Chapter xxxx Effective models for charge transport in DNA nanowires

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Effective Models for Charge Transport in DNA Nanowires

Rafael Gutierrez and Gianaurelio Cuniberti

Summary

Rapid progress in the field of molecular electronics has led to increasing interest in DNA oligomers as possible components of electronic circuits at the nanoscale. For this, however, an understanding of charge transfer and transport mechanisms in this molecule is required. Experiments show that a large number of factors may infiuence the electronic properties of DNA. Although full first-principle approaches are the ideal tool for a theoretical characterization of the structural and electronic properties of DNA, the structural complexity of this molecule limits the usefulness of these methods. Consequently, model Hamiltonian approaches, which filter out single factors infiuencing charge propagation in the double helix, are highly valuable. In this chapter, we review the different DNA models that are thought to capture the infiuence of some of these factors. We will specifically focus on static and dynamic disorder.

Key Words: Correlated disorder; dissipation; DNA conduction; electron-vibron interaction; static disorder.

1. INTRODUCTION

The increasing demands on the integration densities of electronic devices are considerably limiting conventional semiconductor-based electronics. As a result, new possibilities have been explored in the last decade, leading to the emergence of molecular electronics, which basically relies on the idea of using single molecules or molecular groups as elements of electronic devices. A new conceptual idea advanced by molecular electronics is the switch from a top-down approach, where the devices are extracted from a single large-scale building block, to a bottom-up approach, in which the whole system is composed of small basic building blocks with recognition and self-assembly properties.

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A molecule that has recently attracted the attention of both experimentalists and theoreticians is DNA. The observation of electron transfer between intercalated donor and acceptor centers in DNA oligomers in solution over unexpectedly long distances *(1)* led to a revival of interest in the conduction properties of this molecule. Although the idea that DNA might be conducting is rather old *(2)*, there was never any conclusive proof that it could support charge transfers over long distances. This is, however, a critical issue when considering, for example, damage repair during the replication process *(3)*. Apart from the relevance of these and similar experiments for biology and genetics, they also suggested that by appropriately adjusting the experimental conditions, DNA molecules might be able to carry an electrical current. Further, DNA oligomers might be useful as templates in molecular electronic circuits if their self-assembling and self-recognition properties are exploited *(4–6)*. Although many technical and theoretical problems must still be surmounted, it is now possible to carry out transport experiments on single molecules connected to metallic electrodes.

However, despite the many expectations put on DNA as a potential ingredient of molecular electronic circuits, transport experiments on this molecule have revealed some very intriguing and partly contradictory behavior. Thus, it has been found that DNA may be insulating *(7,8)*, semiconducting *(9,10)*, or metallic *(11,12)*. These results demonstrate the high sensitivity of DNA transport to different factors affecting charge motion, such as the quality of the contacts to the metal electrodes, the base-pair sequence, the charge injection into the molecule, or environmental effects (dry vs aqueous environments), among others.

Theoretically, knowledge of the electronic structure of the different building units of a DNA molecule (base pairs, sugar and phosphate groups) is essential for clarifying the most effective transport mechanisms. First-principle approaches are the most suitable tools for this goal. However, the huge complexity of DNA makes *ab initio* calculations still very demanding, so that only comparatively few investigations have been performed *(13–21)*. Further, environmental effects such as the presence of hydration shells and counterions make *ab initio* calculations even more challenging *(14,15,22)*.

In this chapter, we will review a complementary (to first-principle approaches) way to look at DNA, namely, model Hamiltonians. They play a significant role in filtering out possible charge transfer and transport mechanisms as well as in guiding the more involved first-principle investigations. We are not aiming at a thorough review of Hamiltonian-based theories. In fact, because the authors belong to the "physical community," model approaches for charge transfer formulated in the "chemical community" will not be the scope of this chapter. The interested reader can consult refs. *23–28*. We are

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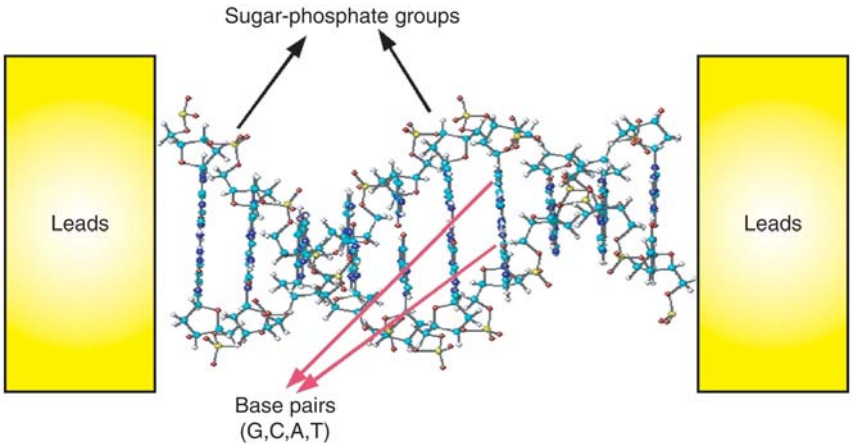

Fig. 1. Schematic representation of a double-stranded DNA oligomer with an arbitrary base-pair sequence and connected to left and right electrodes.

also not considering the infiuence of electron–electron interactions on charge transport, an issue that needs further clarification *(29,30)*. In the next two sections, we discuss models describing the infiuence of static disorder and dynamic effects on charge propagation in DNA. For the sake of presentation, we discuss both factors in different sections. Nevertheless, the reader should be aware that, realistically, the interplay between them is expected to be closer.

2. STATIC DISORDER

DNA oligomers consist of four building blocks (oligonucleotides): adenine (A), thymine (T), cytosine (C), and guanine (G). As is well known, they have specific binding properties, i.e., only A-T and G-C pairs are possible (*see* Fig. 1). Sugar and phosphate groups ensure the mechanical stability of the double helix and protect the base pairs. Because the phosphate groups are negatively charged, the topology of the duplex is only conserved if it is immersed in an aqueous solution containing counterions (Na^+, Mg^+) that neutralize the phosphate groups. Thus, experimenting on "dry" DNA usually means that the humidity has been greatly reduced, but there are still water molecules and counterions attached to the sugar–phosphate mantle.

The specific base-pair sequence is obviously essential for DNA to fulfill its function as a carrier of the genetic code. However, this same fact can be detrimental to charge transport. The apparently random way in which the DNA sequence is composed strongly suggests that a charge propagating along the double helix may basically feel a random potential, leading to

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backscattering. It is well known that in a one-dimensional (1D) system with uncorrelated disorder, all electronic states are completely localized (Anderson localization). However, correlated disorder with, for example, power-law correlations *(31)* may lead to delocalized states within some special energy windows in the thermodynamic limit, the exact structure of the spectrum being determined by the so-called scaling exponent α. This quantity describes the correlation properties of a random process *(31,32)*, specifically, the length-dependence of the position autocorrelation function: $C(l) \sim l^{-\alpha}$. Thus, $\alpha = 0.5$ corresponds to a pure random walk, whereas other values indicate the presence of long-range correlations and hence, the absence of relevant length scales in the problem (self-similarity).

Some of the main issues to be addressed when investigating the role of disorder in DNA are, in our view, the following. First, is the specific base-pair sequence in DNA completely random (Anderson-like) or do there exist (long-or short-range) correlations? Second, a measure for the degree of confinement of the electronic wave function is given by the localization length ζ *(33)*. Are the resulting localization lengths larger or smaller than the actual length L of the DNA segments studied in transport experiments? For $\zeta >> L$, the system may appear to be effectively conducting, despite the presence of disorder, although in the thermodynamic limit, all states may remain localized. Clarification of these issues requires close cooperation between experimentalists and theoreticians. In what follows, we review some theoretical studies addressing these problems.

The simplest way to mimic a DNA wire is by assuming that after charge injection, the electron (hole) will basically propagate along one of the strands (the inter-strand coupling being much smaller), so that 1D tight-binding chains can be a good starting point to minimally describe a DNA wire. Roche *(34)* investigated such a model for poly(GC) and λ-phage DNA, with on-site disorder (resulting from the differences in the ionization potentials of the base pairs) and bond disorder $\sim \cos \theta_{n,n+1}$ related to the twisting motion of nearest-neighbor bases along the strand, $\theta_{n,n+1}$ being independent Gaussian-distributed random variables. Poly(GC) displays two electronic bands and thermal fiuctuations reduce the transmission peaks and also, slightly, the band widths. The effect of disorder does not appear to be very dramatic. In the case of λ-phage, however, the transmission peaks are considerably diminished in intensity and in number with increasing chain length at zero temperature, because only a few electronic states are not backscattered by the random potential profile of the chain. Interestingly, the average Ljapunov exponent, which is related to the localization length, increases with increasing temperature, indicating that despite thermal fiuctuations, many states are still contributing to charge transport.

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In an early paper, Roche et al. *(35)* used scaling coefficients (Hurst exponents), which usually indicate the existence of long-range correlations in disordered systems. Their results showed that, e.g., DNA built from Fibonacci sequences has a very small Hurst exponent (indicating strong correlations). Uncorrelated random sequences show strong fragmentation and suppression of transmission with increasing length, whereas in correlated sequences, several states appear to be rather robust against the increasing rate of backscattering. Hence, it may be expected that correlated disorder will be more favorable for long-distance carrier transport in DNA wires.

Another typical example of correlated disorder was presented by Alburquerque et al. *(36)* within a 1D tight-binding model. The authors investigated the quasi-periodic Rudin-Shapiro sequence as well as the human genome Ch22. As expected, the transmission bands became more and more fragmented with increasing number of nucleotides. Although for very long chain lengths, all electronic states did tend to be completely localized, long-range correlations yielded large localization lengths and thus transport might still be supported for special energy points on rather long wires.

Zhu et al. *(37)* formulated an effective tight-binding model including only HOMO and LUMO of poly(GC) together with on-site Coulomb interactions. On-site and off-diagonal disorder, related to fiuctuations of the local electrostatic potential *(38)* and to the twisting motion of the base pairs at finite temperatures, respectively, were also included. The main effect of the Coulomb interaction was to first reduce the band gap, so that the system goes over to a metallic state, but finally the gap reappears as a Coulomb-blockade gap. Twisting disorder was apparently less relevant for short wires and low temperatures.

A very detailed study of the localization properties of electronic states in two minimal models of different DNA oligomers [poly(GC), λ-DNA, telomeric DNA] was presented by Klotsa et al. *(39)*: a fishbone model *(40–42)* and a ladder model. Both models fulfill the minimal requirement of showing a band gap in the electronic spectrum, mirroring the existence of a HOMO-LUMO gap in isolated DNA molecules. However, the ladder model allows for the inclusion of interstrand effects as well as of the specific base-complementarity typical of the DNA duplex, an issue that cannot be fully captured by the first model. The authors were mainly interested in environmentally induced disorder. Hence, they assumed that only the backbone sites are affected by it, while the nucleotide core is well screened. Nevertheless, as shown by a decimation procedure *(39)*, disorder in the backbone sites can induce local fiuctuations of the on-site energies on the base pairs (gating effect). Uniform disorder (where the on-site energies of the backbones continuously vary over an interval [−W, W], W being the disorder strength)

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is shown to continuously reduce the localization length, as expected. For binary disorder (on-site energies take only two posible values, ±W/2), as it may arise by the binding of counterions to the backbone sites, the situation is similar up to some critical disorder strength W_c. However, further increase of W leads to unexpected behavior: the localization length on the electronic side bands is suppressed but a new band around the mid-gap with *increasing* localization length shows up. Thus, disorder-induced delocalization of the electronic states is observed in some energy window. This result, obtained within a simple model, may be supported by first-principle calculations *(22)*, which clearly show that the environment can introduce additional states in the molecular band gap.

Most of the foregoing investigations considered on-site disorder only. The infiuence of off-diagonal short-range correlations was investigated by Zhang and Ulloa *(43)* in λ-DNA. They showed that this kind of disorder can definitely lead to the emergence of conduction channels in finite systems. For some special ratios of the nearest-neighbor hopping amplitudes, there may even exist extended states in the thermodynamic limit. As a consequence, the authors suggested that λ-DNA may show a finite current at low voltages.

Caetano and Schulz *(44)* investigated a double-strand model with uncorrelated disorder along the single strand, but taking into account the binding specificity of the four bases when considering the complementary strand (A-T and G-C). Participation ratios P(E) were computed, which give a measure of the degree of localization of electronic states. P(E) is, for example, almost zero for localized states in the thermodynamic limit. The results suggest that interstrand correlations may give rise to bands of delocalized states, with a participation ratio that does not appreciably decay with increasing length.

3. DYNAMICAL DISORDER

In the previous section, we presented several studies related to the infiuence of static disorder on the charge-transport properties of different DNA oligomers. Here, we address a second aspect of high relevance, namely the impact of dynamic disorder related to structural fiuctuations on charge propagation. Considering the relative fiexibility of DNA, one may expect that vibrational modes will have a strong infiuence on the charge motion via a modification of electronic couplings.

The markedly small decay rates found in electron-transfer experiments *(1)* have led to the proposal that, besides unistep superexchange mechanisms, phonon-assisted hole-hopping might also be of importance *(26)*. The hole can occupy a specific molecular orbital, localized on a given molecular site; it can also, however, extend over several molecular sites and build a polaron, which is basically a lattice deformation accompanying a propagating

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charge. It results from the energetic interplay of two tendencies: the tendency to delocalize the charge, thus gaining kinetic energy, and the tendency to localize it with a consequent gain in elastic energy. The softness of the DNA molecule and the existence of modes that can appreciably affect the inter-base electronic coupling (like twisting modes or H-stretching bonds) makes this suggestion very attractive *(45,46)*. Conwell and Rakhmanova *(46)* investigated this issue using the Su-Heeger-Schrieffer (SSH) model, which is known to entail rich nonlinear physics and which has been extensively applied to study polaron formation in conducting polymers. The SSH model deals classically with the lattice degrees of freedom while treating the electrons quantum mechanically. The calculations showed that a polaron may be built and be robust within a wide range of model parameters. The infiuence of random base sequences was apparently not strong enough to destroy it. Thus, polaron drifting may constitute a potential transport mechanism in DNA oligomers.

The potential for the lattice displacements was assumed to be harmonic *(45,46)*. Interstrand modes like H-bond stretching are, however, expected to be strongly anharmonic; H-bond fiuctuations can induce local breaking of the double-strand and have thus been investigated in relation to the DNA denaturation problem *(47)*. To investigate this effect, Komineas et al. *(48)* studied a model with strong anharmonic potentials and local coupling of the lattice to the charge density. The strong nonlinearity of the problem led to a *dynamic* opening of bubbles with different sizes that may eventually trap the polaron and thus considerably affect this charge-transport channel.

Zhang et al. *(49,50)* studied a simple model that describes the coupling of torsional excitations (twistons) in DNA to propagating charges and showed that this interaction leads to polaron formation. Twistons modify the interbase electronic coupling, although this effect is apparently weaker than, e.g., in the Holstein model *(51)*, because of the strong nonlinearity of the twistons restoring forces as well as of the twiston–electron coupling. For small restoring forces of the twisting modes and in the nonadiabatic limit ("spring constant" much larger than electronic coupling), the interbase coupling is maximally perturbed and an algebraic band reduction is found that is weaker than the exponential dependence known from the Holstein model. Thus, it may be expected that the polaron will have a higher mobility along the chain.

The observation of two quite different time scales (5 ps and 75 ps) in the decay rates of electron transfer processes in DNA, as measured by femtosecond spectroscopy *(52)*, was the main motivation of Bruinsma et al. *(53)* to investigate the coupling of the electronic system to collective modes of the DNA cage. For this, they considered a tight-binding model of electrons interacting with two modes: a twisting mode, which mainly couples to the

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interbase π-orbital matrix elements, and a linear displacement coupling to the on-site energies of the radical and acting as a local gating of the latter. In the strong-coupling, high-temperature limit, the hopping matrix elements can be treated perturbatively and build the lowest energy scale. Transport has thus a hopping-like character. In analogy with electron-transfer theories, the authors provide a picture where there are basically two reaction coordinates related to the above-mentioned linear and angular modes. The strong thermal fiuctuations associated with the twisting motion are shown to introduce two time scales for electron transfer that can be roughly related to optimal (short) and nonoptimal (long) relative orientation of neighboring base pairs.

In several papers, Hennig et al. *(54,55)* and Yamada *(56)* formulated a model Hamiltonian where only the relative transverse vibrations of bases belonging to the same pair are included. Their calculations showed the formation of stable polarons. Moreover, the authors suggested that poly(GC) should be more effective in supporting polaron-mediated charge transport than poly(AT), because for the latter, the electron-lattice coupling was found to be about one order of magnitude smaller. Although the authors remarked that no appreciable coupling to twisting distortions was found by their semi-empirical quantum chemical calculations, this issue requires further investigation in view of the previously presented results *(49,50,53)*. Disorder did not appear to have a very dramatic infiuence in this model; the localization length only changed quantitatively as a function of the disorder strength *(56)*.

Asai *(57)* proposed a small polaron model to describe the experimental findings of Yoo et al. *(11)* concerning the temperature dependence of the electrical current and of the linear conductance. Basically, he assumed that in poly(GC), completely incoherent polaron hopping dominates whereas in poly(AT), quasi-coherent hopping, i.e., with total phonon number conservation, is more important. As a result, the temperature dependence of the above quantites in both molecules is considerably different.

In complement to the foregoing research, which mainly addressed individual vibrational modes of the DNA cage, other studies have focused on the infiuence of environmental effects. Basko and Conwell *(58)* used a semi-classical model to describe the interaction of an injected hole in DNA, which is placed in a polar solvent. Their basic conclusions pointed out that the main contribution was provided by the interaction with water molecules and not with counterions; further, polaron formation was not hindered by the charge–solvent coupling; rather, the interaction increased the binding energy (self-localization) of the polaron by around half an eV, which is much larger than relevant temperature scales. Li and Yan *(59)* as well as Zhang et al. *(60)* investigated the role of dephasing reservoirs in the spirit

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of the Buettiker-D'Amato-Pastawski model *(61,62)*. Segal et al. showed that a change in the length scaling of the conductance can be induced by the dephasing reservoirs as a result of incoherent phonon-mediated transport, a result known from electron-transfer theories *(63)*. In a similar way, Feng and Xiong *(64)* considered gap-opening a result of the coupling to a set of two-level systems, which simulate low-lying states of the bosonic bath. Gutierrez et al. *(41,42)* discussed electron transport in a "broken-ladder" model in the presence of a strong dissipative environment simulated by a bosonic bath. It was found that the environment can induce virtual polaronic states inside the molecular band gap and thus lead to a change in the low-energy transport properties of the system. In particular, the I-V curves become metallic at low voltages as a result of phonon-assisted hopping. We note that these latter results are quite similar to those found in *ab initio* calculations, showing that water states can appear between the π-π^* gap *(65)*, thus effectively introducing shallow states similar to those in doped bulk semiconductors. These states may support activated hopping at high temperatures.

We finally mention that the role of nonlinear excitations (solitons, breathers) in the process of denaturation of DNA double strands *(47,66,67)* and in the transmission of "chemical" information between remote DNA segments *(68)* was addressed early on in the literature. Because these approaches are not directly connected with the issue of charge transport in DNA wires between electrodes, we do not go into further detail. They may, however, reveal a novel, interesting mechanism for transport and deserve a more careful investigation.

4. CONCLUSIONS

Although much progress has been made in the past decade in clarifying the relevant transport mechanisms in DNA oligomers, a coherent, unifying picture is still lacking. The experimental difficulties involved in giving reliable transport characteristics of this molecule make the formulation of model Hamiltonians quite challenging. The theoretical research presented in this chapter shows that charge transport in DNA is considerably infiuenced by both static and dynamical disorder. Long-range correlated disorder can play a role in increasing the localization length beyond the relevant molecular length scales addressed in experiments, thus making DNA effectively appear to be a conductor. This effect may be supported or contradicted by thermal fiuctuations arising from internal (vibrations) or external (solvent) modes leading to increased charge localization or to incoherent transport.

The presented models only focus on the equilibrium or low-bias limit of transport. However, real transport experiments probe the molecules at finite

voltages and hence, nonequilibrium effects also must be considered. This, of course, makes the mathematical treatment as well as the physical interpretation more involved. Considerable effort has been made recently to deal with this issue *(69–71)*; however, addressing these studies goes beyond the scope of this chapter.

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