughly similar way. Nevertheless, the agreement between theory and lattice results is also quite remarkable.

As discussed at the beginning of this chapter, another important issue regarding the temperature dependence is to what extent it can be approximated by just the scaling of the quark condensate, i.e., whether or not the second term in the Ward Identity in (5.5) can be ignored. This is actually the case if one sticks to $SU(2)$ at NLO in the chiral expansion, what has been used in [171]. In our present work, we are calculating $\chi_{top}(T)$ in $U(3)$ at NNLO, including $SU(3)$ and $SU(2)$ NLO as special cases. Thus, we can provide a much more accurate analysis in that respect. That issue can be also of relevance for lattice analyses. If the quark condensate terms dominate, the combined use of (5.5) and (5.6) may help to relate χ_{top} with quantities much better determined in the lattice. Namely,

$$\chi_{top} = \frac{m_l}{2} \left(2 - \frac{m_l^2}{m_s^2} \right)^{-1} \left[\frac{2}{m_s} \Delta_{l,s} - m_l (\chi_p^{ll} - 2\chi_p^{ss}) \right], \quad (5.37)$$

The relation (5.37) offers a way to measure indirectly χ_{top} , which is alternative to the usual method based on the WI (5.6).

The possible dominance of the quark-condensate term in the WI (5.5) is also relevant

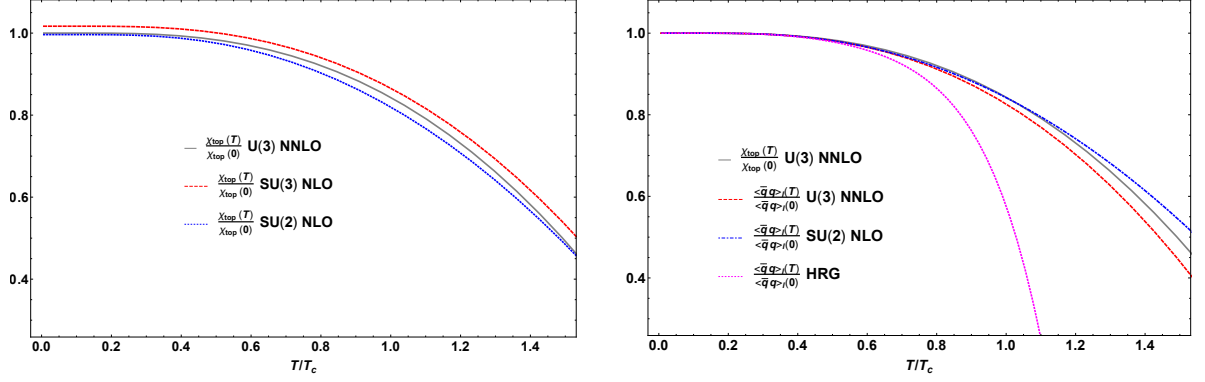


Figure 5.5: Left: comparison of the U(3), SU(3) and SU(2) limits for the topological susceptibility. Right: comparison of the topological susceptibility scaling at finite temperature with various approaches of the light quark condensate scaling.

for a current topic of discussion, which has been actively studied both theoretically and in the lattice [59, 65, 103, 107–113, 115, 118, 119, 169]. Namely, whether the chiral and $U(1)_A$ restoration temperatures are close enough. Since χ_{top} and $\langle \bar{q}q \rangle_l$ are meant to vanish at exact $U(1)_A$ (asymptotically) and chiral $O(4)$ restoration, respectively, their difference, encoded in χ_P^l in (5.5), provides a direct measure of the separation between the two transitions. In this sense, it is useful to recall the behavior of these quantities near the light chiral limit $m_l \rightarrow 0^+ (M_\pi \rightarrow 0^+)$, where the effects of chiral symmetry restoration are meant to be enhanced. In NNLO U(3) ChPT [65], $\chi_{top} = \mathcal{O}(m_l)$, while $\langle \bar{q}q \rangle_l(T)$ and $\chi_P^l(T)$ are both $\mathcal{O}(1)$ quantities in the $m_l \rightarrow 0^+$ limit. Thus, in the equation

$$\frac{\chi_{top}}{m_l} = -\frac{1}{4} [\langle \bar{q}q \rangle_l + m_l \chi_P^l] , \quad (5.38)$$

only the quark condensate contribution survives in the right-hand side of (5.38) in the chiral limit, which supports its dominance at low temperatures. However, near the transition $\langle \bar{q}q \rangle_l(T) \rightarrow 0^+$ in the chiral limit, while $\chi_P^l(T)$ changes much more slowly, since it is controlled by a term proportional to T^2/M_{0K}^2 . Thus, it brings up the question as to whether near the transition the χ_P^l term can become important enough for physical masses.

In Fig. 5.5, we compare the temperature dependence of the full U(3) topological susceptibility with the scaling of the light quark condensate calculated in the same framework, which would correspond to neglect the χ_u term in the WI (5.5) and (5.38). The values of the LECs and other parameters involved are the same as those used in Fig. 5.4. In the same figure, we also show the simple NLO SU(2) scaling used in [171],

corresponding just to the NLO ChPT quark condensate, namely

$$\frac{\chi_{top}^{SU(2),NLO}(T)}{\chi_{top}^{SU(2),NLO}(0)} = \frac{\langle \bar{q}q \rangle_l^{SU(2),NLO}(T)}{\langle \bar{q}q \rangle_l^{SU(2),NLO}(0)} = 1 - \frac{3}{2F_\pi^2} g_1(M_\pi, T) . \quad (5.39)$$

The results in Fig. 5.5 show that the contribution from the additional χ_u term in the WI, although not large, may be significant as T approaches the transition point. The simple $SU(2)$ description remains also close to the full $U(3)$ one, which is a test of its robustness despite its simplicity. However, it is very important to point out that, although the topological susceptibility may be well described within a ChPT analysis including only the lightest degrees of freedom, that is definitively not the case for the quark condensate. To show this explicitly, we have plotted in Fig. 5.5 the quark condensate resulting from the HRG approximation provided in [73], which includes hadron states with masses up to 2 GeV and provides a very good fit to lattice condensate data. One can see clearly a much larger departure from the scaling of the topological susceptibility than the one observed with the ChPT expressions for the quark condensate, which happen to remain close to the topological susceptibility. In this sense, we remark that the addition of degrees of freedom is expected to reduce drastically the chiral condensate, as expected from approximate chiral restoration at T_c . Nevertheless, that may not be the case for the topological susceptibility, whose behavior is not directly related to chiral symmetry restoration but includes $U(1)_A$ restoration features, describing lattice data just with the light degrees of freedom. Thus, in a full description of the hadron gas we do expect large deviations from the quark condensate scaling and hence significant contributions from the second term in (5.5), which becomes large close to the transition point. This also indicates that the $U(1)_A$ symmetry is still sizeably broken at the chiral transition for physical quark masses. This analysis should prevent from the use of the topological susceptibility to extract the quark condensate at finite temperature.

5.6 Conclusions

In this chapter we have provided a full calculation of the topological susceptibility and the fourth-order cumulant up to NNLO in $U(3)$ Chiral Perturbation Theory. Our result allows one to consider the effect of the η' meson consistently, as well as the $\eta - \eta'$ mixing angle dependence. As limits of interest, we recover the $SU(2)$ and $SU(3)$ results when $M_0 \rightarrow \infty$. In addition, we have discussed the large- N_c corrections to both quantities. In the case of the topological susceptibility, we have provided the $\mathcal{O}(1/N_c)$ correction to

the Witten-Veneziano formula up to $\mathcal{O}(\delta^2)$ in the $U(3)$ ChPT expansion, and so on for the $\mathcal{O}(1/N_c^2)$ and $\mathcal{O}(1/N_c^3)$ corrections to the fourth-order cumulant.

We have estimated the η' corrections to χ_{top} and c_4 at zero temperature, which turn out to be of the same order as the K and η contributions. Furthermore, it provides results compatible with lattice analyses, consistently with the idea that the QCD topological charge is an observable well described by the expansion around the chiral limit provided by ChPT.

Including the dominant isospin breaking effect in the vacuum misalignment, we have provided both χ_{top} and the fourth cumulant c_4 of the vacuum energy density expansion in the θ parameter to LO in the $U(3)$ ChPT expansion. Numerical corrections due to isospin breaking remain below the 5% level for $\chi_{top}^{1/4}$ and $(-c_4)^{1/4}$.

Finally, we have calculated χ_{top} and c_4 at finite temperature up to NNLO in $U(3)$ ChPT. The temperature dependence obtained for the topological susceptibility is consistent with lattice data, supporting again that this quantity is well described by a gas made only of light mesons, unlike for instance the quark condensate. We have also discussed the relation between these two quantities, which are connected through a Ward Identity valid at all temperatures. Although the quark condensate calculated within the same ChPT formalism seems to scale quite similarly to χ_{top} , we argue that this cannot be the case for the full hadron gas. It reveals a sizable gap between the chiral transition and the $U(1)_A$ one for physical quark masses, even though recent theoretical analysis show that those transition tend to coincide near the chiral limit for exact chiral restoration.

Chiral perturbation theory for nonzero chemical potentials

6.1 Construction of the Effective Lagrangian

The construction of the most general, model-independent, effective Lagrangian can be carried out within the framework of the external source method. Within this formalism, the building blocks are the meson fields U and the external sources v, a, s, p, θ and $Q_{R,L}$ which transform under local transformations of the chiral $SU_L(N_f) \times SU_R(N_f)$ group so that the action is invariant, up to anomalies. The use of the EOMs to a given order, as well as operator identities, allow to express the Lagrangian in terms of the minimum number of operators [34,35,192]. The effective Lagrangian formalism should be such that the ultraviolet divergences at a given order can be absorbed by the LECs multiplying the different operators, whose finite part can be fixed by the phenomenological analysis of lattice or experimental data. In addition, this formalism is well defined around the low-energy limit of the theory.

As any chemical potential can be expressed as an external source, the external source method allows us to incorporate any chemical potential. Several of these are of interest for lattice and heavy-ion phenomenology, such as the axial μ_5 , baryon μ_B , charge μ_Q or isospin μ_I chemical potentials, or including strangeness μ_S for three flavors. The low-energy ChPT effective Lagrangian framework has been used for analyzing the effect of some of those chemical potentials [193–197].

Two important additional aspects should be taken into account in the derivation of the effective Lagrangian in the presence of a chemical potential: first, in the original

works [34, 35], the external sources r_μ and l_μ were considered as traceless $SU(N_f)$ fields and therefore those results are not directly applicable to an arbitrary case. The effective Lagrangian with spurions fields included was derived in [198] for $SU(3)$ and in [41, 199] for $SU(2)$. The main interest of those works was to apply it to the EM field following previous ideas in [200]. To construct the Lagrangian in that case, the spurion fields mentioned in Subsection 1.1.8 are introduced.

The second observation has to do with covariant derivatives, which for the case (1.47) read

$$d_\mu U = \partial_\mu U - i(v_\mu + a_\mu + Q_R A_\mu)U + iU(v_\mu - a_\mu + Q_L A_\mu) \quad (6.1)$$

$$c_{\mu I} Q_I = \partial_\mu Q_I - i[G_{\mu I}, Q_I] \quad (6.2)$$

with $I = L, R$, $G_{\mu R} = v_\mu + a_\mu + Q_R A_\mu$ and $G_{\mu L} = v_\mu - a_\mu + Q_L A_\mu$. The field strength tensors of $G_{\mu R, L}$ are

$$G_{\mu\nu I} = \partial_\mu G_{\nu I} - \partial_\nu G_{\mu I} - i[G_{\mu I}, G_{\nu I}] \quad (6.3)$$

Summarizing, the most general Lagrangian at a given order is constructed out of the U , $d_\mu U$ and χ fields mentioned in Subsection 1.2.3 and the following fields, where we indicate their chiral power counting:

$$G_{\mu\nu I}, c_{\mu I} Q_I = \mathcal{O}(p^2), \quad Q_I = \mathcal{O}(p), \quad (6.4)$$

which transform under chiral rotations as [198]:

$$\begin{aligned} Q_I &\rightarrow g_I Q_I g_I^\dagger \quad (I = L, R) \\ G_{\mu I} &\rightarrow g_I G_{\mu I} g_I^\dagger + i g_I \partial_\mu g_I^\dagger \\ c_{\mu I} Q_I &\rightarrow g_I c_{\mu I} Q_I g_I^\dagger \quad (I = L, R) \end{aligned} \quad (6.5)$$

where $g_{L, R} \in SU(N_f)$ with $N_f = 2, 3$ light flavors. The Lagrangian is constructed demanding the same invariance properties as the QCD one with external sources, namely under chiral rotations, Lorentz covariance and P, C symmetries [198]:

$$\begin{aligned} Q_L &\xleftrightarrow{P} Q_R, & Q_L &\xleftrightarrow{C} Q_R^T \\ G_{\mu L} &\xleftrightarrow{P} G_{\mu R}^\mu, & G_{\mu L} &\xleftrightarrow{C} (G_{\mu R})^T \\ c_{\mu L} &\xleftrightarrow{P} c_{\mu R}, & c_{\mu L} &\xleftrightarrow{C} c_{\mu R}^T \end{aligned} \quad (6.6)$$

Moreover, using the standard identity $\text{tr}(U^\dagger \partial_\mu U) = 0$ for $SU(N_f)$ fields [192] we have that $\text{tr}(U^\dagger d_\mu U) = -\text{tr}(U d_\mu U^\dagger)$ is not equal to zero for arbitrary $Q_{L, R}$. Therefore, the

operator $\text{tr}(U^\dagger d_\mu U)$ has to be considered as an additional operator for constructing the Lagrangian to a given order, unlike in standard ChPT or in the EM case $Q_L = Q_R = Q$ where that operator vanishes.

Keeping $Q_{L,R}$ arbitrary within the external source method, transforming according to (6.5) and (6.6), ensures that one is taking into account all possible terms. After using EOMs and operator identities, we will replace in the end the $Q_{L,R}$ fields by a particular choice.

In turn, with this procedure, we will be constructing the most general Lagrangian for arbitrary $Q_{L,R}$. Such Lagrangian will be a generalization of that considered for the EM case in [41, 198, 199], which we will reobtain as a consistency check in the case $Q_L = Q_R$.

6.1.1 The leading order $\mathcal{O}(p^2)$ Lagrangian

It is not difficult to see that the lowest nontrivial order Lagrangian that one can construct through the previous procedure is the same as in the standard case, i.e., $\mathcal{O}(p^2)$. Thus, at $\mathcal{O}(p^0)$, the only ingredient that we can use is the field U , and then all possible terms are constants, independent of $Q_{R,L}$ and then irrelevant for our purposes, while at $\mathcal{O}(p)$, the only nontrivial operator with the allowed symmetries and arbitrary $Q_{L,R}$ is

$$\mathcal{L}_1 \rightarrow \text{tr}(Q_L + Q_R) \quad (6.7)$$

To $\mathcal{O}(p^2)$, we have, on the one hand, the standard Lagrangian (1.69) in terms of the covariant derivative in (6.1). In addition to this we must add the term coupling the Q and U fields needed to explain the electromagnetic mass difference of pions [34, 41, 198]:

$$\text{tr}[Q_R U Q_L U^\dagger] \quad (6.8)$$

On the other hand, according to our above discussion, the following operators are also allowed to this order:

$$\text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U), \quad \text{tr}[Q_L^2 + Q_R^2], \quad \text{tr}[Q_L]^2 + \text{tr}[Q_R]^2, \quad \text{tr}[Q_L] \text{tr}[Q_R], \quad (6.9)$$

Summarizing, the $\mathcal{O}(p^2)$ Lagrangian with explicit $Q_{L,R}$ for $N_f = 2$ fields is:

$$\begin{aligned} \mathcal{L}_2 = & \frac{F^2}{4} \text{tr}[d_\mu U^\dagger d^\mu U + 2B_0 \mathcal{M}(U + U^\dagger)] + C \text{tr}[Q_R U Q_L U^\dagger] \\ & + C_1 \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) + C_2 \text{tr}[Q_L^2 + Q_R^2] + C_3 (\text{tr}[Q_L]^2 + \text{tr}[Q_R]^2) + C_4 \text{tr}[Q_L] \text{tr}[Q_R] \end{aligned} \quad (6.10)$$

We recall that the above equation is valid for arbitrary Q_L and Q_R . Taking the EM limit $Q_L = Q_R = Q$, one can relate the constant C with the EM pion mass difference as $M_{\pi^+}^2 - M_\pi^2 = 2Ce^2/F^2$ at tree level.

Finally, we remark that the equations of motion to $\mathcal{O}(p^2)$ are:

$$\begin{aligned} (d_\mu d^\mu U^\dagger)U - U^\dagger d_\mu d^\mu U &= \chi^\dagger U - U^\dagger \chi + \frac{1}{N_f} \text{tr} [U^\dagger \chi - \chi^\dagger U] \\ &\quad - \frac{4C}{F^2} (U^\dagger Q_R U Q_L - Q_L U^\dagger Q_R U) \end{aligned} \quad (6.11)$$

6.1.2 Next to leading order: the $\mathcal{O}(p^4)$ Lagrangian

Before discussing the $\mathcal{O}(p^4)$ we should check first if there are $\mathcal{O}(p^3)$ terms. The list of all possible terms of that order allowed by the symmetries is

- χQ -like terms:

$$\begin{aligned} &\text{tr} [Q_L (U^\dagger \chi + \chi^\dagger U) + Q_R (U \chi^\dagger + \chi U^\dagger)] \\ &\quad \text{tr} [\chi^\dagger U + \chi U^\dagger] \text{tr} [Q_L + Q_R] \end{aligned} \quad (6.12)$$

- QQQ terms:

$$\begin{aligned} &\text{tr} [Q_R^2 U Q_L U^\dagger + Q_L^2 U^\dagger Q_R U] \\ &\quad \text{tr} [Q_R^3 + Q_L^3] \\ &\text{tr} [Q_L + Q_R] \text{tr} [Q_R U Q_L U^\dagger] \\ &\quad \text{tr} [Q_L + Q_R] \text{tr} [Q_R^2 + Q_L^2] \\ &\quad \text{tr} (Q_L - Q_R) \text{tr} (Q_L^2 - Q_R^2) \\ &\text{tr}^2 [Q_L] \text{tr} (Q_R) + \text{tr}^2 [Q_R] \text{tr} (Q_L) \\ &\quad \text{tr}^3 [Q_L] + \text{tr}^3 [Q_R] \end{aligned} \quad (6.13)$$

- Qdd terms:

$$\begin{aligned} &\text{tr} [Q_L + Q_R] \text{tr} [d_\mu U^\dagger d^\mu U] \\ &\text{tr} [Q_L d_\mu U^\dagger d^\mu U + Q_R d_\mu U d^\mu U^\dagger] \\ &\text{tr} [Q_L + Q_R] \text{tr} (U^\dagger d_\mu U) \text{tr} (U^\dagger d^\mu U) \end{aligned} \quad (6.14)$$

Terms of the form $\text{tr} [(c_{\mu L} Q_L) U^\dagger d^\mu U]$, $\text{tr} [(c_{\mu R}) Q_R U d^\mu U^\dagger]$ are not possible since there is no combination of them which can be made P and C invariant (using $U d_\mu U^\dagger = -d_\mu U U^\dagger$) and so on for terms $\text{tr} [c_{\mu L, R} Q_{L, R}] \text{tr} [U^\dagger d^\mu U]$.

Another important comment regards the Wess-Zumino-Witten (WZW) anomalous part of the Lagrangian, which is also $\mathcal{O}(p^4)$. In $SU(2)$, the WZW Lagrangian is independent of the singlet axial field [201]. However, in the presence of nonzero vector

fields, such as the magnetic field needed to study the Chiral Magnetic Effect (CME), the WZW would play an essential role [202].

Let us then follow the same procedure as before, now to $\mathcal{O}(p^4)$. The Lagrangian to this order will consist of the usual $SU(2)$ terms in equation (1.77) with the covariant derivative d_μ in (6.1), plus new terms constructed out of the Q operators and the operator $\text{tr}(U^\dagger d_\mu U)$, as commented above. The LECs associated to those new terms will be labelled k'_i and the resulting Lagrangian is given in equation (6.15) below. Let us explain the origin of the different terms in that equation. For that purpose, it is convenient to classify the different operators contributing according to the number of Q fields.

Gdd terms like

$$\text{tr}[U^\dagger d_\mu U] \text{tr}[U^\dagger d^\nu U] [\text{tr}(G_{\mu\nu}^L) + \text{tr}(G_{\mu\nu}^R)], \quad \text{tr}[d_\mu U^\dagger d_\nu U] [\text{tr}(G_{\mu\nu}^L) + \text{tr}(G_{\mu\nu}^R)],$$

and so on, in principle could contribute after partial integration moving the derivative acting on the Q fields to the other fields and using the equations of motion (6.11).

Terms without Q fields include the usual chiral Lagrangian at this order (1.77) plus new terms which will contain $\text{tr}(U^\dagger d_\mu U)$. In Appendix F.2 we list all the possible terms of this type. Using the equations of motion, all possible terms with two or more derivatives acting on the same field can be rewritten in terms of those with single derivatives. The latter holds also for terms with derivatives acting on the χ fields, which after partial integration and the use of the EOMs can be reduced to those in (F.23). In addition, as discussed in Appendix F, $SU(2)$ operator identities allow to reduce the number of independent terms.

After these considerations, the Lagrangian without explicit Q fields is the usual one plus the new contributions given by the k'_{1-5} terms in (6.15). In the l_4 term as is customary [192, 203] we can transform the l_4 contribution from [41] by using partial integration, the EOMs (6.11) and the identity (F.5), which give rise to the terms containing l_4 plus terms to be absorbed in the k'_4 , k'_5 and k'_{16} operators in (6.15).

As for terms with two Q fields, the possible contributions are of the form $ddQQ$ and χQQ . Once again, trace identities can be used to eliminate some of the operators. In particular, we have used eqns. (F.6)-(F.11) and (F.21). The different operators of this kind contributing to the Lagrangian are those multiplied by the LEC k'_{6-25} in (6.15). We have followed [41] as a guide and for notation, although, as explained, new terms appear with respect to that work which vanish for $Q_L = Q_R$.

Apart from the above, one could in principle have the $(cQ)Qd$ and $(cQ)(cQ)$ operators appearing in Appendix F.3 and F.4 and listed in equations (F.24) and (F.25) respectively.

Finally, we have to consider terms with four explicit Q fields. The relevant trace identities to be used are now (F.12)-(F.18) and the operators contributing are those multiplying the new LECs k'_{27-37} in (6.15).

According to our previous discussion the $SU(2)$ Lagrangian containing the new operators is finally:

$$\begin{aligned}
 \mathcal{L}'_4 = & k'_1 \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) \text{tr}(d^\nu U^\dagger d_\nu U) + k'_2 \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d_\nu U) \text{tr}(d^\mu U^\dagger d^\nu U) \\
 & + k'_3 \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) \text{tr}(U^\dagger d_\nu U) \text{tr}(U^\dagger d^\nu U) + k'_4 \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) \text{tr}(\chi^\dagger U + U^\dagger \chi) \\
 & + k'_5 \text{tr}(U^\dagger d_\mu U) \text{tr}[U^\dagger d_\mu U (\chi^\dagger U + U^\dagger \chi)] + k'_6 \Lambda^2 \text{tr}(d^\mu U^\dagger d_\mu U) [\text{tr}(Q_L^2) + \text{tr}(Q_R^2)] \\
 & + k'_7 \Lambda^2 \text{tr}(d^\mu U^\dagger d_\mu U) \text{tr}(Q_R U Q_L U^\dagger) \\
 & + k'_8 \Lambda^2 [\text{tr}(d^\mu U^\dagger Q_R U) \text{tr}(d_\mu U^\dagger Q_R U) + \text{tr}(d^\mu U Q_L U^\dagger) \text{tr}(d_\mu U Q_L U^\dagger)] \\
 & + k'_9 \Lambda^2 \text{tr}(d^\mu U^\dagger Q_R U) \text{tr}(d_\mu U Q_L U^\dagger) + k'_{10} \Lambda^2 \text{tr}(d^\mu U^\dagger d_\mu U) [\text{tr}^2(Q_L) + \text{tr}^2(Q_R)] \\
 & + k'_{11} \Lambda^2 \text{tr}(d^\mu U^\dagger d_\mu U) \text{tr}(Q_L) \text{tr}(Q_R) + k'_{12} \Lambda^2 \text{tr}(\chi^\dagger U + U^\dagger \chi) [\text{tr}(Q_L^2) + \text{tr}(Q_R^2)] \\
 & + k'_{13} \Lambda^2 \text{tr}(\chi^\dagger U + U^\dagger \chi) \text{tr}(Q_R U Q_L U^\dagger) \\
 & + k'_{14} \Lambda^2 \text{tr}[(\chi U^\dagger + U \chi^\dagger) Q_L + (\chi^\dagger U + U^\dagger \chi) Q_R] \text{tr}(Q_L + Q_R) \\
 & + k'_{15} \Lambda^2 \text{tr}[(\chi^\dagger U + U^\dagger \chi) Q_L - (\chi U^\dagger + U \chi^\dagger) Q_R] \text{tr}(Q_L - Q_R) \\
 & + k'_{16} \Lambda^2 \text{tr}[(\chi^\dagger U - U^\dagger \chi) Q_L U^\dagger Q_R U + (\chi U^\dagger - U \chi^\dagger) Q_R U Q_L U^\dagger] \\
 & + k'_{17} \Lambda^2 \text{tr}(\chi^\dagger U + U^\dagger \chi) [\text{tr}^2(Q_L) + \text{tr}^2(Q_R)] + k'_{18} \Lambda^2 \text{tr}(\chi^\dagger U + U^\dagger \chi) \text{tr}(Q_L) \text{tr}(Q_R) \\
 & + k'_{19} \Lambda^2 \text{tr}(U^\dagger d_\mu U) \text{tr}(U d^\mu U^\dagger Q_R^2 - U^\dagger d_\mu U Q_L^2) \\
 & + k'_{20} \Lambda^2 \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) \text{tr}(Q_L^2 + Q_R^2) + k'_{21} \Lambda^2 \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) \text{tr}(Q_R U Q_L U^\dagger) \\
 & + k'_{22} \Lambda^2 \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) [\text{tr}^2(Q_L) + \text{tr}^2(Q_R)] + k'_{23} \Lambda^2 \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) \text{tr}(Q_R) \text{tr}(Q_L) \\
 & + k'_{24} \Lambda^2 \text{tr}(U^\dagger d_\mu U) [\text{tr}(Q_R U d^\mu U^\dagger) \text{tr}(Q_R) - \text{tr}(Q_L U^\dagger d_\mu U) \text{tr}(Q_L)] \\
 & + k'_{25} \Lambda^2 \text{tr}(U^\dagger d_\mu U) [\text{tr}(Q_R U d^\mu U^\dagger) \text{tr}(Q_L) - \text{tr}(Q_L U^\dagger d_\mu U) \text{tr}(Q_R)] \\
 & + k'_{26} \Lambda^4 [\text{tr}^2(Q_L^2) + \text{tr}^2(Q_R^2)] + k'_{27} \Lambda^4 \text{tr}(Q_L^2) \text{tr}(Q_R^2) + k'_{28} \Lambda^4 \text{tr}(Q_L^2 + Q_R^2) \text{tr}(Q_L) \text{tr}(Q_R) \\
 & + k'_{29} \Lambda^4 \text{tr}(Q_L^2 + Q_R^2) (\text{tr}^2 Q_L + \text{tr}^2 Q_R) + k'_{30} \Lambda^4 \text{tr}(Q_R^2 - Q_L^2) (\text{tr}^2 Q_L - \text{tr}^2 Q_R) \\
 & + k'_{31} \Lambda^4 [\text{tr}^3(Q_L) + \text{tr}^3(Q_R)] \text{tr}(Q_L + Q_R) + k'_{32} \Lambda^4 [\text{tr}^3(Q_L) - \text{tr}^3(Q_R)] \text{tr}(Q_L - Q_R) \\
 & + k'_{33} \Lambda^4 [\text{tr}^2(Q_L) \text{tr}(Q_R) + \text{tr}^2(Q_R) \text{tr}(Q_L)] \text{tr}(Q_L + Q_R) \\
 & + k'_{34} \Lambda^4 \text{tr}(Q_R U Q_L U^\dagger) [\text{tr}^2(Q_L) + \text{tr}^2(Q_R)] + k'_{35} \Lambda^4 \text{tr}(Q_R U Q_L U^\dagger) \text{tr}(Q_R) \text{tr}(Q_L) \\
 & + k'_{36} \Lambda^4 \text{tr}(Q_R U Q_L U^\dagger) \text{tr}(Q_R^2 + Q_L^2) + k'_{37} \Lambda^4 \text{tr}^2(Q_R U Q_L U^\dagger)
 \end{aligned}$$

so that the full $\mathcal{O}(p^4)$ Lagrangian relevant for our analysis at this order reads $\mathcal{L}_4 = \mathcal{L}_{4,SU(2)}^0 + \mathcal{L}'_4$ with $\mathcal{L}_{4,SU(2)}^0$ in (1.77). The parameter Λ has been introduced in order to

get dimensionless k'_i constants. The choice of this parameter Λ is irrelevant, as it should, since it will be absorbed in the new independent LECs involved, which will have to be determined.

For the chemical potential cases which we are going to study in the next sections, the axial and isospin chemical potentials, the Gdd terms vanish for our choices of $G_{\mu I}$ after such partial integration. Also by partial integration, the $(cQ)Qd$ and $(cQ)(cQ)$ operators can be brought for the axial and isospin chemical potentials either to a vanishing contribution or to some of the $ddQQ$ and χQQ contributions. This is why no such terms have been included in the Lagrangian (6.15).

The k'_i constants above are dimensionless and can be compared with the EM LECs k_i by taking from the general expressions above $Q_L = Q_R = Q$ with $Q = e \text{diag}(2/3, -1/3)$ as considered in [41], which implies in particular $(\text{tr } Q)^2 = (1/5)\text{tr}(Q^2)$, $\text{tr}(Q)\text{tr}(Q^3) = (9/25)\text{tr}^2(Q^2)$, $\text{tr}(Q^4) = (17/25)\text{tr}^2(Q^2)$. Thus, we get:

$$\begin{aligned}
2k'_6 + \frac{1}{5}(2k'_{10} + k'_{11}) &= \frac{F^2}{\Lambda^2}k_1 & 2k'_{12} + \frac{1}{5}(2k'_{17} + k'_{18}) &= \frac{F^2}{\Lambda^2}k_5 \\
k'_7 &= \frac{F^2}{\Lambda^2}k_2 & k'_{13} &= \frac{F^2}{\Lambda^2}k_6 \\
k'_8 &= \frac{F^2}{\Lambda^2}k_3 & k'_{14} &= \frac{F^2}{\Lambda^2}\frac{k_7}{2} \\
k'_9 &= \frac{F^2}{\Lambda^2}k_4 & k'_{16} &= \frac{F^2}{\Lambda^2}k_8 \\
2k'_{25} + k'_{27} + \frac{2}{5}k'_{28} + \frac{4}{5}k'_{29} + \frac{4}{25}k'_{31} + \frac{4}{25}k'_{33} &= \frac{F^4}{\Lambda^4}k_{12} & \frac{2}{5}k'_{34} + \frac{1}{5}k'_{35} + 2k'_{36} &= \frac{F^4}{\Lambda^4}k_{13} \\
k'_{37} &= \frac{F^4}{\Lambda^4}k_{14} & &
\end{aligned} \tag{6.15}$$

Note that the combinations of k'_i constants that will appear in the different observables in a certain case will be different in general than those in (6.15). Therefore, we will not be able to determine all the LECs appearing in the Q -dependent terms in terms of previously known ones. As we will explain below, one can use recent lattice analysis to estimate some of those constants, which one would expect that remain within the same order of magnitude than the k_i ones, from the previous expression (6.15).

6.2 Chiral imbalance

The possibility of the existence of space-time regions where parity is violated locally in QCD has attracted a lot of attention over recent years, mostly motivated by appealing

theoretical proposals such as the Chiral Magnetic Effect [202, 204, 205]. Thus, local metastable P -breaking configurations can be created out of the QCD vacuum, still preserving global P conservation, giving rise to observable effects when coupled to the magnetic field created in heavy-ion collisions. This Local Parity Breaking phenomenon can be attributed to the difference between the number densities of right- and left-handed chiral fermions, the so-called chiral imbalance. The same effect can lead to interesting applications in condensed matter physics [205]. The presence of such local P -breaking configurations can influence other observables in heavy-ion collisions, such as the dilepton spectrum [206, 207].

As we mentioned in subsection 1.1.7, the non-abelian nature of the strong interaction gives rise to a complicated vacuum. As a result, the vacuum state can accommodate multiple topological sectors that are separated by high energy barriers. In the presence of a hot medium, sphaleron transitions can connect these configurations through quantum fluctuations of the vacuum state [208]. Actually, a topological charge may arise in the fireball as a result of a HIC. Such charge can be defined as the space integral of the Chern-Simons current, as follows

$$T_5 = \int_{vol} d^3\vec{x} J_0^{CS}(x), \quad (6.16)$$

$$J_0^{CS}(x) = \frac{g^2}{32\pi^2} \epsilon_{\nu\rho\sigma} \text{Tr} \left(G^\nu \partial^\rho G^\sigma - i \frac{2}{3} G^\nu G^\rho G^\sigma \right)$$

where the integration is over a given region within the fireball volume.

Thus, introducing into the QCD Lagrangian a chemical potential μ_{CS} in a gauge invariant way, i.e. adding $\Delta\mathcal{L} = \mu_{CS}\Delta T_5$, with

$$\Delta T_5 = T_5(t_f) - T_5(0) = \frac{g^2}{32\pi^2} \int_0^{t_f} dt \int_{vol} d^3\vec{x} G_{\mu\nu}^a \tilde{G}^{a\mu\nu} \quad (6.17)$$

it is possible to trigger the value of $\langle\Delta T_5\rangle$.

For u and d quarks, the characteristic time of left and right quark oscillations, which is of the order $1/m_q$ [209] is significantly larger than the typical duration of the fireball. This observation suggests that, during the lifetime of the fireball, the chiral charge Q_5 associated with the light u and d quarks may remain approximately constant in a typical heavy-ion collision, since the oscillation can be neglected.

We can associate a non-zero topological charge with a non-trivial quark axial charge

Q_5 integrating the PCAC relation over a finite space volume

$$\frac{d}{dt}(Q_5 - 2N_f T_5) = 2i \int_{vol} d^3\vec{x} \bar{q} \mathcal{M} \gamma_5 q \quad (6.18)$$

$$Q_5 = \int_{vol} d^3\vec{x} \bar{q} \gamma_0 \gamma_5 q \quad (6.19)$$

Thus, using the well-known Atiyah-Singer index theorem, which establishes a relationship between the topological charge of the gauge field and the right N_R and left N_L zero-eigenstates of the Dirac operator we get

$$2N_f T_5 = N_L - N_R \quad (6.20)$$

Therefore, for light u, d quarks for which both the $L - R$ oscillations and the mass terms in (6.19) are negligible [209], one can assign, as customary, a constant axial chemical potential μ_5 in order to parameterize a source of parity breaking or chiral imbalance, which couples in the QCD Lagrangian to the timelike component of the $U(1)_A$ abelian axial current, i.e.,

$$\mathcal{L}_{QCD} \rightarrow \mathcal{L}_{QCD} + \mu_5 \bar{q} \gamma_5 \gamma^0 q \quad (6.21)$$

where $\mu_5 = \mu_{CS}/(2N_f)$, which is equivalent to consider

$$a_\mu + \frac{1}{2} A_\mu (Q_R - Q_L) = \mu_5 \delta_{\mu 0} \mathbb{1} \quad (6.22)$$

in the QCD generating functional given in equation (1.27). Equivalently, one can perform a $U(1)_A$ rotation on the quark fields $q \rightarrow q' = \exp[i\beta(x)\gamma_5] q$ and choose $\beta(x) = \frac{\theta(x)}{2N_f}$, which allows to trade the axial and θ terms in the absence of additional vector or axial sources:

$$Z_{QCD}[0, 0, \mathcal{M}, 0, \theta(x)] = Z_{QCD} \left[0, \frac{1}{2N_f} \partial_\mu \theta(x) \mathbb{1}, \mathcal{M} \cos[\theta(x)/N_f], \mathcal{M} \sin[\theta(x)/N_f], 0 \right] \quad (6.23)$$

Thus, in the chiral limit $\mathcal{M} = 0$, the chemical potential term is equivalent to a non-constant θ source $\theta(t) = \mu_5 t + \theta_0$.

In this context, it is important to provide theoretical support for the behaviour of QCD and hadronic observables in the presence of chiral imbalanced matter, specially regarding the finite-temperature and finite-volume dependence around the QCD phase diagram, given its importance for heavy-ion collisions.

Different models have been considered recently to address this problem, including the Polyakov loop Linear Sigma Model [210], NJL-like models [211–218] and a generalized

sigma model including all the members of the scalar/pseudoscalar multiplets of isospin $I = 0, 1$ and the η' [219]. In those works, several relevant properties have been discussed, such as phase diagram features, the topological susceptibility, the chiral density, the quark condensate and the meson dispersion relation. However, the results are not fully in agreement between different models, as we discuss below, in particular regarding the behaviour of chiral symmetry restoration with increasing axial chemical potential.

On the other hand, there have been a few analyses trying to reproduce such parity-breaking effects in the lattice. Although the pion masses used so far are still large and the continuum extrapolation is not entirely understood, there are promising results which may help to disentangle between model predictions if more precision is achieved in the near future. Thus, in [220] the chiral charge density and the CME have been investigated, while the dependence of the chiral restoration temperature with μ_5 has been studied through the chiral condensate, scalar susceptibility and Polyakov loop for $N_c = 2$ [221] and $N_c = 3$ [222]. The chiral anomaly in the lattice has been also studied in [223] while in more recent lattice analysis, updated results for $N_f = 2$ are provided on the chiral charge density, as well as the topological susceptibility and charge [224].

One of the puzzles which is still not fully understood is that the lattice results clearly show growing condensate and T_c with μ_5 [221, 222] while theoretical analyses yield contradictory results. Thus, within the NJL framework, some works [210–212] found the opposite behaviour, i.e. a decreasing $T_c(\mu_5)$ while others [215, 216] agree with the lattice results. This contradiction seems to be related to the choice of the regularization scheme [214, 225]. In addition, the sigma model approach in [210] is also in disagreement with the lattice, while an analysis based on Schwinger-Dyson equations gives rise also to an increasing $T_c(\mu_5)$ behaviour [226]. The general arguments given in [227] as well as the growing of the constituent mass with μ_5 found in [213] support also a growing quark condensate.

In subsection 6.2.1 we provide the most general low-energy effective Lagrangian including an axial chemical potential μ_5 up to $\mathcal{O}(p^4)$. Although this requires by definition that the applicability range is restricted to low μ_5 and low temperatures, which poses certain limits e.g. on chiral restoration, our analysis will serve as a guideline for models and lattice analyses, which should satisfy the behaviour found here in such low μ_5 regime. In particular, we will derive the main phenomenological consequences in terms of observables such as the energy density, the meson dispersion relation, the quark condensate and the topological susceptibilities. The theoretical tools developed above

can be extended to include heavier degrees of freedom, although, as explained above, the main ideas behind considering the μ_5 term are better supported for two light flavours. That is why we will concentrate on the $SU(2)$ effective Lagrangian.

The analysis of the main phenomenological consequences is carried out in subsection 6.2.2, where we will analyze the pion dispersion relation, the vacuum energy density, chiral symmetry restoration observables, the chiral charge density, the topological susceptibility, the pressure, the speed of sound and the pion scattering. We will compare our results with previous works in the literature and we will try to extract as much phenomenological information as possible from lattice simulations, as well as providing some numerical determinations for the new LECs.

6.2.1 The chiral Lagrangian

In our present case, from (6.22) we can choose, without loss of generality,

$$v_\mu = a_\mu = 0, Q_L = -Q_R = \frac{\mu_5}{\Lambda} \mathbb{1}, \quad A_\mu = \Lambda \delta_{\mu 0}. \quad (6.24)$$

consistently with our power counting as long as $\mu_5 \ll \Lambda$. In [228] we normalized with F for an easier comparison with previous works dealing with the EM case [41, 198]. Note also that we place the μ_5 term in the Q part, to be consistent with the convention of power counting for the Q fields followed in those works.

At $\mathcal{O}(p)$, the only nontrivial operator allowed by the symmetries (6.7) vanishes exactly for the particular choice given by (6.24).

The most general $\mathcal{O}(p^2)$ Lagrangian at nonzero μ_5 is given by

$$\mathcal{L}_2 = \frac{F^2}{4} \text{tr} [\partial_\mu U^\dagger \partial^\mu U + 2B_0 \mathcal{M} (U + U^\dagger)] + 2\mu_5^2 F^2 (1 + \kappa_0) \quad (6.25)$$

where the κ_0 constant accounts for the operators in (6.10). Therefore, at this order, the only modification to the chiral Lagrangian is a constant term, which will contribute to the vacuum energy density and to the chiral charge density, as we discuss below.

Regarding renormalization, it is important to point out that κ_0 should be finite, since there are no loop divergences to cancel out at this order. We will get back to the renormalization of the new LECs in the following.

It is not difficult to see that there are no surviving Gdd terms. Those terms vanish for our choice of $G_{\mu I}$ after such partial integration. Terms of the form $\text{tr} (G_{\mu\nu}^{R,L} G^{\mu\nu R,L})$ and $\text{tr} (G_{\mu\nu}^R U G^{L\mu\nu} U^\dagger)$ do not contribute either for our present case. Thus, the l_5, l_6, h_2 terms in (1.77) vanish because they contain $G_{\mu\nu}^{L,R}$. Apart from that, by partial integration, the

$(cQ)Qd$ and $(cQ)(cQ)$ operators can be brought in our present case either to a vanishing contribution or to some of the $ddQQ$ and χQQ contributions already considered.

Next, let us replace the choice (6.24) in the above Lagrangian (6.15) in order to get the form of the explicit μ_5 -corrections. We obtain

$$\mathcal{L}_4(\mu_5) = \mathcal{L}_4^0(\mu_5 = 0) + \kappa_1 \mu_5^2 \text{tr}(\partial^\mu U^\dagger \partial_\mu U) + \kappa_2 \mu_5^2 \text{tr}(\partial_0 U^\dagger \partial_0 U) + \kappa_3 \mu_5^2 \text{tr}(\chi^\dagger U + U^\dagger \chi) + \kappa_4 \mu_5^4 \quad (6.26)$$

with

$$\kappa_1 = 4l_1 - 16k'_1 + 4k'_6 - 2k'_7 + 8k'_{10} - 4k'_{11} \quad (6.27)$$

$$\kappa_2 = 4l_2 - 16k'_2 \quad (6.28)$$

$$\kappa_3 = l_4 - 16k'_4 - 8k'_5 + 4k'_{12} - 2k'_{13} + 8k'_{15} + 8k'_{17} - 4k'_{18} \quad (6.29)$$

$$\begin{aligned} \kappa_4 = & -128k'_1 - 128k'_2 + 256k'_3 + 32k'_6 - 16k'_7 - 32k'_8 - 16k'_9 + 64k'_{10} - 32k'_{11} + 32k'_{19} - 64k'_{20} \\ & + 32k'_{21} + 32k'_{22} - 128k'_{23} + 64k'_{24} - 64k'_{25} + 8k'_{26} + 4k'_{27} - 16k'_{28} + 32k'_{29} + 64k'_{32} - 16k'_{34} \\ & + 8k'_{35} - 8k'_{36} + 4k'_{37} \end{aligned} \quad (6.30)$$

A word about renormalization is also in order here: the k'_i or the κ_i LECs have to be renormalized in order to absorb the divergences coming from loops, in the same way as the l_i and the k_i [34, 41], namely:

$$\kappa_i = \kappa_i^r(\mu) + \beta_i R \quad (6.31)$$

in dimensional regularization, where the superscript “ r ” denotes the finite part and R defined in (1.79).

The values of the β_i coefficients will be determined through the analysis of the various observables in the subsection below and will imply then conditions on the renormalization of the k'_i showing up in the combinations (6.27)-(6.30). In the case of κ_0 in (6.25), since it shows up at $\mathcal{O}(p^2)$, there is no counterterm associated to that constant, so that $\beta_0 = 0$.

6.2.2 Physical consequences

Pion dispersion relation

Let us start by analyzing the corrections to the kinetic part of the Lagrangian coming from the $\mathcal{O}(p^4)$ μ_5 -dependent corrections in (6.26). The $\mathcal{O}(\pi^2)$ part of $\mathcal{L}_4$ in (6.26) is given by:

$$\begin{aligned} \mathcal{L}_4^{\pi^2} = & \frac{2l_4 M_{0\pi}^2 + 4(\kappa_1 + \kappa_2)\mu_5^2}{F^2} \frac{1}{2} \partial_0 \pi^a \partial^0 \pi^a - \frac{2l_4 M_{0\pi}^2 + 4\kappa_1 \mu_5^2}{F^2} \frac{1}{2} \partial_j \pi^a \partial_j \pi^a \\ & - \frac{2(l_3 + l_4) M_{0\pi}^2 + 4\kappa_3 \mu_5^2}{F^2} \frac{1}{2} M_{0\pi}^2 \pi^a \pi_a \end{aligned} \quad (6.32)$$

The different coefficient for the $\text{tr}(\partial_0 U \partial_0 U^\dagger)$ and $\text{tr}(\partial_i U \partial_i U^\dagger)$ terms translate into different values for the spatial and time components of the pion decay constant, as would be generally expected in a Lorentz covariance breaking scenario [229]. In our present case we have, up to NLO in ChPT,

$$(F_\pi^t)^2(\mu_5) = F_\pi^2(0) + 4(\kappa_1 + \kappa_2)\mu_5^2 \quad (6.33)$$

$$(F_\pi^s)^2(\mu_5) = F_\pi^2(0) + 4\kappa_1 \mu_5^2, \quad (6.34)$$

F_π^t and F_π^s being respectively the generalization of F_π for the timelike and spacelike components of the axial current through the PCAC theorem [229]. At tree level, they arise directly from the coefficients of the $\text{tr}(\partial_0 U \partial_0 U^\dagger)$ and $\text{tr}(\partial_i U \partial_i U^\dagger)$ terms in the Lagrangian. In the above equation we are including in $F_\pi^2(0)$ the one-loop and l_i standard ChPT corrections at $\mu_5 = 0$. Here, it is important to remark that $F_\pi^t/F_\pi^s \neq 1$ implies a reduction of the velocity of propagation of pions [229] as we are about to see.

When taking into account the above corrections to the derivative terms together with the κ_3 correction to the mass term in (6.26), one ends up with the following dispersion relation to this order:

$$p_0^2 - (1 + \delta_s - \delta_t) |\vec{p}|^2 - (1 + \delta_M - \delta_t) M_{0\pi}^2 = 0 \quad (6.35)$$

where

$$\delta_t = 2l_4 \frac{M_{0\pi}^2}{F^2} + A\Delta + 4(\kappa_1 + \kappa_2) \frac{\mu_5^2}{F^2} \quad (6.36)$$

$$\delta_s = 2l_4 \frac{M_{0\pi}^2}{F^2} + A\Delta + 4\kappa_1 \frac{\mu_5^2}{F^2} \quad (6.37)$$

$$\delta_M = 2(l_3 + l_4) \frac{M_{0\pi}^2}{F^2} - B\Delta + 4\kappa_3 \frac{\mu_5^2}{F^2} \quad (6.38)$$

Here, A, B are the coefficients of the loop contributions renormalizing the p^2 and $M_{0\pi}^2$ terms of the dispersion relation at $\mu_5 = 0$, where $\Delta = G(M_\pi, T)/F^2$ is the tadpole contribution. The divergent part of Δ is absorbed in DR in the standard renormalization of the l_i [34].

The two main physical consequences of the above dispersion relation are, on the one hand, a modification of the relativistic pion velocity for massless pions, which at this order is purely a μ_5 effect, namely,

$$v_\pi(\mu_5) = \left. \frac{|\vec{p}|}{p_0} \right|_{M_{0\pi}=0} = 1 - \frac{1}{2}(\delta_s - \delta_t) = 1 + 2\kappa_2 \frac{\mu_5^2}{F^2} \quad (6.39)$$

On the other hand, the loss of Lorentz covariance implies also a different result for the pion mass, depending on whether we take $|\vec{p}| = 0$ (static/pole mass) or $p_0 = 0$ (screening mass):

$$[M_\pi^2]^{pole}(\mu_5) = M_{0\pi}^2(1 + \delta_M - \delta_t) = M_\pi^2(0) - 4(\kappa_1 + \kappa_2 - \kappa_3) \frac{\mu_5^2}{F^2} M_{0\pi}^2 \quad (6.40)$$

$$[M_\pi^2]^{scr}(\mu_5) = M_{0\pi}^2(1 + \delta_M - \delta_s) = M_\pi^2(0) - 4(\kappa_1 - \kappa_3) \frac{\mu_5^2}{F^2} M_{0\pi}^2 \quad (6.41)$$

where $M_\pi^2(0)$ is the $\mu_5 = 0$ mass at this order including one-loop and l_i terms.

Regarding renormalization, the finiteness of the observables (6.33), (6.34), (6.39), (6.40), (6.41) require

$$\beta_1 = \beta_2 = \beta_3 = 0 \quad (6.42)$$

The above renormalization conditions highlight the importance of including properly the new terms in the Lagrangian (6.15). For instance, the presence of the k_2' term is crucial to guarantee $\beta_2 = 0$ once the relation with l_2 in (6.28) is taken into account, since that condition would not be fulfilled by l_2 only, whose renormalization is given in equation (1.78).

As for the numerical values of the LECs $\kappa_1, \kappa_2, \kappa_3$ involved, there is no information available from the lattice regarding the pion dispersion relation at $\mu_5 \neq 0$. Measuring screening masses for light mesons is, in principle, feasible in the lattice, so it would be useful to have such measurements for $\mu_5 \neq 0$ available in the near future. However, we can have some insight from physical requirements. Hence, requiring that the pion velocity in (6.39) remains smaller than the speed of light for any μ_5 yields

$$\kappa_2 < 0. \quad (6.43)$$

The additional requirement that the two squared pion masses in (6.40) and (6.41) remain positive would lead to $\kappa_1 - \kappa_3 < 0$. However, that may be a too restrictive condition, since a decreasing pion mass for low and moderate values of μ_5 does not

necessarily imply a tachyonic mode, given that higher order corrections may change this behaviour. In any case, a tachyonic mode is not necessarily related to an unphysical spectrum [219] and it could indicate for instance phases of pion condensation [194, 195]. We will actually come back to the issue of the sign of that particular LEC combination below, in connection with chiral restoration and the chiral charge density.

Just to obtain a rough estimate of the above results, we plot in Fig. 6.1 the dependence of v_π and M_π^2 with μ_5 expected within the numerical range of LECs around their so-called natural values $1/(16\pi^2)$ which is their expected size from loop corrections [41, 198]. For the numerical values of the standard low-energy parameters, we will take the recent results quoted in [191] and references therein. Thus, we take $F_\pi(0) = 92.2$ MeV, its physical value, $F = 85.93$ MeV, $M_\pi(0) = 140$ MeV, $M_{0\pi} = 130.96$ MeV. For the results showed in this figure, we have replaced for simplicity $F^2 \rightarrow F_\pi^2(0)$ in the right hand side of (6.33) and (6.34), and $M_{0\pi}^2 \rightarrow M_\pi^2(0)$ in (6.40) and (6.41), which is perturbatively equivalent to this order. Thus, as long as we remain within natural values for the corresponding LECs involved, the estimated band for $[M_\pi^2]^{pole,scr}(\mu_5)/M_\pi^2(0)$ and $[F_\pi^2]^{t,s}(\mu_5)/F_\pi^2(0)$ look the same.

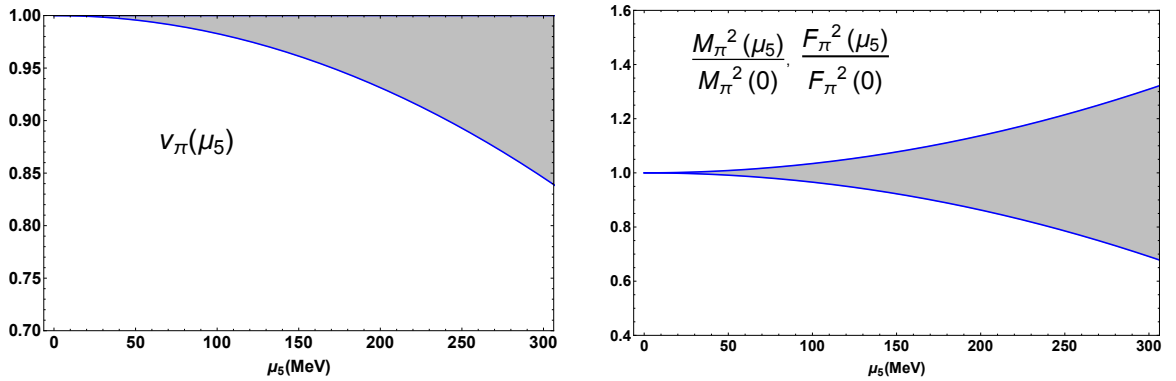


Figure 6.1: μ_5 dependence of pion velocity, pion mass and pion decay constant, to leading order in ChPT. The grey bands correspond to the uncertainties of the LEC within natural values, namely $0 \leq \kappa_2 \leq \frac{1}{16\pi^2}$ in (6.39), and $|\kappa_1 + \kappa_2| \leq \frac{1}{16\pi^2}$, $|\kappa_1| \leq \frac{1}{16\pi^2}$, $|\kappa_1 + \kappa_2 - \kappa_3| \leq \frac{1}{16\pi^2}$, $|\kappa_1 - \kappa_3| \leq \frac{1}{16\pi^2}$, in (6.33), (6.34), (6.40) and (6.41) respectively.

It is worth mentioning also the comparison of our results with previous model analysis. The results in [219] within a generalized sigma model, show a decreasing behaviour of the pion mass with μ_5 after diagonalizing a $\pi - a_0$ μ_5 -dependent interaction. Actually, tachyonic modes appear in that work for high enough μ_5 and pion momentum. The results of that paper are compatible with ours for the μ_5 range showed in Fig.6.1. In addition, the increase in F_π^2 found in [219] would correspond to positive κ_1 according to

our present analysis and is also numerically compatible with our results in Fig.6.1. Our analysis for other observables below will show that the lattice results support $\kappa_1 > 0$, $\kappa_1 + \kappa_2 > 0$, $\kappa_1 - \kappa_3 > 0$, hence compatible with the results in [219], although the sign of $\kappa_1 + \kappa_2 - \kappa_3$ is not determined.

The vacuum energy density

Let us analyze the vacuum energy density defined in equation (1.95) with $Z(T, \mu_5) = Z(0, a_0 = \mu_5 \mathbf{1}, \mathcal{M}, 0, 0)$ the Euclidean QCD partition function. Relevant global observables can be derived from ϵ , such as the light quark condensate and the scalar susceptibility signaling chiral symmetry restoration, as well as the chiral charge density corresponding to the chiral charge (6.19). The μ_5 corrections come from the Lagrangian up to $\mathcal{O}(p^4)$ given in subsection 6.1.1 and 6.1.2 within ChPT. As customary, let us write $\epsilon = \epsilon_2 + \epsilon_4 + \dots$ where ϵ_k denotes the $\mathcal{O}(p^k)$ contribution.

At $\mathcal{O}(p^2)$, it only contributes the constant (field-independent) part of the $\mathcal{L}_2$ Lagrangian in (6.25). This is symbolized by the first contribution in Fig. 6.2 labelled “2” (we follow a similar notation as [49]) which yields the following contribution independent of temperature and volume:

$$\epsilon_2(\mu_5) = -F^2 M_{0\pi}^2 - 2\mu_5^2 F^2 (1 + \kappa_0) \quad (6.44)$$

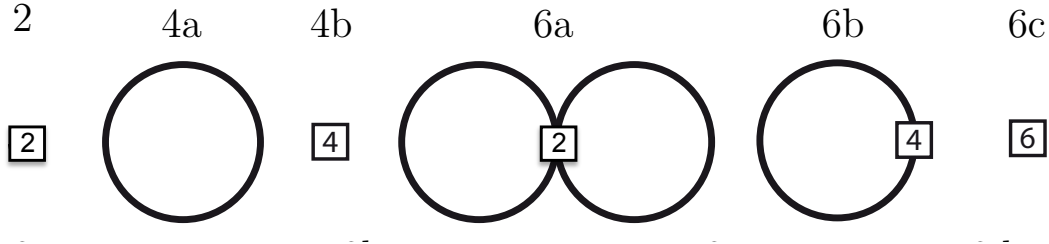


Figure 6.2: Diagrams contributing to the energy density up to $\mathcal{O}(p^6)$

The $\mathcal{O}(p^4)$ includes, on the one hand, the contribution from the kinetic $\mathcal{O}(\pi^2)$ part in (6.25), which is nothing but the energy density of a free pion gas given by equation (1.119). This is the closed loop diagram labelled “4a” in Fig.6.2, which is μ_5 -independent. On the other hand, the diagram “4b” refers to the field-independent terms from $\mathcal{L}_4$ in (1.77) and (6.26). Up to an irrelevant constant, we have in the isospin limit

$$\epsilon_{4a}(T) = 3\frac{T}{V} \sum_{k_i} \log [1 - e^{-\omega_k/T}] + M_{0\pi}^4 \epsilon_{4div} \xrightarrow{V \rightarrow \infty} -\frac{3}{2} g_0(M_{0\pi}, T) + M_{0\pi}^4 \epsilon_{4div}, \quad (6.45)$$

$$\epsilon_{4b}(\mu_5) = -(l_3 + h_1) M_{0\pi}^4 - 4\kappa_3 \mu_5^2 M_{0\pi}^2 - \kappa_4 \mu_5^4, \quad (6.46)$$

where we have displayed explicitly the volume and temperature dependence of ϵ_{4a} as well as its temperature dependence in the infinite volume limit, with $\omega_k^2 = k^2 + M_{0\pi}^2$, $k^2 = (2\pi/L) \sum_{i=1}^3 k_i^2$ ($k_i \in \mathbb{Z}$). The contribution ϵ_{4div} in (6.45) contains a divergent part proportional to R in (1.79). In particular, using (G.2) in Appendix G,

$$\epsilon_{4div} \xrightarrow{V \rightarrow \infty} \frac{3}{2} \left[R + \frac{1}{32\pi^2} \log \frac{M_{0\pi}^2}{\mu^2} - \frac{1}{64\pi^2} \right] \quad (6.47)$$

which is T -independent and whose divergent part is also V independent. The divergent R contribution in ϵ_{4div} cancels with that of the LEC combination in (6.46) with the renormalization of those LECs provided in (1.78).

Up to $\mathcal{O}(p^4)$, the only temperature (and volume) dependence of the energy density is contained in the $\mu_5 = 0$ part, namely in the free pion gas contribution (6.45). For some of our subsequent analysis it will be interesting to analyze the nontrivial T and V dependence arising at the $\mathcal{O}(p^6)$, although the price will be to introduce more unknown LECs.

The diagrams contributing to ϵ_6 are also depicted in Fig.6.2. The “6a” contribution stands for the two-loop closed diagram with four-pion vertices coming from $\mathcal{L}_2$, which is therefore μ_5 independent and has been calculated in [49]:

$$\epsilon_{6a}(T) = \frac{3M_{0\pi}^2}{8F^2} [G(M_{0\pi}, T)]^2 \quad (6.48)$$

with G the euclidean free pion propagator given in equation(1.128) where the divergent part is contained in the $T = 0$ contribution, which for $V \rightarrow \infty$ it is given in (G.1).

The contribution from diagram “6b” stands for the $\mathcal{O}(\pi^2)$ part of the $\mathcal{L}_4$ Lagrangian given in (6.32) and is the one containing the combined μ_5 and T dependence. Following similar steps as above, the sum of diagrams 4a and 6b is written in terms of

$$\frac{3}{2} \frac{T}{V} \sum_n \sum_{k_i} \log [a\omega_n^2 + bk^2 + cM_{0\pi}^2] \quad (6.49)$$

with ω_n the Matsubara frequencies and

$$\begin{aligned}
 a &= 1 + \frac{2l_4 M_{0\pi}^2 + 4(\kappa_1 + \kappa_2)\mu_5^2}{F^2}, \\
 b &= 1 + \frac{2l_4 M_{0\pi}^2 + 4\kappa_1 \mu_5^2}{F^2}, \\
 c &= 1 + \frac{2(l_3 + l_4)M_{0\pi}^2 + 4\kappa_3 \mu_5^2}{F^2}
 \end{aligned} \tag{6.50}$$

Up to order $\mathcal{O}(p^6)$ in the energy density, we can expand the expression in (6.49) up to first order in $a - 1$, $b - 1$, $c - 1$, or, equivalently up to first order in $1/F^2$. Thus, performing the Matsubara sums $\sum_n$, we get

$$\begin{aligned}
 \epsilon_{6b}(T, \mu_5) &= \frac{3}{2} \frac{T}{V} \sum_n \sum_{k_i} \frac{(a-1)\omega_n^2 + (b-1)k^2 + (c-1)M_{0\pi}^2}{\omega_n^2 + \omega_k^2} \\
 &= \epsilon_{6bdiv}^{(0)} + \epsilon_{6bdiv}^{(2)} \mu_5^2 + \frac{3}{2} \frac{1}{V} \sum_{k_i} \frac{1}{\omega_k} \frac{1}{e^{\omega_k/T} - 1} [(b-a)k^2 + (c-a)M_{0\pi}^2] \\
 &\xrightarrow{V \rightarrow \infty} \epsilon_{6bdiv}^{(0)} + \epsilon_{6bdiv}^{(2)} \mu_5^2 + \frac{9}{4} (b-a) g_0(M_{0\pi}, T) + \frac{3}{2} (c-a) M_{0\pi}^2 g_1(M_{0\pi}, T) \\
 &= \epsilon_{6bdiv}^{(0)} + \epsilon_{6bdiv}^{(2)} \mu_5^2 - 9\kappa_2 \frac{\mu_5^2}{F^2} g_0(M_{0\pi}, T) \\
 &+ \frac{3[l_3 M_{0\pi}^2 + 2(\kappa_3 - \kappa_1 - \kappa_2)\mu_5^2]}{F^2} M_{0\pi}^2 g_1(M_{0\pi}, T)
 \end{aligned} \tag{6.51}$$

where $\epsilon_{6bdiv}^{(0)}$ and $\epsilon_{6bdiv}^{(2)}$ are μ_5 and T independent divergent contributions in DR. In the $V \rightarrow \infty$ limit they can be obtained from the integral (G.3) in Appendix G. We get

$$\epsilon_{6bdiv}^{(0)} \xrightarrow{V \rightarrow \infty} 6 \frac{M_{0\pi}^6}{F^2} l_3 \left[R + \frac{1}{32\pi^2} \log \frac{M_{0\pi}^2}{\mu^2} \right] \tag{6.52}$$

$$\epsilon_{6bdiv}^{(2)} \xrightarrow{V \rightarrow \infty} -3 \frac{M_{0\pi}^4}{F^2} \mu_5^2 \left[(4(\kappa_1 - \kappa_3) + \kappa_2) \left(R + \frac{1}{32\pi^2} \log \frac{M_{0\pi}^2}{\mu^2} \right) - \frac{\kappa_2}{64\pi^2} \right] \tag{6.53}$$

Finally, the “6c” contribution collects the field-independent contributions coming from $\mathcal{L}_6$, which involves three new LEC for the μ_5 -dependent part, namely

$$\epsilon_{6c}(\mu_5) = c \frac{M_{0\pi}^6}{F^2} + \gamma_0 \frac{\mu_5^6}{F^2} + \gamma_1 \frac{\mu_5^4 M_{0\pi}^2}{F^2} + \gamma_2 \frac{\mu_5^2 M_{0\pi}^4}{F^2} \tag{6.54}$$

Note that the divergent part coming from the crossed $G(M_{0\pi}, 0)g_1$ term in ϵ_{6a} in equation(6.48) cancels with the l_3 contribution in (6.51), while the $G(M_{0\pi}, T=0)^2$ term in (6.48) and the $\epsilon_{6bdiv}^{(0)}$ term in (6.51) cancel with the c contribution in (6.54) with the renormalization $c = c^r(\mu) - 6l_3^r(\mu)R + (3/2)R^2$.

As for the μ_5 -dependent contributions, the $\epsilon_{6div}^{(2)}\mu_5^2$ contribution in (6.51) is absorbed in the renormalization of γ_2 in (6.54) with

$$\gamma_2 = \gamma_2^r(\mu) + 3[4(\kappa_1 - \kappa_3) + \kappa_2]R. \quad (6.55)$$

The energy density up to the order calculated here is therefore finite and scale-independent with the renormalization of the LECs that we have just explained, which is a welcomed consistency check. One immediate conclusion is that the LECs γ_0 , γ_1 in (6.54) are not renormalized. Also, since the energy density has to remain finite for any M , the κ_4 contribution in (6.46) does not get renormalized either, so that

$$\beta_4 = 0 \quad (6.56)$$

In addition, we have checked that the $\mu_5 = 0$ part of the energy density as given here agrees with [49] up to $\mathcal{O}(p^6)$.

In the following we will consider different observables that can be obtained from the energy density, and comment on their determination in lattice analysis, which will allow us to gain some information about the κ_i LECs involved.

Chiral symmetry restoration: the quark condensate and the scalar susceptibility

Our main purpose in this section will be to study the evolution of chiral restoration for nonzero μ_5 , and hence of the quark condensate and the scalar susceptibility and for such purpose the ChPT treatment will be enough to reach the main conclusions, in particular regarding the role of the κ_i LECs and the comparison with lattice analyses.

From the results in the previous section, we see that the first μ_5 correction to the quark condensate is temperature independent and changes the $T = 0$ value of $\langle \bar{q}q \rangle_l$ with the term coming from the κ_3 contribution in (6.46), so that the leading and next-to-leading orders for the ChPT quark condensate are given by,

$$\langle \bar{q}q \rangle_l^{LO} = -2B_0F^2 \quad (6.57)$$

$$\begin{aligned} \langle \bar{q}q \rangle_l^{NLO}(T, \mu_5) &= -4B_0M_{0\pi}^2 \left[l_3^r(\mu) + h_1^r(\mu) - \frac{3}{64\pi^2} \log \frac{M_{0\pi}^2}{\mu^2} \right. \\ &\quad \left. + 2\kappa_3 \frac{\mu_5^2}{M_{0\pi}^2} - \frac{3}{4M_{0\pi}^2} g_1(M_{0\pi}, T) \right] \end{aligned} \quad (6.58)$$

That is, up to this order, the sign of κ_3 determines whether the quark condensate $|\langle \bar{q}q \rangle_l|$ increases ($\kappa_3 > 0$) or decreases ($\kappa_3 < 0$) with μ_5 and so on for the transition temperature T_c estimated from the vanishing of the condensate at this order. As commented above, lattice analyses at finite temperature favor an increasing behaviour. As for the scalar susceptibility, since the μ_5 corrections to the condensate in (6.58) are mass independent, χ_S is independent of μ_5 at this order. The latter is consistent with the smooth μ_5 dependence observed in the lattice [221].

The modification to the $T = 0$ condensate value at nonzero μ_5 provided by (6.112) allows us to make a rough estimate of a typical μ_5 validity range for the present analysis. Actually, such modification is of the same order as those considered for the pion masses, so we expect typically that corrections remain below 20% for up to $\mu_5 \simeq 300 - 400$ MeV.

Nevertheless, in order to improve the precision in the T and μ_5 range, we consider the next to next leading order in the energy density, by including the ϵ_6 contributions. The full result for the quark condensate up to that order is given by:

$$\begin{aligned} \langle \bar{q}q \rangle_l^{NNLO}(T, \mu_5) &= \langle \bar{q}q \rangle_l^{NNLO}(T, \mu_5 = 0) + \frac{B_0}{F^2} \mu_5^2 \left\{ \frac{M_{0\pi}^2}{4\pi^2} [3(\kappa_3 - \kappa_1) + 16\pi^2 \gamma_2^r(\mu)] \right. \\ &\quad - \frac{3M_{0\pi}^2}{8\pi^2} [4(\kappa_1 - \kappa_3) + \kappa_2] \log \frac{M_{0\pi}^2}{\mu^2} - 6 [2(\kappa_1 - \kappa_3) - \kappa_2] g_1(M_{0\pi}, T) \\ &\quad \left. + 12M_{0\pi}^2 (\kappa_1 - \kappa_3 + \kappa_2) g_2(M_{0\pi}, T) + 2\gamma_1 \mu_5^2 \right\} \end{aligned} \quad (6.59)$$

with

$$\begin{aligned} \langle \bar{q}q \rangle_l^{NNLO}(T, \mu_5 = 0) &= \frac{3B_0 M_{0\pi}^4}{1024\pi^4 F^2} \left\{ 128\pi^2 [16\pi^2 c^r(\mu) + l_3^r(\mu)] \right. \\ &\quad + (384\pi^2 l_3^r(\mu) + 2) \log \frac{M_{0\pi}^2}{\mu^2} + 3 \log^2 \frac{M_{0\pi}^2}{\mu^2} \Big\} \\ &\quad + \frac{B_0}{F^2} \left\{ \frac{3}{4} [g_1(M_{0\pi}, T)]^2 - \frac{3}{2} M_{0\pi}^2 g_1(M_{0\pi}, T) g_2(M_{0\pi}, T) \right. \\ &\quad + \frac{3M_{0\pi}^2}{32\pi^2} \left[1 + 128l_3^r(\mu)\pi^2 + 2 \log \frac{M_{0\pi}^2}{\mu^2} \right] g_1(M_{0\pi}, T) \\ &\quad \left. - \frac{3M_{0\pi}^4}{32\pi^2} \left[64l_3^r(\mu)\pi^2 + \log \frac{M_{0\pi}^2}{\mu^2} \right] g_2(M_{0\pi}, T) \right\} \end{aligned} \quad (6.60)$$

We have checked that the previous expression for $\mu_5 = 0$ coincides with that given in [90, 188], where the renormalization convention for the LEC is slightly different.

We see that the leading T and μ_5 dependent corrections to the condensate show up in the g_1 and g_2 terms in the r.h.s. of (6.59), multiplied by different combinations of

the $\kappa_{1,2,3}$ constants, whose sign will determine the condensate evolution with μ_5 . Recall that the $\mu_5 = 0$ condensate is negative, $g_{1,2}$ are positive increasing functions of T and $\kappa_2 < 0$ according to our previous discussion.

Although, as we have stated above, the ChPT series for the quark condensate cannot provide quantitative reliable predictions around chiral restoration, we expect it to show its main features, especially near the chiral limit, which would correspond to the high temperature $T \gg M_{0\pi}$ of the previous expressions. Thus, in order to provide more quantitative conclusions, let us focus on $T_c(\mu_5)$ determined as the value for which the light quark condensate vanishes. For that purpose, it is very conveniente to consider the chiral series for the ratio

$$\begin{aligned}
\frac{\langle \bar{q}q \rangle_l(T, \mu_5)}{\langle \bar{q}q \rangle_l(0, \mu_5)} &= 1 - \frac{3}{2F^2} g_1(M_{0\pi}, T) - \frac{1}{4B_0 F^4} \{ 3g_1(M_{0\pi}, T) \langle \bar{q}q \rangle_l^{NLO}(0, \mu_5) \\
&\quad + 2F^2 [\langle \bar{q}q \rangle_l^{NNLO}(T, \mu_5) - \langle \bar{q}q \rangle_l^{NNLO}(0, \mu_5)] \} + \mathcal{O}\left(\frac{1}{F^6}\right) = \\
&= 1 - \frac{3}{2F^2} g_1(M_{0\pi}, T) - \frac{3}{4F^4} \left\{ \frac{1}{2} [g_1(M_{0\pi}, T)]^2 - M_{0\pi}^2 g_1(M_{0\pi}, T) g_2(M_{0\pi}, T) \right. \\
&\quad - \left[\frac{M_{0\pi}^2}{16\pi^2} \left[-1 + 64\pi^2 (h_1^r(\mu) - l_3^r(\mu)) - 5 \log \frac{M_{0\pi}^2}{\mu^2} \right] + 4\mu_5^2 (2\kappa_1 - \kappa_2) \right] g_1(M_{0\pi}, T) \\
&\quad - \left. \left[\frac{M_{0\pi}^2}{16\pi^2} \left[64\pi^2 l_3^r(\mu) + \log \frac{M_{0\pi}^2}{\mu^2} \right] - 8\mu_5^2 (\kappa_1 + \kappa_2 - \kappa_3) \right] M_{0\pi}^2 g_2(M_{0\pi}, T) \right\} \\
&\quad + \mathcal{O}\left(\frac{1}{F^6}\right)
\end{aligned} \tag{6.61}$$

since the dependence on the $\mathcal{O}(p^6)$ condensate at $T = 0$ cancels, in particular the constants c^r and γ_2^r drop out. Note also that for the above ratio, the κ_i dependence reduces to the combinations

$$\kappa_a = 2\kappa_1 - \kappa_2, \quad \kappa_b = \kappa_1 + \kappa_2 - \kappa_3, \tag{6.62}$$

where κ_b latter is precisely the combination renormalizing the pion pole mass in (6.40). Noter also that the μ_5 dependence is just quadratic, which in particular implies a quadratic dependence also for $T_c(\mu_5) = T_c(0) [1 + k\mu_5^2/F^2]$ for small μ_5 , in accordance with what is found in lattice analysis [221, 222].

In the chiral limit, the previous condensate ratio becomes particularly simple, depending only on κ_a , namely,

$$\left. \frac{\langle \bar{q}q \rangle_l(T, \mu_5)}{\langle \bar{q}q \rangle_l(0, \mu_5)} \right|_{M_{0\pi}=0} = 1 - \frac{T^2}{8F^2} \left[1 - 2\kappa_a \frac{\mu_5^2}{F^2} \right] - \frac{T^4}{384F^4} + \mathcal{O}\left(\frac{1}{F^6}\right) \tag{6.63}$$

which yields the following $T_c(\mu_5)$ dependence:

$$[T_c(\mu_5)]^2 = 24F^2 \left[\sqrt{\frac{2}{3} + \left[1 - 2\kappa_a \frac{\mu_5^2}{F^2}\right]^2} - 1 + 2\kappa_a \frac{\mu_5^2}{F^2} \right] \quad (M_{0\pi} = 0) \quad (6.64)$$

which for small μ_5 reduces to

$$T_c(\mu_5) = T_c(0) \left[1 + \sqrt{\frac{3}{5}} \kappa_a \frac{\mu_5^2}{F^2} \right] \quad (M_{0\pi} = 0) \quad (6.65)$$

with $T_c(0) = 2\sqrt{2(\sqrt{15} - 3)}F$ in the chiral limit.

In Fig. 6.3 we plot on the one hand, the expected uncertainty band for $T_c(\mu_5)/T_c(0)$ within the range of natural values for $\kappa_{a,b}$. We take $l_3^r(\mu = 770) = 0.21 \times 10^{-3}$ [191] while for the contact LEC h_1^r , which cannot be determined from direct fits, we use the resonance saturation approximation [200] $H_2^r = 2L_8^r$ for those $SU(3)$ LEC, together with the conversion between $SU(2)$ and $SU(3)$ LEC in [35] and the L_6^r , L_8^r and kaon and eta tree masses extracted from [191]. That gives $h_1^r(\mu = 770) = 6.8 \times 10^{-3}$. The same approximation has been used in [90, 188]. We show also in that figure the lattice points corresponding to the $N_c = 2$ analysis in [221] (with $M_\pi = 330$ MeV) and the $N_c = 3$ one in [222] (with $M_\pi = 550$ MeV) which follow similar trends.

Once we normalize T_c to the corresponding $T_c(0)$ for each case, we see that ChPT curve for the physical pion mass lies very close to the chiral limit one and that the lattice points clearly fall into the uncertainty given by the natural values range of $\kappa_{a,b}$. This confirms that the main features are captured by the ChPT approach for the ratio $T_c(\mu_5)/T_c(0)$. Actually, we have performed some fits of the lattice results in order to try to pin down the value of the involved $\kappa_{a,b}$ constants. The results of those fits are given in Fig. 6.4 and in Table 6.1. The uncertainty bands and parameter errors correspond to the 95% confidence level of the fits. We have chosen the set of points obtained in [221] since they provide more points in the low μ_5 regime, where our approach is meant to be more applicable. We see that the chiral limit approach in (6.64), as commented already, yields a very good description of those lattice data for the ratio $T_c(\mu_5)/T_c(0)$. A fit with only two $\mu_5 \neq 0$ points in the chiral limit is shown (fit 1) while for three points (fit 2) we get a smaller error and still a very good fit. When compared to the massive case (fit 3) fixing the κ_a parameter to that of fit 2, we get little sensitivity to κ_b (which is compatible with zero) showing again that the chiral limit approach with just one parameter κ_a is a robust approximation, at least for this particular observable. Actually, setting the two

parameters κ_a, κ_b free does not improve over the results we present here. Finally, we also show a fit with only the parabolic chiral limit μ_5^2 expression in (6.65) (fit 4) which provides a very decent approximation for this μ_5 range. The values quoted for the κ_a parameter in Table 6.1 are all compatible within errors and constitute a rather solid prediction of our present analysis, while for κ_b the error quoted in fit 3 is narrower than the natural values range but shows a larger uncertainty than κ_a .

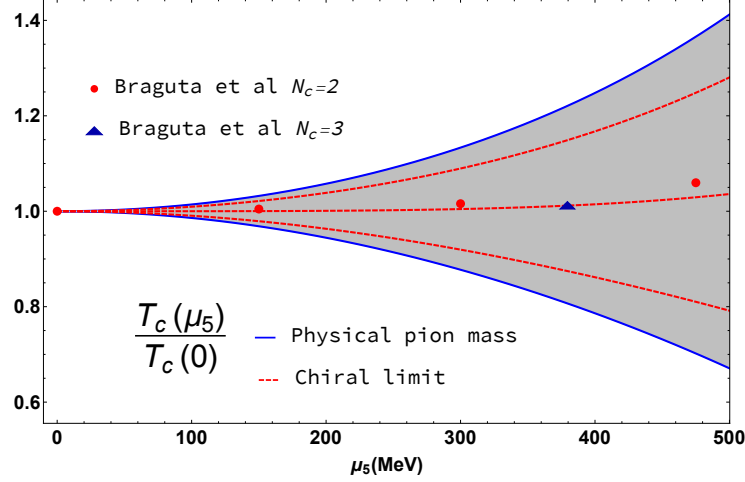


Figure 6.3: μ_5 dependence of the chiral transition temperature extracted from the vanishing of the quark condensate. We show the uncertainty bands corresponding to $|\kappa_a| \leq \frac{1}{16\pi^2}$ and $|\kappa_b| \leq \frac{1}{16\pi^2}$ with $\kappa_{a,b}$ defined in (6.62) and where only κ_a contributes in the chiral limit. We include the lattice points from [221] ($N_c = 2$) and [222] ($N_c = 3$), as explained in the main text. The corresponding $T_c(0)$ values are 227.1 MeV, and 301.0 MeV for the chiral limit and physical mass curves, and $T_c(0) = 195.8$ MeV for [221].

FIT	$\kappa_a \times 10^3$	$\kappa_b \times 10^3$	χ^2/dof	R^2	# points $\mu_5 \neq 0$
Fit 1 ($M_{0\pi} = 0$)	1.7 ± 0.6	—	0.01	1.00	2
Fit 2 ($M_{0\pi} = 0$)	2.3 ± 0.4	—	1.41	0.99	3
Fit 3	2.3 (fixed)	0 ± 1	1.36	0.99	3
Fit 4 ($M_{0\pi} = 0$ $\mathcal{O}(\mu_5^2)$)	2.5 ± 0.4	—	1.85	0.99	3

Table 6.1: Numerical values of the parameters corresponding to the fits in Fig.6.4. The last column indicates the number of lower μ_5 points considered

We end by providing the result for the scalar susceptibility as defined in (1.138). The leading nonvanishing order $\mathcal{O}(1)$ for χ_S comes from the mass derivative of $\langle \bar{q}q \rangle_i^{NLO}$ in (6.58) which, as stated, above, is μ_5 independent. The next to leading order in χ_S is $\mathcal{O}(1/F^2)$ and corresponds to the derivative of $\langle \bar{q}q \rangle_i^{NNLO}$ in (6.59). We get

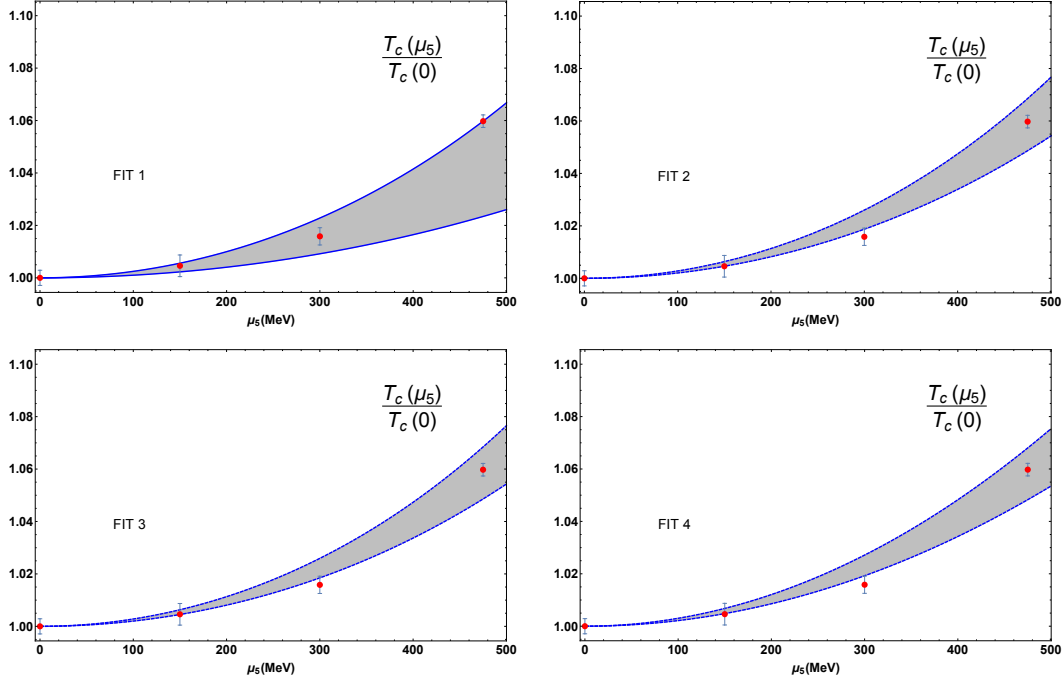


Figure 6.4: Fits of $T_c(\mu_5)/T_c(0)$ from the ChPT framework. The lattice points used for the fit are those for $N_c = 2$ in [221] while those for $N_c = 3$ in [222] are showed for reference. The $T_c(0)$ values are the same as in Fig.6.3.

$$\begin{aligned}
 \chi_S(T, \mu_5) &= \chi_S(T, 0) + B_0^2 \frac{\mu_5^2}{\pi^2 F^2} \left\{ \frac{3}{4} [6(\kappa_1 - \kappa_3) + \kappa_2] - 8\pi^2 \gamma_2^r(\mu) \right. \\
 &\quad + 24\pi^2 M_{0\pi}^2 [\kappa_1 - \kappa_3 + \kappa_2] g_3(M_{0\pi}, T) \\
 &\quad \left. + \frac{1}{4} [4(\kappa_1 - \kappa_3) + \kappa_2] \left[-48\pi^2 g_2(M_{0\pi}, T) + 3 \log \frac{M_{0\pi}^2}{\mu^2} \right] \right\} + \mathcal{O}\left(\frac{1}{F^4}\right) \quad (6.66)
 \end{aligned}$$

with $\chi_S(T, 0)$ given in [90, 188]. As explained above, it is not obvious how to extract useful information about the transition from χ_S calculated in ChPT, since the ChPT approach solely does not reproduce the expected maximum around T_c . However, retaining only the leading terms in the chiral or infrared limit $M_{0\pi} \rightarrow 0^+$, the divergent contribution for χ_S is meant to carry the essential information regarding chiral restoration [64]. In that limit, we obtain

$$\chi_S(T, \mu_5) = \frac{3B_0^2}{4} \frac{T}{\pi M_{0\pi}} \left\{ 1 + \frac{1}{F^2} \left[\frac{T^2}{16} - 6(\kappa_1 - \kappa_3) \mu_5^2 \right] \right\} + \mathcal{O}(\log M_{0\pi}^2) + \mathcal{O}\left(\frac{1}{F^4}\right) \quad (6.67)$$

Interestingly, the coefficient that regulates the dependence of χ_S with μ_5 near the chiral limit is precisely $\kappa_1 - \kappa_3$, appearing in the pole and screening pion mass corrections

in (6.40) and (6.41). The lattice data indicate that χ_S decreases with μ_5 below the transition [221], consistently with the peak of χ_S signaling the transition moving towards higher values of T . This favors the sign $\kappa_1 - \kappa_3 > 0$, in agreement with the results in [219] on the pion mass. Once more, it becomes clear that lattice measurements on the pion masses would be important to determine at least the sign of the μ_5 corrections, connected as we have just seen with the chiral restoring behaviour. The temperatures considered in [221] are too high to trust a fit based on our previous ChPT chiral susceptibility for a pion gas, as commented above.

The chiral charge density and $\mu_5 = 0$ stability

Another quantity whose μ_5 dependence has been studied in the lattice is the chiral charge density [220, 224], defined as

$$\rho_5(T, \mu_5) = \langle (J_A)^0 \rangle = \langle \bar{q} \gamma^0 \gamma_5 q \rangle = -\frac{\partial \epsilon(T, \mu_5)}{\partial \mu_5} \quad (6.68)$$

From our expressions in section 6.2.2 we get, up to $\mathcal{O}(p^6)$ in the free energy,

$$\rho_5(T, \mu_5) = \rho_5^{(1)}(T) \mu_5 + \rho_5^{(3)} \mu_5^3 + \rho_5^{(5)} \mu_5^5 + \mathcal{O}(1/F^4), \quad (6.69)$$

with

$$\begin{aligned} \rho_5^{(1)}(T) = & 4F^2 \left(1 + \kappa_0 + 2\kappa_3 \frac{M_{0\pi}^2}{F^2} \right) + \frac{1}{32\pi^2 F^2} \left\{ 6 [4(\kappa_1 - \kappa_3) + \kappa_2] M_{0\pi}^4 \log \frac{M_{0\pi}^2}{\mu^2} \right. \\ & + 576\pi^2 \kappa_2 g_0(M_{0\pi}, T) + 384\pi^2 (\kappa_1 - \kappa_3 + \kappa_2) M_{0\pi}^2 g_1(M_{0\pi}, T) \\ & \left. - M_{0\pi}^4 [3\kappa_2 + 64\pi^2 \gamma_2^r(\mu)] \right\}, \end{aligned} \quad (6.70)$$

$$\rho_5^{(3)} = 4 \left(\kappa_4 - \frac{M_{0\pi}^2}{F^2} \gamma_1 \right), \quad (6.71)$$

$$\rho_5^{(5)} = -6 \frac{\gamma_0}{F^2} \quad (6.72)$$

The above expressions provide the ChPT prediction for the chiral charge density, which as in the previous observables discussed, should be applicable at low and moderate values of T and μ_5 . Note that the thermal functions above are multiplied by precisely the same κ_i combinations showing up in the pion dispersion relation analysis and that $\kappa_2 < 0$, and therefore the thermal contribution increases the coefficient of the linear term above in the chiral limit. The sign of $\kappa_b = \kappa_1 + \kappa_2 - \kappa_3$ is not clear, as we have already discussed. Note that the chiral charge density satisfies $\rho_5(\mu_5 = 0) = 0$, which is consistent with the Vafa-Witten theorem stating that parity cannot be spontaneously

broken in the absence of axial sources [230]. A way out of this theorem is to consider for instance nonzero baryon density [213, 231].

From the recent lattice analysis in [224] performed for $N_f = 2$, one concludes that for low and moderate values of μ_5 , $\rho_5(\mu_5)$ is very insensitive to the quark masses and its behaviour is pretty much dominated by the linear term $\rho_5 \propto \mu_5$. This is consistent with our results above since the dominant $\mathcal{O}(F^2)$ term shows up only in the linear term (6.70) and is mass independent. Actually, in [224], that term is estimated simply as $4F_\pi^2$, which is adequate regarding its order of magnitude, but as we have seen in detail here, at that order the contribution from the κ_0 term have to be considered in addition to that of the pion decay constant. Another relevant comment in this context is that the temperature and volume corrections might have to be considered in future lattice analyses. Actually, in [224] the total four-volume of the lattice is fixed at around $(1.7 \text{ fm})^4$ which would amount to an effective temperature $T \sim 116 \text{ MeV}$. According to our expressions above, that would affect mostly the linear term $\rho_5^{(1)}$, although we expect that the corrections are small at those temperatures since they appear at the NNLO $\mathcal{O}(1/F^2)$ (see below). The lattice analysis in [220] is performed at very high temperatures $T > 400 \text{ MeV}$ and then our present ChPT-based analysis is less appropriate to describe those results. Nevertheless, the almost linear growth of $\rho_5(\mu_5)$ also holds in [220].

Let us then perform a fit of $\rho_5(\mu_5)$ to the lowest values of μ_5 provided in [224], similarly to what we did before for the critical temperature ratio. For that purpose, and in view of our previous discussion, it makes sense to consider only the chiral limit of our previous expressions for ρ_5 , since we do not expect to extract any useful information about the constants multiplying the mass terms, to which ρ_5 is much less sensitive. We get

$$\rho_5(T, \mu_5)|_{M_0\pi=0} = 4F^2\mu_5 \left(1 + \kappa_0 + \kappa_2 \frac{\pi^2 T^4}{10F^4} \right) + 4\kappa_4\mu_5^3 - 6\frac{\gamma_0}{F^2}\mu_5^5 + \mathcal{O}(1/F^4). \quad (6.73)$$

With the previous expression, we have performed the fits showed in Fig.6.5 and Table 6.2, for which the uncertainty bands and parameter errors correspond to the 95% confidence level. Lattice errors are not provided in [224] for ρ_5 . In both fits, we have not included the temperature dependent term proportional to κ_2 in (6.73). Actually, we get $\kappa_2 \frac{\pi^2 T^4}{10F^4} \sim 6 \times 10^{-3}(1 + \kappa_0)$ with the κ_0 values quoted in Table 6.2 and setting the natural value $\kappa_2 = 1/(16\pi^2)$ and $T = 116 \text{ MeV}$ (as corresponds to [224]). Thus, for these fits it is completely justified to ignore the volume or temperature dependence, as

expected. That contribution is relatively much smaller than the typical error quoted in Table 6.2 and therefore no useful conclusion about that value of κ_2 can be inferred from this analysis.

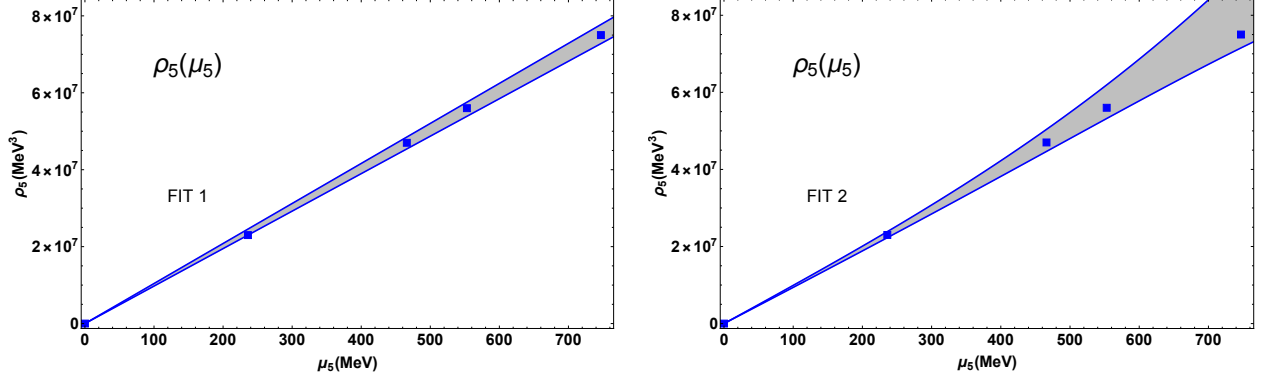


Figure 6.5: Fits of $\rho_5(\mu_5)$ using the chiral limit expression (6.73) for $\kappa_2 = 0$. The lattice points used for the fit are those in [224].

FIT	κ_0	$\kappa_4 \times 10^3$	$\gamma_0 \times 10^5$	R^2	# points $\mu_5 \neq 0$
Fit 1	2.4 ± 0.1	0 (fixed)	0 (fixed)	0.99	3
Fit 2	2.3 ± 0.1	7.1 ± 3.6	4.6 ± 2.4	0.99	4

Table 6.2: Numerical values of the parameters corresponding to the fits in Fig.6.5. The last column indicates the number of lower μ_5 points considered

The results show that the simple linear dependence setting $\kappa_4 = \gamma_0 = 0$ (fit 1) already fits very well the lowest μ_5 lattice points. The prediction for κ_0 is consistent with the fit allowing the three parameters $\kappa_0, \kappa_4, \gamma_0$ to be free (fit 2) which allow to include an additional point, expected to be more sensitive to the nonlinear dependence. Recall that the numerical value for κ_0 is not expected to lie within natural values $1/(16\pi^2)$ since it is a low-energy constant of the $\mathcal{L}_2$ Lagrangian. As a consequence of the dominance of the linear term, for the numerical values of κ_2 and γ_0 in fit 2 are affected by larger errors. Our ChPT-based approach essentially captures then the main features of the lattice results.

A relevant issue related to the previous ρ_5 analysis has to do with the stability of the $\mu_5 = 0$ solution. One may wonder whether the free energy admits minima with $\mu_5 \neq 0$, which would define a characteristic "expected" value for the axial chemical potential, at least within the present low-energy approach. The temperature and volume dependence of such solution is relevant since it could be achieved within a heavy-ion collision and/or lattice environment.

Thus, writing the free energy as $\epsilon(\mu_5) = \epsilon(0) - \frac{1}{2}\rho_5^{(1)}\mu_5^2 - \frac{1}{4}\rho_5^{(3)}\mu_5^4 + \dots$ with the $\rho_5^{(i)}$ coefficients defined in our previous analysis of the chiral charge density, the behaviour of $\epsilon(\mu_5)$ around $\mu_5 = 0$ is controlled by the coefficient of the μ_5^2 term, which according to our previous discussion satisfies $\rho_5^{(1)} > 0$ to ensure the growing behaviour of $\rho_5(\mu_5)$ observed in the lattice, which appears to be pretty independent of the temperature and volume.

Therefore, $\epsilon(\mu_5)$ would have a maximum at $\mu_5 = 0$, which opens up the interesting possibility that the energy density develops a minimum at a nonzero (and not very large) value of μ_5 , which would require $\rho_5^{(3)} < 0$ and would be given by $[\mu_5^2]_{min} = -\rho_5^{(1)}/\rho_5^{(3)}$. At the order we are calculating here, $\rho_5^{(3)}$ is dominated by κ_4 in (6.71) since the γ_1 contribution is expected to be suppressed, as well as the $\gamma_0 \mathcal{O}(\mu_5^6)$ term in the free energy given by (6.72). On the other hand, our previous fits to lattice data suggest $\kappa_4 > 0$. In any case, even setting a negative value for κ_4 of the expected size 10^{-3} , would give $[\mu_5]_{min} \simeq 30F \simeq 2600$ MeV, much higher than the typical applicability range of our present approach. Therefore, our present analysis does not favor a $\mu_5 \neq 0$ minimum for the free energy for low and moderate values of μ_5 . This conclusion is independent of temperature and volume, at least at the order considered here.

The topological susceptibility

The topological susceptibility for $\mu_5 \neq 0$ has also been recently analyzed in the lattice [224] and it might provide additional information about the κ_i LECs. it is defined as

$$\chi_{top} = \left. \frac{\partial^2 \epsilon(\theta)}{\partial^2 \theta} \right|_{\theta=0} \quad (6.74)$$

where $\epsilon(\theta)$ is the vacuum energy when the θ -term is included in the QCD Lagrangian. From our μ_5 -dependent effective Lagrangian, we can calculate the topological susceptibility by noting that a constant θ term amounts to a complex quark mass matrix according to (6.23). This is actually the way that χ_{top} has been calculated within the effective theory ChPT framework for $SU(2)$ and $SU(3)$ [170, 177]. It is important to remark that the quark mass dependence of χ_{top} favors the dominance of light quarks, being proportional to M_π^2 in the $SU(2)$ limit $m_{u,d} \ll m_s$. Actually, this would explain why the ChPT predictions remain close to the lattice analysis.

Following then the procedure in [170, 177], one considers a nontrivial unitary vacuum configuration different from $U = 1$ where U is the Goldstone boson matrix field, namely $U_0 = \text{diag}(e^{i\varphi}, e^{-i\varphi})$ where φ minimizes $\epsilon(\theta)$ with $m_u \neq m_d$. Now, the only μ_5 -dependent

term up to $\mathcal{L}_4$ proportional to the quark mass is the κ_3 contribution in (6.26), which has precisely the same form as the mass term in $\mathcal{L}_2$. Therefore, at this order this amounts to a redefinition $F^2 \rightarrow F^2 + 4\mu_5^2\kappa_3$ in $\epsilon_2(\theta) = -F^2 M_{0\pi}^2 [1 + \frac{1}{8}(\hat{\epsilon}^2 - 1)\theta^2 + \mathcal{O}(\theta^4)]$ with $\hat{\epsilon} = (m_u - m_d)/(m_u + m_d)$ [177] so that we get

$$\chi_{top}(\mu_5) = \chi_{top}(0) + \kappa_3 \mu_5^2 M_{0\pi}^2 (1 - \hat{\epsilon}^2) + \mathcal{O}(p^6/F^2) \quad (6.75)$$

with $\chi_{top}(0)$ given in [170, 177].

Note that the above results imply in particular that for $\theta = 0$ the solution $\phi = 0$ is still the vacuum energy minimum at $\mu_5 \neq 0$, which is compatible with the absence of a pion condensate at the order we are calculating here.

Therefore, the dependence of χ_{top} with low and moderate μ_5 is controlled by the κ_3 constant. We could try to fix it with lattice data. However, the only available results in [224] lack of a solid continuum limit and are therefore quite noisy. The effect of heavy pion masses in the lattice is also expected to be more distorting for χ_{top} than for other observables, due to its mass dependence commented above, and actually there is a high sensitivity to m_π in the results in [224]. At most, one can infer from those results a growing tendency $\chi_{top}(\mu_5)$ for large μ_5 , which is not so clear for lower values.

Nevertheless, the previous uncertainties reduce considerably by considering the ratio $\chi_{top}(\mu_5)/\chi_{top}(0)$ for which the expected $M_{0\pi}^2$ dependence is expected to cancel out, as can be seen in Fig. 6.6, where the lattice data for different masses are compatible within errors. Also, the band of natural values for κ_3 covers widely the lattice points, so it is meaningful to fit the lowest data points with the ChPT curve, which at this order is given by

$$\frac{\chi_{top}(\mu_5)}{\chi_{top}(0)} = 1 + 4 \frac{\kappa_3 \mu_5^2}{F^2} + \mathcal{O}(1/F^4) \quad (6.76)$$

for $m_u = m_d$, where we have used that $\chi_{top}(0) = M_{0\pi}^2 F^2/4 + \mathcal{O}(F^0)$ in $SU(2)$ [122, 170, 177].

FIT	$\kappa_3 \times 10^3$	R^2	χ^2/dof	# points $\mu_5 \neq 0$
Fit 1	0.1 ± 1.4	0.99	1.20	2 ($M_\pi = 410$ MeV)+2 ($M_\pi = 580$ MeV)
Fit 2	0.5 ± 0.9	0.99	1.13	3 ($M_\pi = 410$ MeV)+3 ($M_\pi = 580$ MeV)

Table 6.3: Numerical values of the parameters corresponding to the fits in Fig.6.7. The last column indicates the number of lower μ_5 points considered

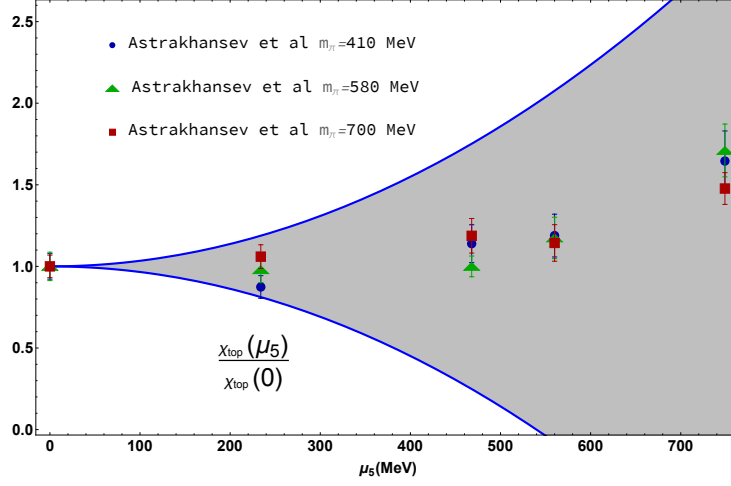


Figure 6.6: μ_5 dependence of the topological susceptibility chiral transition temperature extracted from the vanishing of the quark condensate. We show the uncertainty bands corresponding to $|\kappa_3| \leq \frac{1}{16\pi^2}$. We include the lattice points from [224] for $a = 0.0856$.

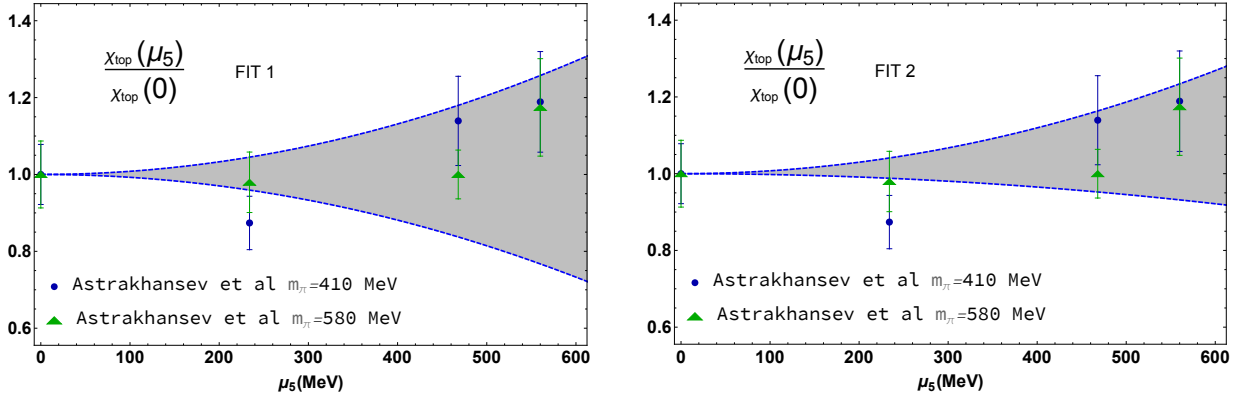


Figure 6.7: Fits of $\chi_{top}(\mu_5)/\chi_{top}(0)$ using the ChPT expression (6.76). The lattice points used for the fit are those in [224].

The results of the best fits are showed in Fig. 6.7 and Table 6.2, where we have selected two sets for the lowest masses in [224]. The results for κ_3 are compatible with zero but the error bands corresponding to the 95% confidence level of the fits are much narrower than the natural values showed in Fig. 6.6.

Pressure and speed of sound

It is interesting to explore the consequences of the μ_5 corrections and the new LECs involved, as far as other thermodynamical quantities are concerned. The thermodynamic pressure P , the entropy density s , the specific heat c_v , and the speed of sound squared c_s^2 can be obtained from the energy density as customary.

From our expressions from the energy density derived before, we obtain for the pressure

$$P(T, \mu_5) = \frac{3}{2}g_0(M_{0\pi}, T) \left(1 + 6\kappa_2 \frac{\mu_5^2}{F^2}\right) - \frac{3M_{0\pi}^2}{8F^2} \{[g_1(M_{0\pi}, T)]^2 + 8g_1(M_{0\pi}, T) \left[M_{0\pi}^2 \left(l_3^r(\mu) + \frac{1}{64\pi^2} \log \frac{M_{0\pi}^2}{\mu^2}\right) - 2\mu_5^2 \kappa_b\right]\} + \mathcal{O}\left(\frac{1}{F^4}\right) \quad (6.77)$$

which in the chiral limit reduces to

$$P(T, \mu_5)|_{M_{0\pi}=0} = \frac{\pi^2 T^4}{15} \left(1 + 6\kappa_2 \frac{\mu_5^2}{F^2}\right) \quad (6.78)$$

Thus, the μ_5 corrections to the pressure are parametrized by κ_2 and the combination κ_b in (6.62), only the first one surviving in the chiral limit, which corresponds to the ultrarelativistic free pion gas corrected by the κ_2 term. In Fig. 6.8 we represent the pressure for two reference values of $\mu_5 = 150$ MeV and $\mu_5 = 300$ MeV for which our approach can be considered valid, with the bands corresponding to natural values for κ_2, κ_b , keeping $\kappa_2 > 0$ as explained in section 6.2.2. The main source of uncertainty in the pressure comes actually from the κ_2 term, the result remaining almost unchanged if using for instance the uncertainty for κ_b given in Table 6.1.

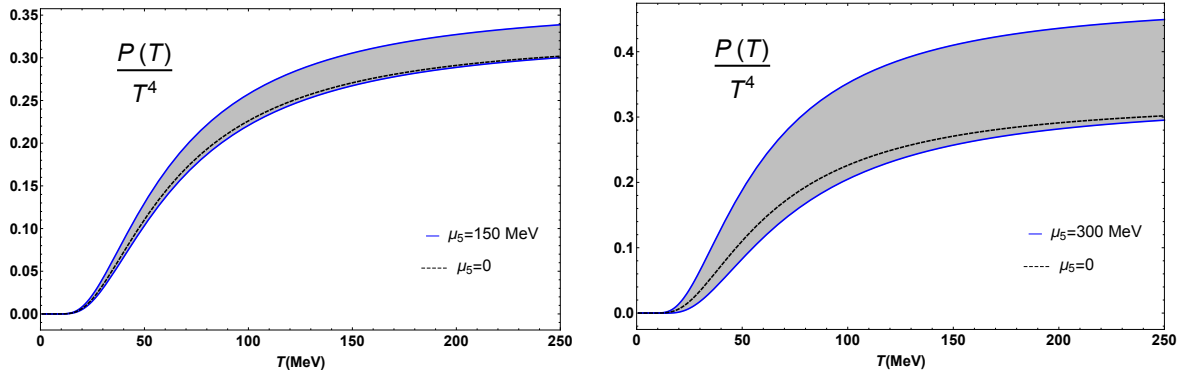


Figure 6.8: Pressure for $\mu_5 = 150$ MeV and $\mu_5 = 300$ MeV compared to the $\mu_5 = 0$ case. The uncertainty bands correspond to $0 \leq \kappa_2 \leq \frac{1}{16\pi^2}, |\kappa_b| \leq \frac{1}{16\pi^2}$.

It is particularly interesting to study the speed of sound and whether the μ_5 corrections may affect the physical limitations for this quantity. The analytic result for $M_{0\pi} \neq 0$ is given by

$$\begin{aligned}
 c_s^2(T, \mu_5) = & \frac{1}{T g_0''(M_{0\pi}, T)} \left\{ g_0'(M_{0\pi}, T) + \frac{M_{0\pi}^2}{2F^2 g_0''(M_{0\pi}, T)} \left[(g_1'(M_{0\pi}, T))^2 g_0'(M_{0\pi}, T) \right. \right. \\
 & + \left. \left(g_1(M_{0\pi}, T) + 4M_{0\pi}^2 \left(l_3^r(\mu) + \frac{1}{64\pi^2} \log \frac{M_{0\pi}^2}{\mu^2} \right) - 8\kappa_b \mu_5^2 \right) \right. \\
 & \times \left. \left. (g_0'(M_{0\pi}, T) g_1''(M_{0\pi}, T) - g_1'(M_{0\pi}, T) g_0''(M_{0\pi}, T)) \right] \right\} + \mathcal{O}\left(\frac{1}{F^4}\right) \quad (6.79)
 \end{aligned}$$

where g_i' and g_i'' denote derivatives with respect to T . Note that the κ_2 contribution cancels in c_s^2 which then depends only on μ_5 upon the κ_b combination. In addition, at this order in the chiral limit one just gets $c_s^2 \rightarrow 1/3$, i.e., the ultrarelativistic limit of a free boson gas, which is meant to be reached asymptotically as the temperature increases, i.e., for $T \gg M_{0\pi}$. This is clearly seen in Fig. 6.9 where c_s^2 remains below $1/3$ with the μ_5 corrections included. The uncertainty band for κ_b actually narrows as T increases, consistent with the chiral limit being μ_5 -independent for this quantity at this order. Therefore, having no lattice results available to compare with, the analysis of pressure and the speed of sound poses no extra requirements on the κ_i LEC.

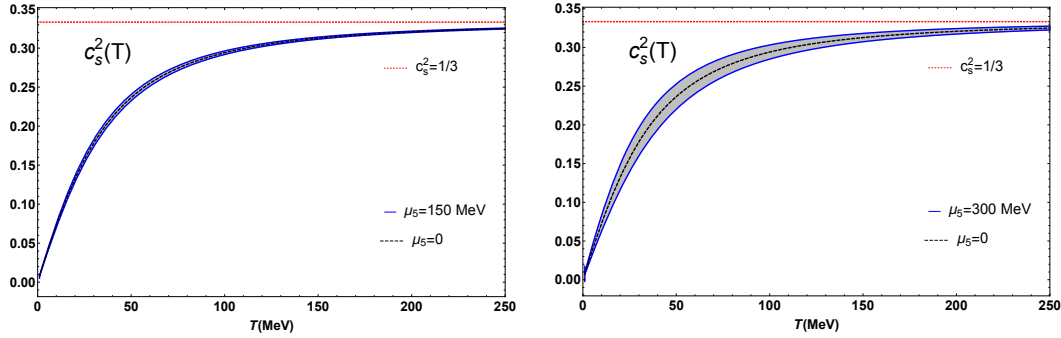


Figure 6.9: Speed of sound squared for $\mu_5 = 150$ MeV and $\mu_5 = 300$ MeV compared to the $\mu_5 = 0$ case. The uncertainty bands correspond to $|\kappa_b| \leq \frac{1}{16\pi^2}$.

Pion scattering

Here we will extend the analysis described before for the critical temperature by calculating the pion-pion elastic scattering amplitude with the $\mu_5 \neq 0$ Lagrangian, up to NLO, i.e. $\mathcal{O}(p^4)$, within the ChPT framework and unitarizing it in order to obtain the lightest resonant states $f_0(500)/\sigma$ and $\rho(770)$. The μ_5 corrections to the amplitude come from the following sources:

- i) The $\mathcal{O}(p^4)$ tree level order amplitude, which can be extracted directly from the four-pion terms in the Lagrangian (6.26), corresponding to the topology of Fig.1.16b.

We get:

$$\mathcal{T}_{4,tree}(\mathbf{S}, \mathbf{T}, \mathbf{U}; \mu_5) = \frac{4\mu_5^2}{3F^4} [3\kappa_1 s + M_{0\pi}^2(\kappa_3 - 4\kappa_1) + \tilde{\kappa}_2(2S_0^2 - T_0^2 - U_0^2)] \quad (6.80)$$

- ii) The correction coming from the $\mathcal{O}(p^4)$ dispersion relation modification arising from the two-pion fields in (6.26), represented by diagrams d,e in Fig.1.16.

At the order we are considering, including the contributions of diagrams d,e in Fig.1.16 is equivalent to consider for the external legs the $\mathcal{O}(p^4)$ renormalized pion propagator. The pole of this propagator yields the μ_5 -dependent modification of the pion dispersion relation at this order.

Since the μ_5 modifications to the dispersion relation in (6.35) are $\mathcal{O}(p^4)$, when setting the external legs on-shell it only affects the LO amplitude. Thus, let us consider the tree level contribution $\mathcal{T}_2$ in Fig.1.16a off the mass-shell, i.e., without specifying the dispersion relation for the external legs, which is given by

$$\mathcal{T}_{2,off-shell} = \frac{3s - \sum_{i=1}^4 p_i^2 + M_{0\pi}^2}{3F^2} \quad (6.81)$$

Replacing then the dispersion relation (6.35) in (6.81) gives rise to the following $\mathcal{O}(p^4)$ μ_5 -dependent correction to the amplitude:

$$\mathcal{T}_{4,dr}(\mathbf{S}, \mathbf{T}, \mathbf{U}; \mu_5) = \frac{4\mu_5^2}{3F^4} [\kappa_2(S_0^2 + T_0^2 + U_0^2) + 4(\kappa_1 - \kappa_3)M_{0\pi}^2] \quad (6.82)$$

- iii) The $\mathcal{O}(p^4)$ correction coming from the residue of the LSZ formula application.

As explained above, including properly the dressed external lines as given in Fig. 1.16d,e, amounts to consider scattering of pions with the modified dispersion relation (6.35). According to the LSZ formalism, we must then amputate those dressed external legs by multiplying the 4-point Green function by the adequate momentum function removing the pole for each leg and extracting the corresponding residue.

One can follow the same steps as in [78] considering asymptotic external fields satisfying a generic dispersion relation $p_0^2 = f(|\vec{p}|^2)$, which in our present case (6.35) corresponds at this order to

$$f(|\vec{p}|^2) = |\vec{p}|^2 + M_\pi^2(0) - \frac{4\mu_5^2}{F^2} \kappa_2 |\vec{p}|^2 + \frac{4\mu_5^2}{F^2} (\kappa_3 - \kappa_1 - \kappa_2) M_{0\pi}^2 \quad (6.83)$$

In the end one has just to modify the standard LSZ amputation prescription as

$$\left\{ \left\{ \prod_{i=1}^n [-p_i^2 + M_\pi^2] \right\} G(p_1, \dots, p_n) \right\}_{OS} \rightarrow \left\{ \left\{ \prod_{i=1}^n [-(p_i^0)^2 + f(|\vec{p}|^2)] \right\} G(p_1, \dots, p_n) \right\}_{OS} \quad (6.84)$$

for n external legs, with G the n -point connected Green function with all momenta set as incoming and where "OS" means the mass shell condition $(p_i^0)^2 = f(|\vec{p}_i|^2)$.

Therefore, in our case, from (6.84) and (6.83), we are left with the following correction factor with respect to the $\mu_5 = 0$ case, coming from the amputation of the external legs, at the order we are considering here:

$$\begin{aligned} [-(p_1^0)^2 + f(|\vec{p}_1|^2)] G(p_1) &= \frac{p_1^2 - M_\pi^2(0) + \frac{4\mu_5^2}{F^2} [\kappa_2 |\vec{p}_1|^2 - (\kappa_3 - \kappa_1 - \kappa_2) M_{0\pi}^2]}{p_1^2 - M_\pi^2(0) + \frac{4\mu_5^2}{F^2} [\kappa_1 p_1^2 + \kappa_2 (p_1^0)^2 - \kappa_3 M_{0\pi}^2]} = \\ &= 1 - 4 \frac{\mu_5^2}{F^2} (\kappa_1 + \kappa_2) + \mathcal{O}(p^6) \end{aligned} \quad (6.85)$$

being p_1 a particular external four-momentum. As in the dispersion relation modification, the above correction affects at this order only the LO amplitude, giving rise to the following $\mathcal{O}(p^4)$ correction:

$$\mathcal{T}_{4,LSZ}(\mathbf{S}, \mathbf{T}, \mathbf{U}; \mu_5) = -16\mu_5^2(\kappa_1 + \kappa_2) \frac{s - M_0^2}{F^4} \quad (6.86)$$

where the factor of 4 comes from the four external legs.

Therefore, collecting the results in (6.80), (6.82) and (6.86), the total amplitude is given by:

$$\begin{aligned} \mathcal{T}(\mathbf{S}, \mathbf{T}, \mathbf{U}; T, \mu_5) &= \mathcal{T}(\mathbf{S}, \mathbf{T}, \mathbf{U}; T, \mu_5 = 0) \\ &+ \frac{4\mu_5^2}{3F^4} \{ -3(3\kappa_1 + 4\kappa_2)s + 3\kappa_2 S_0^2 + 3[4(\kappa_1 + \kappa_2) - \kappa_3] M_{0\pi}^2 \} \end{aligned} \quad (6.87)$$

The μ_5 corrections to the lowest angular momentum perturbative ChPT partial waves read:

$$\Delta t^{00} = -\frac{4\mu_5^2}{32\pi F^4} [\kappa'_1 s + \kappa'_2 M_{0\pi}^2], \quad (6.88)$$

$$\Delta t^{11} = -\frac{4\mu_5^2}{96\pi F^4} (s - 4M_{0\pi}^2) \kappa'_3, \quad (6.89)$$

$$\Delta t^{20} = \frac{4\mu_5^2}{32\pi F^4} [\kappa'_4 s - 2M_{0\pi}^2 \kappa'_5], \quad (6.90)$$

with the following combinations of κ_i constants

$$\begin{aligned} \kappa'_1 &= 6\kappa_1 + 5\kappa_2, & \kappa'_2 &= -8\kappa_1 - 4\kappa_2 + 5\kappa_3, & \kappa'_3 &= 3\kappa_1 + 4\kappa_2, \\ \kappa'_4 &= 3\kappa_1 + 4\kappa_2, & \kappa'_5 &= 2\kappa_1 + 4\kappa_2 + \kappa_3. \end{aligned} \quad (6.91)$$

From the previous analysis, a consistent picture with lattice data emerges, allowing to determine some LEC combinations with acceptable precision. Taking the average values of the κ_a and κ_3 fits performed above and whose results are given in tables 6.1 and 6.3, one gets $\kappa_1 \simeq 0.8 \times 10^{-3}$, $\kappa_2 \simeq -0.5 \times 10^{-3}$, $\kappa_3 \simeq 0.3 \times 10^{-3}$ although with uncertainties of order 10^{-3} , i.e., larger than for particular combinations such as κ_a , inherited from the uncertainty in κ_b . Nevertheless, it is remarkable to observe that those mean values obey the expected sign conditions discussed above, namely $\kappa_2 < 0$ and $\kappa_1 - \kappa_3 > 0$.

Now, we are going to obtain the critical temperature $T_c(\mu_5)$ by saturating the scalar susceptibility, as we showed in chapter 2. Our present analysis provides new interesting possibilities for determining the $\kappa_{1,2,3}$ constants from lattice data. Thus, on the one hand, the prediction for $T_c(\mu_5)$ from the peak of the saturated scalar susceptibility is much more reliable as a truly transition temperature than the prediction from the ChPT quark condensate, as confirmed by the numerical values for T_c given below. Besides, note that in the lattice works [221, 222] $T_c(\mu_5)$ is determined precisely from the peak of the scalar susceptibility. On the other hand, Δt^{00} in (6.88) and hence T_c depend on the combinations κ'_1 and κ'_2 in (6.91), which are different from $\kappa_{a,b}$ appearing in the quark condensate. Thus, a fit of those combinations combined with the analysis described above should allow for a better individual determination of $\kappa_{1,2,3}$.

The pion scattering amplitude and poles depend in addition on the LEC $\bar{l}_{1,2,3,4}$ of the $\mu_5 = 0$ Lagrangian in equation (1.77). We will take here the values of $\bar{l}_{1,2}$ LEC fitted in [96] to scattering data, namely $\bar{l}_1 = -0.1 \pm 0.2$, $\bar{l}_2 = 5.8 \pm 0.2$. For $\bar{l}_3$ we take the estimate $\bar{l}_3 = 3.4 \pm 0.8$ in [191] for the sake of an easier comparison with the results obtained before, where $\bar{l}_3$ was fixed to that value and it was the only one of the $\bar{l}_i$ showing up in the fits. That $\bar{l}_3$ value is fully compatible with the value used in [96], which is not fitted but taken directly from [34]. For $\bar{l}_4$ we take $\bar{l}_4 = 4.4 \pm 0.9$, the same value as in [96] and [34] whose central value coincides with the estimate in [191].

With the above $\bar{l}_i$ set, we obtain for the peak position of the saturated scalar susceptibility (6.66), $T_c(0) = 158.5$ MeV, which, as advanced, is remarkably close to the lattice prediction $T_c = 156 \pm 1.5$ MeV [232], the uncertainties of the LEC yielding compatibility with lattice results [233].

As a first analysis, we have fitted only the critical temperature obtained using the saturated scalar susceptibility leaving κ'_1 and κ'_2 as fit parameters. We have considered the lattice points provided in [221] for the critical temperature ratio. In the physical

limit, the sensitivity of the fit to κ'_1 turns out to be much stronger than to the constant proportional to the pion mass, i.e. κ'_2 . Indeed, trying to fit the lattice data, one can see that the error in κ'_2 is very large. In that sense, the behaviour of our present theoretical result is similar to that in [228] based on the quark condensate and one could think of fitting the lattice points with the chiral limit result only, as in that work.

However, there is an important qualitative difference between the two approaches regarding the chiral limit. The ChPT quark condensate merely reduces its value in that limit, and consequently T_c is also reduced, but the qualitative form of the curve is similar and, as mentioned, the ratio $T_c(\mu_5)/T_c(0)$ is almost unaffected. In fact, since it is based on the ChPT perturbative approach, it does not reproduce the expected inflection point at T_c in the physical limit. However, the susceptibility approach we are discussing here, based on thermal scattering, resembles more accurately the expected shape, i.e., a peak at T_c in the physical limit, turning into a divergence in the chiral limit at $T_c^{chiral}(\mu_5 = 0) = 125.5$ MeV, also quite close to the lattice predictions [136]. Such strong qualitative change in the chiral limit is expected to show somehow in the sensitivity of the fit. This is indeed the case: if we perform the fit in the chiral limit we obtain $\kappa'_1 = (7.7 \pm 0.8) \times 10^{-3}$ and a $\chi^2/\text{dof} = 3.90$, where the uncertainty corresponds to the 95% confidence level of the fit. This result is compatible with $\kappa'_1 = (2.3 \pm 7.8) \times 10^{-3}$ estimated from the fits previously performed for T_c and χ_{top} because of the large error in κ_i . However, the mean values are quite far from each other. Thus, we conclude that although the dependence with κ'_1 is larger than with κ'_2 , it is crucial to consider the mass of the pion, and thus the constant κ'_2 , to accurately determine the critical temperature and fit the selected lattice points in the approach based on the saturated scalar susceptibility.

Therefore, in order to reduce the error of the κ'_2 constant and to incorporate further lattice results, we will perform a combined fit with $\kappa_{1,2,3}$ as fit parameters and where the fitted observables will be, on the one hand, $T_c(\mu_5)/T_c(0)$ with the two methods already discussed, i.e., the ChPT condensate and the scalar susceptibility obtained here, and, on the other hand, the topological susceptibility χ_{top} given by (6.75). We have used the full $M_\pi \neq 0$ ChPT expression (6.61) for the condensate and we have checked that using the chiral limit expression instead does not alter significantly the obtained κ_i parameters nor their uncertainties, as expected from our previous comments.

The result of such combined fit is showed in Table 6.4, where we provide the κ_i and their uncertainties for a 95% confidence level. The error contours obtained are shown in

Fig.6.10 and in Fig.6.11 we display the results of the fit for the T_c ratio and χ_{top} . Lattice points are perfectly compatible with both T_c determinations and confirm the growing behaviour of $T_c(\mu_5)$. In fact, we have checked that $T_c(\mu_5)$ also grows within the same range when using the present T_c determination but with the central κ_i values obtained in the previous analyses. As mentioned, the T_c determination is quite different in both approaches. Namely, $T_c^{ChPT\bar{q}q}(0) = 301$ MeV and $T_c^{latt}(0) = 195.8$ MeV for the lattice work we are considering [221], which, due to the higher pion mass, is notably higher than the standard value measured in the physical limit [232]. The error band of the topological susceptibility is similar to that showed in fig. 6.7, since the uncertainty of κ_3 obtained from our present fit is indeed of the same order as their value, as it can be seen in table 6.4.

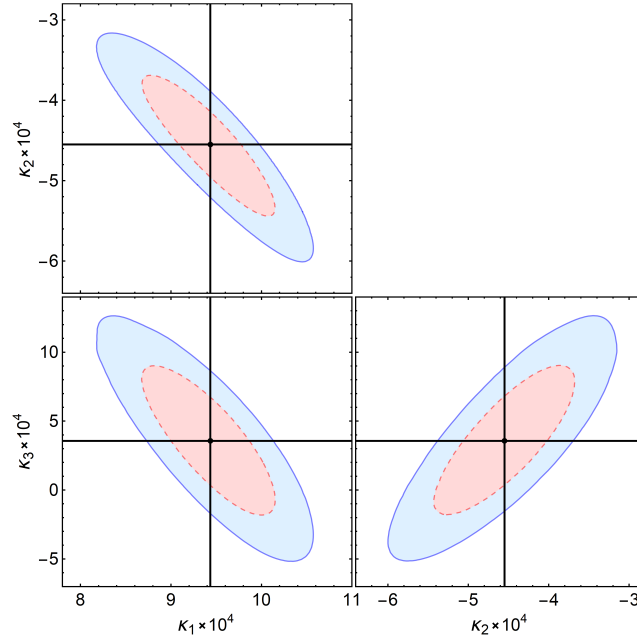


Figure 6.10: Error contours for the fit discussed in the main text. The black lines show the ‘best fit’ locations and the contours correspond to the 68% (red) and 95% (blue) confidence levels.

The fit value we have obtained here for κ_2 , provided in Table 6.4 remains negative within uncertainties, while the central value of $\kappa_1 - \kappa_3 \sim (6 \pm 9) \times 10^{-4}$ is positive, although the larger κ_3 uncertainty affects the sign of that combination. Additional lattice data for the topological susceptibility would be needed to achieve a smaller uncertainty, since this is the observable most sensitive to κ_3 , as explained.

Our results for the pole parameters as a function of μ_5 for $T = 0$ are displayed in Fig. 6.12. The uncertainty bands corresponding to those of the κ_i in Table 6.4 are

	$\kappa_1 \times 10^4$	$\kappa_2 \times 10^4$	$\kappa_3 \times 10^4$	χ^2/dof
This work (combined fit)	$9.4^{+1.1}_{-1.3}$	$-4.5^{+1.5}_{-1.4}$	$3.6^{+9.1}_{-8.7}$	1.37
Estimated from T_c and χ_{top} fits in tables 6.1 and 6.3	8 ± 10	-5 ± 10	3 ± 10	$1.1(T_c)$ $1.4(\chi_{top})$

Table 6.4: Numerical values of the κ_i parameters with the fit discussed in the main text. We also display for comparison the estimated values obtained in [228].

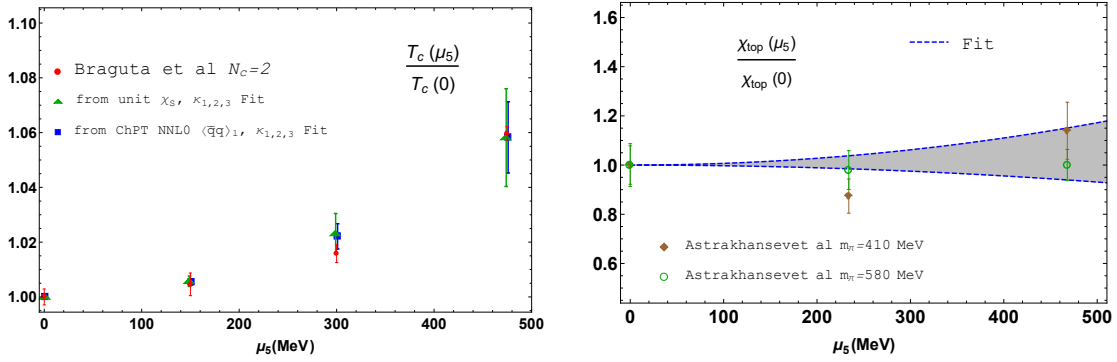


Figure 6.11: Combined fit of $T_c(\mu_5)/T_c(0)$ (left) determined from the NNLO ChPT quark condensate [228] and the present analysis using the saturated scalar susceptibility, and the topological susceptibility (right) with the ChPT result [228]. We also show the lattice results from [221], [224] and their uncertainties. All the results are plotted with the κ_i set corresponding to our present combined fit, given in Table 6.4.

showed, confirming, as mentioned above, that our results are predictive for low and moderate values of μ_5 . It is worth pointing out that in general, we expect a much softer dependence with the fourth-order LEC for the pole in the $I = J = 0$ channel than in the $I = J = 1$ one [80]. That explains the narrower uncertainty bands for the $f_0(500)/\sigma$ in Fig.6.12 even though the $I = J = 1$ amplitude depends only on one single κ_i combination, as given in (6.89).

In Fig.6.13 we plot the $f_0(500)$ saturated scalar susceptibility temperature dependence for $\mu_5 = 0, 300, 475$ MeV. Apart from the shift of the peak position corresponding to the increasing of T_c , χ_S is significantly larger with increasing μ_5 , notably around T_c . This qualitative behaviour is confirmed by the lattice analysis in [221] although the higher pion mass used in those simulations does not allow for a direct comparison with the result in Fig.6.13.

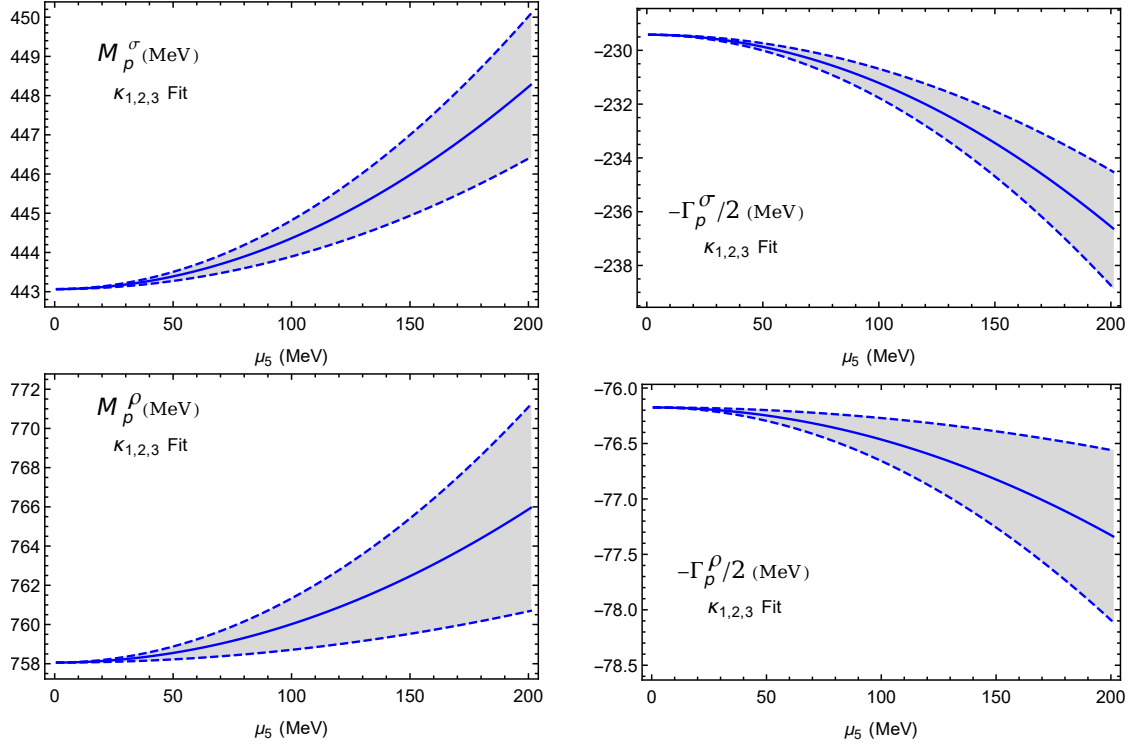


Figure 6.12: Corrections to the M_p and Γ_p parameters of the $f_0(500)$ and $\rho(770)$ resonances due to μ_5 at $T = 0$.

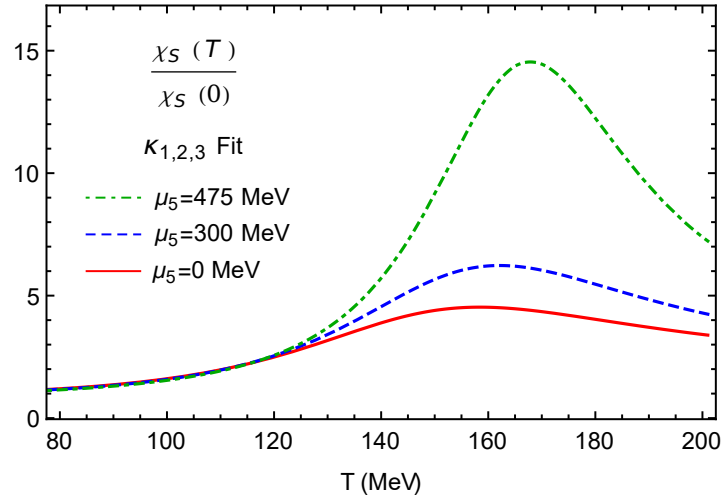


Figure 6.13: Scalar susceptibility for different values of μ_5 .

6.3 Isospin chemical potential

The case of isospin chemical potential μ_I has become particularly interesting. As it was first showed in [234] within a leading-order Chiral Perturbation Theory effective theory approach, QCD at increasing μ_I exhibits a second-order phase transition from the normal vacuum phase to a Bose-Einstein Condensation (BEC) phase for the charged

pion modes. The transition point μ_c predicted by ChPT analyses is at the physical pion mass, including next-to-leading order corrections [196, 235] which have extended to three flavours in [236]. For high enough μ_I , the system would enter a BCS-like phase [234] where effective theory approaches based on the low-density regime, such as ChPT, are expected to break down [237, 238].

Other recent analyses at $\mu_I \neq 0$ have included finite temperature corrections, allowing to study the effects on the QCD transition [195, 235, 239–241]. Temperature effects are expected to smooth out the BEC transition, increasing the value of the critical μ_I value for BEC and setting an upper temperature limit for which the BEC phase does no longer take place. In addition, the QCD transition temperature T_c is expected to drop with increasing μ_I . Other effects considered in this context have been $\mu_B \neq 0$ [242] and $\mu_S \neq 0$ [197, 243] corrections. A recent analysis within the NJL model confirms the ChPT results, showing some deviations for $\mu_I \gtrsim 2M_\pi$ [244].

Lattice works have confirmed most of the previous findings. In particular, in [237] the energy density as a function of the isospin density n_I , as well as n_I versus μ_I were investigated at a small but nonzero temperature of around $T \sim 20$ MeV. Significant deviations from the ChPT prediction take place for $\mu_I \gtrsim 2M_\pi$ and the ratio of the energy density with the Stefan-Boltzmann energy density corresponding to free quarks exhibits a maximum around $\mu_I \simeq 1.3 M_\pi$, which was interpreted in [237] as the onset of the BEC phase. Such peak behaviour is well reproduced both within the ChPT and NJL approaches [244]. The apparent plateau of that ratio above $\mu_I = 3M_\pi$ might indicate a BEC-BCS crossover.

On the other hand, lattice simulations at finite temperature and nonzero isospin chemical potential confirm the decreasing behaviour of T_c with μ_I as well as the increase of the BEC onset with temperature [245, 246]. Recent analyses provide results for the pion and quark condensates from $T = 113$ MeV up to the QCD transition temperature, confirming those trends for the $T - \mu_I$ phase diagram [247, 248]. Lattice results for n_I as a function of μ_I for low temperatures are provided in [249]. Recent comparisons between lattice data and the ChPT and NJL model approaches can be found respectively in [250] and [251].

In this section we will discuss some new relevant aspects related to the formulation of the effective ChPT Lagrangian at nonzero isospin density. The usual approach to construct the effective Lagrangian follows from considering the isospin contribution in the QCD Lagrangian as an external constant vector source in the τ_3 direction and using

the well-know external source method [34, 35] so that the chemical potential enters through covariant derivatives rendering the theory locally invariant under the chiral symmetry. However, since the μ_I term in QCD is not invariant under isospin rotations in the $\tau_{1,2}$ directions, the most general effective Lagrangian may include additional terms with such symmetry-breaking pattern, which would be multiplied by additional low-energy constants.

6.3.1 The chiral Lagrangian at finite isospin density

We start from the QCD Lagrangian including a nonzero isospin chemical potential, corresponding to the grand-canonical partition function. The fermionic part of the Lagrangian reads

$$\mathcal{L}_{QCD} = \bar{q} (i \not{D} - \mathcal{M}) q + \frac{\mu_I}{2} \bar{q} \gamma_0 \tau_3 q \quad (6.92)$$

As we mentioned before, the $\mu_I = 0$ Lagrangian is invariant under the isospin symmetry $SU(2)_V$. However, for nonzero μ_I , the latter symmetry breaks down to $U(1)_{I_3}$ since the μ_I term is only invariant under vector transformations in the τ_3 direction. Note also that Lorentz invariance is also broken by the inclusion of the μ_I term, as a consequence of the preferred reference frame of the thermal bath at rest. In addition the isospin chemical potential term breaks C invariance, since it is essentially a charge operator.

The Lagrangian in (6.92) corresponds to the particular choice $v_\mu + \frac{1}{2} A_\mu (Q_R + Q_L) = \frac{\mu_I}{2} \tau_3$, $a_\mu = 0$, $s = \mathcal{M}$ and $p = 0$. Thus, after the general effective Lagrangian is constructed, we will choose, without loss of generality,

$$v_\mu = 0, \quad A_\mu = \Lambda \delta_{\mu 0}, \quad Q = Q_R = Q_L = \frac{\mu_I}{2\Lambda} \tau_3 \quad (6.93)$$

introducing a constant Λ in the same way that we did in the axial chemical potential case. The important point is to include μ_I in the Q contribution, consistently with the counting $\mu_I = \mathcal{O}(p)$. In addition, we have kept a nonzero pseudoscalar source $p(x)$ in order to derive expectation values of pionic fields, such as the pion condensate. As customary, we will write $p(x) = j\tau_1$ so that taking derivatives with respect to j we reproduce expectation values of the π_1 field, which is the direction we have chosen for the condensed field. Thus, the standard χ matrix appearing in the ChPT Lagrangian is in this case $\chi = M_{0\pi}^2 + 2iB_0 j\tau_1$.

Next, let us replace the choice (6.93) in the Lagrangian (6.10). The most general $\mathcal{O}(p^2)$ Lagrangian at nonzero μ_I is given by

$$\mathcal{L}_2 = \frac{F^2}{4} \text{tr} \left[d_\mu U d^\mu U^\dagger + \chi^\dagger U + \chi U^\dagger + \frac{1}{2} a_1 \mu_I^2 U \tau_3 U^\dagger \tau_3 \right] + \frac{1}{4} a_2 F^2 \mu_I^2 \quad (6.94)$$

where a_1 and a_2 are new low-energy constants to be determined below and we have included a F^2 factor in front of the new terms just to render the new LEC dimensionless. As our analysis in subsection 6.3.3 below will show, physical constraints imply that the actual chiral order of those constants has to be parametrically $a_{1,2} = \mathcal{O}(1/F^2)$ so that, as we just have explained, the contributions proportional to those constants will be formally of NLO.

One can check that the $\mathcal{O}(p^3)$ in (6.12), (6.13) and (6.14) vanish for $d_\mu U$ and U in $SU(2)$ and Q in (6.93) as long as we remain in the isospin limit $m_u = m_d$, as we will do here consistently with isospin conservation. The first term in (6.12) is actually proportional to $\text{tr}(\tau_3 \mathcal{M}) = m_u - m_d$.

Evaluating the effective chiral Lagrangian constructed in (6.15) for the choice (6.93), we have that the explicit μ_I contribution to the $\mathcal{O}(p^4)$ Lagrangian is

$$\begin{aligned} \mathcal{L}_4^Q &= q_1 \Lambda^2 \text{tr} (d_\mu U d^\mu U^\dagger) \text{tr} (Q^2) + q_2 \Lambda^2 \text{tr} (d_\mu U d^\mu U^\dagger) \text{tr} (QUQU^\dagger) \\ &+ q_3 \Lambda^2 [\text{tr} (d_\mu U QU^\dagger) \text{tr} (d^\mu U QU^\dagger) + \text{tr} (d_\mu U^\dagger QU) \text{tr} (d^\mu U^\dagger QU)] \\ &+ q_4 \Lambda^2 \text{tr} (d_\mu U^\dagger QU) \text{tr} (d^\mu U QU^\dagger) + q_5 \Lambda^2 \text{tr} (\chi^\dagger U + \chi U^\dagger) \text{tr} (Q^2) \\ &+ q_6 \Lambda^2 \text{tr} (\chi^\dagger U + \chi U^\dagger) \text{tr} (QUQU^\dagger) + q_7 \Lambda^2 \text{tr} [(\chi^\dagger U - U^\dagger \chi) QU^\dagger QU] \\ &+ (\chi U^\dagger - U \chi^\dagger) QUQU^\dagger + q_8 \Lambda^4 [\text{tr} (Q^2)]^2 + q_9 \Lambda^4 \text{tr} (QUQU^\dagger) \text{tr} (Q^2) \\ &+ q_{10} \Lambda^4 [\text{tr} (QUQU^\dagger)]^2 \end{aligned} \quad (6.95)$$

with Q in (6.93). In addition to those terms, at $\mathcal{O}(p^4)$ we have to include the standard $\mathcal{L}_4^0$ Lagrangian, which depends on μ_I due to the covariant derivative.

Now, following also the derivation in [196, 234, 235, 241], we allow for a nontrivial vacuum configuration of the NGB field, which will parametrize the pion condensed phase. Namely, we write

$$\begin{aligned} U(x) &= A \exp \left[i \frac{\tau^a \pi^a(x)}{F} \right] A \\ A &= \cos(\alpha/2) \mathbb{1} + i \sin(\alpha/2) \tau_1 \end{aligned} \quad (6.96)$$

with π^a the pion fields, so that the condensed phase is characterized by a nonzero value of the α angle, which is determined by minimizing the vacuum energy density at a given

chiral order, from which we will actually obtain the main properties of interest here.

The μ_I dependence of different observables will be analyzed in detail in the next subsections. The observables of interest we can calculate in both phases are the quark condensate defined in equation(1.137), and the pion condensate and the isospin density which are given by

$$\langle i\bar{q}\gamma_5\tau_1 q \rangle(\mu_I) = \frac{\partial\epsilon(\mu_I, j)}{\partial j} \quad (6.97)$$

$$n_I(\mu_I) = -\frac{\partial\epsilon(\mu_I, j)}{\partial\mu_I} \quad (6.98)$$

6.3.2 Leading order results

Let us consider the static, linear and quadratic terms in the pion field, from the $\mathcal{L}_2$ Lagrangian in (6.94):

$$\mathcal{L}_2^{stat} = \frac{F^2}{4} [\mu_I^2 (1 + a_2 - (1 - a_1) \cos(2\alpha)) + 4M_{0\pi}^2 \cos \alpha + 8B_0 j \sin \alpha], \quad (6.99)$$

$$\begin{aligned} \mathcal{L}_2^{lin} &= -F \sin \alpha [M_{0\pi}^2 - (1 - a_1) \mu_I^2 \cos \alpha] \pi_1(x) \\ &+ F \mu_I \partial_0 \pi_2(x) \sin \alpha + 2B_0 F j \pi_1(x) \cos \alpha, \end{aligned} \quad (6.100)$$

$$\begin{aligned} \mathcal{L}_2^{quad} &= \frac{1}{2} \partial_\mu \pi^a \partial^\mu \pi_a + \frac{1}{2} m_{12} [\pi_1(x) \partial_0 \pi_2(x) - \pi_2(x) \partial_0 \pi_1(x)] \\ &- \frac{1}{2} [m_1^2 \pi_1^2(x) + m_2^2 \pi_2^2(x) + m_3^2 \pi_3^2(x)], \end{aligned} \quad (6.101)$$

where, following the notation in [196], we have

$$m_{12} = 2\mu_I \cos \alpha, \quad (6.102)$$

$$m_1^2 = M_{0\pi}^2 \cos \alpha - (1 - a_1) \mu_I^2 \cos(2\alpha) + 2B_0 j \sin \alpha, \quad (6.103)$$

$$m_2^2 = M_{0\pi}^2 \cos \alpha - (1 - a_1) \mu_I^2 \cos^2 \alpha + 2B_0 j \sin \alpha, \quad (6.104)$$

$$m_3^2 = M_{0\pi}^2 \cos \alpha + (1 - a_1) \mu_I^2 \sin^2 \alpha + 2B_0 j \sin \alpha. \quad (6.105)$$

The lowest order of the energy density, ϵ_2 , parametrically of $\mathcal{O}(F^2)$, is given just by minus the constant part of the $\mathcal{L}_2$ Lagrangian in (6.94)

$$\epsilon_2(\mu_I, j) = -\frac{F^2}{4} [\mu_I^2 (1 + a_2 - (1 - a_1) \cos(2\alpha)) + 4M_{0\pi}^2 \cos \alpha + 8B_0 j \sin \alpha] \quad (6.106)$$

The value α_0^{LO} minimizing ϵ_2 with respect to α is given for $j = 0$ by

$$\cos \alpha_0^{LO} = \begin{cases} 1 & \text{for } \mu_I < \mu_c = \frac{M_{0\pi}}{\sqrt{1 - a_1}} \\ \frac{M_{0\pi}^2}{(1 - a_1) \mu_I^2} & \text{for } \mu_I > \mu_c \end{cases} \quad (6.107)$$

Therefore, at this order, the constant a_1 displaces the critical BEC value μ_c from the pion mass. We will see below that this is perfectly compatible, both with the effective Lagrangian framework and with lattice results, which will constrain the a_1 value and its uncertainty. In addition, as we will see in the next subsection, the constraint $\mu_c = M_\pi$ can actually be maintained formally to LO and NLO. Note also that the upper bound $a_1 < 1$ arises here from the very existence of a BEC phase.

Now, we follow the same steps as in [196] to obtain the pion dispersion relation in terms of the parameters $m_{12}, m_{1,2,3}^2$. Note that to leading order, we can replace $\alpha = \alpha_0^{LO}$, which in particular cancels the contribution proportional to $\pi_1(x)$ in (6.100) so that such linear Lagrangian becomes a total derivative in the condensed phase and vanishes in the normal phase. Therefore, at this order, the linear Lagrangian does not play any role for the dispersion relation nor in the vacuum energy density. As we will see, this does no longer hold to NLO, so that term will have to be included.

We then get for the dispersion relation of charged and neutral pions to leading order, respectively,

$$E_\pm^2(p) = p^2 + \frac{1}{2} (m_1^2 + m_2^2 + m_{12}^2) \pm \frac{1}{2} \sqrt{4p^2 m_{12}^2 + (m_1^2 + m_2^2 + m_{12}^2)^2 - 4m_1^2 m_2^2}, \quad (6.108)$$

$$E_0^2(p) = p^2 + m_3^2, \quad (6.109)$$

where $p \equiv |\vec{p}|$. Now, setting $\alpha = \alpha_0^{LO}$ given in (6.107) and $p = 0$ we get then the dependence of the static pion masses on the isospin chemical potential, now including the correction from the a_1 term, which for $j = 0$ read

$$\mu_I < \mu_c \begin{cases} M_\pm^2 &= M_{0\pi}^2 + (1 + a_1)\mu_I^2 \pm 2\mu_I \sqrt{M_{0\pi}^2 + a_1\mu_I^2}, \\ M_0^2 &= M_{0\pi}^2, \end{cases} \quad (6.110)$$

$$\mu_I > \mu_c \begin{cases} M_+^2 &= (1 - a_1)\mu_I^2 + \frac{3 + a_1}{(1 - a_1)^2} \frac{M_{0\pi}^4}{\mu_I^2} \\ M_-^2 &= 0 \\ M_0^2 &= (1 - a_1)\mu_I^2 \end{cases} \quad (6.111)$$

In fact, lysisevious analysis of the dispersion relation, we realize that the displacement of the critical point to LO produced by the a_1 term can be understood as folllows, consistently within the effective Lagrangian framework. From general grounds, the BEC critical point is that where the particle energy at $p = 0$ equals the chemical potential, so that the Bose-Einstein distribution diverges. That is $\mu_c = \tilde{M}_-$ with $\tilde{M}_- = \tilde{E}_-(p = 0)$

and $\tilde{E}_-(p)$ the π^- particle mass and energy respectively below the critical point. In other words, $M_-(\mu_c) = 0$ with $M_-(\mu_I) = \tilde{M}_- - \mu_I$. In usual scalar models, including Ginzburg-Landau type, and in standard ChPT to LO, $\mu_c = M_\pi$ follows from that condition. However, within the effective Lagrangian framework, one has μ_I -dependent interactions, which in particular enter in the particle dispersion relation and may then modify the critical point. This is the case for $a_1 \neq 0$, for which we expect the same modification in the charged pion mass as in the case of EM interactions. Actually, from (6.110), we see that the effect of the new a_1 term below μ_c amounts to the shift $M_{0\pi}^2 \rightarrow M_{0\pi}^2 + a_1 \mu_I^2$ which we readily recognize as the same effect as the charged pion mass shift $M_{0\pi}^2 \rightarrow M_{0\pi}^2 + 2C \frac{e^2}{F^2}$ which takes place when EM interactions are included, coming from the term $\Delta \mathcal{L}_2^{EM} = C \text{tr}(QUQU^\dagger)$ with Q the quark charge matrix [41, 198–200]. The origin of that mass shift is in both cases the Lagrangian contribution breaking isospin only in the charged pion directions, so it does not affect the neutral pion mass.

Therefore, from $M_{0\pi}^2 + a_1 \mu_c^2 = \mu_c^2$ we would readily have the shifted $\mu_c = M_{0\pi}/\sqrt{1 - a_1}$. Actually, one can check that $M_-(\mu_c) = 0$ with M_- in (6.110) for any a_1 . Thus, as in the $a_1 = 0$ case, the vanishing mass of one of the charged pions signals the onset of BEC condensation, as a Goldstone mode corresponding to the $U(1)_{I_3}$ spontaneous symmetry breaking of the vacuum in that phase, i.e, with a nonzero pion expectation value. The above mass dependence is plotted in Fig. 6.14 for a sample value of $a_1 = -0.1$, compared to the $a_1 = 0$ case, the qualitative dependence with μ_I being quite similar, although note that a_1 introduces a non-polynomial dependence below μ_c .

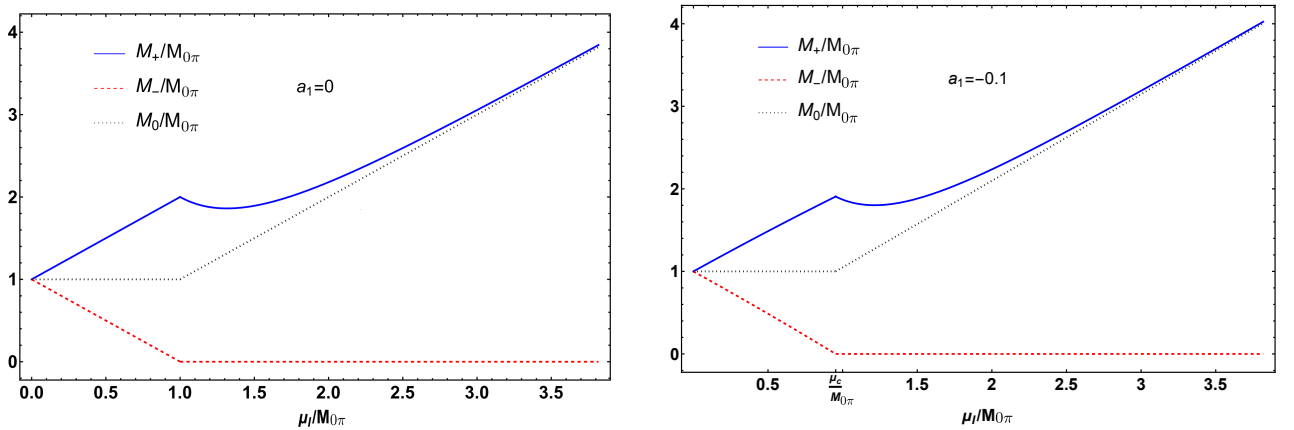


Figure 6.14: Dependence of pion masses with isospin chemical potential to leading order in ChPT with and without the extra term, for a sample value $a_1 = -0.1$.

From the energy density in (6.106) we get the LO to the quark and pion condensates and the isospin density. Namely, from (1.137), (6.97), (6.98), we get, replacing $\alpha = \alpha_0$

and for $j = 0$,

$$\langle \bar{q}q \rangle_l^{LO}(\mu_I) = \begin{cases} -2B_0F^2 & \mu_I < \mu_c \\ \frac{-2B_0F^2M_{0\pi}^2}{(1-a_1)\mu_I^2} & \mu_I > \mu_c \end{cases} \quad (6.112)$$

$$\langle i\bar{q}\gamma_5\tau_1q \rangle^{LO}(\mu_I) = \begin{cases} 0 & \mu_I < \mu_c \\ -2B_0F^2\sqrt{1 - \frac{M_{0\pi}^4}{(1-a_1)^2\mu_I^4}} & \mu_I > \mu_c \end{cases} \quad (6.113)$$

$$n_I^{LO}(\mu_I) = \begin{cases} \frac{1}{2}(a_1 + a_2)F^2\mu_I & \mu_I < \mu_c \\ \frac{1}{2}F^2\mu_I \left(2 - a_1 + a_2 - \frac{2M_{0\pi}^4}{(1-a_1)\mu_I^4} \right) & \mu_I > \mu_c \end{cases} \quad (6.114)$$

Note that the only dependence with a_2 shows up in the pion density, which should remain zero below the BEC point. Therefore, with that physical requirement we fix

$$a_2 = -a_1 + \mathcal{O}(1/F^2) \quad (6.115)$$

up to higher order corrections, which leaves us only with one free parameter at this order.

The condition (6.115) is an example of the physical conditions implying LEC relations, mentioned in subsection 6.3.1. It has to be understood as a constraint on $a_{1,2}$ relative size under the chiral power counting. As explained, this is not contradictory with the effective Lagrangian framework, where at the Lagrangian level the field operators corresponding to $a_{1,2}$ are indeed independent. In subsection 6.3.3 we will discuss additional constraints at NLO. In fact, we will see that when all contributions from ϵ_4 are properly taken into account, one gets actually $a_{1,2} = \mathcal{O}(1/F^2)$ so that all a_1 corrections to the energy density fall formally into the NLO.

Now, we will discuss more quantitatively the effects of the new terms to leading order, by contrasting the results for different observables with those obtained in the lattice. For that purpose, we have considered the most recent lattice results. In particular, we will use the lattice points provided in [235] at $T = 0$, coming from the collaboration [249], for the quark and pion condensates. The latter are given for a finite pionic source. We take $j = 0.00517054M_\pi$, one of the two values considered in [235]. As for the isospin density, we compare with the results quoted in [249] for $j = 0$ and T small enough to

provide an accurate enough description of the $T = 0$ case. We also fix the numerical values of $M_\pi = 131$ MeV, $F_\pi = 90.51$ MeV and $m_l = 3.47$ MeV for an easier comparison with the results in [235, 249]. In addition, we assign a characteristic uncertainty of 5% to the lattice data, following again [235, 249].

As discussed above, the new LO contributions considered here in the Lagrangian are parametrized only in the constant a_1 . A relevant question is then whether $a_1 \neq 0$ is preferred for lattice results over the standard choice $a_1 = 0$. In that context, recall that $a_1 \neq 0$ implies in particular a displacement in the critical value μ_c with respect to the pion mass. In fact, $\mu_c = M_\pi$ is not actually a prediction of lattice analyses. In some of those works, like [248], that condition is imposed invoking ChPT, as part of the continuum extrapolation within the procedure to reduce the uncertainty around the critical point. On the other hand, the results in [249] are compatible with a nonzero value for the isospin density below $\mu_I = M_\pi$, which would call for $\mu_c < M_\pi$ and then $a_1 < 0$ according to (6.107). In fact, as we are about to see, fits to lattice points consistently favor a negative nonzero value for a_1 .

Thus, we show here the results of three different fits, which are summarized in Table 6.5 and Figs. 6.15, 6.16 and 6.17. The uncertainty bands in the figures and the uncertainty range for the a_1 parameter correspond to the 95% confidence level.

Those results lead to the following partial conclusions. First, the quark and pion condensates can be reasonably fitted with $a_1 = 0$ within the uncertainties considered (fit 1). Fitting only the quark (pion) condensate favors a positive (negative) a_1 value, still compatible with zero. However, the conclusion is very different when fitting the isospin density in fit 2, for which we have included only the lattice points with $\mu_I > M_\pi$. As explained in [249], the lattice uncertainty for $\mu_I \sim M_\pi$ is actually much higher, although we have still plotted the first lattice point below μ_I and given in [249]. As mentioned above, that point lies below M_π with a nonzero isospin density central value, which is actually favored by our present analysis with negative a_1 . In fact, as can be seen from the results in Table 6.5, the lattice results for n_I are much better fitted with a negative value for a_1 than for $a_1 = 0$, as the values of the corresponding χ^2/dof clearly show. The same conclusion is reached when performing a combined fit of the three observables (fit 3), with significant corrections from the $a_1 = 0$ case. Note also that the fits for n_I reproduce quite well the two ends of the lattice points, i.e., the closest points to $\mu_I = M_\pi$ and those for larger $\mu_I > M_\pi$, improving over the $a_1 = 0$ case.

In Fig. 6.18 we show the results for α_0^{LO} , i.e., the solution of the equation $\frac{\partial \epsilon_2}{\partial \alpha} = 0$,

FIT	a_1	χ^2/dof	$\chi^2/\text{dof}, a_1 = 0$
1: $\langle i\bar{q}\gamma_5\tau_1 q \rangle, \langle \bar{q}q \rangle$	$0.000^{+0.036}_{-0.038}$	0.64	0.64
2: n_I	-0.020 ± 0.007	1.39	7.30
3: $\langle i\bar{q}\gamma_5\tau_1 q \rangle, \langle \bar{q}q \rangle, n_I$	-0.019 ± 0.007	0.84	2.03

Table 6.5: Results for the a_1 constant in different fits to quark and pion condensates and isospin density.

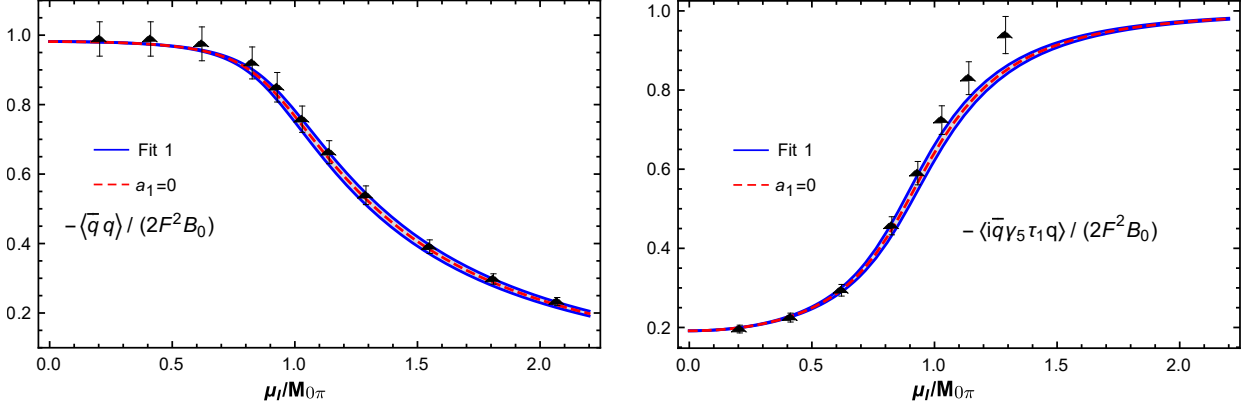


Figure 6.15: Combined fit of the quark condensate (left) and the pion condensate (right) for $j = 0.00517054M_\pi$. Lattice points are taken from [235].

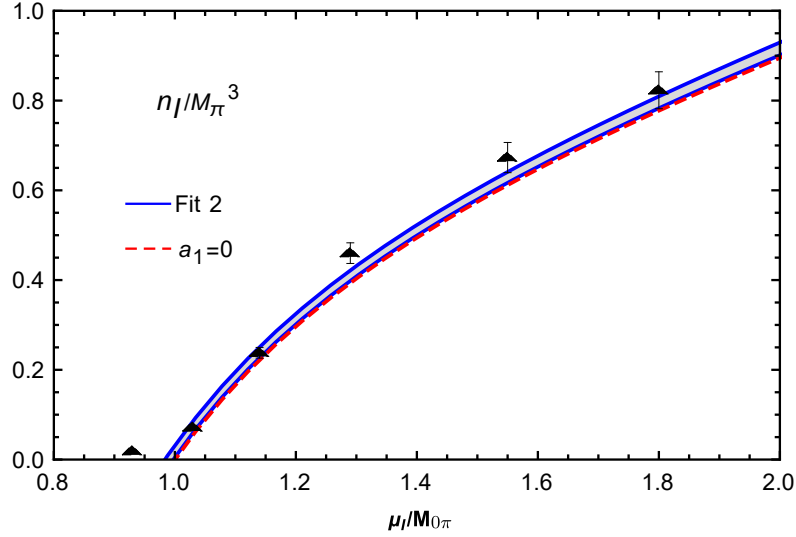


Figure 6.16: Fit of the isospin density for $j = 0$. Lattice points are taken from [249].

for the value of a_1 obtained in the joint fit 3, both for $j = 0$ and for the value of j used here. The explicit expression of α_0^{LO} is given in (6.107). While for $j = 0$, the a_1 contribution changes the transition point to the BEC phase, as already commented, for

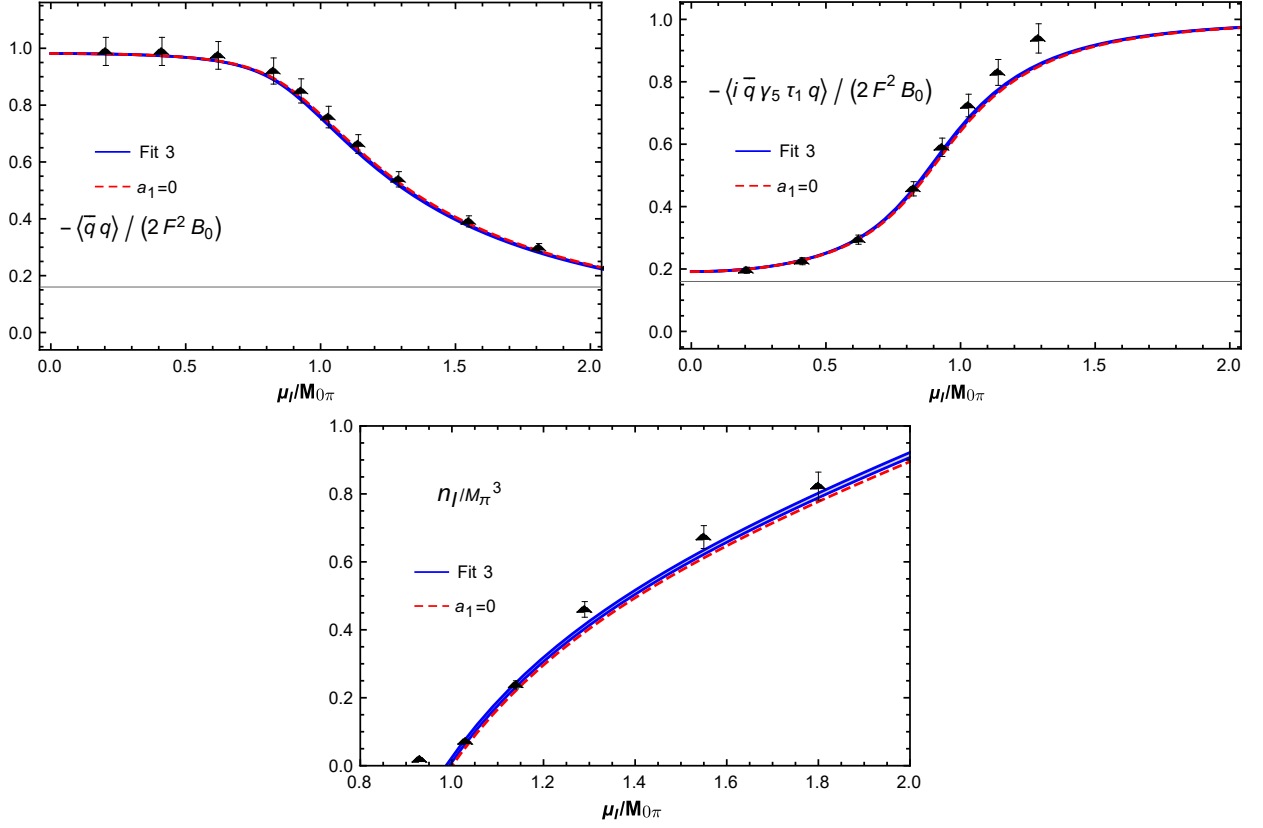


Figure 6.17: Combined fit of the quark condensate (upper left panel), the pion condensate (upper right panel) and the isospin density (lower panel). Lattice points are the same as in Figs 6.15 and 6.16.

$j \neq 0$ the transition is a crossover and a_1 merely modifies the inflection point of the α_0^{LO} function.

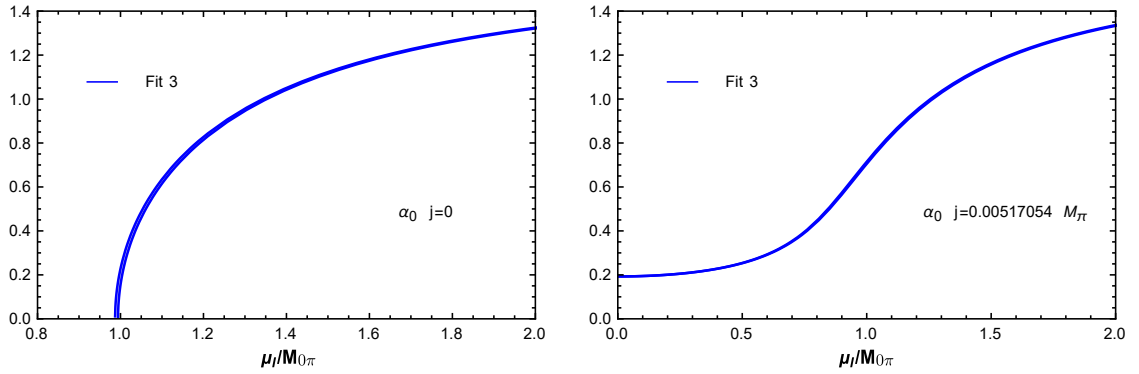


Figure 6.18: α_0^{LO} as a function of $\mu_I/M_{0\pi}$ for $j = 0$ (left) and $j = 0.00517054 M_\pi$ (right).

To summarize this section, lattice results are perfectly compatible with a coefficient $a_1 \neq 0$, which actually improves the description of the isospin density and the overall description of n_I and the two condensates.

6.3.3 Next to leading order results

The next to leading corrections ϵ_4 to the energy density come from three different sources. The first is the one-loop contribution coming from the quadratic field terms (6.101) in the $\mathcal{L}_2$ Lagrangian, which can be obtained in a similar fashion as to the standard free-field contributions to the partition function in vacuum, including now the μ_I -corrections to the pion dispersion relation [196]. The second is given by the constant terms coming from the $\mathcal{L}_4$. The LEC coming from this contribution, including the new ones coming from $\mathcal{L}_4^Q$, will be renormalized to absorb the loop divergences. The last contribution come from the linear field terms, which appear in the $\mathcal{L}_2$ and are given in (6.100).

Loop contributions

Following the same steps as in previous works [196] we can write the one-loop contribution to the energy density as

$$\epsilon_4^{loop} = \frac{1}{2} \int_p [E_+(p) + E_-(p)] + \frac{1}{2} \int_p E_0(p) \quad (6.116)$$

with $E_\pm(p)$ and $E_0(p)$ in (6.108)-(6.109) and, following the notation in [196],

$$\int_p = \mu^{2\epsilon} \int \frac{d^{D-1}p}{(2\pi)^{D-1}} \quad (6.117)$$

with $D = 4 - 2\epsilon$ and $\epsilon \rightarrow 0^+$ and μ the Dimensional Regularization scale.

The treatment of the above integrals, separating their UV divergent contribution in DR follows the same steps as in [196] except for the modifications proportional to a_1 in equations (6.102)-(6.105). The contribution from the charged pions to the one-loop energy density can be written as

$$\frac{1}{2} \int_p [E_+(p) + E_-(p)] = \epsilon_{4,+-}^{div} + \epsilon_{4,+-}^{fin} \quad (6.118)$$

with

$$\epsilon_{4,+-}^{div} = \frac{1}{2} \int_p [E_1(p) + E_2(p)] \quad (6.119)$$

$$\epsilon_{4,+-}^{fin} = \frac{1}{2} \int_p [E_+(p) + E_-(p) - E_1(p) - E_2(p)] \quad (6.120)$$

and where we have introduced the quantities $E_{1,2}(p)$ given by

$$\begin{aligned}
 E_{1,2}(p) &= \sqrt{p^2 + \hat{m}_{1,2}^2} \\
 \hat{m}_1^2 &= (M_{0\pi}^2 + \mu_I^2 \cos \alpha) \cos \alpha - (1 - a_1) \mu_I^2 \cos 2\alpha + 2B_0 j \sin \alpha \\
 \hat{m}_2^2 &= (M_{0\pi}^2 + a_1 \mu_I^2 \cos \alpha) \cos \alpha + 2B_0 j \sin \alpha \\
 \hat{m}_3^2 &= m_3^2 = M_{0\pi}^2 \cos \alpha + (1 - a_1) \mu_I^2 \sin^2 \alpha + 2B_0 j \sin \alpha
 \end{aligned} \tag{6.121}$$

Separating in this way the divergent part of the charged contribution, $\epsilon_{4,+}^{div}$ in (6.119) has the form of the neutral part in (6.116) and is easier to handle in DR. Actually, note that the large- p behavior of $E_1 + E_2$ is the same as the sum $E_+ + E_-$. The finite contribution (subtraction integral) $\epsilon_{4,+}^{fin}$ can be calculated numerically. Thus, in DR we get for the full divergent part

$$\left(\epsilon_4^{loop} \right)_{div} = \frac{1}{2} \int_p [E_1(p) + E_2(p)] + \frac{1}{2} \int_p E_0(p) = - \sum_{i=1}^3 \frac{\hat{m}_i^4}{4(4\pi)^2} \left[N_\epsilon + \frac{3}{2} + \log \left(\frac{\mu^2}{\hat{m}_i^2} \right) \right] \tag{6.122}$$

with $N_\epsilon = \frac{1}{\epsilon} - \gamma + \log(4\pi)$ and γ the Euler constant.

Fourth order Lagrangian and renormalization

The contributions to the energy density coming from the constant part in the fourth order Lagrangian are respectively given by

$$\begin{aligned}
 \epsilon_4^{40} &= - (l_1 - l_2) \mu_I^4 \sin^4 \alpha - l_4 M_{0\pi}^2 \mu_I^2 \cos \alpha + l_4 M_{0\pi}^2 \mu_I^2 \cos^3 \alpha - 2l_4 B_0 \mu_I^2 j \sin \alpha \\
 &+ 2l_4 B_0 \mu_I^2 j \sin \alpha \cos^2 \alpha - (h_1 - l_4) M_{0\pi}^4 - (l_3 + l_4) M_{0\pi}^4 \cos^2 \alpha \\
 &- 2B_0 j (l_3 + l_4) M_{0\pi}^2 \sin(2\alpha) - 4B_0^2 j^2 [h_1 - l_4 + (l_3 + l_4) \sin^2 \alpha]
 \end{aligned} \tag{6.123}$$

$$\begin{aligned}
 \epsilon_4^{4Q} &= -\hat{q}_1 \mu_I^4 \sin^4 \alpha - \frac{1}{2} \hat{q}_2 M_{0\pi}^2 \mu_I^2 \cos \alpha - \frac{1}{2} \hat{q}_3 M_{0\pi}^2 \mu_I^2 \cos^3 \alpha - \hat{q}_4 B_0 \mu_I^2 j \sin \alpha \\
 &- \hat{q}_5 B_0 \mu_I^2 j \sin \alpha \cos^2 \alpha - \hat{q}_6 \mu_I^4 \cos^2 \alpha - \hat{q}_7 \mu_I^4
 \end{aligned} \tag{6.124}$$

with

$$\begin{aligned}
 \hat{q}_1 &= q_{10} - 2q_2 - 2q_3 - q_4 & \hat{q}_5 &= 8(q_6 + q_7) \\
 \hat{q}_2 &= 4q_5 - 2q_6 - 8q_7 & \hat{q}_6 &= \frac{1}{2}(-2q_1 + 2q_{10} - 2q_2 + q_9) \\
 \hat{q}_3 &= 4(q_6 + 2q_7) & \hat{q}_7 &= \frac{1}{4}(4q_1 - 3q_{10} + 4q_2 + q_8 - q_9) \\
 \hat{q}_4 &= 4(q_5 - q_6)
 \end{aligned}$$

Comparing (6.124) with (6.123), we see that new terms introduce μ_I -dependent corrections as follows: $\hat{q}_1$ shifts the $(l_1 - l_2)\mu_I^4$ contribution, $\hat{q}_{2,3,4,5}$ modify respectively the four $l_4\mu_I^2$ terms, whereas $\hat{q}_{6,7}$ introduce new μ_I^4 terms. Of those new seven independent LECs appearing in the energy density, $\hat{q}_4$ and $\hat{q}_5$ will not contribute for $j = 0$ and the $\hat{q}_7$ term is independent of α so it does not contribute to the energy density minimum.

The new LECs will precisely absorb the new loop divergences dependent on a_1 included in (6.122). Thus, the renormalized energy density at NLO resulting of adding all the contributions mentioned before can be written as

$$\begin{aligned}
 \epsilon_4^{loop} + \epsilon_4^{40} + \epsilon_4^{4Q} = & -\frac{1}{(4\pi)^2} \left[\frac{3}{2} - \bar{l}_3 + 4\bar{l}_4 + \log \left(\frac{M_{0\pi}^2}{\hat{m}_2^2} \right) + 2 \log \left(\frac{M_{0\pi}^2}{\hat{m}_3^2} \right) \right] \left[\frac{1}{4} M_{0\pi}^4 \cos^2 \alpha \right. \\
 & + B_0^2 j^2 \sin^2 \alpha + \frac{1}{2} M_{0\pi}^2 B_0 j \sin(2\alpha) \left. \right] - \frac{1}{2(4\pi)^2} \left\{ \frac{1}{2} + \frac{1}{3} \bar{l}_1 + \frac{2}{3} \bar{l}_2 + 2(4\pi)^2 \hat{q}_1^r \right. \\
 & - \frac{a_1}{2} \left[3(1 - a_1) + 4(1 - a_1) \log \left(\frac{\mu^2}{\hat{m}_1^2} \right) - a_1 \log \left(\frac{\mu^2}{\hat{m}_2^2} \right) + (2 - a_1) \log \left(\frac{\mu^2}{m_3^2} \right) \right] \left. \right\} \\
 & - \frac{M_{0\pi}^2 \mu_I^2}{(4\pi)^2} \left\{ \frac{1}{2} + \bar{l}_4 + \frac{(4\pi)^2}{2} \hat{q}_2^r - \frac{a_1}{2} \left[1 + \log \left(\frac{\mu^2}{\hat{m}_1^2} \right) + \log \left(\frac{\mu^2}{m_3^2} \right) \right] + \log \left(\frac{M_{0\pi}^2}{m_3^2} \right) \right\} \cos \alpha \\
 & + \frac{M_{0\pi}^2 \mu_I^2}{(4\pi)^2} \left\{ \frac{1}{2} + \bar{l}_4 - \frac{(4\pi)^2}{2} \hat{q}_3^r - \frac{a_1}{2} \left[2 + 2 \log \left(\frac{\mu^2}{\hat{m}_1^2} \right) + \log \left(\frac{\mu^2}{\hat{m}_2^2} \right) + \log \left(\frac{\mu^2}{m_3^2} \right) \right] \right\} \cos^3 \alpha \\
 & - \frac{2B_0 j \mu_I^2}{(4\pi)^2} \left\{ \frac{1}{2} + \bar{l}_4 + \frac{(4\pi)^2}{2} \hat{q}_4^r - \frac{a_1}{2} \left[1 + \log \left(\frac{\mu^2}{\hat{m}_1^2} \right) + \log \left(\frac{\mu^2}{m_3^2} \right) \right] + \log \left(\frac{M_{0\pi}^2}{m_3^2} \right) \right\} \sin \alpha \\
 & + \frac{2B_0 j \mu_I^2}{(4\pi)^2} \left\{ \frac{1}{2} + \bar{l}_4 - \frac{(4\pi)^2}{2} \hat{q}_5^r - \frac{a_1}{2} \left[2 + 2 \log \left(\frac{\mu^2}{\hat{m}_1^2} \right) + \log \left(\frac{\mu^2}{\hat{m}_2^2} \right) + \log \left(\frac{\mu^2}{m_3^2} \right) \right] \right\} \sin \alpha \cos^2 \alpha \\
 & + \frac{\mu_I^2}{(4\pi)^2} \log \left(\frac{M_{0\pi}^2}{m_3^2} \right) \left[2B_0 j \sin \alpha \cos^2 \alpha + M_{0\pi}^2 \cos^3 \alpha - \frac{1}{2} \mu_I^2 \sin^4 \alpha \right] \\
 & - \frac{1}{2(4\pi)^2} \left\{ 2(4\pi)^2 \hat{q}_6^r - \frac{a_1}{2} \left[1 - 3a_1 + 2(1 - 2a_1) \log \left(\frac{\mu^2}{\hat{m}_1^2} \right) - 2a_1 \log \left(\frac{\mu^2}{\hat{m}_2^2} \right) \right] \right\} \mu_I^4 \cos^2 \alpha \\
 & - \frac{1}{2(4\pi)^2} \left\{ 2(4\pi)^2 \hat{q}_7^r + \frac{a_1}{2} \left[1 - 2a_1 + (2 - 3a_1) \log \left(\frac{\mu^2}{\hat{m}_1^2} \right) - a_1 \log \left(\frac{\mu^2}{\hat{m}_2^2} \right) \right] \right\} \mu_I^4 \\
 & - \frac{1}{(4\pi)^2} (\bar{h}_1 - \bar{l}_4) [M_{0\pi}^2 + 4B_0^2 j^2] + \epsilon_{4,+}^{fin}
 \end{aligned} \tag{6.125}$$

where the renormalized and scale-independent $\bar{l}_i, \bar{h}_i$ are the standard ones given in (1.80) while the new LECs are renormalized as

$$\hat{q}_i = \hat{q}_i^r(\mu) - \eta_i \frac{\mu^{-2\epsilon}}{2(4\pi)^2} [N_\epsilon + 1] \tag{6.126}$$

with

$$\begin{aligned}
\eta_1 &= -3a_1 + 3a_1^2 & \eta_5 &= 8a_1 \\
\eta_2 &= -4a_1 & \eta_6 &= -a_1 + 3a_1^2 \\
\eta_3 &= 8a_1 & \eta_7 &= a_1 - 2a_1^2 \\
\eta_4 &= -4a_1 & &
\end{aligned} \tag{6.127}$$

where, as usual, the μ -dependence of the renormalized LECs cancels with that of the loops, rendering the energy density finite and scale independent. In the following we will analyze the effect of these new LECs on the μ_I -dependence of the different observables obtained from the energy density.

The numerical values we will use for the $\bar{l}_i$ as well as for the physical pion mass and decay constant will be the same as the previous works on this subject [235, 250] for an easier comparison. Thus, we will take the central values of the $\bar{l}_i, \bar{h}_i$ from [252]:

$$\bar{l}_1 = -0.4, \quad \bar{l}_2 = 4.3, \quad \bar{l}_3 = 2.9, \quad \bar{l}_4 = 4.4, \quad \bar{h}_1 - \bar{l}_4 = -1.5, \tag{6.128}$$

which have been used to study the quark and pion condensates in [235] and the isospin density in [250] at zero temperature.

As for the physical M_π, F_π , as commented above, we are considering those used in the lattice simulations, which using the one-loop standard ChPT expressions (1.81) and (1.82) give rise for the following values of the tree-level $M_{0\pi}, F$ appearing in our previous expressions for the energy density:

$$M_\pi = 131 \text{ MeV}, \quad M_{0\pi} = 132.49 \text{ MeV}, \quad F_\pi = 90.51 \text{ MeV}, \quad F = 84.93 \text{ MeV}. \tag{6.129}$$

Recall that the $\bar{l}_i, \bar{h}_i$, although scale-independent are mass-dependent and therefore there might be slight numerical variations from the values (6.128) when taking the masses in (6.129). Those variations are logarithmic and therefore numerically negligible, so for our purposes of comparing with previous works we will still use the values in (6.128).

As for the $\hat{q}_i$ constants, for simplicity we will consider them within natural values, defined as a characteristic ChPT uncertainty range [41, 199] as

$$|\hat{q}_i^r| \leq \frac{1}{16\pi^2} \tag{6.130}$$

at a typical chiral scale, which we will set as $\mu = M_\rho \simeq 770$ MeV from now on. Recall that all our results are independent of the scale μ .

Linear terms

The solution for the angle minimizing the energy density to leading order, given in (6.107) for $j = 0$, is such that the linear term in (6.100) proportional to $\pi_1(x)$ vanishes so the linear terms can be ignored since the derivative term in (6.100) does not contribute to the vacuum energy density. However, this is not necessarily true to higher orders. That is, if we consider a perturbative deviation of the LO minimizing angle,

$$\alpha = \alpha_0^{LO} + \delta\alpha_0 \quad (6.131)$$

with $\alpha_0^{LO} = \mathcal{O}(1)$, $\delta\alpha_0 = \mathcal{O}(1/F)$ in the chiral expansion, we can write

$$\mathcal{L}_2^{lin} = f'(\alpha_0^{LO})(\alpha - \alpha_0^{LO})\pi_1(x) + \mathcal{O}(1/F) + \dots \quad (6.132)$$

where the dots denote derivative terms and, according to (6.100),

$$f(\alpha) = -F \sin \alpha \left[M_{0\pi}^2 - (1 - a_1)\mu_I^2 \cos \alpha \right] + 2B_0 F j \cos \alpha \quad (6.133)$$

The above linear contribution to NLO can be reabsorbed into a redefinition of the π_1 field, over which we are integrating to get the energy density. Namely,

$$\pi_1 \rightarrow \pi_1 + \frac{f'(\alpha_0^{LO})}{m_1^2(\alpha_0^{LO})}(\alpha - \alpha_0^{LO}) \quad (6.134)$$

The above shift eliminates the linear term at this order and completing squares generates the following additional $\mathcal{O}(1)$ perturbative contribution to the NLO energy density:

$$\epsilon_4^{lin} = -\frac{1}{2} \frac{[f'(\alpha_0^{LO})]^2}{m_1^2(\alpha_0^{LO})} (\alpha - \alpha_0^{LO})^2 \quad (6.135)$$

with m_1^2 in (6.103), which added to the contributions given in (6.116), (6.123) and (6.124) has to be minimized with respect to α , around α_0^{LO} , to find α_0^{NLO} . Moreover, it must be taken into account to calculate different observables because of its m , j and μ_I

dependences:

$$\Delta\langle\bar{q}q\rangle_{lin}^{NLO} = \frac{\partial\epsilon_4^{lin}}{\partial m} = -B_0 F^2 \cos(\alpha_0^{LO}) (\alpha - \alpha_0^{LO})^2 \quad (6.136)$$

$$\Delta\langle i\bar{q}\gamma_5\tau_1 q\rangle_{lin}^{NLO} = \frac{\partial\epsilon_4^{lin}}{\partial j} = -B_0 F^2 \sin(\alpha_0^{LO}) (\alpha - \alpha_0^{LO})^2 \quad (6.137)$$

$$\Delta(n_I)_{lin}^{NLO} = -\frac{\partial\epsilon_4^{lin}}{\partial\mu_I} = -\mu_I F^2 (1 - a_1) \cos(2\alpha_0^{LO}) (\alpha - \alpha_0^{LO})^2 \quad (6.138)$$

To have a more quantitative idea of the effect of this correction, we have plotted in Fig. 6.19 the result for the minimizing angle α_0 , comparing the LO contribution with the NLO with and without including the linear term contribution (6.135). For easier comparison with previous works, we have not included in that plot the new contributions coming from the a_1 and q_i terms and we have used the LEC given in (6.128). We consider both the $j = 0$ and $j \neq 0$ situations. As we can see in that figure, the inclusion of the linear term may generate sizable differences between the NLO and LO results. Actually, for some values of the constants involved, those linear corrections can be such that the effective potential stops having a minimum above a certain μ_I value. We can actually see this behaviour in the plot showed in Fig. 6.19 for which that limiting value is $\mu_I \simeq 300$ MeV for $j = 0$ and $\mu_I \simeq 340$ MeV for the $j \neq 0$ value considered. The deviations with respect to the LO indicate that we are reaching the borderline of the ChPT validity limit where in particular the very same approximation followed in (6.131) and (6.132) would fail. This is actually consistent with lattice analyses showing that deviations from ChPT around those μ_I values signal the onset of the BCS phase [237]. Nevertheless, it should be taken into account that the actual value of such validity limit depends also on the rest of the LEC involved, as we will discuss in detail below.

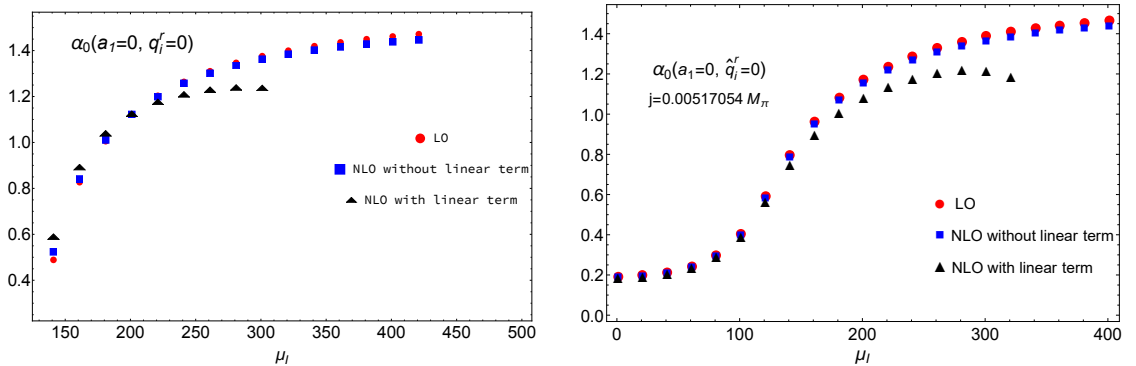


Figure 6.19: Effect of the linear term in the minimizing angle α_0 for $j = 0$ (left) and $j \neq 0$ (right).

NLO constraints

First, let us discuss the constraints that arise for the LEC from the condition of vanishing isospin density for $\mu_I < \mu_c$, i.e., the extension to NLO of the LO constraint (6.115). Thus, let us denote $\mu_c^{LO} = \frac{M_{0\pi}}{\sqrt{1-a_1}}$ and μ_c^{NLO} the NLO value for μ_c which will be determined explicitly below and which depends on the $\hat{q}_i^r$ constants.

Note that by definition, $\alpha^{NLO}(\mu_I < \mu_c^{NLO}) = 0$. In addition, the linear term correction (6.135) vanishes for μ_I below μ_c^{NLO} and μ_c^{LO} since $\alpha^{LO}(\mu_I < \mu_c^{LO}) = 0$ but it would survive for $\mu_c^{LO} < \mu_I < \mu_c^{NLO}$ provided $\mu_c^{LO} < \mu_c^{NLO}$. Therefore, taking the derivative with respect to μ_I and setting $j = \alpha = 0$ in our previous expressions for the energy density, we get,

$$\begin{aligned} \bullet \quad \mu_c^{LO} > \mu_c^{NLO} &\Rightarrow n_I(\mu_I < \mu_c^{NLO}) = n_0(\mu_I) \\ \bullet \quad \mu_c^{LO} < \mu_c^{NLO} &\Rightarrow n_I(\mu_I < \mu_c^{NLO}) = \begin{cases} n_0(\mu_I) + n_1(\mu_I) & \mu_c^{LO} < \mu_I < \mu_c^{NLO} \\ n_0(\mu_I) & \mu_I < \mu_c^{LO} \end{cases} \end{aligned}$$

with

$$\begin{aligned} n_0(\mu_I) &= \frac{F^2}{2}(a_1 + a_2)\mu_I + M_{0\pi}^2(\hat{q}_2^r + \hat{q}_3^r)\mu_I + 4(\hat{q}_6^r + \hat{q}_7^r)\mu_I^3 \\ &\quad + \frac{a_1}{8\pi^2(M_{0\pi}^2 + a_1\mu_I^2)} \left[\frac{M_{0\pi}^4}{4}\mu_I + (M_{0\pi}^2 + a_1\mu_I^2)^2 \log\left(\frac{\mu^2}{M_{0\pi}^2 + a_1\mu_I^2}\right) \right] + \mathcal{O}\left(\frac{1}{F^2}\right) \\ n_1(\mu_I) &= \frac{1}{2} \frac{\partial}{\partial \mu_I} \left[\frac{\alpha_0^{LO}(\mu_I) f'_0[\alpha_0^{LO}(\mu_I)]}{m_1(\mu_I)} \right]^2 + \mathcal{O}\left(\frac{1}{F^2}\right) \end{aligned} \tag{6.139}$$

where $f_0 = f(j=0)$ with f in (6.133) and we have followed [196] for the calculation of the loop integrals.

Thus, since the μ_I dependence of the n_1 function above (coming from the linear term) is non-polynomial, the only way to ensure that n_I vanishes for all μ_I below μ_c^{NLO} is that the $\hat{q}_i^r$ satisfy the constraint

$$\mu_c^{NLO}(\hat{q}_i^r) < \mu_c^{LO} \tag{6.140}$$

On the other hand, the condition that the n_0 function in (6.139) vanishes, together with (6.115), implies at this order:

$$a_1, a_2 = \mathcal{O}\left(\frac{1}{F^2}\right) \quad (6.141)$$

$$a_1 + a_2 = -\frac{2M_{0\pi}^2}{F^2} [\hat{q}_2^r(\mu) + \hat{q}_3^r(\mu)] + \mathcal{O}\left(\frac{1}{F^4}\right) \quad (6.142)$$

$$\hat{q}_6^r(\mu) + \hat{q}_7^r(\mu) = \mathcal{O}\left(\frac{1}{F^2}\right) \quad (6.143)$$

The constraints (6.142) and (6.143) allow us to eliminate the dependence on two of the LEC involved in terms of the remaining ones. In fact, note that equation (6.142) is actually the explicit expression for the $\mathcal{O}(1/F^2)$ in (6.115). We also remark that the condition (6.141) is fully consistent with having obtained a numerical value $|a_1| \ll 1$ in our fit study in section 6.3.2. The situation is similar to the EM corrections in ChPT, where there are operators which are formally $\mathcal{O}(p^2)$, such as (6.8), but multiplied by e^2 which is a numerically small parameter. Actually, in view of the above considerations, if we had normalized $a_{1,2} = \frac{M_{0\pi}^2}{F^2} \hat{a}_{1,2}$ so that the $\hat{a}_i$ would be parametrically of the same order as the $\hat{q}_i$, then conditions such as (6.142) or (6.148) below would translate into mass-independent relations. As commented in subsection 6.3.2, we are following the standard convention of ordering the Lagrangians according to the chiral order of the field operators, but from the above results we could have equally considered formally the $a_{1,2}$ terms as part of the fourth order Lagrangian. On the other hand, equation (6.142) provides the explicit expression for the $\mathcal{O}(1/F^2)$ corrections in (6.115), while the condition (6.143) will be applied in what follows to eliminate the dependence on $\hat{q}_7$ and a_2 .

Now, let us evaluate the effect of the NLO corrections to the critical value μ_c . Since $\frac{\partial \epsilon^{NLO}}{\partial \alpha}|_{\alpha=0} = 0$, μ_c can be determined as the value for which $\alpha = 0$ flips from a local minimum to a local maximum. Therefore, expanding the energy density around $\alpha = 0$,

$$\epsilon = \beta_0(\mu_I) + \beta_2(\mu_I)\alpha^2 + \mathcal{O}(\alpha^4) \quad (6.144)$$

we have

$$\beta_2(\mu_I)|_{\mu_I=\mu_c} = 0 \quad (6.145)$$

From the energy density discussed above, we find

$$\begin{aligned} \beta_2(\mu_I) = & \frac{1}{2}F_\pi^2 [M_\pi^2 - (1 - a_1)\mu_I^2] + \frac{1}{4}\mu_I^2 [M_{0\pi}^2 (\hat{q}_2^r + 3\hat{q}_3^r) + 4\hat{q}_6^r\mu_I^2] \\ & - \frac{F^2(\mu_I^4 - M_{0\pi}^4)}{2\mu_I^2} + \mathcal{O}\left(\frac{1}{F^2}\right) \end{aligned} \quad (6.146)$$

where M_π and F_π are the NLO pion decay constant and mass given in equations (1.82) and (1.81) respectively and where we have made use of the condition (6.141) so that the a_1 dependence in the NLO has been ignored. The last term in (6.146), proportional to F^2 , comes from the linear-field contribution (6.135). Note that we are interested in the expansion around $\alpha = 0$ only in order to determine μ_c^{NLO} . Therefore, μ_I lies around $\mu_c^{LO} = M_{0\pi} [1 + \mathcal{O}(F^{-2})]$ so that the linear-field contribution just mentioned remains of NLO, as it should.

From the previous expression, we see that only $\hat{q}_{2,3,6}^r$ and a_1 modify the critical BEC value. We show in Table 6.6 the value of μ_c^{NLO} expected within the range of natural values for those constants in (6.130) and taking $a_1 = -0.019$, the central value of fit 3 to lattice results in subsection 6.3.2. In addition, we have highlighted in the table the values for which the condition (6.140) holds. As explained, $\hat{q}_i^r$ values not satisfying that condition are not acceptable, since they give rise to a nonzero isospin density below the critical value. Note that, as happened at LO, our results support $\mu_c < M_\pi$, which, as showed in section 6.3.2, is compatible with lattice results.

Anyhow, we remark that, due to the condition (6.141), parametrically we have at leading order

$$\mu_c^{LO} = M_{0\pi} + \mathcal{O}\left(\frac{1}{F^2}\right) = M_\pi + \mathcal{O}\left(\frac{1}{F^2}\right) \quad (6.147)$$

while at next-to-leading order, from (6.146), the condition $\mu_c = M_\pi$ could be satisfied by imposing an additional constraint relating $\hat{q}_{2,3,6}^r$ and a_1 , namely,

$$\mu_c^{NLO} = M_\pi \Rightarrow a_1 F_\pi^2 + \frac{M_\pi^2}{2} \left[\hat{q}_2^r + 3\hat{q}_3^r + 4\hat{q}_6^r + \frac{\bar{l}_3}{8\pi^2} \right] = \mathcal{O}\left(\frac{1}{F^2}\right) \quad (6.148)$$

where $\bar{l}_3$ arises from the $M_\pi^2 - M_{0\pi}^2$ difference [34] and we have replaced $M_{0\pi}$ by M_π in the NLO when the difference is of higher order. Since $M_\pi < M_{0\pi}$, the consistency condition in eq.(6.140) is compatible with (6.148), ensuring a vanishing isospin density below μ_c . If the constraint (6.148) is imposed, a further LEC could be eliminated.

It is important to observe, from (6.148), that maintaining $\mu_c^{NLO} = M_\pi$ requires at least one nonzero value for the new LEC $a_1, \hat{q}_i$, which comes from the fact that

$\beta_2(\mu_c = M_\pi) \neq 0$ for $a_1 = \hat{q}_i = 0$, with β_2 in (6.146) due to the linear term contribution. That is, taking into account also the above results, the presence of the linear term implies that the conditions $n_I(\mu_I < \mu_c) = 0$ and $\mu_c = M_\pi$ can be mutually satisfied at NLO only if the new terms considered here are taken into account. Recall that in previous ChPT studies [196, 235] those conditions hold but the linear term was not considered.

As explained in section 6.3.2, $\mu_c \neq M_\pi$ is theoretically allowed when interactions are included within the most general effective Lagrangian formalism, and is indeed consistent with lattice. Nevertheless, we will evaluate numerically the different observables to NLO in the following section with and without using the constraint (6.148), which physically amounts to impose that the system still behaves as a noninteracting Bose gas as far as the critical point is concerned. In any case, deviations will be small, consistently with (6.147).

μ_c^{NLO}/M_π	$\hat{q}_6^r = \frac{1}{16\pi^2}$		$\hat{q}_6^r = -\frac{1}{16\pi^2}$	
	$\hat{q}_3^r = \frac{1}{16\pi^2}$	$\hat{q}_3^r = -\frac{1}{16\pi^2}$	$\hat{q}_3^r = \frac{1}{16\pi^2}$	$\hat{q}_3^r = -\frac{1}{16\pi^2}$
$\hat{q}_2^r = \frac{1}{16\pi^2}$	1.007	0.935	0.916	0.803
$\hat{q}_2^r = -\frac{1}{16\pi^2}$	1.005	0.873	0.874	0.773

Table 6.6: Critical value of the BEC transition for natural values of $\hat{q}_2^r$, $\hat{q}_3^r$ and $\hat{q}_6^r$. The highlighted values are those fulfilling the condition (6.140).

NLO Results for different observables

We will consider now the NLO evolution of chiral observables for nonzero μ_I , in particular regarding the role of the $\hat{q}_i^r$ LEC and the comparison with lattice analyses. From the results in the previous sections, we see that the NLO energy density depends on seven independent new LECs, namely $a_1, \hat{q}_{1-6}^r$ whose numerical values will then influence the μ_I dependence of the observables. Note that all the observables considered depend on $\hat{q}_{1-6}^r$ since, in addition to the explicit $\hat{q}_i^r$ dependence one must consider that in α_0^{NLO} . We will represent our results for the range of natural values (6.130) at the scale $\mu = M_\rho$ and setting $a_1 = -0.019$ (the mean value obtained in Fit 3). Thus, we have 3^6 points for each μ_I , corresponding to the three values $0, \pm 1/(16\pi^2)$. In doing so, we discard those $\hat{q}_i^r$ violating the condition (6.140) and we calculate the mean square error of the results which provides a dispersion estimation. Note that, as commented before, due to the linear term, the minimum could disappear above a given μ_I . Thus, the uncertainty bands in the following figures for a given $\mu_I > \mu_c$ correspond to those $\hat{q}_i^r$ combinations

for which the minimum exists. The effect of the linear term will be actually showed separately in the figures in order to calibrate better its effect. In addition, as we have just mentioned, we will show separately the results with and without imposing the NLO condition $\mu_c = M_\pi$ in (6.148).

First, in Fig. 6.20, we show α_0^{NLO} , i.e., the angle minimizing the energy density including NLO corrections. We see that including all the corrections discussed here implies sizable deviations above μ_c with respect to the LO, larger than in previous analyses [196, 235]. Note in particular the tail below $\mu_I = M_\pi$ coming from the reduction in the numerical value of μ_c^{NLO} as Table 6.6 shows.

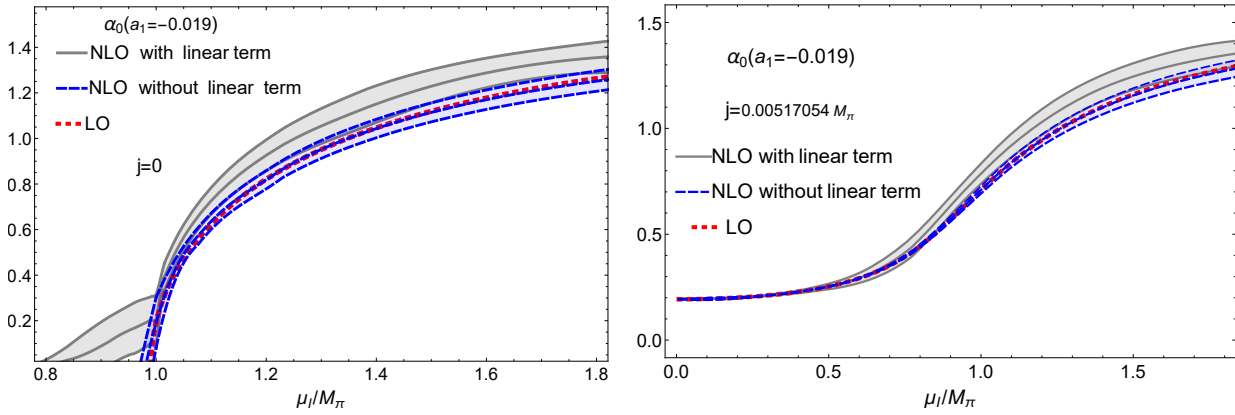


Figure 6.20: Results for the minimizing angle α_0 at NLO for finite source $j = 0$ (left) and $j = 0.00517054 M_\pi$ (right), with $a_1 = -0.019$ and natural values for $\hat{q}_{1-6}^r$.

We plot in Fig. 6.21 the quark and pion condensate deviations (as defined in [235]) at NLO for natural values of $\hat{q}_i^r$ with and without linear term, comparing with lattice results. The NLO corrections are again significant and remain within the uncertainties of lattice points, taking into account that we are not performing a NLO fit so there would be still room for improvement. The NLO corrections actually improve over the LO fit for the pion condensate for high μ_I values, whereas in the case of the quark condensate, with the inclusion of the linear term, the theoretical curve seems to depart from the lattice points with respect to the LO.

Finally, we study the isospin density at NLO for $j = 0$. The result, including the uncertainty bands of $\hat{q}_i^r$ natural values, are showed in Fig. 6.22. As for previous observables, the NLO with the new terms considered in this work provides significant deviations from the LO as μ_I increases, still accommodating the lattice results.

As explained above, for the NLO analysis we have fixed a_1 to the LO fit and consider the new $\hat{q}_i^r$ within natural values. In view of the results in Figs. 6.21 and 6.22, we would

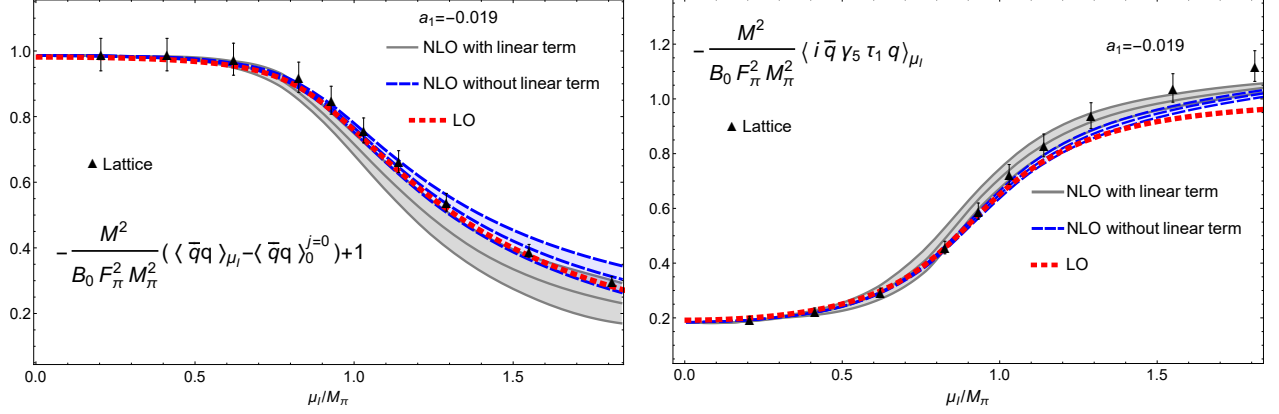


Figure 6.21: Results for the quark condensate deviation (left) and pion condensate deviation (right) as a function of μ_I/M_π at NLO for finite source $j = 0.005170554M_\pi$, $a_1 = -0.019$ and natural values for $\hat{q}_i^r$. The lattice data are from [235].

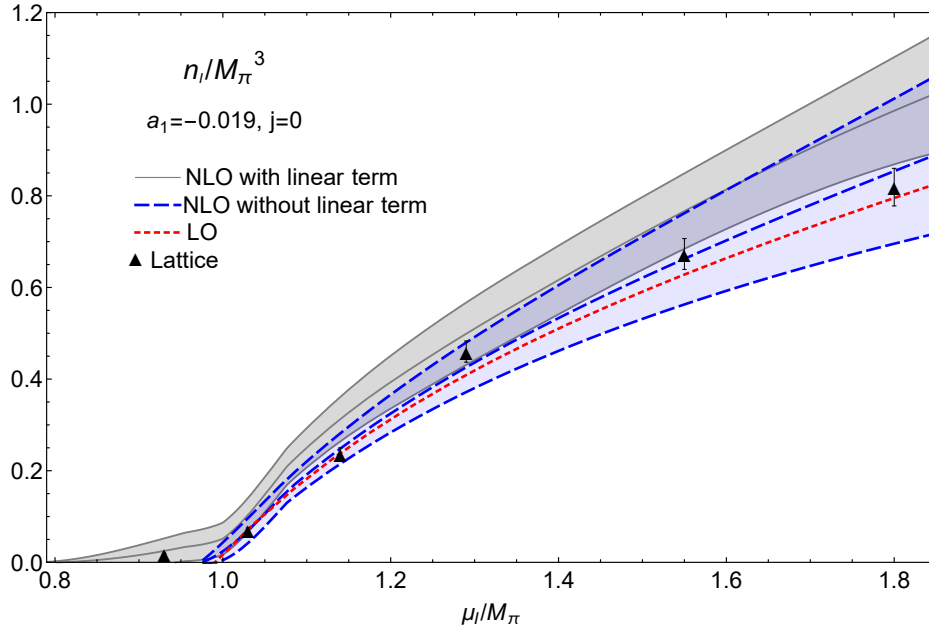


Figure 6.22: Normalized isospin density as a function of μ_I/M_π at NLO with and without the linear term. Lattice points are taken from [249].

surely have obtained a much better description of lattice results by keeping a_1 and the $\hat{q}_i^r$ as fit parameters with the NLO curves, but such precision analysis is outside the scope of this work.

Finally, in Fig. 6.23 we show the same observables as in Figs. 6.21 and 6.22 but using equation (6.148) to fix $\mu_c = M_\pi$ and eliminate the constant $\hat{q}_3^r$ in terms of a_1 , $\hat{q}_2^r$ and $\hat{q}_6^r$. The pion and quark condensate corrections at NLO fixing $\mu_c = M_\pi$ remain very close to the corrections calculated without setting the critical value and, as in that case, most of the lattice data fall into the uncertainty bands. As for the isospin density, fixing

$\mu_c = M_\pi$ narrows the uncertainty band around the pion mass since n_I vanishes in that case below M_π , remaining compatible with lattice data.

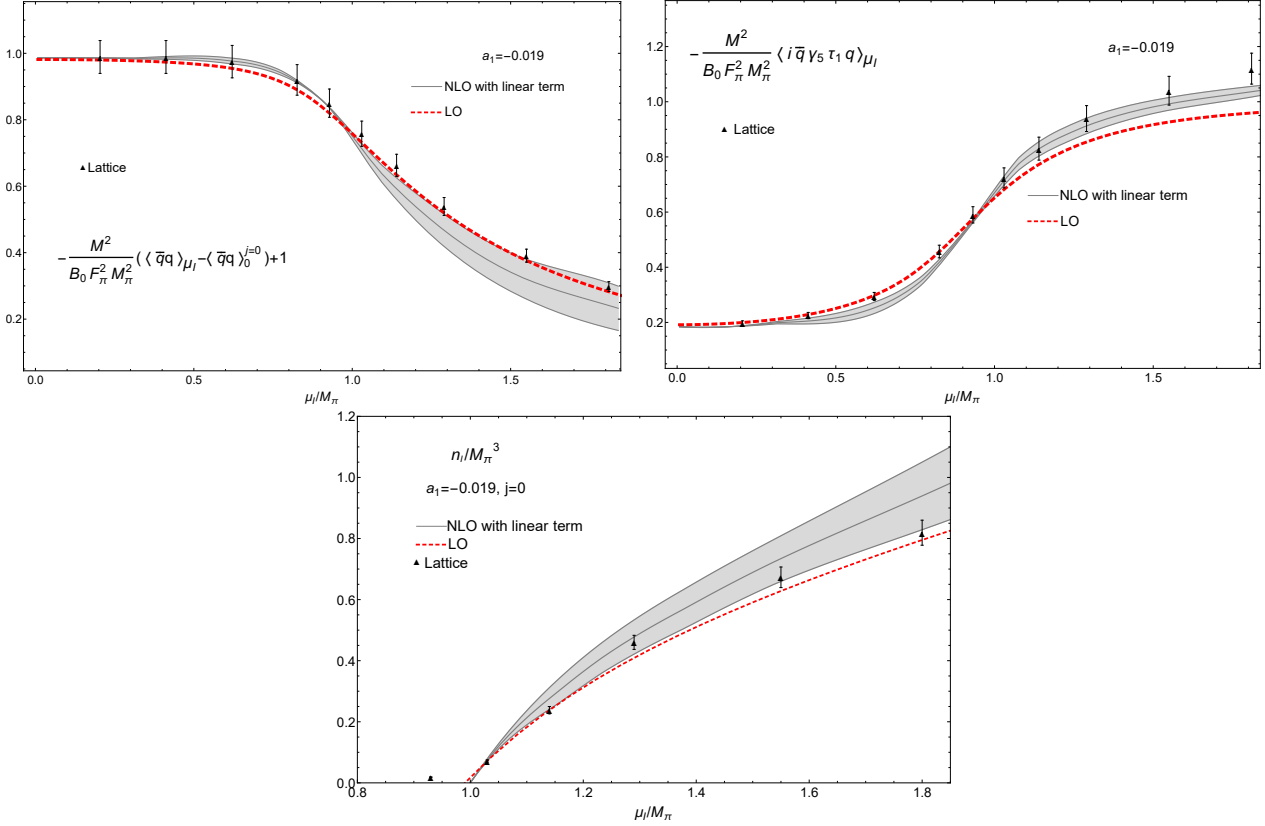


Figure 6.23: Results for the quark condensate (upper left panel), pion condensate (upper right panel) and isospin density (lower panel) deviations as a function of μ_I/M_π at NLO for $a_1 = -0.019$ and fixing $\mu_I = M_\pi$. We show the expected uncertainty bands within the range of natural values for $\hat{q}_{1,2,4,5,6}^T$ and $\hat{q}_3^T$ fixed by the constraint given in (6.148). The value of j for the quark and pion condensates is the same as in Fig.6.21. The lattice data are from [235].

6.4 Conclusions

In this chapter we have constructed the most general Lagrangian up to fourth order, following the technique of external sources extended to include nonzero chemical potentials. The technique of external sources including spurion fields allows to account for all possible operators respecting the symmetry breaking problem at hand. In the Lagrangian construction, two different types of operators arise: those coming from the covariant derivative and new terms allowed by the symmetry, carrying new LEC.

First, we have analyzed the effective chiral Lagrangian for nonzero chiral imbalance for two light flavours, through its dependence with the axial chemical potential μ_5 . Our

analysis provides a consistent framework for the behaviour at low and moderate values of μ_5 , which would be useful for physical systems where local parity breaking is at work, as in relativistic heavy ion collisions. We have also explored the main phenomenological consequences, paying special attention to the comparison with existing lattice results.

The second-order Lagrangian $\mathcal{L}_2$ only receives a constant (field independent) μ_5 -dependent contribution, which affects the free energy. It contains a new low-energy constant κ_0 . At fourth order, there are two derivative-like terms in $\mathcal{L}_4$, one of them breaking Lorentz covariance (broken by the choice of a_μ^0), a mass term and a constant term. All of them are multiplied by combinations of standard and new LEC, giving rise to four undetermined constants $\kappa_{1,\dots,4}$, whose renormalization ensures that the μ_5 -dependent corrections to observables are finite.

Regarding the phenomenological consequences, we have analyzed several observables and the dependence of their μ_5 corrections with the κ_i constants. The main results are the following:

- The pion dispersion relation is modified through a reduction in the pion velocity due to the Lorentz breaking effect. The same effect implies that the screening and pole pion masses become different, both receiving μ_5 corrections. The LEC involved are κ_2 for the pion velocity, which should be negative to ensure that pions do not become tachyonic, and both κ_2 and $\kappa_1 - \kappa_3$ for the masses. At present, there are no available lattice data to confront here, the screening mass being the most feasible one, which we leave here as a suggestion for future lattice analysis.
- We have calculated the μ_5 corrections to the vacuum energy density up to sixth order, which includes three new LEC coming from the sixth-order Lagrangian. We have shown that the energy density is finite and scale independent once the LEC renormalization is properly accounted for. From the energy density, several observables can be extracted, such as the quark condensate, the scalar susceptibility and the chiral charge density.
- Chiral restoration properties at finite temperature have been explored through the light quark condensate and the scalar susceptibility in ChPT. The transition temperature approximated from the vanishing of the quark condensate turns out to behave quite according to lattice analysis when the ratio $T_c(\mu_5)/T_c(0)$ is considered in the chiral limit. Actually, this allows to provide a rather trustable numerical value for the combination $\kappa_a = 2\kappa_1 - \kappa_2$ by fitting lattice data. That ratio is

pretty insensitive to mass corrections. Actually, including those corrections in the fit gives a worse determined numerical value for the combination $\kappa_b = \kappa_1 + \kappa_2 - \kappa_3$, appearing for $M \neq 0$. The analysis of the scalar susceptibility χ_S shows that for low μ_5 it is controlled by the same combination $\kappa_1 - \kappa_3$ appearing in the screening mass. A positive sign for that combination would be consistent with the lattice observation of χ_S decreasing with μ_5 below the transition.

- The chiral charge density ρ_5 follows essentially a linear behaviour with μ_5 , consistently with lattice data. The constant κ_0 appearing in the linear term can actually be well fixed by fitting the lattice points with the chiral limit ChPT expression, since lattice data for $N_f = 2$ are almost insensitive to the pion mass. Thermal corrections are small here and reduce the size of the linear term in the chiral limit. The fourth-order constant κ_4 and the sixth-order one γ_0 enter in the cubic and fifth-order terms respectively, and can also be reasonably determined. This observed behaviour of ρ_5 in the lattice is at odds with the possibility of a $\mu_5 \neq 0$ minimum for the free energy for low and moderate values of μ_5 .
- The topological susceptibility χ_{top} dependence with μ_5 has also been determined recently in the lattice, although it is subject to more uncertainties than the previously considered observables. Our ChPT analysis predicts that the lowest order corrections to χ_{top} are of order μ_5^2 controlled by the κ_3 constant. The pion mass dependence uncertainty of lattice points is reduced by taking the ratio $\chi_{top}(\mu_5)/\chi_{top}(0)$, which allows to obtain a decent determination of κ_3 , albeit with larger errors than other combinations.
- The pressure and the speed of sound are also affected by μ_5 corrections, which at the order considered depend on κ_2 and κ_b for the pressure, while for the speed of sound the κ_2 dependence disappears. The ultrarelativistic limit $T \gg M$ is reached for both quantities as temperature increases and corresponds to the chiral limit. In the case of the speed of sound, that limit is the $1/3$ value independent of μ_5 which is not violated by the μ_5 corrections at nonzero M .
- The calculation of the ratio $T_c(\mu_5)/T_c(0)$ from the $f_0(500)$ saturated scalar susceptibility allows to improve the determination of the low-energy constants κ_i of the $\mu_5 \neq 0$ Lagrangian. That ratio is actually pretty insensitive to the pion mass, which makes it a suitable quantity to compare with our theoretical predictions.

We have been actually able to reduce the uncertainties of $\kappa_{1,2,3}$ by fitting lattice points for $T_c(\mu_5)/T_c(0)$ and the topological susceptibility. An important difference of the $T_c(\mu_5)$ determination from the saturated analysis with respect to that from the quark condensate is that the chiral limit expressions alone are not enough to fit accurately the lattice results, since the behaviour of the susceptibility in that limit is qualitatively very different from the massive case, corresponding to a divergence near T_c . Moreover, for the κ_i values obtained in our main fit, our results consistently show that both the critical temperature calculated with the NNLO ChPT quark condensate and with the saturated approach increase with μ_5 , in agreement with the lattice results.

- Our results for the resonance pole parameters M_p , Γ_p of the $f_0(500)$ and $\rho(770)$ increase with μ_5 , showing a behaviour compatible with chiral restoration in the $IJ = 00$ case and with previous analysis on dilepton production in the $IJ = 11$ one. Furthermore, our results are predictive for low and moderate values of μ_5 . The $f_0(500)/\sigma$ has smaller uncertainty band than the $f_0(500)$ for the $m\mu_5$ dependence of M_p and Γ_p .

Apart from describing the observed lattice trends for the observables mentioned above, our analysis points to decreasing pion mass and increasing pion decay constant consistently with recent model analyses. Further lattice observables, such as the screening masses, or improving the precision over existing determinations, would certainly help to narrow this picture.

Summarizing, our present study provides a solid setup for the analysis of chirally imbalanced matter for two light flavours, at low and moderate values of μ_5 , typically $\mu_5 \lesssim 500$ MeV. A rigorous construction of the effective Lagrangian has been developed and the main physical effects have been analyzed and compared to existing lattice data, which allows for a first determination of the new low-energy constants involved. Thus, within its applicability range, the present analysis is meant to provide a useful benchmark for model and lattice analysis.

On the other hand, we have analyzed the most general effective chiral Lagrangian for nonzero isospin chemical potential for two light flavours up to $\mathcal{O}(p^4)$. The effect of the new Lagrangian terms in the free energy density has been calculated up to next-to-leading order. In addition, we have calculated a new NLO contribution to the free energy density coming from terms linear in the pion fields. The main results are the

following:

- In the second-order Lagrangian $\mathcal{L}_2$ two new-independent terms have to be considered, whose corresponding low-energy constants a_1 , a_2 are related from the constraint of vanishing isospin density below the critical BEC value μ_c . The constant a_1 contributes in particular to a shift in μ_c with respect to the pion mass, although our complete NLO analysis shows that parametrically $\mu_c = M_\pi$ still holds at leading order. To estimate the preferred value of a_1 , we have performed several fits to lattice results for the quark and pion condensates (for nonzero pionic source j) as well as for the isospin density (for $j = 0$), which favor $a_1 < 0$ (and therefore $\mu_c < M_\pi$) with $|a_1| \ll 1$, consistently with its parametric NLO dependence. When comparing to the $a_1 = 0$ results, a small nonzero negative value for a_1 improves the description of lattice results, specially for the isospin density.
- The $\mathcal{O}(p^4)$ Lagrangian $\mathcal{L}_4$ contains seven new terms with new low-energy constants $\hat{q}_i$, which we have consistently renormalized to absorb the divergences coming from loops with vertices of the new $\mathcal{L}_2$ terms. As mentioned above, the NLO free energy density includes also an additional contribution coming from a term in $\mathcal{L}_2$ linear in the pion fields. That term comes from the NLO corrections to the angle minimizing the free energy density. The effect of the linear term is qualitatively important, since it eventually makes the minimum of the free energy density disappear, which sets a natural limit of validity for the ChPT framework consistent with lattice analyses.
- Imposing that the isospin density vanishes below μ_c to NLO gives rise to additional constraints, involving now the $a_1, a_2, \hat{q}_i^r$ LEC. Those constraints imply on the one hand that the $a_{1,2}$ contributions belong are parametrically to the NLO, consistently with the small value for a_1 found in our fits. On the other hand, the dependence on one of the seven new LEC can be eliminated. In addition, the critical BEC value to NLO must remain below the LO one, which restricts further the admissible values for the $\hat{q}_i^r$. If $\mu_c = M_\pi$ is demanded also to NLO, a further constraint arises, which could not be satisfied if all the new LEC would vanish, due to the correction to μ_c coming from the linear term.
- We have estimated the effect of the new LEC and the linear term to NLO by keeping the $\hat{q}_i^r$ within natural values and using for a_1 our fitted value. The results

for the different observables show again consistency with the lattice points, leaving room for improvement with respect to the LO within the $\hat{q}_i^r$ uncertainty.

In summary, our present analysis establishes systematically the most general way to describe low-energy QCD at nonzero isospin density, consistently with lattice results and complementing previous theoretical analyses. We believe that these results will be useful towards a better understanding of the QCD phase diagram and we leave for future works its extension to three flavours and finite temperature.

Conclusions

Throughout this thesis we have studied chiral and $U(1)_A$ symmetry restoration. First, we have analyzed some thermal resonances as the $f_0(500)$ and the $K_0^*(700)$ and their connection with chiral symmetry and $U(1)_A$ restoration. We have also estimated the η' corrections to χ_{top} and c_4 at zero temperature and at finite temperature up to NNLO in ChPT, which play a direct role in the discussion about $O(4)$ and $U(1)_A$ restoration since the vanishing of χ_{top} signals also $O(4) \times U(1)_A$ restoration. Finally, we have analyzed the effective chiral lagrangian for nonzero chemical potential, and from this we have studied several observables and the dependence of their chemical potential corrections with the new LECs for axial and isospin chemical potentials.

The main conclusions of this thesis are

- We have analyzed the importance of thermal corrections to the $f_0(500)$ resonance spectral parameters characterising the scalar susceptibility χ_S around the region of chiral symmetry restoration. We have used the LSM to establish a direct link between the scalar susceptibility and the propagator of the lightest scalar state at zero momentum. The susceptibility saturated by the σ propagator exhibits a more substantial growth compared to the purely perturbative approach, thus aligning better with lattice data. That analysis have been used to check the validity of the UChPT saturation approach. That approach gives an accurate description of the $f_0(500)$ parameters and reproduces the cross-over behaviour of χ_S . On the other hand, taking into account the LEC uncertainty we have found a susceptibility that is compatible with the lattice data, at least below and around T_c . Finally we have tested the robustness of the saturation approach changing the unitariza-

tion method. The thermal $f_0(500)$ state is crucial for correctly describing scalar susceptibility and understanding the chiral restoration transition. The analyses (LEC, unitarization method, LSM) confirms that the thermal $f_0(500)$ saturation approach is robust from the theoretical point of view. We have also compared the thermal $f_0(500)$ description with one based on the HRG. In order to compare both approaches, we performed various fits incorporating a normalization factor. The HRG tends to give a better description of the data below the maximum, as expected, but the saturated approach can better account for the data around the transition peak.

- We have investigated the interplay between chiral and $O(4) \times U(1)_A$ restoration using Ward Identities, lattice data, and UChPT to derive scalar and pseudoscalar susceptibilities in the $I = 1/2$ channel. At low temperatures, the scalar susceptibility κ increases proportionally to the light quark condensate. In the physical limit and for $N_f = 2 + 1$, a peak appears above the chiral transition. Beyond this point, the strange quark condensate gains importance, causing the susceptibility to decrease and tend towards degeneracy with the K susceptibility. The existence of the χ_S^κ peak and the degeneration $\chi_S^\kappa - \chi_P^K$ has been confirmed using Ward Identities and lattice data to reconstruct the $I = 1/2$ susceptibilities. In the physical case, the position of the peak was found to fall within the $O(4) \times U(1)_A$ restoration region. The susceptibility peak also appears when the scalar susceptibility κ is saturated with the thermal pole of the $K_0^*(700)$ or κ , calculated using UChPT at finite temperature. Using this approach, the peak was observed to occur in both the chiral and $SU(3)$ limits. Our analysis suggests that the $O(4)$ and $O(4) \times U(1)_A$ transitions coincide at T_c when the $N_f = 2$ limit ($m_l/m_s \rightarrow 0$) is reached. In the limit $m_l/m_s \rightarrow 1$, corresponding to $SU(3)$, χ_S^κ is expected to degenerate with χ_S . As the kaon mass decreases, approaching the $SU(3)$ limit in UChPT, χ_S^κ behaves similarly to that of χ_S : the peak grows and shifts towards lower temperatures.
- We have calculated the temperature corrections to the πK scattering amplitude within ChPT. In addition to the standard $T = 0$ cuts, the amplitude shows $T \neq 0$ Landau cuts. From this we have extended the thermal unitarity relation for unequal-mass meson-meson scattering. The thermal behaviour of the $K_0^*(700)$ and $K^*(890)$ poles has been calculated through the one-loop IAM. The mass of the $K_0^*(700)$ decreases for temperatures above 75 MeV, while its width increases

at low temperatures. On the other hand, the $K^*(892)$ pole position shows a softer temperature dependence. For the $m_l/m_s \rightarrow 1$ limit, which we have studied by reducing the kaon mass, the width of the $K^*(892)$ increases significantly with the temperature. As in chapter 3, where we related the pole of the $K_0^*(700)$ to the scalar susceptibility in the $I = 1/2$ channel, here we have analyzed the saturated susceptibility calculated using the full IAM and we have obtained a similar temperature dependence for the saturated susceptibility.

- We shown the results of the topological susceptibility and the fourth-order cumulant calculated up to NNLO in $U(3)$ ChPT, taking into account the influence of the η' meson and the $\eta - \eta'$ mixing angle. At $T = 0$, the η' corrections to the topological susceptibility and the fourth cumulant are provided. These corrections are shown to be comparable in magnitude to the K and η ones introduced in the $SU(3)$ approach, and the results are consistent with findings from lattice analyses. Furthermore, we have included the relevant isospin-breaking corrections to LO in the $U(3)$ ChPT expansion. Numerical corrections due to isospin breaking remain below the 5% level. The temperature dependence of χ_{top} , derived from the $U(3)$ ChPT analysis, is consistent with lattice data. We have compared the topological susceptibility with the quark condensate, which are linked by a Ward Identity. When these quantities are computed using the same ChPT formalism, their scaling is remarkably similar. However, the quark condensate calculated from the HRG shows a clear deviation from χ_{top} , which is dominated by the light degrees of freedom around T_c . This is consistent with a gap between chiral and $U(1)_A$ restorations for physical quark masses. Additionally, the existence of this gap is also in agreement with WIs.
- We provide a model-independent approach, constructing the most general effective Lagrangian for the lightest degrees of freedom in the presence of a nonzero chemical potential source.

For the chemical potential associated to nonzero chemical imbalance, we have studied several observables related to the vacuum energy density and the dependence of their μ_5 corrections with the κ_i constants. Besides this we have compared our results with existing lattice data and we have performed several fits to obtain the values of the new κ_i LECs that appear in the Lagrangian. Requiring that the pion velocity remains smaller than the speed of light for any μ_5 , the constrain

$\kappa_2 < 0$ is obtained. On the other hand, in order to the square pion mass remains positive, $\kappa_1 - \kappa_3 < 0$. On the other hand, we have calculated $\pi\pi$ scattering to one loop in ChPT at nonzero temperature and nonzero chiral imbalance chemical potential μ_5 . From this, using a saturated scalar susceptibility approach, we have indeed managed to reduce the uncertainties of $\kappa_{1,2,3}$ by performing a joint fit of $T_c(\mu_5)/T_c(0)$ and χ_{top} to lattice points. Moreover, the results obtained consistently demonstrate the growth of T_c with μ_5 .

For the isospin chemical potential case, the second-order Lagrangian $\mathcal{L}_2$, introduces two new LECs, denoted as a_1 and a_2 . Through various fits to lattice data, specifically for quark and pion condensates, as well as isospin density, a preference for $a_1 < 0$ emerges, which implies that $\mu_c < M_\pi$. This preference notably enhances the agreement with lattice results, particularly concerning isospin density. The fourth-order Lagrangian $\mathcal{L}_4$, contains seven new with additional LECs ($\hat{q}_i$). Furthermore, the NLO free energy density incorporates an extra contribution from a term in $\mathcal{L}_2$ that is linear in the pion fields. The qualitative significance of this linear term is notable. When enforcing the condition of vanishing isospin density below μ_c at NLO, it is observed that the contributions of $a_{1,2}$ are parametrically NLO, and we can eliminate the dependence of one of the seven new LECs. The NLO results for the quark and pion condensate and the isospin density within natural values for the new LECs show agreement with the lattice data improving the LO results.

Appendix A

Matsubara frequency Sums

We will focus on evaluating sums over the Matsubara frequencies. Suppose we want to evaluate a frequency sum of the form

$$T \sum_{n=-\infty}^{\infty} f(i\omega_n) \quad (\text{A.1})$$

Note that the hyperbolic cotangent function $\coth(\beta z/2)$ produces a collection of poles at $z = i\omega_n$. Thus, using the Cauchy's residue theorem, the above sum can be evaluated by performing the integral in the complex z plane as

$$T \sum_{n=-\infty}^{\infty} f(i\omega_n) = \frac{T}{2\pi i} \oint_{C_1} f(z) \frac{\beta}{2} \coth\left(\frac{\beta z}{2}\right) \quad (\text{A.2})$$

where the contour C_1 is the contour in Figure A.1. This can be deformed into C_2 (which covers the entirety of the complex plane, with the exception of the imaginary axis) and, therefore, the equation (A.2) can be expressed as

$$-\frac{1}{2\pi i} \int_{-i\infty-\epsilon}^{i\infty-\epsilon} dz f(z) \coth\left(\frac{\beta z}{2}\right) + \frac{1}{2\pi i} \int_{-i\infty+\epsilon}^{i\infty+\epsilon} dz f(z) \coth\left(\frac{\beta z}{2}\right) \quad (\text{A.3})$$

In so doing, expressing the hyperbolic cotangent in the form of combination of exponential functions and regrouping these terms in a convenient way, we have the following result

$$T \sum_{n=-\infty}^{\infty} f(i\omega_n) = \frac{1}{2\pi i} \left\{ \int_{-i\infty}^{i\infty} dz f(z) + \int_{-i\infty+\epsilon}^{i\infty+\epsilon} dz f(z) n_B(z) - \int_{i\infty-\epsilon}^{-i\infty-\epsilon} dz f(z) n_B(-z) \right\} \quad (\text{A.4})$$

which is correct if the function $f(z)$ has no singularities along the imaginary axis. In this way, we have separate the zero temperature part from the finite temperature part. The T dependence is included in $n_B(x)$ that is the Bose-Einstein distribution given by

$$n_B(x) = \frac{1}{e^{\beta x} - 1} \quad (\text{A.5})$$

Thus, the temperature dependent integrals can be computed by deforming the contour to C_3 , which covers the whole complex plane except the imaginary axis. Due that

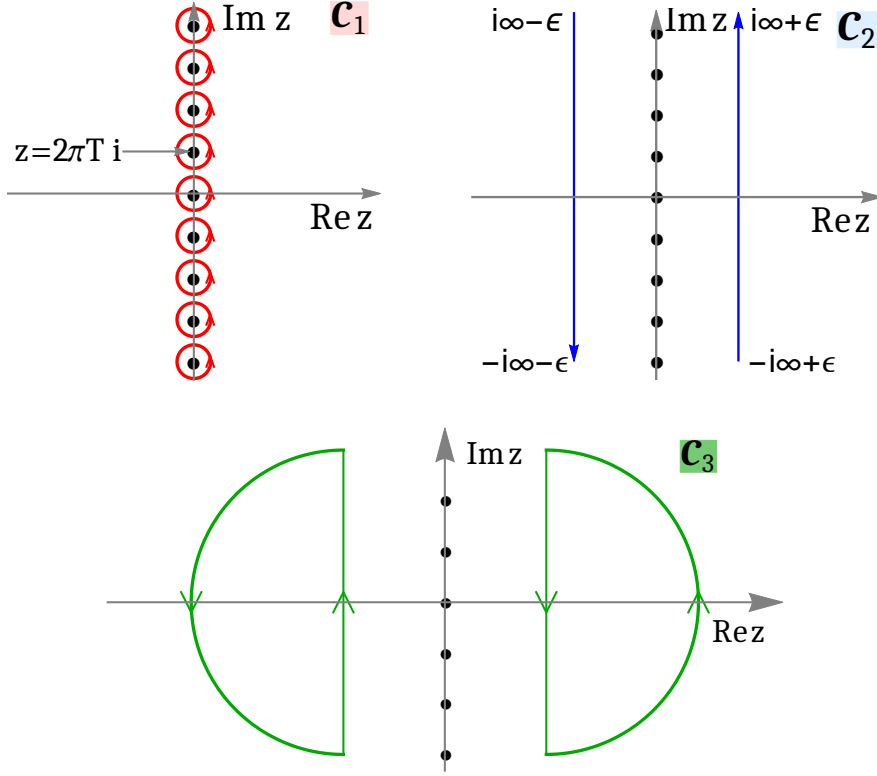


Figure A.1: Integration contours for doing the Matsubara sums.

the hyperbolic cotangent function does not produce poles off the imaginary axis, the relevant poles here are those of $f(z)$.

Taking into account that the function $f(z)n_B(z)$ tends to zero as $|z| \rightarrow \infty$, it is easy to demonstrate that the integrals over the semicircles in the Figure A.1 cancel out. Therefore, we only need to consider the closed contours defined by C_3 . The contour C_3 runs in the opposite direction of C_2 so we have to introduce a negative sign.

Finally, we identify all the poles generated by $f(z)$ and compute their residue in order to obtain the initial frequency sum

$$\begin{aligned}
 T \sum_{n=-\infty}^{\infty} f(i\omega_n) &= \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} dz f(z) \\
 &\quad - \sum_{i=\text{poles}(\text{Re} z_i > 0)} \text{Res}(f, z_i) n_B(z_i) + \sum_{i=\text{poles}(\text{Re} z_i < 0)} \text{Res}(f, z_i) n_B(-z_i)
 \end{aligned}
 \tag{A.6}$$

Now, for example, if we want to evaluate a sum with $f(i\omega_n) = -1/[(i\omega_n)^2 - \vec{p}^2 - m^2]$ for which the $f(z)$ poles are $z = \pm(\vec{p}^2 + m^2)^{1/2} = \pm E_p$ we obtain

$$-T \sum_{n=-\infty}^{\infty} \frac{1}{(i\omega_n)^2 - \vec{p}^2 - m^2} = \frac{1}{2E_p} [1 + 2n_B(E_p)] \quad (\text{A.7})$$

Also notice that, defining $p_4 = iz$ in the first integral of equation (A.4) we can identify it with the standard result of $T = 0$ field theory in four Euclidean dimensions. Thus,

$$\int \frac{d^3\vec{p}}{(2\pi)^3} \left(\frac{1}{2\pi i} \int_{-i\infty}^{i\infty} dz f(z) \right) = \int \frac{d^3\vec{p}}{(2\pi)^3} \int \frac{dp_4}{2\pi} \frac{1}{p_4^2 + \vec{p}^2 + m^2}. \quad (\text{A.8})$$

Another case is

$$f(i\omega_n) = \frac{1}{(i\omega_n)^2 - E_1^2} \frac{1}{(i\omega_n - i\omega_m)^2 - E_2^2} \quad (\text{A.9})$$

where we have four poles located at $p_0 = i\omega_n = \pm E_1, i\omega_m \pm E_2$. Summing the residuals

$$\begin{aligned} T \sum_{n=-\infty}^{\infty} f(i\omega_n) &= -\frac{1}{4E_1E_2} \left(\frac{1}{i\omega_m - E_1 - E_2} - \frac{1}{i\omega_m + E_1 + E_2} \right) \\ &\quad - \frac{1}{2E_1} \frac{1}{(E_1 - i\omega_m)^2 - E_2^2} n_B(E_1) \\ &\quad + \frac{-1}{2E_1} \frac{1}{(-E_1 - i\omega_m)^2 - E_2^2} n_B(E_1) \\ &\quad - \frac{1}{2E_2} \frac{1}{(i\omega_m + E_2)^2 - E_1^2} n_B(i\omega_m + E_2) \\ &\quad + \frac{-1}{2E_2} \frac{1}{(i\omega_m - E_2)^2 - E_1^2} n_B(-i\omega_m + E_2) \end{aligned} \quad (\text{A.10})$$

Taking into account that the external momentum corresponds to a bosonic particle, that means $\exp(i\beta\omega_m) = 1$, the value of the frequency sum is

$$\begin{aligned} T \sum_{n=-\infty}^{\infty} f(i\omega_n) &= -\frac{1}{4E_1E_2} \left[(1 + n_B(E_1) + n_B(E_2)) \left(\frac{1}{i\omega_m - E_1 - E_2} - \frac{1}{i\omega_m + E_1 + E_2} \right) \right. \\ &\quad \left. + (n_B(E_2) - n_B(E_1)) \left(\frac{1}{i\omega_m - E_1 + E_2} - \frac{1}{i\omega_m + E_1 - E_2} \right) \right] \end{aligned} \quad (\text{A.11})$$

Appendix B

Ward Identities for susceptibilities and condensates

We will first proceed to the formal derivation of the relevant Ward identities from QCD. Lets start by writing the expected value of a local operator $O(x_1, \dots, x_n)$ from the QCD generating functional as:

$$\langle O(y) \rangle = Z_{\text{QCD}}^{-1} \int [dG] [d\bar{q}] [dq] O(y) e^{i \int d^4x \mathcal{L}_{\text{QCD}}} \quad (\text{B.1})$$

We consider an infinitesimal local axial transformation on the quark fields

$$q'(x) \rightarrow \left(1 - i\alpha_A^a \frac{\lambda^a}{2} \gamma_5 \right) q(x) + \mathcal{O}[(\alpha_A^a)^2] \quad (\text{B.2})$$

where λ^a are the Pauli matrices for $SU(2)$ and the Gell-Mann matrices for $SU(3)$ (with $a = 1, \dots, 8$) and $\lambda^0 = \sqrt{2/3} \mathbf{1}$. Thus, from (B.1), linearly in α_A^a we get:

$$\left\langle \frac{\delta O(y)}{\delta \alpha_A^a(x)} \right\rangle + \left\langle O(y) \frac{\delta S_{\text{QCD}}}{\delta \alpha_A^a(x)} \right\rangle + \left\langle O(y) \frac{\delta \log \mathcal{J}}{\delta \alpha_A^a(x)} \right\rangle = 0 \quad (\text{B.3})$$

where

$$\left\langle O(y) \frac{\delta S_{\text{QCD}}}{\delta \alpha_A^a(x)} \right\rangle = i \partial_\mu^x \langle O(y) (J_A)^{a\mu} \rangle + \langle O(y) \partial^\mu (J_A)_\mu^a \rangle \quad (\text{B.4})$$

The QCD expectation value of an operator O in terms of the transformed fields leads to [103, 137]

$$\left\langle \frac{\delta O(y)}{\delta \alpha_A^a(x)} \right\rangle = - \left\langle O(y) \bar{q}(x) \left\{ \frac{\lambda^a}{2}, \mathcal{M} \right\} q(x) \right\rangle + i \frac{\delta^{a0}}{\sqrt{6}} \langle O(y) A(x) \rangle \quad (\text{B.5})$$

so, as we can see, the identities involving the singlet ($a = 0$) lead to the presence of the $U(1)_A$ anomalous term.

B.1 Susceptibilities

Ward Identities derived from the QCD generating functional can be used to relate susceptibilities and quark condensates in different channels. We will define as usual the

associated scalar, pseudoscalar and anomalous susceptibilities with the quark bilinears defined in (3.1),(3.2) and (3.3):

$$\chi_S^{ab} \equiv \delta^{ab} \chi_S^\delta = \int_T \langle \mathcal{T} \delta^a(x) \delta^b(0) \rangle \quad (a, b = 1, 2, 3) \quad (\text{B.6})$$

$$\chi_S^{ab} \equiv \delta^{ab} \chi_S^\kappa = \int_T \langle \mathcal{T} \kappa^a(x) \kappa^b(0) \rangle \quad (a, b = 4, 5, 6, 7) \quad (\text{B.7})$$

$$\chi_S^{ll} \equiv \int_T \langle \mathcal{T} \sigma_l(x) \sigma_l(0) \rangle \quad (\text{B.8})$$

$$\chi_S^{ss} \equiv \int_T \langle \mathcal{T} \sigma_s(x) \sigma_s(0) \rangle \quad (\text{B.9})$$

$$\chi_S^{ls} \equiv \int_T \langle \mathcal{T} \sigma_l(x) \sigma_s(0) \rangle \quad (\text{B.10})$$

$$\chi_P^{ab} \equiv \delta^{ab} \chi_P^\pi = \int_T \langle \mathcal{T} \pi^a(x) \pi^b(0) \rangle, \quad (a, b = 1, 2, 3) \quad (\text{B.11})$$

$$\chi_P^{ab} \equiv \delta^{ab} \chi_P^K = \int_T \langle \mathcal{T} K^a(x) K^b(0) \rangle, \quad (a, b = 4, 5, 6, 7) \quad (\text{B.12})$$

$$\chi_P^{ll} \equiv \int_T \langle \mathcal{T} \eta_l(x) \eta_l(0) \rangle \quad (\text{B.13})$$

$$\chi_P^{ss} \equiv \int_T \langle \mathcal{T} \eta_s(x) \eta_s(0) \rangle \quad (\text{B.14})$$

$$\chi_P^{ls} \equiv \int_T \langle \mathcal{T} \eta_l(x) \eta_s(0) \rangle \quad (\text{B.15})$$

$$\chi_P^{0A} \equiv \int_T \langle \mathcal{T} P^0(x) A(0) \rangle, \quad (\text{B.16})$$

$$\chi_P^{8A} \equiv \int_T \langle \mathcal{T} P^8(x) A(0) \rangle, \quad (\text{B.17})$$

$$\chi_P^{AA} \equiv \int_T \langle \mathcal{T} A(x) A(0) \rangle, \quad (\text{B.18})$$

where $P^{0,8}$ pseudoscalar states (or equivalently $\eta^{0,8}$) are related to the η_l and η_s bilinears as follows:

$$P^0 = \sqrt{\frac{2}{3}} (\eta_l + \eta_s), \quad P^8 = \frac{1}{\sqrt{3}} (\eta_l - \eta_s) \quad (\text{B.19})$$

Remember that the mixing of η^0 and η^8 results in the physical η and η' . In the 0, 8 state basis we have

$$\chi_P^{00} \equiv \int_T \langle \mathcal{T} P^0(x) P^0(0) \rangle \quad (\text{B.20})$$

$$\chi_P^{88} \equiv \int_T \langle \mathcal{T} P^8(x) P^8(0) \rangle \quad (\text{B.21})$$

$$\chi_P^{80} \equiv \int_T \langle \mathcal{T} P^8(x) P^0(0) \rangle \quad (\text{B.22})$$

B.2 Ward Identities

Here, we will analyze the channels corresponding to the quantum numbers of the π , K and $\eta - \eta'$. First of all, let us take $O = \pi^a$. In the isospin limit, $\{\frac{\tau^a}{2}, \mathcal{M}\} = m_l \tau^a$, $\{\tau^a, \tau^b\} = 2\delta^{ab}$ and the $SU(2)$ expression of (B.5) reduces to:

$$\delta^{ab} \langle \bar{q}q \rangle_l = -m_l \chi_P^{ab}, \quad (a = 1, 2, 3) \quad (\text{B.23})$$

In the $I = \frac{1}{2}$ channel, we have now $\{\frac{1}{2}\lambda^a, \mathcal{M}\} = \frac{m_l + m_s}{2}\lambda^a$ and the Gell Mann matrices satisfy the anti-commutation relations

$$\left\{ \frac{\lambda^a}{2}, \frac{\lambda^b}{2} \right\} = \frac{4}{3} \delta^{ab} \mathbf{1} + 2 \sum_c d_{abc} \lambda^c, \quad (\text{B.24})$$

with d_{abc} the structure constants. Thus, applying (B.5) to $O = K^b$ one obtains

$$\delta^{ab} [\langle \bar{q}q \rangle_l + 2\langle \bar{s}s \rangle] = -(m_l + m_s) \chi_P^{ab}, \quad (a, b = 4, 5, 6, 7) \quad (\text{B.25})$$

and taking $O = \kappa^b$ we get

$$\delta^{ab} [\langle \bar{q}q \rangle_l - 2\langle \bar{s}s \rangle] = -(m_l - m_s) \chi_S^{ab} \quad (\text{B.26})$$

Now, let us consider the case $O = P^8$. For $a = 8$ and $a = 0$ in (B.5) we have:

$$a = 8 : \quad \langle \bar{q}q \rangle_l + 4\langle \bar{s}s \rangle = -(m_l + 2m_s) \chi_P^{88} - \sqrt{2}(m_l - m_s) \chi_P^{80} \quad (\text{B.27})$$

$$a = 0 : \quad \langle \bar{q}q \rangle_l - 2\langle \bar{s}s \rangle = -(m_l - m_s) \chi_P^{88} - \frac{(2m_l - m_s)}{\sqrt{2}} \chi_P^{80} - \frac{\sqrt{3}}{2} \chi_P^{8A} \quad (\text{B.28})$$

Taking now $O = P^0$ and $a = 0, 8$:

$$a = 8 : \quad \langle \bar{q}q \rangle_l - 2\langle \bar{s}s \rangle = -\frac{(m_l + 2m_s)}{\sqrt{2}} \chi_P^{80} - (m_l - m_s) \chi_P^{00} \quad (\text{B.29})$$

$$a = 0 : \quad \langle \bar{q}q \rangle_l + \langle \bar{s}s \rangle = -\frac{(2m_l + m_s)}{2} \chi_P^{00} - \frac{(m_l - m_s)}{\sqrt{2}} \chi_P^{80} - \frac{\sqrt{6}}{4} \chi_P^{0A} \quad (\text{B.30})$$

We can also calculate a relations for χ_P^{AA} . This is done by considering $O = A$:

$$a = 8 : \quad \chi_P^{8A} = \sqrt{2} \frac{m_s - m_l}{(2m_s + m_l)} \chi_P^{0A} \quad (\text{B.31})$$

$$a = 0 : \quad \chi_P^{AA} = -\frac{2}{\sqrt{3}}(m_l - m_s) \chi_P^{8A} - \frac{2}{\sqrt{6}}(m_s + 2m_l) \chi_P^{0A} \quad (\text{B.32})$$

Appendix C

Loop integrals at finite temperature for unequal-mass meson-meson scattering

C.1 General expressions and relations

At finite temperature, the following relations hold for the different combinations of loop integrals with momenta in the numerator (with $p_0 = 2\pi nT$, $\mathcal{Q}_0 = 2\pi mT$ and Euclidean metric $(-, -, -, -)$):

$$\oint_p \frac{p_i}{(p^2 - M_a^2)((p - \mathcal{Q})^2 - M_b^2)} = -\frac{\mathcal{Q}_i}{|\vec{\mathcal{Q}}|^2} \left[\mathcal{Q}_0 J_1 + \frac{(\mathcal{Q}^2 + \Delta_{ab})}{2} J_0 + \frac{1}{2} (G_b - G_a) \right], \quad (\text{C.1})$$

$$\oint_p \frac{p_\mu \mathcal{Q}^\mu}{(p^2 - M_a^2)((p - \mathcal{Q})^2 - M_b^2)} = \frac{(\mathcal{Q}^2 + \Delta_{ab})}{2} J_0 + \frac{1}{2} (G_b - G_a), \quad (\text{C.2})$$

$$\oint_p \frac{p_0 p_i}{(p^2 - M_a^2)((p - \mathcal{Q})^2 - M_b^2)} = -\frac{\mathcal{Q}_i}{|\vec{\mathcal{Q}}|^2} \left[\mathcal{Q}_0 J_2 + \frac{(\mathcal{Q}^2 + \Delta_{ab})}{2} J_1 + \frac{\mathcal{Q}_0}{2} G_b \right], \quad (\text{C.3})$$

$$\oint_p \frac{p_i p_j}{(p^2 - M_a^2)((p - \mathcal{Q})^2 - M_b^2)} = \mathcal{Q}_i \mathcal{Q}_j I_{ab} + g_{ij} \hat{I}_{ab}, \quad (\text{C.4})$$

$$\oint_p \frac{p_0(p \cdot p)}{(p^2 - M_a^2)((p - \mathcal{Q})^2 - M_b^2)} = \mathcal{Q}_0 G_b + M_a^2 J_1, \quad (\text{C.5})$$

$$\oint_p \frac{p_i(p \cdot p)}{(p^2 - M_a^2)((p - \mathcal{Q})^2 - M_b^2)} = \mathcal{Q}_i G_b - M_a^2 \frac{\mathcal{Q}_i}{|\vec{\mathcal{Q}}|^2} \left[\mathcal{Q}_0 J_1 + \frac{1}{2} (\mathcal{Q}^2 + \Delta_{ab}) J_0 + \frac{1}{2} (G_b - G_a) \right], \quad (\text{C.6})$$

$$\oint_p \frac{(p \cdot p)^2}{(p^2 - M_a^2)((p - \mathcal{Q})^2 - M_b^2)} = (\mathcal{Q}^2 + \Sigma_{ab}) G_b + M_a^4 J_0, \quad (\text{C.7})$$

$$\begin{aligned}
 I_{ab} = & \frac{1}{(D-2)|\vec{Q}|^4} \left\{ \left[(D-1)\mathcal{Q}_0^2 + |\vec{Q}|^2 \right] J_2 + (D-1)\mathcal{Q}_0(\mathcal{Q}^2 + \Delta_{ab})J_1 \right. \\
 & + \left[\frac{D-1}{4}(\mathcal{Q}^2 + \Delta_{ab})^2 + M_a^2|\vec{Q}|^2 \right] J_0 + \left[\left(\frac{\mathcal{Q}^2}{2} + \mathcal{Q}_0^2 \right) (D-1) + |\vec{Q}|^2 \right] G_b \\
 & \left. + \frac{D-1}{4}(\mathcal{Q}^2 + \Delta_{ab})(G_b - G_a) \right\}, \quad (C.8)
 \end{aligned}$$

$$\begin{aligned}
 \hat{I}_{ab} = & \frac{1}{(D-2)|\vec{Q}|^2} \left\{ -\mathcal{Q}^2 J_2 + \mathcal{Q}_0(\mathcal{Q}^2 + \Delta_{ab})J_1 + \left[\frac{1}{4}(\mathcal{Q}^2 + \Delta_{ab})^2 + M_a^2|\vec{Q}|^2 \right] J_0 \right. \\
 & \left. - \frac{\mathcal{Q}^2}{2}G_b + \frac{1}{4}(\mathcal{Q}^2 + \Delta_{ab})(G_b - G_a) \right\}. \quad (C.9)
 \end{aligned}$$

with $G_a \equiv G(M_a, T)$ and J_k defined in (1.128) and (1.182) respectively. The symbol $\sum_p$ was introduced in equation (1.125).

In the CM frame where $|\vec{Q}| = 0$, the following additional simplifications take place:

$$J_1^{ab}(\mathcal{Q}_0, 0; T) = \frac{1}{2\mathcal{Q}_0} [G_a - G_b - (-\mathcal{Q}_0^2 + \Delta_{ab}) J_0(\mathcal{Q}_0, 0; T)], \quad (C.10)$$

$$J_2^{ab}(\mathcal{Q}_0, 0; T) = -\frac{G_b}{2} + \frac{(-\mathcal{Q}_0^2 + \Delta_{ab})}{4\mathcal{Q}_0^2} [G_b - G_a + (-\mathcal{Q}_0^2 + \Delta_{ab}) J_0(\mathcal{Q}_0, 0; T)], \quad (C.11)$$

C.2 Particular cases of interest for the scattering amplitude

Here we provide useful expressions for the thermal loop integrals corresponding to the scattering diagrams in Fig. 1.16 according to the center of mass kinematics.

C.2.1 *S*-channel in CM frame

In this case, in the CM frame, we are interested in $\mathcal{Q}_0^2 = s \geq 0, |\vec{Q}| = 0$ in (4.1). To derive the imaginary part in (4.2), remember that the solution to $[E_1(p) \pm E_2(p)]^2 = s$ is given by $p = p_{CM}(s; M_a, M_b)$ in (1.166) and $E_1 = |s + \Delta_{ab}|/(2\sqrt{s})$, $E_2 = |s - \Delta_{ab}|/(2\sqrt{s})$. In particular, note that $E_1 = E_2$ for $M_a = M_b$. Therefore,

$$(E_1 + E_2)^2 = s \Leftrightarrow E_1 = \frac{s + \Delta_{ab}}{2\sqrt{s}}, \quad E_2 = \frac{s - \Delta_{ab}}{2\sqrt{s}} \quad (s \geq (M_a + M_b)^2), \quad (C.12)$$

$$(E_1 - E_2)^2 = s \Leftrightarrow E_1 = \frac{s + \Delta_{ab}}{2\sqrt{s}}, \quad E_2 = \frac{\Delta_{ab} - s}{2\sqrt{s}} \quad (0 \leq s \leq (M_a - M_b)^2) \quad (C.13)$$

where we are choosing the masses so that $M_a \geq M_b$, so that $\Delta_{ab} \geq 0$ and $E_1 \geq E_2$ for $s \geq 0$. Note that in this frame, the lower limit for the Landau cut is at $s = 0$, in accordance with Fig. 1.7. In this way, this cut vanishes for $M_a = M_b$ in the CM frame.

Therefore, solving for the corresponding δ functions in (4.2) we get

$$\begin{aligned} \text{Im } J_k^{ab}(\mathcal{Q}_0, 0; T) &= \\ &= \text{sgn}(\mathcal{Q}_0)^{k+1} \frac{\sigma_{ab}(s)}{16\pi} \left(\frac{s + \Delta_{ab}}{2\sqrt{s}} \right)^k \times \\ &\times \left\{ \left[1 + n_B \left(\frac{s + \Delta_{ab}}{2\sqrt{s}} \right) + n_B \left(\frac{s - \Delta_{ab}}{2\sqrt{s}} \right) \right] \theta [s - (M_a + M_b)^2] \right. \\ &+ \left. \left[n_B \left(\frac{\Delta_{ab} - s}{2\sqrt{s}} \right) - n_B \left(\frac{s + \Delta_{ab}}{2\sqrt{s}} \right) \right] \theta [(M_a - M_b)^2 - s] \theta(s) \right\}, \quad (\text{C.14}) \end{aligned}$$

with $s = \mathcal{Q}_0^2$ and where we can readily identify the unitary and Landau contributions. The above structure has direct implications for thermal unitarity, as discussed in section 4.1.

For the extension of the thermal amplitude to the s or $\mathcal{Q}_0$ complex plane, we need an expression for the thermal integrals manifestly analytic in $\mathcal{Q}_0 + i\epsilon$. One can use the relation

$$\Delta J_0^{ab}(s, 0; T) = -\frac{1}{2\pi^2} \int_{M_a}^{\infty} dy \sqrt{y^2 - M_a^2} \frac{s + \Delta_{ab}}{(s + \Delta_{ab})^2 - 4sy^2} n_B(y) + (M_a \leftrightarrow M_b) \quad (\text{C.15})$$

where $s = (\mathcal{Q}_0 + i\epsilon)^2 = s + \text{sgn}(\mathcal{Q}_0)i\epsilon$ with $\epsilon \rightarrow 0^+$, so that the above expression allows one for the analytical continuation to the upper (lower) s plane for $\mathcal{Q}_0 > 0$ ($\mathcal{Q}_0 < 0$). Since $J_0(s)$ is real in the real axis for $(M_a - M_b)^2 \leq s \leq (M_a + M_b)^2$, we can extend the analytical continuation from one half-plane to the other through Schwarz's reflection principle $J_0(\bar{s}) = \overline{J_0(s)}$. Note that the corresponding analytic functions for $J_{1,2}(s)$ in the CM frame can be obtained from (C.15) through the relations (C.10) and (C.11).

The expressions in (C.14) and (C.15) reduce to that in [54] for the case of equal masses $M_a = M_b$. In particular, as mentioned above, the Landau cut contribution in (C.14) vanishes in that case.

C.2.2 T -channel in CM frame

In this channel we have $\mathcal{Q}_0 = T_0 = 0$ and $|\vec{\mathcal{Q}}|^2 = |\vec{T}|^2 = -t(s, \theta)$.

First, from (4.2), we realize that the thermal imaginary part corresponding to the Landau cut in the t variable vanishes in this channel since it is proportional to $\int [n_B(E_1) - n_B(E_2)] \delta(E_1 - E_2)$, which corresponds to the lower end of the Landau cut

in Fig. 1.7. As for the unitary cut, it requires $t \geq (M_a + M_b)^2$, so that from (1.166) we conclude that it is present only for $s < 0$, as in the $T = 0$ case.

Therefore, in the physical region $s \geq (M_a + M_b)^2$, where $|\vec{T}| > 0$ and $t < 0$, the $J_k(0, |\vec{T}| = \sqrt{-t}; T)$ are real. In particular, from (4.1), we have for $t < 0$

$$\begin{aligned}\Delta J_0^{ab}(0, \sqrt{-t}; T) &= -\frac{1}{4\pi^2} \text{P} \int_{-1}^1 dx \int_0^\infty dp \frac{p^2}{E_1(p)} \frac{n_B[E_1(p)]}{t + 2qx\sqrt{-t} + \Delta_{ab}} + (M_a \leftrightarrow M_b) \\ &= \frac{1}{8\pi^2 \sqrt{-t}} \int_0^\infty dp \frac{p n_B[E_1(p)]}{E_1(p)} \log \left| \frac{t + \Delta_{ab} - 2q\sqrt{-t}}{t + \Delta_{ab} + 2p\sqrt{-t}} \right| + (M_a \leftrightarrow M_b), \\ J_1^{ab}(0, \sqrt{-t}; T) &= 0, \\ \Delta J_2^{ab}(0, \sqrt{-t}; T) &= \frac{1}{8\pi^2 \sqrt{-t}} \int_0^\infty dp p E_1(p) n_B[E_1(p)] \log \left| \frac{t + \Delta_{ab} - 2p\sqrt{-t}}{t + \Delta_{ab} + 2p\sqrt{-t}} \right| + (M_a \leftrightarrow M_b),\end{aligned}\tag{C.16}$$

where P denotes Cauchy's principal value and where we have performed the change of variable $\vec{p} \rightarrow -\vec{p} + \vec{T}$ in the integrals containing $n_B(E_2)$ in (4.1).

The above expressions generalize those obtained in [54, 88] for $M_a = M_b$. Actually, in the present work, only J_{aa} integrals appear in the T channel, so we refer to [88] for the analytical continuation of those integrals to the complex s - or t -plane beyond the real $t < 0$ region.

C.2.3 U -channel in CM frame

Now we have $\mathcal{Q}_0 = U_0$ and $|\vec{\mathcal{Q}}|^2 = |\vec{U}|^2$. Thus, in principle, one has both the Landau and unitary cut contributions in this channel. Performing as before the change $\vec{q} \rightarrow -\vec{q} + \vec{U}$ in the integrals containing $n_B(E_2)$, for real values of U_0 and $|\vec{U}| > 0$, we have from (4.1)

$$\begin{aligned}\Delta J_0^{ab}(U_0, |\vec{U}|; T) &= -\frac{1}{4\pi^2} \int_0^\infty dp \frac{p^2 n_B[E_1(p)]}{E_1(p)} \times \\ &\int_{-1}^1 dx \frac{u + 2p|\vec{U}|x + \Delta_{ab}}{(U_0 + i\epsilon)^4 - 2(U_0 + i\epsilon)^2 (2p^2 + |\vec{U}|^2 - 2p|\vec{U}|x + \Sigma_{ab}) + (\Delta_{ab} - |\vec{U}|^2 + 2p|\vec{U}|x)^2} \\ &+ (M_a \leftrightarrow M_b),\end{aligned}\tag{C.17}$$

$$\begin{aligned}\Delta J_1^{ab}(U_0, |\vec{U}|; T) &= \frac{U_0}{4\pi^2} \int_0^\infty dp p^2 \int_{-1}^1 dx \\ &\left\{ -2n_B[E_1(p)] \frac{E_1(p)}{(U_0 + i\epsilon)^4 - 2(U_0 + i\epsilon)^2 (2p^2 + |\vec{U}|^2 - 2p|\vec{U}|x + \Sigma_{ab}) + (\Delta_{ab} - |\vec{U}|^2 + 2p|\vec{U}|x)^2} \right. \\ &+ \left. \frac{n_B[\tilde{E}_2(p)]}{\tilde{E}_2(p)} \frac{2p^2 - u - 2p|\vec{U}|x + \Sigma_{ab}}{(U_0 + i\epsilon)^4 - 2(U_0 + i\epsilon)^2 (2p^2 + |\vec{U}|^2 - 2p|\vec{U}|x + \Sigma_{ab}) + (-\Delta_{ab} - |\vec{U}|^2 + 2p|\vec{U}|x)^2} \right\},\end{aligned}\tag{C.18}$$

$$\begin{aligned} \Delta J_2^{ab}(U_0, |\vec{U}|; T) = & -\frac{1}{4\pi^2} \int_0^\infty dp p^2 \int_{-1}^1 dx \\ & \left\{ n_B [E_1(p)] \frac{E_1(p)(u + 2p|\vec{U}|x + \Delta_{ab})}{(U_0 + i\epsilon)^4 - 2(U_0 + i\epsilon)^2 (2p^2 + |\vec{U}|^2 - 2p|\vec{U}|x + \Sigma_{ab}) + (\Delta_{ab} - |\vec{U}|^2 + 2p|\vec{U}|x)^2} \right. \\ & \left. + \frac{n_B [\tilde{E}_2(p)]}{\tilde{E}_2(p)} \frac{[(\tilde{E}_2^2(p) - U_0^2)^2 - (\tilde{E}_2^2(p) + U_0^2)(E_1^2(p) + |\vec{U}|^2 - 2p|\vec{U}|x)]}{(U_0 + i\epsilon)^4 - 2(U_0 + i\epsilon)^2 (2p^2 + |\vec{U}|^2 - 2p|\vec{U}|x + \Sigma_{ab}) + (-\Delta_{ab} - |\vec{U}|^2 + 2p|\vec{U}|x)^2} \right\}, \end{aligned} \quad (\text{C.19})$$

with $\tilde{E}_2^2(p) = p^2 + M_b^2$.

The previous expressions can be evaluated numerically and extended to complex U_0 and $|\vec{U}|$ values when needed. Actually, using these expressions, we have checked numerically that the general cut structure depicted in Fig. 1.7 is fulfilled.

Appendix D

Complete expression for the thermal $K^+\pi^+ \rightarrow K^+\pi^+$ amplitude

Here we list the expressions of the temperature-dependent corrections of the pion-kaon scattering amplitude to one loop in ChPT, with $\mathcal{T}_4^{F,J}(\mathbf{S}, \mathbf{T}, \mathbf{U}; T) = \mathcal{T}_4^{F,J}(s, t, u; T = 0) + \Delta\mathcal{T}_4^{F,J}(\mathbf{S}, \mathbf{T}, \mathbf{U}; T)$ and $\Delta f(T) \equiv f(T) - f(0)$,

$$\begin{aligned}
& \Delta\mathcal{T}_4^F(\mathbf{S}, \mathbf{T}, \mathbf{U}; T) = \\
& = \frac{1}{F^4} \left\{ -\frac{(\vec{k} \cdot \vec{T})(\vec{p} \cdot \vec{T})}{2|\vec{T}|^4} (3t + 4|\vec{T}|^2) \left(\Delta G_\pi + \frac{1}{2} \Delta G_K \right) - \frac{(\vec{k} \cdot \vec{T})}{|\vec{T}|^2} \left(\frac{1}{18} (7|\vec{T}|^2 - 18p_0 T_0) \Delta G_\pi \right. \right. \\
& + \frac{1}{6} (|\vec{T}|^2 - 3p_0 T_0) \Delta G_K \Big) + \frac{(\vec{p} \cdot \vec{T})}{|\vec{T}|^2} \left(\frac{1}{18} (7|\vec{T}|^2 + 18k_0 T_0) \Delta G_\pi + \frac{1}{6} (|\vec{T}|^2 + 3k_0 T_0) \Delta G_K \right) \\
& + \frac{(\vec{k} \cdot \vec{U})(\vec{p} \cdot \vec{U})}{16|\vec{U}|^4} \left(-3(3(-M_K^2 + M_\pi^2 + u) + 8|\vec{U}|^2) \Delta G_\pi + 9(M_\eta^2 - 2M_K^2 + M_\pi^2 - 2u) \Delta G_K \right. \\
& - 3(3(M_\eta^2 - M_K^2 + u) + 8|\vec{U}|^2) \Delta F_{\beta\eta} \Big) + \frac{(\vec{k} \cdot \vec{U})}{12|\vec{U}|^2} \left(\frac{1}{2} (-4|\vec{U}|^2 + 3(M_K^2 + M_\pi^2 - u + 6p_0 U_0)) \Delta G_\pi \right. \\
& + (3M_\eta^2 - M_K^2 - 2M_\pi^2 - 3u) \Delta G_K - \frac{1}{2} (6M_\eta^2 + M_K^2 - M_\pi^2 - 9u + 12|\vec{U}|^2 - 18p_0 U_0) \Delta G_\eta \Big) \\
& + \frac{(\vec{p} \cdot \vec{U})}{12|\vec{U}|^2} \left((7|\vec{U}|^2 - 3(M_K^2 - 2M_\pi^2 + 2u - 3k_0 U_0)) \Delta G_\pi - \frac{1}{2} (3M_\eta^2 - 16M_K^2 + 13M_\pi^2 - 12u) \Delta G_K \right. \\
& + \frac{1}{2} (3M_\eta^2 - 10M_K^2 + M_\pi^2 + 6|\vec{U}|^2 + 18k_0 U_0) \Delta G_\eta \Big) + \frac{t(\vec{p} \cdot \vec{k})}{2|\vec{T}|^2} \left(\Delta G_\pi + \frac{1}{2} \Delta G_K \right) \\
& + \frac{3(\vec{p} \cdot \vec{k})}{16|\vec{U}|^2} \left(-(M_K^2 - M_\pi^2 - u) \Delta G_\pi - (M_\eta^2 - 2M_K^2 + M_\pi^2 - 2u) \Delta G_K + (M_\eta^2 - M_K^2 + u) \Delta G_\eta \right) \\
& + \frac{1}{72} [M_K^2 - 47M_\pi^2 + 7s - 21t - 20u + 28k_0 T_0 - 28p_0 T_0 + 12k_0 U_0 - 42p_0 U_0] \Delta G_\pi \\
& - \frac{1}{180} [15M_\eta^2 + 8M_K^2 + 33M_\pi^2 - 14s + 16t - 14u - 30k_0 T_0 + 30p_0 T_0] \Delta G_K \\
& + \frac{1}{360} [39M_\eta^2 - 199M_K^2 + 46M_\pi^2 + 21s + 21t - 114u + 180k_0 U_0 - 90p_0 U_0] \Delta G_\eta \Big\} \quad (D.1)
\end{aligned}$$

$$\begin{aligned}
 \Delta\mathcal{T}^J(\mathbf{S}, \mathbf{T}, \mathbf{U}; T) = & \\
 = & \frac{1}{F^4} \left\{ \frac{1}{4} (M_K^2 + M_\pi^2 - s)^2 \Delta J_0^{K\pi}(S) - \frac{\vec{k} \cdot \vec{p}}{4|\vec{T}|^2} \left[(t^2 + 4M_\pi^2 |\vec{T}|^2) \Delta J_0^{\pi\pi}(T) - 4tT_0 \Delta J_1^{\pi\pi}(T) \right. \right. \\
 & + 4t \Delta J_2^{\pi\pi}(T) + \frac{1}{2} (t^2 + 4M_K^2 |\vec{T}|^2) \Delta J_0^{KK}(T) - 2tT_0 \Delta J_1^{KK}(T) + 2t \Delta J_2^{KK}(T) \Big] \\
 & + 6 \frac{(\vec{k} \cdot \vec{T})(\vec{p} \cdot \vec{T})}{|\vec{T}|^4} \left[\frac{1}{36} (27t^2 + 36(M_\pi^2 + t) |\vec{T}|^2 + 14|\vec{T}|^4) \Delta J_0^{\pi\pi}(T) - (3t + 2|\vec{T}|^2) T_0 \Delta J_1^{\pi\pi}(T) \right. \\
 & - (|\vec{T}|^2 - 3T_0^2) \Delta J_2^{\pi\pi}(T) + \frac{1}{24} (9t^2 + 4(3M_K^2 + 2t) |\vec{T}|^2) \Delta J_0^{KK}(T) - \frac{1}{6} (9t + 4|\vec{T}|^2) T_0 \Delta J_1^{KK}(T) \\
 & - \frac{1}{2} (|\vec{T}|^2 - 3T_0^2) \Delta J_2^{KK}(T) \Big] + \frac{(\vec{k} \cdot \vec{T})}{|\vec{T}|^2} \left[\frac{1}{36} (6t(t - 4p_0T_0) + |\vec{T}|^2(3M_\pi^2 + 2t - 14p_0T_0)) \Delta J_0^{\pi\pi}(T) \right. \\
 & + \frac{1}{3} (-tT_0 + p_0(3t + 2|\vec{T}|^2 - 4T_0^2)) \Delta J_1^{\pi\pi}(T) - 2p_0T_0 \Delta J_2^{\pi\pi}(T) - \frac{t}{12} (3t + 4|\vec{T}|^2) \Delta J_0^{KK}(T) \\
 & + \frac{1}{6} ((3t + 4|\vec{T}|^2)p_0 + 3tT_0) \Delta J_1^{KK}(T) - p_0T_0 \Delta J_2^{KK}(T) - \frac{1}{12} M_\pi^2 |\vec{T}|^2 \Delta J_0^{\eta\eta}(T) \Big] \\
 & + 6 \frac{(\vec{p} \cdot \vec{T})}{|\vec{T}|^2} \left[\frac{1}{18} (3t(t - 2p_0T_0) + |\vec{T}|^2(5t - 7p_0T_0)) \Delta J_0^{\pi\pi}(T) + \frac{1}{3} (-tT_0 + k_0(3t + 4|\vec{T}|^2 - 2T_0^2)) \Delta J_1^{\pi\pi}(T) \right. \\
 & - 2k_0T_0 \Delta J_2^{\pi\pi}(T) - \frac{t}{12} (t + 4k_0T_0) \Delta J_0^{KK}(T) + \frac{1}{6} (tT_0 + k_0(3t - 4T_0^2)) \Delta J_1^{KK}(T) - k_0T_0 \Delta J_2^{KK}(T) \Big] \\
 & - \frac{3\vec{k} \cdot \vec{p}}{16|\vec{U}|^2} \left[((M_K^2 - M_\pi^2 + u)^2 + 4M_K^2 |\vec{U}|^2) \Delta J_0^{K\pi}(U) - 4U_0(M_K^2 - M_\pi^2 + u) \Delta J_1^{K\pi}(U) + 4u \Delta J_2^{K\pi}(U) \right. \\
 & + ((-M_\eta^2 + M_K^2 + u)^2 + 4M_K^2 |\vec{U}|^2) \Delta J_0^{K\eta}(U) + 4U_0(M_\eta^2 - M_K^2 - u) \Delta J_1^{K\eta}(U) + 4u \Delta J_2^{K\eta}(U) \Big] \\
 & + \frac{3(\vec{k} \cdot \vec{U})(\vec{p} \cdot \vec{U})}{16|\vec{U}|^4} \left[(3(M_K^2 - M_\pi^2 + u)^2 + 4M_K^2 |\vec{U}|^2) \Delta J_0^{K\pi}(U) - 12U_0(M_K^2 - M_\pi^2 + u) \Delta J_1^{K\pi}(U) \right. \\
 & - 4(|\vec{U}|^2 - 3U_0^2) \Delta J_2^{K\pi}(U) + (3(-M_\eta^2 + M_K^2 + u)^2 + 4M_K^2 |\vec{U}|^2) \Delta J_0^{K\eta}(U) \\
 & - 12U_0(-M_\eta^2 + M_K^2 + u) \Delta J_1^{K\eta}(U) - 4(|\vec{U}|^2 - 3U_0^2) \Delta J_2^{K\eta}(U) \Big] \\
 & - \frac{(\vec{k} \cdot \vec{U})}{8|\vec{U}|^2} \left[(-M_K^4 + (M_\pi^2 - u)^2) \Delta J_0^{K\pi}(U) - 2(3(M_K^2 - M_\pi^2 + u)p_0 - (M_K^2 + M_\pi^2 - u)U_0) \Delta J_1^{K\pi}(U) \right. \\
 & + 12p_0U_0 \Delta J_2^{K\pi}(U) - \frac{1}{3} (6M_\eta^2 + M_K^2 - M_\pi^2 - 9u)(M_\eta^2 - M_K^2 - u) \Delta J_0^{K\eta}(U) \\
 & + \frac{2}{3} (9(M_\eta^2 - M_K^2 - u)p_0 + (-6M_\eta^2 - M_K^2 + M_\pi^2 + 9u)U_0) \Delta J_1^{K\eta}(U) + 12p_0U_0 \Delta J_2^{K\eta}(U) \Big] \\
 & - \frac{(\vec{p} \cdot \vec{U})}{4|\vec{U}|^2} \left[(M_K^4 - 3M_K^2(M_\pi^2 - u) + 2(M_\pi^2 - u)^2) \Delta J_0^{K\pi}(U) \right. \\
 & - (3(M_K^2 - M_\pi^2 + u)k_0 + 2(M_K^2 - 2M_\pi^2 + 2u)U_0) \Delta J_1^{K\pi}(U) \\
 & + 6k_0U_0 \Delta J_2^{K\pi}(U) + \frac{1}{6} (3M_\eta^2 - 10M_K^2 + M_\pi^2)(M_\eta^2 - M_K^2 - u) \Delta J_0^{K\eta}(U) \\
 & + \frac{1}{3} (9(M_\eta^2 - M_K^2 - u)k_0 + (3M_\eta^2 - 10M_K^2 + M_\pi^2)U_0) \Delta J_1^{K\eta}(U) + 6k_0U_0 \Delta J_2^{K\eta}(U) \Big] \\
 & + \frac{1}{4} (M_\pi^2 - u)(M_K^2 + M_\pi^2 - u) \Delta J_0^{K\pi}(U) - \frac{1}{4} ((-M_K^2 + M_\pi^2 - u)k_0 + 2(M_K^2 - 2M_\pi^2 + 2u)p_0) \Delta J_1^{K\pi}(U) \\
 & + \frac{3}{3} k_0p_0 \Delta J_2^{K\pi}(U) - \frac{1}{216} (3M_\eta^2 - 10M_K^2 + M_\pi^2)(6M_\eta^2 + M_K^2 - M_\pi^2 - 9u) \Delta J_0^{K\eta}(U) \\
 & - \frac{1}{12} ((6M_\eta^2 + M_K^2 - M_\pi^2 - 9u)k_0 - (3M_\eta^2 - 10M_K^2 + M_\pi^2)p_0) \Delta J_1^{K\eta}(U) - \frac{3}{2} \Delta J_2^{K\eta}(U) \\
 & + \frac{t}{36} ((-3M_\pi^2 + 4t - 10p_0T_0) + k_0T_0(3M_\pi^2 + 2t - 14p_0T_0)) \Delta J_0^{\pi\pi}(T) + \frac{1}{3} (tp_0 + k_0(t + 6p_0T_0)) \Delta J_1^{\pi\pi}(T) \\
 & + 2k_0p_0 \Delta J_2^{\pi\pi}(T) + \frac{t}{12} (t + 4k_0T_0) \Delta J_0^{KK}(T) - \frac{1}{6} (tp_0 + k_0(3t - 4p_0T_0)) \Delta J_1^{KK}(T) + k_0p_0 \Delta J_2^{KK}(T) \\
 & - \frac{1}{36} M_\pi^2 (3M_\eta^2 + M_\pi^2 - 3t - 3k_0T_0) \Delta J_0^{\eta\eta}(T) \Big\} ,
 \end{aligned}$$

with $k_\mu = (p_K)_\mu$ and $p_\mu = (p_\pi)_\mu$.

Appendix E

Results for χ_{top} at NLO and NNLO in U(3) ChPT in the isospin limit

We provide here the full results for the topological susceptibility in the U(3) ChPT formalism at NLO and NNLO in the δ expansion.

$$\begin{aligned}
& \chi_{top}^{U(3),NLO} = \\
& = \frac{1}{9M_{0\eta'}^4} \left\{ F^2 \Lambda_2 M_0^2 c_\theta \left[2M_{0K}^2 (c_\theta - \sqrt{2}s_\theta) + M_{0\pi}^2 (2\sqrt{2}s_\theta + c_\theta) \right] (M_0^2 c_\theta^2 - M_{0\eta'}^2) \right. \\
& + 8M_0^4 c_\theta^2 L_8^r \left[4M_{0K}^4 (2s_\theta^2 + c_\theta^2 - 2\sqrt{2}s_\theta c_\theta) \right. \\
& - 4M_{0\pi}^2 M_{0K}^2 (2s_\theta^2 + c_\theta^2 - 2\sqrt{2}s_\theta c_\theta) + 3M_{0\pi}^4 \left. \right] \left. \right\} \\
& + \frac{1}{9M_{0\eta}^4} \left\{ F^2 \Lambda_2 M_0^4 s_\theta^3 \left[2M_{0K}^2 (s_\theta + \sqrt{2}c_\theta) + M_{0\pi}^2 (s_\theta - 2\sqrt{2}c_\theta) \right] \right. \\
& + 8M_0^4 s_\theta^2 L_8^r \left[4M_{0K}^4 (s_\theta^2 + 2c_\theta^2 + 2\sqrt{2}s_\theta c_\theta) \right. \\
& - 4M_{0\pi}^2 M_{0K}^2 (s_\theta^2 + 2c_\theta^2 + 2\sqrt{2}s_\theta c_\theta) + 3M_{0\pi}^4 \left. \right] \left. \right\} \\
& + \frac{1}{9M_{0\eta}^2 M_{0\eta'}^2} \left\{ F^2 \Lambda_2 M_0^2 s_\theta \left[(2M_{0K}^2 (s_\theta + \sqrt{2}c_\theta) + M_{0\pi}^2 (s_\theta - 2\sqrt{2}c_\theta)) (M_0^2 c_\theta^2 - M_{0\eta'}^2) \right. \right. \\
& + M_0^2 s_\theta c_\theta \left[2M_{0K}^2 (c_\theta - \sqrt{2}s_\theta) + M_{0\pi}^2 (2\sqrt{2}s_\theta + c_\theta) \right] \left. \right] \\
& + 64M_0^4 s_\theta c_\theta M_{0K}^2 (M_{0K}^2 - M_{0\pi}^2) L_8^r (-\sqrt{2}s_\theta^2 + \sqrt{2}c_\theta^2 - s_\theta c_\theta) \left. \right\} \tag{E.1}
\end{aligned}$$

$$\begin{aligned}
 \chi_{top}^{U(3),NNLO} = & -\frac{16M_0^2\Lambda_2L_8^r}{27M_{0\eta}^6M_{0\eta'}^6} \left\{ 8M_{0K}^6 \left[c_\theta \left(c_\theta^3\sqrt{2}s_\theta c_\theta^2 + 6s_\theta^2 c_\theta \right. \right. \right. \\
 & - 2\sqrt{2}s_\theta^3 \left. \left. \left(2c_\theta^2 M_0^2 - M_{0\eta'}^2 \right) M_{0\eta}^6 M_{0\eta'}^2 \left(2c_\theta \left(c_\theta^5 + 2\sqrt{2}s_\theta c_\theta^4 \right. \right. \right. \right. \\
 & - 7s_\theta^2 c_\theta^3 - 2\sqrt{2}s_\theta^3 c_\theta^2 + 7s_\theta^4 c_\theta - \sqrt{2}s_\theta^5 \left. \left. \right) M_0^2 \right. \right. \\
 & + \left. \left(-2c_\theta^4 - \sqrt{2}s_\theta c_\theta^3 + 6s_\theta^2 c_\theta^2 + \sqrt{2}s_\theta^3 c_\theta - 2s_\theta^4 \right) M_{0\eta'}^2 \right) M_{0\eta}^4 \\
 & + s_\theta M_{0\eta'}^4 \left(2 \left(\sqrt{2}c_\theta^5 + 7s_\theta c_\theta^4 + 2\sqrt{2}s_\theta^2 c_\theta^3 - 7s_\theta^3 c_\theta^2 - 2\sqrt{2}s_\theta^4 c_\theta + s_\theta^5 \right) M_0^2 \right. \\
 & - \left. \left(2\sqrt{2}c_\theta^3 + 6s_\theta c_\theta^2 + 3\sqrt{2}s_\theta^2 c_\theta + s_\theta^3 \right) M_{0\eta'}^2 \right) M_{0\eta}^2 \\
 & + 2s_\theta^3 \left(2\sqrt{2}c_\theta^3 + 6s_\theta c_\theta^2 + 3\sqrt{2}s_\theta^2 c_\theta + s_\theta^3 \right) M_0^2 M_{0\eta'}^6 \left. \right] \\
 & - 4M_{0\pi}^2 M_{0K}^4 \left[c_\theta \left(c_\theta^3 - 6\sqrt{2}s_\theta c_\theta^2 + 18s_\theta^2 c_\theta - 8\sqrt{2}s_\theta^3 \right) \left(2c_\theta^2 M_0^2 - M_{0\eta'}^2 \right) M_{0\eta}^6 \right. \\
 & + 2M_{0\eta'}^2 \left(c_\theta \left(4c_\theta^5 + 2\sqrt{2}s_\theta c_\theta^4 - 25s_\theta^2 c_\theta^3 + 4\sqrt{2}s_\theta^3 c_\theta^2 + 22s_\theta^4 c_\theta \right. \right. \\
 & - 4\sqrt{2}s_\theta^5 \left. \left. \right) M_0^2 + \left(-4c_\theta^4 + \sqrt{2}s_\theta c_\theta^3 + 9s_\theta^2 c_\theta^2 - \sqrt{2}s_\theta^3 c_\theta - 4s_\theta^4 \right) M_{0\eta'}^2 \right) M_{0\eta}^4 \\
 & + M_{0\eta'}^4 s_\theta \left(2 \left(4\sqrt{2}c_\theta^5 + 22s_\theta c_\theta^4 - 4\sqrt{2}s_\theta^2 c_\theta^3 - 25s_\theta^3 c_\theta^2 - 2\sqrt{2}s_\theta^4 c_\theta + 4s_\theta^5 \right) M_0^2 \right. \\
 & - \left. \left(8\sqrt{2}c_\theta^3 + 18s_\theta c_\theta^2 + 6\sqrt{2}s_\theta^2 c_\theta + s_\theta^3 \right) M_{0\eta'}^2 \right) M_{0\eta}^2 \\
 & + 2s_\theta^3 \left(8\sqrt{2}c_\theta^3 + 18s_\theta c_\theta^2 + 6\sqrt{2}s_\theta^2 c_\theta + s_\theta^3 \right) M_0^2 M_{0\eta'}^6 \left. \right] \\
 & + 2M_{0\pi}^4 M_{0K}^2 \left[c_\theta \left(c_\theta^3 - 3\sqrt{2}s_\theta c_\theta^2 + 15s_\theta^2 c_\theta - 11\sqrt{2}s_\theta^3 \right) \left(2c_\theta^2 M_0^2 - M_{0\eta'}^2 \right) M_{0\eta}^6 \right. \\
 & + M_{0\eta'}^2 \left(c_\theta \left(8c_\theta^5 - 5\sqrt{2}s_\theta c_\theta^4 - 38s_\theta^2 c_\theta^3 + 32\sqrt{2}s_\theta^3 c_\theta^2 + 38s_\theta^4 c_\theta \right. \right. \\
 & - 11\sqrt{2}s_\theta^5 \left. \left. \right) M_0^2 - 4 \left(2c_\theta^4 - 2\sqrt{2}s_\theta c_\theta^3 - 3s_\theta^2 c_\theta^2 + 2\sqrt{2}s_\theta^3 c_\theta + 2s_\theta^4 \right) M_{0\eta'}^2 \right) M_{0\eta}^4 \\
 & + s_\theta M_{0\eta'}^4 \left(\left(11\sqrt{2}c_\theta^5 + 38s_\theta c_\theta^4 - 32\sqrt{2}s_\theta^2 c_\theta^3 - 38s_\theta^3 c_\theta^2 \right. \right. \\
 & + 5\sqrt{2}s_\theta^4 c_\theta + 8s_\theta^5 \left. \left. \right) M_0^2 - \left(11\sqrt{2}c_\theta^3 + 15s_\theta c_\theta^2 + 3\sqrt{2}s_\theta^2 c_\theta + s_\theta^3 \right) M_{0\eta'}^2 \right) M_{0\eta}^2 \\
 & + 2s_\theta^3 \left(11\sqrt{2}c_\theta^3 + 15s_\theta c_\theta^2 + 3\sqrt{2}s_\theta^2 c_\theta + s_\theta^3 \right) M_0^2 M_{0\eta'}^6 \left. \right] \\
 & + 3M_{0\pi}^6 \left[c_\theta \left(c_\theta + 2\sqrt{2}s_\theta \right) \left(2c_\theta^2 M_0^2 - M_{0\eta'}^2 \right) M_{0\eta}^6 \right. \\
 & + 2c_\theta s_\theta \left(-\sqrt{2}c_\theta^2 + s_\theta c_\theta + \sqrt{2}s_\theta^2 \right) M_0^2 M_{0\eta'}^2 M_{0\eta}^4 + 2s_\theta^3 \left(s_\theta - 2\sqrt{2}c_\theta \right) M_0^2 M_{0\eta'}^6 \\
 & + s_\theta M_{0\eta'}^4 \left(2c_\theta \left(-\sqrt{2}c_\theta^2 + s_\theta c_\theta + \sqrt{2}s_\theta^2 \right) M_0^2 + \left(2\sqrt{2}c_\theta - s_\theta \right) M_{0\eta'}^2 \right) M_{0\eta}^2 \left. \right] \left. \right\} \\
 & - \frac{128M_0^4(L_8^r)^2}{27F^2M_{0\eta}^6M_{0\eta'}^6} \left\{ 16M_{0K}^8 \left[c_\theta^2 \left(c_\theta^4 - 4\sqrt{2}s_\theta c_\theta^3 + 12s_\theta^2 c_\theta^2 - 8\sqrt{2}s_\theta^3 c_\theta + 4s_\theta^4 \right) M_{0\eta}^6 \right. \right. \\
 & + c_\theta \left(2c_\theta^2 - s_\theta^2 \right) \left(c_\theta^3 - 6s_\theta^2 c_\theta + 4\sqrt{2}s_\theta^3 \right) M_{0\eta'}^2 M_{0\eta}^4 \\
 & + s_\theta \left(c_\theta^2 - 2s_\theta^2 \right) \left(4\sqrt{2}c_\theta^3 + 6s_\theta c_\theta^2 - s_\theta^3 \right) M_{0\eta'}^4 M_{0\eta}^2 \\
 & + s_\theta^2 \left(4c_\theta^4 + 8\sqrt{2}s_\theta c_\theta^3 + 12s_\theta^2 c_\theta^2 + 4\sqrt{2}s_\theta^3 c_\theta + s_\theta^4 \right) M_{0\eta'}^6 \left. \right] \\
 & - 32M_{0\pi}^2 M_{0K}^6 \left[c_\theta^2 \left(c_\theta^4 - 4\sqrt{2}s_\theta c_\theta^3 + 12s_\theta^2 c_\theta^2 - 8\sqrt{2}s_\theta^3 c_\theta + 4s_\theta^4 \right) M_{0\eta}^6 \right.
 \end{aligned}$$

$$\begin{aligned}
& + c_\theta (2c_\theta^2 - s_\theta^2) \left(c_\theta^3 - 6s_\theta^2 c_\theta + 4\sqrt{2}s_\theta^3 \right) M_{0\eta'}^2 M_{0\eta}^4 \\
& + s_\theta (c_\theta^2 - 2s_\theta^2) \left(4\sqrt{2}c_\theta^3 + 6s_\theta c_\theta^2 - s_\theta^3 \right) M_{0\eta'}^4 M_{0\eta}^2 \\
& + s_\theta^2 \left(4c_\theta^4 + 8\sqrt{2}s_\theta c_\theta^3 + 12s_\theta^2 c_\theta^2 + 4\sqrt{2}s_\theta^3 c_\theta + s_\theta^4 \right) M_{0\eta'}^6 \Big] \\
& + 8M_{0\pi}^4 M_{0K}^4 \left[c_\theta^2 \left(5c_\theta^4 - 14\sqrt{2}s_\theta c_\theta^3 + 33s_\theta^2 c_\theta^2 - 22\sqrt{2}s_\theta^3 c_\theta + 14s_\theta^4 \right) M_{0\eta}^6 \right. \\
& + c_\theta \left(4c_\theta^5 + 3\sqrt{2}s_\theta c_\theta^4 - 29s_\theta^2 c_\theta^3 + 16\sqrt{2}s_\theta^3 c_\theta^2 + 9s_\theta^4 c_\theta - 11\sqrt{2}s_\theta^5 \right) M_{0\eta'}^2 M_{0\eta}^4 \\
& + s_\theta \left(11\sqrt{2}c_\theta^5 + 9s_\theta c_\theta^4 - 16\sqrt{2}s_\theta^2 c_\theta^3 - 29s_\theta^3 c_\theta^2 - 3\sqrt{2}s_\theta^4 c_\theta + 4s_\theta^5 \right) M_{0\eta'}^4 M_{0\eta}^2 \\
& \left. + s_\theta^2 \left(14c_\theta^4 + 22\sqrt{2}s_\theta c_\theta^3 + 33s_\theta^2 c_\theta^2 + 14\sqrt{2}s_\theta^3 c_\theta + 5s_\theta^4 \right) M_{0\eta'}^6 \right] \\
& - 24M_{0\pi}^6 M_{0K}^2 \left[c_\theta^2 \left(c_\theta^2 - 2\sqrt{2}s_\theta c_\theta + 2s_\theta^2 \right) M_{0\eta}^6 \right. \\
& + c_\theta s_\theta \left(\sqrt{2}c_\theta^2 - s_\theta c_\theta - \sqrt{2}s_\theta^2 \right) M_{0\eta'}^2 M_{0\eta}^4 \\
& + c_\theta s_\theta \left(\sqrt{2}c_\theta^2 - s_\theta c_\theta - \sqrt{2}s_\theta^2 \right) M_{0\eta'}^4 M_{0\eta}^2 + s_\theta^2 \left(2c_\theta^2 + 2\sqrt{2}s_\theta c_\theta + s_\theta^2 \right) M_{0\eta'}^6 \Big] \\
& + 9M_{0\pi}^8 (c_\theta^2 M_{0\eta}^6 + s_\theta^2 M_{0\eta'}^6) \Big\} \\
& + \frac{1}{M_{0\eta}^4 M_{0\eta'}^4} \left\{ (2M_{0K}^2 + M_{0\pi}^2) F^2 v_2^{(2)} [(c_\theta^2 M_0^2 - M_{0\eta'}^2) M_{0\eta}^2 + s_\theta^2 M_0^2 M_{0\eta'}^2] \right\}^2 \\
& + \frac{8L_6^r M_0^4 (2M_{0K}^2 + M_{0\pi}^2)}{9} \left[c_\theta^2 \left(2 \left(c_\theta^2 - 2\sqrt{2}s_\theta c_\theta + 2s_\theta^2 \right) M_{0K}^2 \right. \right. \\
& + \left. \left(c_\theta^2 + 4\sqrt{2}s_\theta c_\theta - s_\theta^2 \right) M_{0\pi}^2 \right) M_{0\eta}^4 \\
& + 4c_\theta s_\theta \left(\sqrt{2}c_\theta^2 - s_\theta c_\theta - \sqrt{2}s_\theta^2 \right) (M_{0K}^2 - M_{0\pi}^2) M_{0\eta'}^2 M_{0\eta}^2 \\
& + s_\theta^2 \left(2 \left(2c_\theta^2 + 2\sqrt{2}s_\theta c_\theta + s_\theta^2 \right) M_{0K}^2 + \left(-c_\theta^2 - 4\sqrt{2}s_\theta c_\theta + s_\theta^2 \right) M_{0\pi}^2 \right) M_{0\eta'}^4 \Big] \\
& + \frac{8C_{19} M_0^4}{3} \left[c_\theta^2 \left(8 \left(c_\theta^2 - 2\sqrt{2}s_\theta c_\theta + 2s_\theta^2 \right) M_{0K}^6 \right. \right. \\
& - 12 \left(c_\theta^2 - 2\sqrt{2}s_\theta c_\theta + 2s_\theta^2 \right) M_{0\pi}^2 M_{0K}^4 \\
& + 6 \left(c_\theta^2 - 2\sqrt{2}s_\theta c_\theta + 2s_\theta^2 \right) M_{0\pi}^4 M_{0K}^2 + \left. \left(c_\theta^2 + 4\sqrt{2}s_\theta c_\theta - s_\theta^2 \right) M_{0\pi}^6 \right) M_{0\eta}^4 \\
& + 4c_\theta s_\theta \left(\sqrt{2}c_\theta^2 - s_\theta c_\theta - \sqrt{2}s_\theta^2 \right) (4M_{0K}^6 - 6M_{0\pi}^2 M_{0K}^4 + 3M_{0\pi}^4 M_{0K}^2 - M_{0\pi}^6) M_{0\eta'}^2 M_{0\eta}^2 \\
& + s_\theta^2 \left(8 \left(2c_\theta^2 + 2\sqrt{2}s_\theta c_\theta + s_\theta^2 \right) M_{0K}^6 - 12 \left(2c_\theta^2 + 2\sqrt{2}s_\theta c_\theta + s_\theta^2 \right) M_{0\pi}^2 M_{0K}^4 \right. \\
& + 6 \left(2c_\theta^2 + 2\sqrt{2}s_\theta c_\theta + s_\theta^2 \right) M_{0\pi}^4 M_{0K}^2 + \left. \left(-c_\theta^2 - 4\sqrt{2}s_\theta c_\theta + s_\theta^2 \right) M_{0\pi}^6 \right) M_{0\eta'}^4 \Big] \\
& + \frac{16C_{31} M_0^4}{9} \left[c_\theta^2 \left(8 \left(c_\theta^2 - 2\sqrt{2}s_\theta c_\theta + 2s_\theta^2 \right) M_{0K}^6 \right. \right. \\
& - 12 \left(c_\theta^2 - 2\sqrt{2}s_\theta c_\theta + 2s_\theta^2 \right) M_{0\pi}^2 M_{0K}^4 \\
& + 6 \left(c_\theta^2 - 2\sqrt{2}s_\theta c_\theta + 2s_\theta^2 \right) M_{0\pi}^4 M_{0K}^2 + \left. \left(c_\theta^2 + 4\sqrt{2}s_\theta c_\theta - s_\theta^2 \right) M_{0\pi}^6 \right) M_{0\eta}^4 \\
& + 4c_\theta s_\theta \left(\sqrt{2}c_\theta^2 - s_\theta c_\theta - \sqrt{2}s_\theta^2 \right) (4M_{0K}^6 - 6M_{0\pi}^2 M_{0K}^4 + 3M_{0\pi}^4 M_{0K}^2 - M_{0\pi}^6) M_{0\eta'}^2 M_{0\eta}^2 \\
& + s_\theta^2 \left(8 \left(2c_\theta^2 + 2\sqrt{2}s_\theta c_\theta + s_\theta^2 \right) M_{0K}^6 - 12 \left(2c_\theta^2 + 2\sqrt{2}s_\theta c_\theta + s_\theta^2 \right) M_{0\pi}^2 M_{0K}^4 \right. \\
& + 6 \left(2c_\theta^2 + 2\sqrt{2}s_\theta c_\theta + s_\theta^2 \right) M_{0\pi}^4 M_{0K}^2 + \left. \left(-c_\theta^2 - 4\sqrt{2}s_\theta c_\theta + s_\theta^2 \right) M_{0\pi}^6 \right) M_{0\eta'}^4 \Big]
\end{aligned}$$

$$\begin{aligned}
 & + \frac{8L_7^r M_0^4}{9} \left[c_\theta^2 (8s_\theta^2 (M_{0K}^2 - M_{0\pi}^2)^2 + c_\theta^2 (2M_{0K}^2 + M_{0\pi}^2)^2 \right. \\
 & + 4\sqrt{2}c_\theta s_\theta (-2M_{0K}^4 + M_{0\pi}^2 M_{0K}^2 + M_{0\pi}^4) \left. \right] M_{0\eta}^4 \\
 & + 2c_\theta s_\theta \left(4 \left(\sqrt{2}c_\theta^2 - s_\theta c_\theta - \sqrt{2}s_\theta^2 \right) M_{0K}^4 \right. \\
 & + 2 \left(-\sqrt{2}c_\theta^2 + 10s_\theta c_\theta + \sqrt{2}s_\theta^2 \right) M_{0\pi}^2 M_{0K}^2 \\
 & + \left(-2\sqrt{2}c_\theta^2 - 7s_\theta c_\theta + 2\sqrt{2}s_\theta^2 \right) M_{0\pi}^4 \left. \right] M_{0\eta'}^2 M_{0\eta}^2 \\
 & + s_\theta^2 \left(8c_\theta^2 (M_{0K}^2 - M_{0\pi}^2)^2 + s_\theta^2 (2M_{0K}^2 + M_{0\pi}^2)^2 + 4\sqrt{2}c_\theta s_\theta (2M_{0K}^4 - M_{0\pi}^2 M_{0K}^2 - M_{0\pi}^4) \right) M_{0\eta'}^4 \Big] \\
 & - \frac{8L_{25}^r M_0^2}{3} \left[c_\theta \left(4 \left(c_\theta - \sqrt{2}s_\theta \right) M_{0K}^4 - 4 \left(c_\theta - \sqrt{2}s_\theta \right) M_{0\pi}^2 M_{0K}^2 + 3c_\theta M_{0\pi}^4 \right) M_{0\eta}^2 \right. \\
 & + s_\theta \left(4 \left(\sqrt{2}c_\theta + s_\theta \right) M_{0K}^4 \right. \\
 & + \left. -4 \left(\sqrt{2}c_\theta + s_\theta \right) M_{0\pi}^2 M_{0K}^2 + 3s_\theta M_{0\pi}^4 \right) M_{0\eta'}^2 \left. \right] \left((c_\theta^2 M_0^2 - M_{0\eta'}^2) M_{0\eta}^2 + s_\theta^2 M_0^2 M_{0\eta'}^2 \right) \Big\} \\
 & - \frac{M_0^4}{54M_{0\eta}^4} \left\{ 4s_\theta^2 \left(2(2\mu_\eta(T) + \mu_{\eta'}(T)) c_\theta^4 + 2\sqrt{2}s_\theta (4\mu_\eta(T) - \mu_{\eta'}(T)) c_\theta^3 \right. \right. \\
 & + 3s_\theta^2 (4\mu_\eta(T) - \mu_{\eta'}(T)) c_\theta^2 + 2\sqrt{2}s_\theta ((2\mu_\eta(T) + \mu_{\eta'}(T)) s_\theta^2 + 3\mu_K(T)) c_\theta \\
 & + 6\mu_K(T) s_\theta^2 + s_\theta^4 (\mu_\eta(T) + 2\mu_{\eta'}(T))) M_{0K}^2 \\
 & + s_\theta^2 M_{0\pi}^2 \left(- (7\mu_\eta(T) + 2\mu_{\eta'}(T)) c_\theta^4 + 2\sqrt{2}s_\theta (\mu_{\eta'}(T) - 10\mu_\eta(T)) c_\theta^3 \right. \\
 & + 3((\mu_{\eta'}(T) - 4\mu_\eta(T)) s_\theta^2 - 2\mu_K(T) + 3\mu_\pi(T)) c_\theta^2 \\
 & - 2\sqrt{2}s_\theta ((8\mu_\eta(T) + \mu_{\eta'}(T)) s_\theta^2 + 6\mu_K(T) + 9\mu_\pi(T)) c_\theta + 18s_\theta^2 \mu_\pi(T) \\
 & \left. \left. + 2s_\theta^4 (\mu_\eta(T) - \mu_{\eta'}(T))) \right\} \right. \\
 & - \frac{M_0^4}{54M_{0\eta'}^4} \left\{ 4M_{0K}^2 c_\theta^2 \left[(2\mu_\eta(T) + \mu_{\eta'}(T)) c_\theta^4 - 2\sqrt{2}s_\theta (\mu_\eta(T) + 2\mu_{\eta'}(T)) c_\theta^3 \right. \right. \\
 & + (6\mu_K(T) - 3s_\theta^2 (\mu_\eta(T) - 4\mu_{\eta'}(T))) c_\theta^2 + 2\sqrt{2}s_\theta (s_\theta^2 (\mu_\eta(T) - 4\mu_{\eta'}(T)) - 3\mu_K(T)) c_\theta \\
 & + 2s_\theta^4 (\mu_\eta(T) + 2\mu_{\eta'}(T))] + M_{0\pi}^2 c_\theta^2 \left[2(\mu_{\eta'}(T) - \mu_\eta(T)) c_\theta^4 \right. \\
 & + 2\sqrt{2}s_\theta (\mu_\eta(T) + 8\mu_{\eta'}(T)) c_\theta^3 + 3((\mu_\eta(T) - 4\mu_{\eta'}(T)) s_\theta^2 + 6\mu_\pi(T)) c_\theta^2 \\
 & + 2\sqrt{2}s_\theta c_\theta (- (\mu_\eta(T) - 10\mu_{\eta'}(T)) s_\theta^2 + 6\mu_K(T) + 9\mu_\pi(T)) \\
 & \left. \left. - s_\theta^2 ((2\mu_\eta(T) + 7\mu_{\eta'}(T)) s_\theta^2 + 6\mu_K(T) - 9\mu_\pi(T)) \right] \right\} \\
 & - \frac{M_0^4}{54M_{0\eta}^2 M_{0\eta'}^2} \left\{ 8c_\theta s_\theta M_{0K}^2 \left[\sqrt{2}(2\mu_\eta(T) + \mu_{\eta'}(T)) c_\theta^4 + s_\theta (2\mu_\eta(T) - 5\mu_{\eta'}(T)) c_\theta^3 \right. \right. \\
 & + 3\sqrt{2}((\mu_{\eta'}(T) - \mu_\eta(T)) s_\theta^2 + \mu_K(T)) c_\theta^2 + s_\theta c_\theta ((2\mu_{\eta'}(T) - 5\mu_\eta(T)) s_\theta^2 + 6\mu_K(T)) \\
 & \left. \left. - \sqrt{2}s_\theta^2 ((\mu_\eta(T) + 2\mu_{\eta'}(T)) s_\theta^2 + 3\mu_K(T)) \right] \right. \\
 & + 2c_\theta s_\theta M_{0\pi}^2 \left[\sqrt{2}(4\mu_\eta(T) + 5\mu_{\eta'}(T)) s_\theta^4 + c_\theta (8\mu_\eta(T) + \mu_{\eta'}(T)) s_\theta^3 \right. \\
 & + 3\sqrt{2}((\mu_\eta(T) - \mu_{\eta'}(T)) c_\theta^2 + 2\mu_K(T) + 3\mu_\pi(T)) s_\theta^2 \\
 & + s_\theta c_\theta ((\mu_\eta(T) + 8\mu_{\eta'}(T)) c_\theta^2 + 6\mu_K(T) + 9\mu_\pi(T)) \\
 & \left. \left. - \sqrt{2}c_\theta^2 ((5\mu_\eta(T) + 4\mu_{\eta'}(T)) c_\theta^2 + 6\mu_K(T) + 9\mu_\pi(T)) \right] \right\} \Big] \quad (E.2)
 \end{aligned}$$

Appendix F

New $O(p^4)$ operators for nonzero chemical potential

F.1 $SU(2)$ operator identities

For arbitrary two-dimensional matrices A_1, A_2, A_3 , Cayley-Hamilton theorem implies [192]:

$$\text{tr}(A_3\{A_1, A_2\}) = \text{tr}(A_1)\text{tr}(A_2A_3) + \text{tr}(A_2)\text{tr}(A_1A_3) + \text{tr}(A_3)\text{tr}(A_1A_2) - \text{tr}(A_1)\text{tr}(A_2)\text{tr}(A_3) \quad (\text{F.1})$$

Using (F.1) we can eliminate single traces of operators in terms of double or triple traces. In particular, the following identities hold:

$$\begin{aligned} \text{tr}(d_\mu U^\dagger d^\mu U d_\nu U^\dagger d^\nu U) &= \frac{1}{2} [\text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) \text{tr}(d^\nu U^\dagger d_\nu U) + \text{tr}^2(d_\mu U^\dagger d^\mu U)] \\ &- \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U d^\nu U^\dagger d_\nu U) \end{aligned} \quad (\text{F.2})$$

$$\begin{aligned} \text{tr}(d_\mu U^\dagger d_\nu U d^\mu U^\dagger d^\nu U) &= -\text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U d^\nu U^\dagger d_\nu U) \\ &+ \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d_\nu U) \text{tr}(d^\mu U^\dagger d^\nu U) + \text{tr}(d_\mu U^\dagger d_\nu U) \text{tr}(d^\mu U^\dagger d^\nu U) \\ &- \frac{1}{2} [\text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) \text{tr}(d^\nu U^\dagger d_\nu U) + \text{tr}^2(d_\mu U^\dagger d^\mu U)] \end{aligned} \quad (\text{F.3})$$

$$\begin{aligned} 2 \text{tr}(U^\dagger d^\mu U d^\nu U^\dagger d_\nu U) &= 2 \text{tr}(U^\dagger d_\nu U) \text{tr}(d_\mu U^\dagger d^\nu U) + \text{tr}(U^\dagger d_\mu U) \text{tr}(d_\nu U^\dagger d^\nu U) \\ &+ \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d_\nu U) \text{tr}(U^\dagger d^\nu U) \end{aligned} \quad (\text{F.4})$$

$$\begin{aligned} \text{tr} [d_\mu U^\dagger d^\mu U (\chi^\dagger U + U^\dagger \chi)] &= \frac{1}{2} \text{tr}(d_\mu U^\dagger d^\mu U) \text{tr}(\chi^\dagger U + U^\dagger \chi) \\ &- \text{tr}(U^\dagger d_\mu U) \text{tr} [U^\dagger d_\mu U (\chi^\dagger U + U^\dagger \chi)] \\ &+ \frac{1}{2} \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) \text{tr}(\chi^\dagger U + U^\dagger \chi) \end{aligned} \quad (\text{F.5})$$

$$\begin{aligned} \text{tr} (d^\mu U^\dagger d_\mu U Q_L^2 + d^\mu U d_\mu U^\dagger Q_R^2) &= \frac{1}{2} \text{tr} (d^\mu U^\dagger d_\mu U) \text{tr} (Q_R^2 + Q_L^2) \\ &- \text{tr} (d^\mu U^\dagger U) \text{tr} (U d_\mu U^\dagger Q_R^2 - U^\dagger d_\mu U Q_L^2) - \frac{1}{2} \text{tr} (d^\mu U^\dagger U) \text{tr} (U^\dagger d_\mu U) \text{tr} (Q_R^2 + Q_L^2) \end{aligned} \quad (\text{F.6})$$

$$\begin{aligned} \text{tr} (d^\mu U^\dagger d_\mu U Q_L + d^\mu U d_\mu U^\dagger Q_R) &= \frac{1}{2} \text{tr} (d^\mu U^\dagger d_\mu U) \text{tr} (Q_R + Q_L) \\ &- \text{tr} (d^\mu U^\dagger U) \text{tr} (U d_\mu U^\dagger Q_R - U^\dagger d_\mu U Q_L) - \frac{1}{2} \text{tr} (d^\mu U^\dagger U) \text{tr} (U^\dagger d_\mu U) \text{tr} (Q_R + Q_L) \end{aligned} \quad (\text{F.7})$$

$$\begin{aligned} \text{tr} (d^\mu U^\dagger d_\mu U Q_L U^\dagger Q_R U + d_\mu U d^\mu U^\dagger Q_R U Q_L U^\dagger) &= \\ \text{tr} (d^\mu U^\dagger d_\mu U) \text{tr} (Q_L U^\dagger Q_R U) + \text{tr} (d^\mu U^\dagger U) \text{tr} (d_\mu U Q_L U^\dagger Q_R - d_\mu U^\dagger Q_R U Q_L) & \quad (\text{F.8}) \\ - \text{tr} (d^\mu U^\dagger U) \text{tr} (U^\dagger d^\mu U) \text{tr} (Q_R U Q_L U^\dagger) \end{aligned}$$

$$\begin{aligned} 2 \text{tr} (d_\mu U Q_L U^\dagger Q_R - d_\mu U^\dagger Q_R U Q_L) &= \text{tr} (U^\dagger d_\mu U) \text{tr} (Q_L U^\dagger Q_R U) \\ &+ \text{tr} (d_\mu U U^\dagger Q_R) \text{tr} (Q_L) + \text{tr} (U^\dagger d_\mu U Q_L) \text{tr} (Q_R) - \text{tr} (U^\dagger d_\mu U) \text{tr} (Q_L) \text{tr} (Q_R) \end{aligned} \quad (\text{F.9})$$

$$\begin{aligned} \text{tr} [(\chi U^\dagger + U \chi^\dagger) Q_R^2 + (\chi^\dagger U + U^\dagger \chi) Q_L^2] &= \frac{1}{2} \text{tr} (\chi^\dagger U + U^\dagger \chi) \text{tr} [(Q_R^2) + (Q_L^2)] \\ &+ \text{tr} [(\chi U^\dagger + U \chi^\dagger) Q_R] \text{tr} (Q_R) + \text{tr} [(\chi^\dagger U + U^\dagger \chi) Q_L] \text{tr} (Q_L) \quad (\text{F.10}) \\ &- \frac{1}{2} [\text{tr}^2 (Q_L) + \text{tr}^2 (Q_R)] \text{tr} (\chi^\dagger U + U^\dagger \chi) \end{aligned}$$

$$\begin{aligned} \text{tr} [(\chi^\dagger U + U^\dagger \chi) Q_L U^\dagger Q_R U + (\chi U^\dagger + U \chi^\dagger) Q_R U Q_L U^\dagger] &= \\ \text{tr} (\chi U^\dagger + U \chi^\dagger) \text{tr} (Q_R U Q_L U^\dagger) + \text{tr} [(\chi U^\dagger + U \chi^\dagger) Q_R] \text{tr} (Q_L) & \quad (\text{F.11}) \\ + \text{tr} [(\chi^\dagger U + U^\dagger \chi) Q_L] \text{tr} (Q_R) - \text{tr} (Q_R) \text{tr} (Q_L) \text{tr} (\chi U^\dagger + U \chi^\dagger) \end{aligned}$$

$$\begin{aligned} \text{tr} [(Q_R U Q_L U^\dagger)^2] &= \text{tr}^2 (Q_R U Q_L U^\dagger) - \text{tr} (Q_R) \text{tr} (Q_L) \text{tr} (Q_R U Q_L U^\dagger) \\ &+ \frac{1}{2} [\text{tr} (Q_R) \text{tr} (Q_R U Q_L^2 U^\dagger) + \text{tr} (Q_L) \text{tr} (Q_R^2 U Q_L U^\dagger)] \quad (\text{F.12}) \\ &- \frac{1}{2} \text{tr} (Q_R^2) \text{tr} (Q_L^2) + \frac{1}{4} \text{tr} (Q_R^2) \text{tr}^2 (Q_L) + \frac{1}{4} \text{tr} (Q_L^2) \text{tr}^2 (Q_R) \end{aligned}$$

$$\begin{aligned} \text{tr} (Q_R^2 U Q_L^2 U^\dagger) &= \frac{1}{2} \text{tr} (Q_R^2) \text{tr} (Q_L^2) - \frac{1}{4} \text{tr} (Q_R^2) \text{tr}^2 (Q_L) - \frac{1}{4} \text{tr} (Q_L^2) \text{tr}^2 (Q_R) \\ &+ \frac{1}{2} [\text{tr} (Q_R) \text{tr} (Q_R U Q_L^2 U^\dagger) + \text{tr} (Q_L) \text{tr} (Q_R^2 U Q_L U^\dagger)] \end{aligned} \quad (\text{F.13})$$

$$\begin{aligned} \text{tr} (Q_R) \text{tr} (Q_R U Q_L^2 U^\dagger) + \text{tr} (Q_L) \text{tr} (Q_R^2 U Q_L U^\dagger) &= 2 \text{tr} (Q_R) \text{tr} (Q_L) \text{tr} (Q_R U Q_L U^\dagger) \\ &- \text{tr}^2 (Q_L) \text{tr}^2 (Q_R) + \frac{1}{2} \text{tr} (Q_R^2) \text{tr}^2 (Q_L) + \frac{1}{2} \text{tr} (Q_L^2) \text{tr}^2 (Q_R) \end{aligned} \quad (\text{F.14})$$

$$\text{tr} (Q_R^3) = \frac{3}{2} \text{tr} (Q_R) \text{tr} (Q_R^2) - \frac{1}{2} \text{tr}^3 (Q_R) \quad (\text{F.15})$$

$$\text{tr}(Q_L^3) = \frac{3}{2}\text{tr}(Q_L)\text{tr}(Q_L^2) - \frac{1}{2}\text{tr}^3(Q_L) \quad (\text{F.16})$$

$$\text{tr}(Q_R^4) = \frac{3}{2}\text{tr}^2(Q_R)\text{tr}(Q_R^2) - \text{tr}^4(Q_R) + \frac{1}{2}\text{tr}^2(Q_R^2) \quad (\text{F.17})$$

$$\text{tr}(Q_L^4) = \frac{3}{2}\text{tr}^2(Q_L)\text{tr}(Q_L^2) - \text{tr}^4(Q_L) + \frac{1}{2}\text{tr}^2(Q_L^2) \quad (\text{F.18})$$

Two useful additional relations are

$$\begin{aligned} d_\mu \text{tr} (d^\mu U^\dagger U Q_L U^\dagger Q_R U) &= \text{tr} (d_\mu d^\mu U^\dagger U Q_L U^\dagger Q_R U) + 2 \text{tr} (d^\mu U^\dagger d_\mu U Q_L U^\dagger Q_R U) \\ &- \text{tr} (d^\mu U Q_L d_\mu U^\dagger Q_R) - \text{tr} (d^\mu U \partial_\mu Q_L U^\dagger Q_R) - \text{tr} (d^\mu U Q_L U^\dagger \partial_\mu Q_R) \end{aligned} \quad (\text{F.19})$$

$$\begin{aligned} d_\mu \text{tr} (U^\dagger d^\mu U Q_L U^\dagger Q_R U) &= \text{tr} (U^\dagger d^\mu d_\mu U Q_L U^\dagger Q_R U) \\ &+ \text{tr} (d^\mu U Q_L d_\mu U^\dagger Q_R) + \text{tr} (d^\mu U \partial_\mu Q_L U^\dagger Q_R) + \text{tr} (d^\mu U Q_L U^\dagger \partial_\mu Q_R) \end{aligned} \quad (\text{F.20})$$

Using that and the equation of motion we obtain

$$\begin{aligned} \text{tr} (d_\mu U^\dagger Q_R d^\mu U Q_L) &= \frac{1}{2}\text{tr} (d_\mu U^\dagger d^\mu U Q_L U^\dagger Q_R U + d_\mu U d^\mu U^\dagger Q_R U Q_L U^\dagger) \\ &+ \frac{1}{4}\text{tr} [(\chi^\dagger U - U^\dagger \chi) Q_L U^\dagger Q_R U + (\chi U^\dagger - U \chi^\dagger) Q_R U Q_L U^\dagger] \\ &- 2Z\text{tr} (Q_R^2 U Q_L^2 U^\dagger) + 2Z\text{tr} [(Q_R U Q_L U^\dagger)^2] \\ &- \frac{1}{2}\text{tr} [d_\mu U \partial^\mu Q_L U^\dagger Q_R + d_\mu U Q_L U^\dagger \partial^\mu Q_R \\ &+ d_\mu U^\dagger \partial^\mu Q_R U Q_L + d_\mu U^\dagger Q_R U \partial^\mu Q_L] \\ &+ \frac{1}{2}d_\mu \text{tr} [d^\mu U Q_L U^\dagger Q_R + d^\mu U^\dagger Q_R U Q_L] \end{aligned} \quad (\text{F.21})$$

F.2 Terms with no Q fields

We begin by considering four-derivative operators. The possible terms are:

$$\begin{aligned}
& [\text{tr} (d_\mu U^\dagger d^\mu U)]^2 \\
& \text{tr} (d_\mu U^\dagger d_\nu U) \text{tr} (d^\mu U^\dagger d_\nu U) \\
& \text{tr} (d_\mu U^\dagger d^\mu U d_\nu U^\dagger d^\nu U) \\
& \text{tr} (d_\mu U^\dagger d_\nu U d^\mu U^\dagger d^\nu U) \\
& \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U d^\nu U^\dagger d_\nu U) \\
& \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) \text{tr}(d^\nu U^\dagger d_\nu U) \\
& \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d_\nu U) \text{tr}(d^\mu U^\dagger d^\nu U) \\
& \text{tr}(U^\dagger d_\mu U) \text{tr}(U^\dagger d^\mu U) \text{tr}(U^\dagger d_\nu U) \text{tr}(U^\dagger d^\nu U)
\end{aligned} \tag{F.22}$$

As customary, one can use $SU(2)$ identities to eliminate some of these operators in favor of the rest. In particular, using the identities (F.2), (F.3) and (F.4) one can eliminate the third, four and fifth terms in (F.22).

As for operators including the χ field, the following terms are allowed for constant χ :

$$\begin{aligned}
& \text{tr} [d_\mu U^\dagger d^\mu U (\chi U^\dagger + U \chi^\dagger)] \\
& \text{tr} (d_\mu U^\dagger d^\mu U) \text{tr} (\chi U^\dagger + U \chi^\dagger) \\
& \text{tr} (U^\dagger d_\mu U) \text{tr} [U^\dagger d^\mu U (\chi U^\dagger + U \chi^\dagger)] \\
& \text{tr} (U^\dagger d_\mu U) \text{tr} (U^\dagger d^\mu U) \text{tr} (\chi U^\dagger + U \chi^\dagger) \\
& \text{tr} [\chi^\dagger U \chi^\dagger U + U^\dagger \chi U^\dagger \chi] \\
& \text{tr}^2 (\chi U^\dagger + U \chi^\dagger) \\
& \text{tr}^2 (\chi U^\dagger - U \chi^\dagger) \\
& \text{tr} (\chi^\dagger \chi) \\
& \text{Re} (\det \chi)
\end{aligned} \tag{F.23}$$

Using (F.5), the first operator on (F.23) can be eliminated.

F.3 (cQ) Qd terms

$$\begin{aligned}
& \text{tr} \left(d_\mu U^\dagger [(c_R^\mu Q_R), Q_R] U + d_\mu U [(c_L^\mu Q_L), Q_L] U^\dagger \right) \\
& \text{tr} \left[d_\mu U^\dagger Q_R U (c_L^\mu Q_L) + d_\mu U Q_L U^\dagger (c_R^\mu Q_R) \right] + \text{tr} \left[U^\dagger Q_R d_\mu U (c_L^\mu Q_L) + U Q_L d_\mu U^\dagger (c_R^\mu Q_R) \right] \\
& \text{tr}(U^\dagger d_\mu U) (\text{tr}[Q_L (c_L^\mu Q_L)] - \text{tr}[Q_R (c_R^\mu Q_R)]) \\
& \text{tr}(U^\dagger d_\mu U) (\text{tr}[(c_L^\mu Q_L) U^\dagger Q_R U] - \text{tr}[(c_R^\mu Q_R) U Q_L U^\dagger]) \\
& \text{tr}(U^\dagger d_\mu U) (\text{tr}(Q_L) \text{tr}(c_L^\mu Q_L) - \text{tr}(Q_R) \text{tr}(c_R^\mu Q_R)) \\
& \text{tr}(U^\dagger d_\mu U) (\text{tr}(Q_L) \text{tr}(c_R^\mu Q_R) - \text{tr}(Q_R) \text{tr}(c_L^\mu Q_L))
\end{aligned} \tag{F.24}$$

F.4 (cQ) (cQ) terms

$$\begin{aligned}
& \text{tr} [(c_R^\mu Q_R) U (c_{\mu L} Q_L) U^\dagger] \\
& \text{tr} [(c_R^\mu Q_R) (c_{\mu R} Q_R) + (c_L^\mu Q_L) (c_{\mu L} Q_L)] \\
& \text{tr}(c_R^\mu Q_R) \text{tr}(c_{\mu R} Q_R) + \text{tr}(c_L^\mu Q_L) \text{tr}(c_{\mu L} Q_L)
\end{aligned} \tag{F.25}$$

Appendix G

Useful integrals in dimensional regularization

We quote here the integrals needed for the renormalization of the vacuum energy density:

$$\int \frac{d^{D-1}k}{(2\pi)^{D-1}} (k^2 + M^2)^{-1} = G(x=0, T=0) = 2M^2 \left[R + \frac{1}{32\pi^2} \log \frac{M^2}{\mu^2} \right] \quad (\text{G.1})$$

$$\int \frac{d^{D-1}k}{(2\pi)^{D-1}} (k^2 + M^2)^{1/2} = M^4 \left[R + \frac{1}{32\pi^2} \log \frac{M^2}{\mu^2} - \frac{1}{64\pi^2} \right] \quad (\text{G.2})$$

$$\int \frac{d^{D-1}k}{(2\pi)^{D-1}} (k^2 + M^2)^{-1/2} (Ak^2 + BM^2) = -M^4 \left[(3A - 4B) \left(R + \frac{1}{32\pi^2} \log \frac{M^2}{\mu^2} \right) + \frac{A}{64\pi^2} \right] \quad (\text{G.3})$$

with R in (1.79).

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