FTUAM/92-39

Instanton-like contributions to the dynamics of Yang-Mills fields on the twisted torus

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January 24, 2004

Abstract

We study $SU(2)$ lattice gauge theory in small volumes and with twist $\vec{m} = (1,1,1)$. We investigate the presence of the periodic instantons of $Q = \frac{1}{2}$ and determine their free energy and their contribution to the splitting of energy flux sectors $E(\vec{e} = (1,1,1)) - E(\vec{e} = (0,0,0))$.

[1]Partially supported by DGA-PIT-2/89 and CICyT: TIC1161/90-E, TIC91-0963-C02, AEN90-0034, AEN90-0272 and AEN90-0030.

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1 Introduction

Yang-Mills theory is an extremely rich Quantum Field Theory. Despite its simple formulation, it gives rise to a wide variety of subtle, beautiful and complicated phenomena, such as asymptotic freedom, confinement, dimensional transmutation and generation of a gap, finite temperature phase transition, etc. As in all QFT's, the structure of the vacuum of the theory encompasses all of its properties. Presumably, the precise value of most of the observables of the theory such as the string tension or the glueball spectra can only be obtained numerically by means of Monte-Carlo simulations of the lattice-regularized version of the theory. However, it seems both desirable and feasible to have a qualitative and semi-quantitative understanding of the structure of the vacuum from which the mentioned numerical values arise. In this respect a good deal of work has been done in the last 20 years.

By now, the possible different phases of the theory are well-known and a compelling numerical evidence shows that at $T = 0$ the (4-dimensional) theory is in the confined phase. The corresponding vacuum structure has been described as dual (electric $\leftrightarrow$ magnetic) to a superconductor [1, 2]. Despite the attractive features of such description there is yet no equivalent to a dual BCS theory. An interesting attempt in this direction has recently been investigated [3, 4].

Different classical configurations have been considered responsible for different properties of the theory. Most notably instantons [5, 6], merons [7], and monopoles [8, 9]. Other type of configurations "fluxons" [10, 11] lie on the basis of the Copenhagen [12, 13, 14] description of the QCD vacuum. All these configurations are important, no doubt, but there is no general consensus on the most relevant piece responsible for the property of confinement.

In this paper we have investigated a new type of classical configuration which is related to fluxons and for $SU(2)$ shares with merons the property of being associated with lumps of topological charge $Q = 1/2$. These configurations are only known numerically [15, 16] and are periodic in space. They emerge quite naturally when considering gauge fields on the torus with twisted boundary conditions. Their role in the QCD vacuum is at present unknown and in this paper we are taking the first steps in the direction of their study. Our results are restricted to the study of their contribution to the path integral on relatively small lattice toruses and for β values where their behaviour would turn out to be described by the semiclassical approximation. The prefactor, which has not been determined analytically, will be estimated as a result of our computations. Although this region is far from the large volume one, where full Yang-Mills vacuum structure is recovered, it can be seen as a second step in the description of the transition from the small volume perturbative region to the large volume confinement region. It forms part of a general program initiated in Ref. [17] and [18] for purely periodic boundary conditions and in Ref. [19] for twisted boundary conditions. For a review see Ref. [20].

At small volumes where, due to asymptotic freedom, perturbation theory is a good approximation, the dynamics depends crucially of the boundary conditions, and results obtained in the large N limit [21] indicate that certain twisted boundary conditions are closer to the infinite volume limit. Since twist can be described as the presence of Z_N magnetic flux in the torus, this fact agrees with the Saviddy-Copenhagen picture of the vacuum [22]

An important observable is given by the energy of a state carrying non-zero Z_2^3 (for $SU(2)$) electric flux [23, 24]. On the torus this is a topologically conserved quantum number described by a vector of integers modulo 2, $\vec{e} = (e_1, e_2, e_3)$. Purely spatial Polyakov loops with winding number $\vec{w}$ create electric flux $\vec{e} = \vec{w}$ (mod 2). Just as magnetic flux in ordinary superconductors, in the Yang-Mills vacuum the minimum energy configuration in the presence of electric flux is one where the flux is squeezed to a tube carrying a fixed energy σ per unit length. To minimise energy, the tube must be a straight line with winding number $\vec{e}$. Due to the boundary conditions, the tube cannot break and decay to the vacuum. Thus we expect

$$E(\vec{e}) - E(\vec{e} = 0) = \ l_s \ \sigma \ \sqrt{|e_1| + |e_2| + |e_3|}, \tag{1}$$

where l_s is the length of the torus in each direction.

When the torus is small, the behaviour is quite different. In the absence of twist the levels are degenerate in perturbation theory [17] and the degeneracy is broken by tunnelling over a barrier generated by quantum fluctuations [18, 25].

In the case of the symmetric twist $\vec{m} = (1, 1, 1)$, there are two spatial configurations (up to gauge transformations) which minimise the potential energy. Thus, in perturbation theory the eight-fold degeneracy of the no-twist case is broken down to a two-fold degeneracy between sectors with $\vec{e}$ and $\vec{e} + \vec{m}$ electric fluxes [26]. Polyakov loops which wind once along each spatial direction will take opposite sign values in each of the classical minima and hence we will refer to them as our order parameters $\Phi(t)$.

The splitting of sectors with $\vec{e} = (0, 0, 0)$ and $\vec{e} = (1, 1, 1)$ occurs beyond perturbation theory as a result from tunnelling between both classical minima mediated by the twisted instanton configurations of Ref. [15, 16]. In the semiclassical approximation one gets

$$\Delta E \equiv E(\vec{e} = (1, 1, 1)) - E(\vec{e} = (0, 0, 0)) = 2\, \frac{\langle \Delta N_I \rangle}{\Delta t}, \tag{2}$$

where the right-hand side is given by twice the mean number of instantons per unit time.

In the rest of the paper we will show the results of our simulations, leading to the computation of the energy splitting, which thus complement the results of Ref. [26] and serve to bridge the gap between perturbation theory and the confinement phase.

2 The Data

We have performed Monte Carlo simulations of the Wilson-action $SU(2)$ Yang-Mills lattice theory with the spatial twist $\vec{m} = (1, 1, 1)$ and no temporal twist, for various lattice sizes $N_s^3 \cdot N_t$ and values of β. The simulations, which employed the heat bath method, were performed on our reconfigurable 64-transputer machine RTN [27]. The code was written in OCCAM language and the parallelization algorithm consisted on distributing the lattice points among the transputers and employing a checkerboard strategy: during the updates, the transputers were organised in a ring and each of them controlled a number of time slices. With this method the parallelization efficiency was very close to 95%. For some values of β the simulations were done in a single 8-transputers board of the type contained in RTN and controlled by a PC.

One of our main concerns has been that of ensuring that our data are appropriately thermalised and that two sequential measurements are sufficiently uncorrelated. As a matter of fact, we are dealing with the dynamics of creation, annihilation and displacement of instantons which extend over various lattice points. The relaxation of these modes with our local updating mechanism is much slower than for local quantities. These autocorrelation times grow with β and rather soon become astronomically large. For example at $\beta = 3$ and $N_s = 4$ a pair of instantons do not annihilate after several hundred thousand sweeps, while none is created if we start from a cold initial configuration with no instantons. This point was noticed some time ago by one of us (A. G-A) and verified in Ref. [28]. An overrelaxation algorithm does not seem to improve things sizably in this case. Fortunately, it turns out that for the values of β which we have used in this paper the autocorrelation times are still small compared with the number of iterations. To check this fact and ensure the thermal character of our measurement sample, we have performed a number of tests. First of all we estimated the autocorrelation times by analysing the evolution of the number of instantons from one measurement to the next. The number of iterations between subsequent measurements Δn was chosen to be larger than twice these autocorrelation times. In increasing order of β values, Δn was equal to 50, 250, 1000 and 3000 for $N_s = 4$, 1000 and 2000 for $N_s = 6$ and 1000 for $N_s = 8$.

As a final check that thermalization was attained, we have performed simulations starting from different initial conditions and compared the compatibility of the final results. Some simulations started from one of the cold configurations with no instantons, and others from hot ones with many instantons.

As mentioned in the introduction, the main quantities which interest us are the purely spatial Polyakov loops with winding number equal to one around each of the three spatial directions, Φ. The corresponding quantum operators carry electric flux $\vec{e} = (1, 1, 1)$ and produce states with the same quantum numbers when acting on the vacuum. Classically these loops take the values ± 1 on the two gauge inequivalent classical vacua. Instantons are configurations which interpolate from one of the values to the other in time. Thus, operationally, we may identify the instanton time locations with those of the sign flips of Φ.

For large β the choice of Φ is irrelevant. The naive choice $\Phi_0(t)$ is the spatial average of a Polyakov loop which is made of a straight line in the x-direction followed by one in the y-direction and then one in the z-direction. In Fig. 1a one can see the structure of $\Phi_0(t)$ as a function of t for a configuration with $N_s = 4$, $N_t = 128$ and $\beta = 15$. The two-level structure and the presence of the instantons is evident.

As β decreases the thermal (quantum) fluctuations produce both a decrease of $|\Phi_0|$ around each of the classical vacua together with an increase in the fluctuations of Φ_0 for each t. The combination of both effects make it very difficult for small β to separate between instantons and fluctuations around the classical vacua. However, the problem is due mainly to very small wavelength fluctuations and can be solved by the use of an improved order-parameter. Such an improved parameter can be obtained by averaging over various paths with equal winding number and starting and ending at the same point. The average is performed by adding the path-dependent matrices themselves and then normalizing the resulting matrix to have determinant equal to 1. Finally the trace is taken and the result divided by 2. It is clear that in this way the value of the order parameter at the classical vacua is still ± 1 provided the path-dependent matrices are taken with the appropriate sign, while the uncorrelated fluctuations decrease like $1/\sqrt{N(\gamma)}$ with $N(\gamma)$ the number of paths. There are various ways of selecting the set of paths. In this paper we have employed the fuzzying algorithm [29, 30]. It amounts to defining blocked links of length 2 as the $SU(2)$-projection of the sum of purely spatial paths of length 2 and 4. Then, applying the same definition as $\Phi_0(t)$ for the resulting $(N_s/2)^3$ blocked lattice and averaging over initial points, we get $\Phi_1(t)$. In the case of $N_s = 4$ and $N_s = 8$, we have applied a new blocking operation to the previous one and obtained $\Phi_2(t)$. For the case of $N_s = 6$, $\Phi_2(t)$ is defined by applying a scale 3 blocking transformation to the configuration giving $\Phi_1(t)$.

In Fig. 1b we show how the use of the new order parameters improves the situation of signal to background ratio. For smaller β and larger N_s, even with the new operators, the fluctuations are non-negligible and contaminate the sample. Identifying the number and locations of the instantons with that of the flips in sign of Φ would tend to overestimate the former. To extract the correct estimate of the number of instantons we have employed two completely different approaches. The first one uses the different temporal distributions of instantons and fluctuations to separate both samples on an statistical basis. Later on we will describe this approach in more detail. The second approach is based in reducing even further the amount of fluctuations by applying a few cooling steps to the configurations [31, 32] and computing Φ_0, Φ_1, Φ_2 from the cooled configurations (Fig. 1c). One might be worried by the possibility that cooling could affect the instanton number and distribution. Indeed, if a large number of cooling steps were performed, one would end up in one of the configurations with no instantons. However, due to its local character, cooling washes away faster short wavelength fluctuations while retaining the instanton structure which is a local minimum of the action. In our case we have applied at most 3 cooling steps and feel confident that the instanton structure has not been appreciably modified. The validity of our final results can be crosschecked by the comparison of both methods of analysis which have completely different sources of error.

3 Analysis of the data

Let us define the variable $\sigma(t) = \mathrm{sign}(\Phi(t))$ where Φ is any of the previously mentioned order-parameters. This is an Ising-like variable which is defined on a one dimensional periodic lattice of length N_t. We can introduce a new Ising variable defined on links $\hat{\sigma}(t+1/2)$ as $\sigma(t)\sigma(t+1)$. In the absence of fluctuations, the presence of $\hat{\sigma}$ taking the value -1 signals the appearance of an instanton at the corresponding link. Thus our most important result, number of instantons per unit time, is given by

$$\frac{1}{N_t}\sum_t \left\langle \frac{1-\hat{\sigma}(t+1/2)}{2} \right\rangle = \frac{\langle N_I \rangle}{N_t}. \tag{3}$$

The expected distribution of the variables $\hat{\sigma}$ is Poisson-like, *i.e.* $\hat{\sigma}(l)$ and $\hat{\sigma}(l')$ are statistically independent variables for $l \neq l'$. Indeed, it deviates from Poisson due to the overall constraint that the number of instantons must be even, and to the discretization of time. We have checked that the distribution is indeed what it should by means of two tests. The first test concerns the distribution of N_I. The expected behaviour is binomial

$$P(N_I) = \mathcal{N} \begin{pmatrix} N_t \\ N_I \end{pmatrix} A^{N_I}, \tag{4}$$

where $\mathcal{N}$ is a normalization factor and A is related to the binomial parameter, x, by: $A = x/(1-x)$. The data for $N_s = 4$, $\beta = 2.44$ and three cooling steps are shown in Fig. 2a compared with the prediction of Formula (4).

A second test of the behaviour concerns the time distribution of instantons:

$$D(l) = \frac{1}{N_t}\sum_t \left\langle \frac{(1-\hat{\sigma}(t+1/2))}{2}\ \frac{(1-\hat{\sigma}(t+l+1/2))}{2} \right\rangle = \frac{\langle N_I \rangle^2}{N_t^2}. \tag{5}$$

Essentially one is checking the l-independence of $D(l)$. In Fig. 2b, we show the plot of $D(l)$ for $N_s = 4$, $\beta = 2.44$. For $l > 2$ the distribution is indeed flat, fitting the data to a constant gives a χ^2 per degree of freedom of 1.4.

It is clear that as β gets small there are fluctuations in the order parameter which induce flips ($\hat{\sigma} = -1$) not due to instantons. Nonetheless these fluctuations have a small correlation length, given by the inverse mass gap in the $\vec{e} = (0,0,0)$ sector. For large β this gap is $2\sqrt{2}\pi/N_s$. The departure from flatness in the plot for $D(l)$ can be attributed to this phenomenon. In all cases this deviation is only appreciable for $l \leq 3$. The only exception is our data point at $N_s = 8$ which is also plotted in this Figure. Since cooling tends to eliminate fluctuations, it should also give a flatter distribution, as can be easily seen in our example of Fig 2b.

A simple model that incorporates fluctuations is to consider that

$$\sigma(t) = \lambda(t) u(t) \tag{6}$$

where λ and u are two new Ising variables. The former $\lambda(t)$ are a bunch of identical independent variables with mean $\langle\lambda\rangle$. The latter is the Ising variable describing the instantons and sharing the Poisson-like distribution mentioned previously. Our physical parameter is related to the mean value $\langle u(t)u(t+1)\rangle$ and should be independent on the order parameter that has been used (blocked or cooled). On the contrary the value of $\langle\sigma(t)\sigma(t+1)\rangle$ does depend on the order parameter, since λ does. In order to extract the number of instantons from our data we need two observables from which to eliminate $\langle\lambda\rangle$ and $\langle N_I\rangle$. We have taken $D(1)$ and $\langle\hat{\sigma}(t+1/2)\rangle$ to obtain our final values of $\langle N_I\rangle/N_t$.

To check the final results we have used an alternative method to determine the number of instantons which is based on imposing a dead time cut. Fluctuations produce flips which are clustered, while instantons are uncorrelated in time. Thus, we will neglect all flips that are within a certain time distance τ from another flip. In this way we end up with widely separated flips which are hence certainly instantons. To obtain the estimate of the mean number of instantons we should simply correct for the missing "phase space" induced by the cut. The method mimics the procedure followed often by experimentalists.

To conclude this section we comment that the quoted errors are obtained by partitioning the data into a few groups, measuring the dispersion of the results between groups and taking the square root of this dispersion divided by the number of groups. We have checked the independence of the errors with respect to group size.

4 Results and Conclusions

Table 1 summarises our results. The value of $\mathcal{A}(N_s)$ follows from the formula

$$\langle N_I\rangle = \frac{N_t}{2}\,\mathcal{A}(N_s)\,\beta^2\,\exp\{-\frac{\beta}{4}S_L(N_s)\}, \tag{7}$$

where the mean value of the number of instantons is obtained in an $N_s^3 \cdot N_t$ lattice and $S_L(N_s)$ is the instanton lattice action. We have $S_L(4) = 37.4927$, $S_L(6) = 38.6376$ and $S_L(8) = 39.0016$ (as N_s grows the value quickly approaches $4\pi^2$). For every value of β, N_s and initial configuration we give several determinations of $\mathcal{A}(N_s)$ obtained through different observables. The first four columns come from estimating the mean number of instantons by substracting from the number of flips in the order parameter, the contributions of fluctuations, according to the prescription given in the previous section. The different values correspond to zero, one, two and three cooling steps if available. The results agree quite nicely among themselves despite the simplicity of the model used to substract fluctuations. One can nevertheless consider that the numbers are affected by, in addition to the quoted statistical error, a systematic error due to the procedure used to substract fluctuations. By the observed dispersion of the different determinations with different coolings, one can see that the size of this systematic error is of the order of the statistical error. An exception is the case of $N_s = 8$, owing perhaps to the fact that the flip correlation function (Fig. 2b) deviates from flatness for up to 5 or 6 time slices, while the model predicts flatness after one time slice. We should nevertheless stress once more that, despite the mentioned systematic errors, our model to substract fluctuations is remarkably successful since the number of flips before cooling is typically 2 to 3 times larger than the number of instantons.

In the Table we have also shown other determinations. The fifth and sixth entries are obtained by counting the number of flips which are separated from other flips more (or equal) than 3 and 5 time-slices (dead-time) respectively. One can determine the Poisson parameter from these numbers without making any hypothesis on the nature of the observed flip clustering. The price to pay for this model independence is an increase in the size of statistical errors.

Finally, the last column is an estimate obtained in terms of the correlator $G(t) = \langle \Phi_2(0)\ \Phi_2(t) \rangle$ by the formula

$$1 - 2\frac{\langle N_I \rangle}{N_t} = \frac{G(t+1)}{G(t)}, \tag{8}$$

Consistent determinations are gotten from different values of t in the range 2 to 10. Errors tend to increase at large separations. The quoted number is a weighted average of time distances 2, 4, 6, and 8. The error given is the smallest of all the errors for fixed t.

In summary, good agreement is obtained between all model independent determinations, yielding an estimate which is normally slightly smaller than the ones obtained from our model of fluctuations. Nonetheless the difference is, except for the $N_s = 8$ case, within one or two standard deviations. No difference is found if for our correlators and dead-time estimates we use the cooled configurations.

Let us now compare the different rows of the table. First of all, there are entries corresponding to the same values of N_s and β, but obtained starting from different initial configurations. The agreement of these estimates within errors provides a check that our data are appropriately thermalised. Next, we compare the results obtained from the different values of β but the same value of N_s. Notice, that our results for $\mathcal{A}(N_s)$ are consistent with each other. This fact means that our data correspond to a region in parameter space where the semiclassical approximation holds and thus expression (7) is well satisfied. One could expect corrections of order $1/\beta$ to this formula to occur but, due to the limited range of explored β values, they do not show up. From the different values of β one can give an average determination of the prefactor $\mathcal{A}(N_s)$:

$$\begin{aligned} \mathcal{A}(4) &= 2.013\ (19)\ 10^8, \\ \mathcal{A}(6) &= 7.43\ (15)\ 10^8, \\ \mathcal{A}(8) &= 15.57\ (66)\ 10^8, \end{aligned} \tag{9}$$

obtained from the last column of Table 1. The numbers could include small $1/\beta$ corrections and may then differ slightly from the asymptotic value which would follow from a one loop computation of fluctuations around the instanton.

Finally, we arrive to a comparison among lattice sizes. The relation among the different values of N_s follows from scaling. In order to show how scaling is reproduced by our results, we have plotted our estimate for $\Delta E \cdot l_s$. This is a dimensionless quantity which on the lattice is determined from our results as

$$\Delta E \cdot l_s = -\log\left(1 - 2\frac{\langle N_I\rangle}{N_t}\right) \cdot N_s. \qquad (10)$$

The lattice quantities do of course depend on N_s and β, but scaling predicts they should depend on the single variable $l_s = N_s a(\beta)$. In Fig. 3 we have plotted $\Delta E \cdot l_s$ as a function of l_s. Since our data are still in a region where asymptotic scaling is not valid, we have taken

$$a(\beta) = 400\ \exp\{-\frac{\log 2}{0.205}\beta\}\ \ \mathrm{fm}, \qquad (11)$$

where the dependence on β is extracted from recent results in the same β range [33].

One can see that our results scale quite well, given the small values of N_s involved. In particular, data from $N_s = 4$ and 6 at $l_s = 0.512$ fm are fairly close to each other and close to our data point at $N_s = 8$ with slightly smaller l_s. The same is true for the region around $l_s = 0.42$ fm. The continuous lines are the prediction of the semiclassical formula (7) with $\mathcal{A}(N_s)$ given by (9). They can be seen to describe pretty well our data points: It seems that the scaling limit is approached from above, since the $N_s = 4$ data lies above the other two curves. The $N_s = 6$ and $N_s = 8$ curves are perfectly consistent within errors. The continuum limit curve for $\Delta E \cdot l_s$ is therefore expected to follow closely the shape of these curves. They can be well approximated by an l_s^3 dependence, lying in between the $l_s^{\frac{11}{3}}$ predicted by the continuum semiclassical approximation and l_s^2 which follows for a finite value of the string tension. If we extrapolate the l_s^3 dependence to larger values of l_s, the curve goes through the data points obtained by Stephenson [28] 2.72(56) at $l_s = 0.68$ fm and 20(6) at $l_s = 1.43$ fm.

To conclude let us summarise our results and mention some open problems. We have studied the occurrence of the twisted instanton configurations of Refs. [15, 16] in SU(2) Yang-Mills theory for volumes $N_s = 4$, 6 and 8 and β values ranging from 2.38 up to 2.6. Our results show that the data in this region follow the semiclassical formulas both in the average number of instantons as in the time distribution and Poisson-like number distribution.

From our results an estimate of the prefactor appearing in the semiclassical expression (7) is obtained. From these values one can determine the splitting ΔE between the $\vec{e} = (1,1,1)$ and $\vec{e} = (0,0,0)$ electric flux sectors (which is zero in perturbation theory) in the region $l_s \in (0.341, 0.512)$ fm. As the size of the torus increases ΔE should approach the confinement prediction $\sqrt{3}\,\sigma l_s$. From different considerations one expects that behaviour to set in for $l_s \approx 1$ fm, where the dilute gas approximation has already broken down and our methods of analysis are not-applicable. It would be very interesting to investigate how the transition to this region is achieved and whether instantons are still present and identifiable. It is encouraging to discover that the extrapolated value of $\Delta E/(l_s \cdot \sqrt{3})$ at 1 fm is $(0.41(2)\ \mathrm{Gev}^{-1})^2$, not far from the infinite volume value.

Table Captions

The values of $\mathcal{A}(N_s)$ appearing in formula (7) are shown for all our different runs with cold and hot initial configurations. The first four estimates are obtained by substracting from the number of flips of the order parameter after c cooling steps, the contribution of fluctuations (Section 3). The eighth and ninth columns come from our dead-time cuts of 3 and 5 respectively. The last column comes from formula (8).

Figure Captions

- Fig. 1
  - a) The order parameter Φ_0 is plotted as a function of lattice time t for a configuration with $\beta = 15$ and $N_s = 4$.
  - b) The order parameters Φ_0 (thin line) and Φ_2 (intermediate line) for $\beta = 2.5$ and $N_s = 4$.
  - c) For $\beta = 2.5$ and $N_s = 6$ we plot Φ_0 (thin line), Φ_2 (intermediate line) and Φ_2 after 3 coolings (thick line).
- Fig. 2
  - a) The histogram of number of instantons observed in our run for $\beta = 2.44$ after 3 coolings, compared with the prediction for a binomial distribution.
  - b) We display the flip correlation function $D(l)$ for 3 configurations: $\beta = 2.6$, $N_s = 8$ (diamonds) and $\beta = 2.44$, $N_s = 4$ before (filled circles) and after 3 cooling steps (empty circles).
- Fig.3

  The results of $\Delta E \cdot l_s$ as a function of the spatial lenght l_s. Circles, triangles and squares come from our data for $N_s = 4, 6$ and 8 respectively. The curves are the predictions of the semiclassical formula (7) with $\mathcal{A}$ given by Eq. (9).

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