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Charge transfer in DNA: effective Hamiltonian approaches

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Abstract. Aperiodic order plays a very significant role in biology, as it determines most informative content of genomes. Amongst the various physical, chemical or biological phenomena that might be inferred from sequence correlations, charge transfer properties deserve particular attention. Indeed, the nature of DNA-mediated charge migration has been related to the understanding of damage recognition process, protein binding, or with the task of engineering biological processes (*e.g.* designing nanoscale sensing of genomic mutations), opening new challenges for emerging nanobiotechnologies. Nevertheless, the solution of Schrödinger's equation with a potential that is given by a one-dimensional array of the double-stranded DNA remains as a main open theme in solid state physics of biological macromolecules. In this contribution, I will shortly review several approaches introduced during the last few years in order to describe charge transfer migration in DNA in terms of tight-binding effective Hamiltonians.

1. Conceptual and physical motivations

During the 1930s, DNA was considered to be merely a tetranucleotide composed of one unit each of deoxy-adenylic, -guanilyc, -thymidylic, and -cytidilic acids (the particular order of appearance of each of these bases being considered as irrelevant). Even when it was subsequently realized that the molecular weight of DNA is actually much higher, it was still widely believed that the tetranucleotide unit was the basic repeating building block of the large DNA polymer, in which the four different kinds of nucleotides recur in periodic sequence *i.e.*, $(GACT)_n$ [1]. Thus, DNA was originally viewed as a trivially periodic macromolecule, unable to store the amount of information required for the governance of cell function. The mystery of the nature of the genetic material attracted some physicists to genetics. Thus, Schrödinger suggested that a gene consists of a long sequence of a few repeating elements exhibiting a well defined order *without* the recourse of periodic repetition, and illustrated the vast combinatorial possibilities of such a structure. In this way, the notion of a one-dimensional *aperiodic solid* was introduced [2], and we can consider Schrödinger was the first person to put forward the notion of a linear genetic code [1]. Hence, Schrödinger's proposal of considering DNA as a one-dimensional aperiodic chain, with four different nucleotides arranged in a way able to store the required genetic information was progressively incorporated into dominant biophysical thinking. In fact, when macromolecules of biological interest are considered from the viewpoint of condensed matter physics, a fundamental question naturally arises regarding the potential role of certain physical properties on their biological functions. In particular, the role of charge migration in DNA mutation repair has been extensively discussed during the last decade, and the possible existence of correlation effects in electrical conductivity due to the presence of long-range spatial correlations in DNA has been also explored in detail. In this way, the field of transport properties in aperiodic systems brings useful concepts and approaches for the fundamental study of the possible relationship between information storage (determined by the order of appearance of nucleotides) and physical properties directly related to the electronic structure of nucleic acids.

Nucleic acids can be classified in several classes. For instance, in addition to the most usual single and double-stranded helical structures consisting of either DNA or RNA, there are also three-stranded (*i.e.*, polyU-polyA-polyU) and four-stranded (mainly based on the formation of G or C quartets) stable complexes which adopt coiled helix geometries as well [3]. In turn, each class can be further split into biological (*i.e.*, samples extracted from living organisms, like viruses, bacteria or eucaryotic cells) and artificially engineered molecules (*e.g.*, polyG-polyC, polyA-polyT, or polyGC-polyCG chains). In addition, fragments of biological DNAs can be further split into coding (the so-called introns) and non-coding ones (exons). In general, synthetic nucleic acids considered so far comprise short oligonucleotides where relatively few base pairs (bps) are periodically arranged. These structures are quite different from the biological ones, in which several thousands to millions of bps are *aperiodically* distributed, exhibiting characteristic scale invariant properties due to the presence of long-range correlations in certain regions. Thus, in the short range, a sequence periodicity of 3 base pairs indicates the presence of protein coding sequences, a feature which can be used to distinguish coding and noncoding DNA regions. Initial ana-

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lysis from human genome show that protein coding regions constitute less than 3% of the total genome. In contrast, about 50% of the human genome consists of repetitive sequences [4, 5]. These repeats are approximate copies of patterns of nucleotides of various lengths disperse throughout the genome. Thus, sequence periodicities of about 10 base pairs reflect DNA bendability, much as the secondary structure of proteins [6]. On the next length scale, correlations in the order of 100 base pairs can explain the nucleosomal structure in eukaryotes [7]. Finally, compositional heterogeneities in the range $10^2 - 10^6$ base pairs are related to the presence of wide specific domains characterized by long-range correlations obeying power laws of the form $y = AN^{\alpha}$, where y is a suitable statistical measure, A is a normalization constant, α is the scaling exponent, and N is the chain length [8, 9]. Accordingly, biological DNAs exhibit a greater chemical complexity, determined by their bp sequencing.

Two kinds of order coexist in DNA, each one related to two separate subsystems in the DNA helix, namely the nucleotide subsystem and the backbone system [10]. Thus, one has periodic structural order at the atomic scale in the sugar-phosphate backbone, which yields discrete Bragg spots in X-ray diffraction patterns, exhibiting a characteristic cross-shaped pattern. On the other hand, one has aperiodic, informative chemical order at the molecular scale, as determined by the base pairs sequence. The chemical order of the bps sequence can be properly characterised by ab-initio quantum chemistry calculations, which nicely highlight the emergence of molecular orbitals beyond the atomic scale. Therefore, from a structural point of view DNA could be classified as a periodic crystal (with helical symmetry!), whereas the nucleobase system electronic structure, defining most basic properties of DNA molecule, is effectively aperiodic. Accordingly, one may think of DNA as a sort of hybrid order system exhibiting both aperiodic (stemming from the nucleobase subsystem) and periodic (corresponding to the sugar-phosphate backbone helix subsystem) order features in its electronic structure. As a consequence, one may then think of probing aperiodic order in DNA (that is reading the bps sequence!) by means of purely physical (as opposed to current chemical based) techniques [11]. In particular, could spectroscopic techniques or transport measurements be able to unveil the aperiodic sequence of bps?

As a general trend, experimental results reported to date indicate that (i) periodic synthetic DNAs transport charge better than aperiodic biological samples, and (ii) double-stranded DNA exhibits electrical conductance values orders of magnitude higher than single-stranded chains of comparable length [12]. The question whether DNA is an insulator, a semiconductor, or a metal is often raised. This terminology originates from the field of solid-state physics and it is intimately related to the electronic structure of the considered system. The electronic structure of periodic DNA chains resembles that of doped semiconductors, in agreement with most current-voltage curves obtained so far. From a theoretical point of view the question is not so clear in the case of aperiodic DNA duplexes of biological interest, though experimental measurements for relatively short chains have shown similar results to those obtained for periodic chains of comparable size [13].

2. DNA ladder quantum models

Charge transfer in DNA has been proven to be mainly conveyed by intrastrand coupling, through either sequential incoherent hopping or coherent tunneling. The latter mechanism might be expected to dominate the conduction in the very low temperature regime, specially in the case of periodic oligonucleotides. At low voltage, the main contribution to the resistance comes from the metal-DNA junction potential mismatch (barrier), whereas for high enough voltage, new conduction channels are provided by the molecular states. In order to properly describe the charge transfer mechanisms we must consider a model Hamiltonian accounting for different scales of time and space by means of an adequate choice of generalized coordinates describing both electronic and dynamic DNA degrees of freedom. In the following we will first present a basic formalism to compute transmission coefficients of DNA chains connected to two external metallic leads [14].

An excellent agreement between the DNA band structures calculated from detailed, fully atomistic, ab-initio calculation and tight-binding chain models has been reported [15]. This result demonstrates that each base pair contributes with one single orbital which interacts negligibly with other orbitals in the pair. In fact, quantum mechanical studies show that hydrogen bonding interaction gives rise to a spatial separation of the HOMO and LUMO in the nucleobase system, so that hole (electron) transfer proceeds through the purine (pyrimidine) bases, where the HOMO (LUMO) carriers are located in polyG-polyC (polyA-polyT), respectively [15, 16]. Thus, as a first approximation, the basic physics of charge transport in DNA molecules can be addressed in terms of relatively simple models with one single orbital per base pair plus transfer parameters describing (i) the coupling between successive nucleobases, (ii) the coupling of these bases with the backbone states, and (iii) hydrogen-bonding between base-pairs. In some previous models a transport channel associated to the possible hopping of charge carriers between successive phosphate groups along the backbone was considered [17, 18]. However, first principle calculations, showing that the phosphate molecular orbitals are systematically below the base related ones, do not favour the presence of such a transport channel [12].

The ladder model Hamiltonian can be expressed in the form,

$$H = \sum_{n=1}^{N} \hat{\boldsymbol{\varepsilon}}_n \boldsymbol{c}_n^{\dagger} \boldsymbol{c}_n - \sum_{n=1}^{N-1} \hat{\boldsymbol{t}}_{n,n+1} (\boldsymbol{c}_n^{\dagger} \boldsymbol{c}_{n+1} + \boldsymbol{c}_{n+1}^{\dagger} \boldsymbol{c}_n) \,, \tag{1}$$

where

$$\boldsymbol{c}_n \equiv \begin{pmatrix} c_n^A \\ c_n^B \end{pmatrix} , \tag{2}$$

are the charge destruction operators at site n in the chain, and

$$\hat{\boldsymbol{\varepsilon}}_n \equiv \begin{pmatrix} \varepsilon_n^A & t \\ t & \varepsilon_n^B \end{pmatrix} , \qquad \hat{\boldsymbol{t}}_{n,n+1} \equiv \begin{pmatrix} t_{n,n+1}^A & 0 \\ 0 & t_{n,n+1}^B \end{pmatrix} , \tag{3}$$

where ε_n^m is the on-site energy of the nucleobase located at site n in the strand $m \in \{A, B\}$, $t_{n,n+1}^m$ is the nearest-neigh-

bor transfer integral between nucleobases located at sites nth and $(n+1)$th in strand m, and t is the interstrand hopping integral describing the hydrogen bonding between complementary Watson-Crick bps. We note that while the intrastrand hopping terms $t^m_{n,n+1}$ (describing the $\pi-\pi$ orbital coupling) are included into the $\hat{\boldsymbol{t}}_{n,n+1}$ matrix, the H-bonding mediated interstrand coupling is incorporated into the $\hat{\varepsilon}_n$ matrix instead. In this way, the algebraic formalism adopted to describe the double-stranded DNA Hamiltonian properly distinguishes the different types of chemical interactions in the macromolecule.

Making use of the transfer-matrix formalism the two coupled Schrödinger equations related to this ladder model can be expressed in the form [17, 19, 20]

$$\begin{aligned}(E-\varepsilon_n^A)\,\psi_n^A &= t^A_{n,n-1}\psi^A_{n-1}+t^A_{n,n+1}\psi^A_{n+1}+t\psi^B_n\\ (E-\varepsilon_n^B)\,\psi_n^B &= t^B_{n,n-1}\psi^B_{n-1}+t^B_{n,n+1}\psi^B_{n+1}+t\psi^A_n\,,\end{aligned}\tag{4}$$

where $\psi_{n,m}$ is the wave function amplitude at site n in the strand $m\in\{A,B\}$. Making use of this approach the charge transfer in DNA has been studied in a number of works. It this way, the very weak distance dependence of charge rates experimentally measured for the DNA sequence $(\mathrm{G:C})(\mathrm{T:A})_k(\mathrm{G:C})_3$, for different k values, was explained in terms of the ability of charge carriers to bridge from one strand to the other depending on the ratio of intra- and interstrand neighboring base-base couplings [19]. The role of the intrinsic DNA correlations, arising from the Watson-Crick base pairing, do not suffice to give rise to the presence of extended states when four values of the on-site energies corresponding to the G, C, T, and A bases are randomly assigned in one of the strands (say ε_n^A), with the same probability, while the sites of the second strand are set to follow Chargaff's complementary rule [20, 21].

3. Helical geometry and dynamical effects

In physiological conditions DNA double helix exhibits a full-fledged three-dimensional geometry, so that every two consecutive bases are twisted by a certain angle ($\theta_0\simeq\pi/5$ in equilibrium conditions). As a result, the orbital overlapping is substantially reduced, yielding smaller values for the $\pi-\pi$ transfer integral values [12, 22]. Therefore, one should expect a significant reduction of the charge transfer efficiency stemming from purely geometrical considerations (dimensionality effect). In addition, at physiological temperatures the relative orientation of neighboring bases becomes a function of time, thereby modifying their mutual overlapping in an oscillatory way (dynamical effect). In that case, the effective model Hamiltonian can be expressed as the sum of two main contributions $H=H_e+H_l$, where H_e describes the charge carrier dynamics over the π-stacked electronic system and H_l describes the duplex DNA dynamics. The electronic degrees of freedom of a double-stranded DNA (including sugar-phosphate and environmental effects) are described in terms of the effective Hamiltonian [23],

$$H_e=\sum_{n=1}^{N}\tilde{\varepsilon}_n(E)\,c_n^{\dagger}c_n-\sum_{n=1}^{N-1}t_{n,n+1}(\theta_n)(c_{n+1}^{\dagger}c_n+H.c.)\,,\tag{5}$$

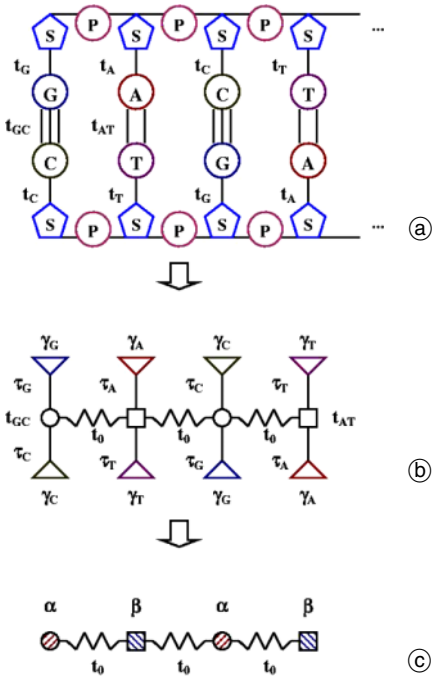

Fig. 1. Sketch illustrating the two step renormalization process mapping the ds-DNA chain into a linear diatomic lattice. (**a**) Starting effective tight-binding model for the polyGACT-polyCTGA unit cell. (**b**) renormalized model after the first decimation step. (**c**) renormalized model after the second decimation step.

corresponding to an equivalent monatomic lattice (Fig. 1), where the renormalized "atoms" correspond to complementary pairs in the original DNA molecule whose on-site energies $\tilde{\varepsilon}_n(E)$ depend on the charge carrier energy, the hopping integral between the sugar's oxygen atom and the base's nitrogen atom, the hydrogen bonding between complementary bases and the presence of water molecules and/or counterions attached to the backbone, according to the overall scheme illustrated in Fig. 2. In addition, the transfer integral $t_{n,n+1}$ explicitly includes the angular dependence of the aromatic base stacking between adjacent nucleotides (θ_n).

When describing the phonon dynamics in DNA one can disregard the inner degrees of freedom of the bases, since we can separate the fast vibrational motions of atoms about their equilibrium positions from the slower motions of molecular groups. In this way, three characteristic vibrational states have been usually considered in

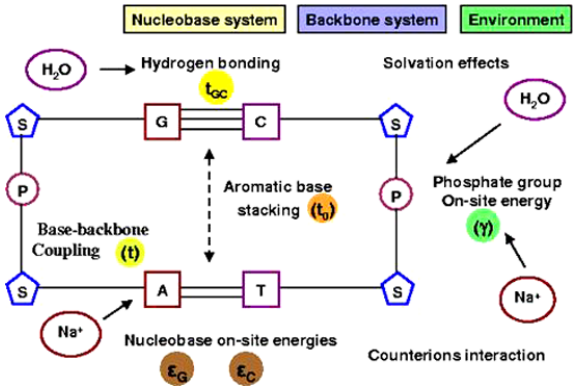

Fig. 2. Sketch illustrating the overall energetics of a double-stranded DNA chain and the different tight-binding parameters included in the DNA model considered in this work.

DNA normal mode calculations, namely, the stretch oscillations of each base back and forth with respect to the center of mass of the system located at the helical axis (radial oscillations), longitudinal oscillations of the bps planes along the helix axis, and twist oscillations of each bp as a whole around the helical axis. In order to get a basic picture of the physical effects related to the coupling between electronic and dynamical degrees of freedom, we shall focus on the low frequency twist mode, hence keeping the DNA radius constant, *i.e.*, $R_0 \simeq 1$ nm $\forall n$. In that case, one can express the lattice Hamiltonian in the form

$$H_l = \sum_{n=1}^{N} \frac{p_n^2}{4\xi^2 m_n} + 4k \sum_{n=1}^{N-1} \left(\sqrt{c^2\phi_n^2 + R_0^2 \sin^2 \phi_n} - \frac{l_0}{2} \right)^2 , \tag{6}$$

where m_n is the base mass, $\phi_n = \theta_n/2$, $\xi = \sqrt{R_0^2 + c^2}$, $c = h_0/\theta_0$, $h_0 \simeq 0.34$ nm being the equilibrium separation between two successive bp planes (B-DNA form), p_n is the angular momentum, k is an effective force constant and l_0 is the equilibrium distance. The low frequency response is obtained linearizing the canonical equations of motion by considering only linear terms of the Taylor expansion. Since $m_G + m_C \simeq m_A + m_T$ (so that the aperiodic order of bps has a little influence on its dynamics) one can consider all the masses to be equal as a first approximation, to obtain

$$\ddot{\theta}_{n+1} - \ddot{\theta}_{n-1} = \omega_0^2(\theta_{n+2} - 3\theta_{n+1} + 3\theta_{n-1} - \theta_{n-2}) , \tag{7}$$

where $\omega_0 \equiv \sqrt{k/m}$ is the natural twist frequency of each base. This expression describes a *correlated* motion involving three consecutive bps (codon unit cell). Searching for solutions in the form of linear waves we plug the ansatz $\theta_{n,k} = \sqrt{2}\theta_0\, e^{i\omega t} \cos\left((n+k)q/2\right)$, where q is the wave number, into Eq. (7) to obtain the dispersion relation $\omega^2 = 4\omega_0^2 \sin^2(q/2)$. Finally, making use of $\theta_{n,k}$ into the Eq. (5) one can express the corresponding Schrödinger equation in the form

$$(E - \tilde{\varepsilon}_n)\, \psi_n - (\tau_0 - B\Omega T_n)\, \Psi_n^+ - 2B\Omega(1 - \Omega^2)\, U_{n-1} \Psi_n^- = 0 , \tag{8}$$

where $\tau_0 \equiv t_0(1 - \chi\theta_0^2)$, $B \equiv t_0\chi\theta_0^2$, with the dimensionless parameter χ measuring the coupling strength between the charge and the lattice system, $\Psi_n^{\pm} \equiv \psi_{n+1} \pm \psi_{n-1}$, and $T_k(\tilde{\Omega})$ and $U_{k-1}(\tilde{\Omega})$ are Chebyshev polynomials of the first and second kinds, respectively, with $\tilde{\Omega} \equiv 2\Omega^2 - 1$, and $\Omega \equiv 1 - \omega^2/2\omega_0^2$ ($\Omega \in [-1, 1]$). From the study of this equation one realizes that the coupling with the low band edge vibrational state results in a significant improvement of the charge transport efficiency through synthetic polyG-polyC DNA chains [23]. In fact, although an ensemble of bps twisting back and forth around the helix axis generally results in a degraded charge transfer efficiency, a significant improvement of charge migration can occur via charge coupling to the lattice modes at low temperatures.

As mentioned before, biological and artificial DNA molecules significantly differ in size, chemical complexity, and the kind of structural order. Consequently, one can hardly expect that results obtained from the study of the oversimplified synthetic molecular systems may be directly extrapolated to understand the physical properties of complex DNA molecules of biological interest. In fact, both the sugar-phosphate backbone and the nucleotide bases sequence are periodically ordered in, say, polyG-polyC chains, whereas in biological DNA the nucleotide bases are aperiodically ordered instead. Current bioengineering techniques allow for the growth of oligonucleotide sequences tailored at will. Thus, a nucleic acid arranged according to the Fibonacci sequence, for instance a (G : C)(A : T)(G : C)(G : C)(A : T)(G : C)(A : T)... oligonucleotide may be easily synthesized. Such a molecule, where complementary Watson-Crick base pairs play the role of *A*s and *B*s in the Fibonacci's substitutional rule, could be properly referred to as a *DNA quasicrystal* approximant.

From general principles one expects the aperiodic nature of the nucleotide sequence distribution would favor localization of charge carriers in biological nucleic acids, reducing charge transfer rate due to backscattering effects. In fact, the main effect of quasiperiodic order in Fibonacci DNA is the emergence of a highly fragmented energy spectrum, introducing a characteristic low-energy scale in the electronic structure of aperiodic DNA chains [24]. Nevertheless, this scenario must be refined in order to take into account correlation effects among nucleotides reported in biological DNA samples, since these correlations can enhance charge transport via resonant effects [25, 26]. Besides its fundamental importance for the progress of biological condensed-matter theory, several properties of biological interest may be directly related to the presence of sequence correlations in genomic DNA, including gene regulation, cell division, or damage recognition processes due to DNA-mediated charge migration. In this sense, the quest for suitable aperiodic substitution sequences, able to mimic relevant features related to long-range correlation effects in natural DNA samples, is an appealing task to further research in the field of aperiodic systems [27]. Quite remarkably, an interesting connection between nucleotide frequencies in human chromosomes and Fibonacci numbers has been recently reported [28], and suitable mathematical approaches have been introduced in order to clarify the evolution of repetitive DNA strings, within the framework of genomic evolution by duplication [29]. In that case, the canonical mechanism of genomic growth is assumed to be performed schematically through a series of replication – excision – concatenation processes which are successively applied in an iterative way.

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