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Charge transport in DNA molecules: Cooperative interplay between the disordered base-pair channel and the ordered backbone

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Charge transport in DNA molecules has raised considerable interest because of its importance in biological processes and potential applications in nanoscale devices. A DNA molecule can be viewed as a quasi-one-dimensional system composed of stacked base pairs (AT, CG) together with backbones of sugar phosphates. Motivated by recent experimental observations on the importance of the backbone integrity, we investigate the interplay between charge transport through the ordered backbone and disordered base stacks with random sequences. By analytical and numerical calculations, we find that the coupling between the backbone and base-pair channels plays an important role in charge transport. The backbone can generate effective hopping constants well beyond the adjacent base pairs, enhancing charge transport through the base-pair channel. The corresponding enhancement of the localization length is nearly independent of the length of the DNA and increases with increasing coupling between backbone and base pair. Our model can explain qualitatively several experimental observations.

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I. INTRODUCTION

DNA molecules are fundamental objects in biological systems. They are composed of paired bases (A-T, C-G) and backbones of sugar phosphates. The specific sequence of base pairs (BPs) carries essential biological information and it may also have significant impact on the charge transport properties of the molecule. The self-recognition and self-assembly properties of BPs provide a promising flexible tool to design specific nanodevices; understanding the electronic properties of DNA is essential for possible applications. Another important element of these molecules is the backbone (BB) and typically considered to play no role on the charge transport along the molecule, given that its levels are distant from the Fermi level. However, there are some indications that apart from maintaining mechanical stability, the BB may also have an important role in charge transport in DNA, contributing to important biological processes such as DNA repair after damage [1,2].

There exists a wide variety of experimental results showing widely different conducting behavior, where the DNA molecule appears to behave as insulator, semiconductor, conductor, and even as proximity-induced superconductor material [3–9] (or see Ref. [1] and references therein). The observed diverse behavior may depend on environmental parameters, on details of the molecular structure, as well as contacts and sample preparation, which may obscure the microscopic mechanisms at play. In fact, several possible conduction mechanisms for charge transport in DNA have been proposed. Cuniberti *et al.* [10] discussed the backbone-induced semiconducting behavior in short poly(G)-poly(C) DNA wires. The effect of specific sequences on charge transport, especially the role of correlations in disordered molecules, has also been explored in significant detail [11–18]. The role of finite temperatures in producing variable range hopping behavior on the ac conductivity has been discussed [19] as the twist angle fluctuations between base pairs qualitatively explain the temperature dependence in long DNA double helix molecules [20]. Microscopic models to study the role of vibrational excitations and polaron dynamics in DNA have been reported recently [19,21–26], demonstrating the importance of these degrees of freedom in the resulting transport properties. Similarly, the role of solvent effects has received a great deal of theoretical attention [27,28], as well as the importance of good-quality contacts [29,30] and dephasing effects [31].

Although the experimental signatures of transport are the result of the complex external environment in the measurement setups or perhaps because of that, the role of the internal structure of the molecule, both static and dynamic, has not been fully established on transport. One of the important intrinsic factors is the specific sequence of BPs that makes the molecule in either different DNA molecules or in different regimes (intron-free coding regime with random sequences and intron-rich noncoding regime with long-range correlated sequences [14]) of a given molecule. The specific structure may yield very different electronic behavior. For example, it is known that in one-dimensional systems with uncorrelated disorder, all electronic eigenstates are spatially localized, clearly resulting in poor conducting behavior (fully insulating in the thermodynamic limit) [32]. This theoretical expectation is in contrast with some experimental observations, which exhibit conducting behavior even for long molecular chains, although significant carrier transfer along *short* chains is not unexpected. Thus, it is important to develop further insight into the theoretical description that explains the observed conducting behavior in DNA molecules with random sequences. There have been many studies on the relevance of the BP channel, as it is associated with the "π way". While relatively much less attention has been paid to the BB transport channel (except for viewing it as a source of dissipation). The BB channel is an interesting structure, as it has a clearly periodic structure *regardless of the BP sequence*, and it hosts the in-principle extended wave functions that arise from Bloch's theorem in such a periodic atomic arrangement. As the energy levels or bands associated with the BB are far away from the Fermi level, it is clear that they do not take *direct* part in charge transport. This may explain the relatively scant attention paid to this part of the molecule, although, as we will show below, the BB does play an important role in charge mobility. In fact, recent beautiful experiments using Auger spectroscopy indicate that a periodic BB in DNA gives rise (or is at least strongly required) to extended states in the molecule [33]. Earlier interesting experiments on "nicked" and repaired DNA have also revealed the importance of BB on charge transport [34].

Based on these experimental observations and considerations, we present in this paper a model that studies the coupling between the ordered BB and the disordered BP stacks with random sequences to investigate charge transport in DNA. Our study pays special attention to the interplay between the BP and the BB channels. We find that the BB channel can *assist* charge transport along the BPs by generating an effective hopping *beyond the adjacent BP*, which enhances the localization length *even though* the BB levels are away from the Fermi energy and they do not take part in the transport directly. The enhancement of conductance could be significant, despite being perturbative second-order processes, as the original BP channel may be highly fractured. We also discuss the dependence on the size of DNA and the degree of disorder. The qualitative explanation of some experimental observations is also given. Our model reveals interesting physics of coupled ordered and disordered systems, which is of intrinsic fundamental interest and is under extensive current research in different areas.

The rest of the paper is organized as follows. In Sec. II, we construct the theoretical model and present a complete analytical analysis and numerical results based on the transfer-matrix method. The results and discussions are given in Sec. III. The paper ends with a brief summary in Sec. IV.

II. THEORETICAL MODEL

We describe a DNA molecule by a quasi-one-dimensional structure with three coupled bands. One band is the π-way BP band, while the others represent the two BBs of the double helix molecule. Notice that in order to obtain a simpler or clearer physical picture, we use a simplified one-band model for the BP channel instead of a double chain for the double BP strands. Nevertheless, we believe our model captures the main physics of the interplay between the *disordered* BP channel and the *ordered* BB channel. Moreover, the two-band BP model can be reduced to a single band BP model with effective parameters. We have also assumed that the effect from the solvent is small and as such neglected, so that extended states in the backbone exist for at least a finite system (i.e., the localization length in the backbone channel is larger than the system size), as demonstrated in experiment [33]. Thus, the Hamiltonian for our system is

$$\begin{aligned} H_S = \sum_j \{ & \varepsilon_{c,j} c_j^+ c_j + t_c (c_j^+ c_{j+1} + c_{j+1}^+ c_j) \\ & + [\varepsilon_0 l_j^+ l_j + t(l_j^+ l_{j+1} + l_{j+1}^+ l_j)] \\ & + [\varepsilon_0 r_j^+ r_j + t(r_j^+ r_{j+1} + r_{j+1}^+ r_j)] \\ & + V_0 [l_j^+ c_j + c_j^+ l_j + r_j^+ c_j + c_j^+ r_j] \}, \end{aligned} \tag{1}$$

where c_j is the annihilation operator for a charge [hole in the highest occupied molecular orbital (HOMO)] at site j in the BP channel and l_j and r_j are the annihilation operators for a charge at site j in the two BB channels; $\varepsilon_{c,j}$ is the on-site energy for each BP with value ε_{AT} for the A-T BP and ε_{CG} for C-G BP; ε_0 is the sugar-phosphate energy level in the BB; t_c and t are the hopping constants within the BP and BB channels; V_0 is the hopping between the BP and BB channels.

This three-band model can be reduced to an effective two-band model by a simple transformation $a_j = \frac{(l_j + r_j)}{\sqrt{2}}$, $b_j = \frac{(l_j - r_j)}{\sqrt{2}}$, which yields $H_S = H + H_b$, where

$$\begin{aligned} H &= H_c + H_a + H_{ac} + H_{ca} \\ &= \sum_j \{ [\varepsilon_{c,j} c_j^+ c_j + t_c (c_j^+ c_{j+1} + c_{j+1}^+ c_j)] \\ &\quad + [\varepsilon_0 a_j^+ a_j + t(a_j^+ a_{j+1} + a_{j+1}^+ a_j)] + V[a_j^+ c_j + c_j^+ a_j] \} \end{aligned} \tag{2}$$

and

$$H_b = \sum_j \{ [\varepsilon_0 b_j^+ b_j + t(b_j^+ b_{j+1} + b_{j+1}^+ b_j)] \}, \tag{3}$$

where $V = \sqrt{2} V_0$ and the channel described by H_b decouples from H. The fishbone model [13] is a limit case of our model for $t = 0$.

In this paper, we focus mainly on the situation where the Fermi energy is in the BP channel. Using a Schrieffer-Wolff transformation, we obtain the effective Hamiltonian for the BP channel $H_{c,\mathrm{eff}} = H_c + H'$, where

$$H' = H_{ca} (E - H)^{-1} H_{ac}. \tag{4}$$

In the case of weak interchannel coupling, H' has the form

$$H' = \sum\nolimits_k \alpha_k c_k^+ c_k = \sum\nolimits_{j,m} \beta_m c_j^+ c_{j+m} + \mathrm{H.c.}, \tag{5}$$

where H.c. represents Hermitian conjugated terms, $c_k = \sum_j e^{-ijk} c_j$ is the Fourier transform of the annihilation operator in the BP channel, $\alpha_k = V^2 / [E - \varepsilon_0(k)]$, and $\beta_m = \sum_k \frac{V^2 e^{ikm}}{E - \varepsilon_0(k)}$, with $\varepsilon_0(k) = \varepsilon_0 + 2t \cos(k)$. Here we see that the BB channel leads to the renormalization of the on-site BP energy $\varepsilon_{c,j} \to \varepsilon_{c,j} + \beta_0$. Since the on-site energy shift is a constant, it will not affect the degree of disorder. However, it may shift the energy of a state relative to the Fermi level. Perhaps most importantly, the coupling to the ordered BB channel results in the renormalization of the hopping between the nearby BPs. This may significantly extend the hopping to the sites beyond the nearest neighbors, which are absent in the original model. Thus the BB may strongly affect the charge transport in the BP channel even if the BB levels are far from the Fermi energy.

Now we calculate β_m. By transforming the integral to the complex plane, we have

$$\beta_m = V^2 \frac{\rho_1^m}{\rho_1 - \rho_2}, \tag{6}$$

where $\rho_{1,2}$ are the two roots of the equation

$$z^2 - 2zx + 1 = 0, \tag{7}$$

with ρ_1 within the unit circle and $|x| \equiv |(E-\varepsilon_0)|/2t > 1$. In this case, β_m decays exponentially with a characteristic length $\lambda = \frac{1}{\ln(1/\rho_1)}$. With increasing V, β_m increases and the transport in the BP channel is enhanced. When ε_0 approaches the BP energy levels or t increases, x decreases. Therefore, the charge transport is improved due to the increasing λ. The physical picture can be described as follows. The charge carriers can hop from the BP to the BB channel, propagate along the ordered BB "for a while" and then come back to the BP. It is this ordered-channel-induced effective hopping beyond the adjacent BP that results in the enhancement of the localization length, improving charge transport along BP. When BP and BB energy levels are closer, the ordered BB channel has a much stronger effect on the disordered BP channel. When x approaches 1 (ρ_1 is on the unit circle), λ diverges. We will not discuss this issue in more details in the present paper, since the energy difference between the BP and BB channels in DNA molecules is large.

Though we are mainly interested in the effects of BB channel on the charge transport through BP channel, it is also of interest to see the influence of disorder in the BP channel *back* on the BB channel. Here, we give a brief discussion on this issue. One can derive an effective Hamiltonian for the BB channel. The interchannel coupling leads to the renormalization of the on-site energy and the hopping between the nearest sugar phosphate in BB. For small V_0, we have $\delta\varepsilon_{a,j} = \frac{V^2}{E-\varepsilon_{j,c}}$ and $\delta t_{j,j+1} = \frac{V^2 t_c}{(E-\varepsilon_{c,j})(E-\varepsilon_{c,j+1})}$ when $t_c \ll V$. Thus the coupling to the disordered BP channel brings about both diagonal and off-diagonal disorders into the BB channel, so that localization may indeed appear in the BB channel.

The analytical perturbative analysis above can give us a picture of the interplay between the BP and BB channels, as well as the possible consequence on charge transport properties. A quantitative nonperturbative calculation is needed for the accurate understanding of the transport mechanism. We use the transfer-matrix method. From Eq. (2), the eigenstates can be found by solving the following equations:

$$\varepsilon_{c,n} A_n + t_c (A_{n+1} + A_{n-1}) + V B_n = E A_n,$$

$$\varepsilon_0 B_n + t (B_{n+1} + B_{n-1}) + V A_n = E B_n, \tag{8}$$

where A_n is the probability amplitude for a charge at site n in the BP channel and B_n is the probability amplitude for a charge at site n in the BB channel. Equation (8) can be written in the matrix form

$$\Phi_{n+1} := \begin{pmatrix} A_{n+1} \\ B_{n+1} \\ A_n \\ B_n \end{pmatrix} = T_n \begin{pmatrix} A_n \\ B_n \\ A_{n-1} \\ B_{n-1} \end{pmatrix} = T_n \Phi_n, \tag{9}$$

where

$$T_n = \begin{pmatrix} \frac{E-\varepsilon_{c,n}}{t_c} & -\frac{V}{t_c} & -1 & 0 \\ -\frac{V}{t} & \frac{E-\varepsilon_0}{t} & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{10}$$

Then we have $\Phi_{N+1} = \hat{T}_N \Phi_1$, where $\hat{T}_N = \Pi_{i=1}^{N} T_i$. The localization length λ at energy E is the inverse of the Lyapunov coefficient ($\gamma > 0$), which is the smallest positive eigenvalue of the limiting matrix $\lim_{N\to\infty} \ln(\hat{T}_N \hat{T}_N^{\dagger})^{1/2N}$ [32]. In the calculations, we have used the reorthogonalization method [35] to obtain reliable values of γ.

III. RESULTS AND DISCUSSIONS

In our calculations, we use parameters mainly from experimental data, first-principles calculations, or a combination of them. There are some unresolved uncertainties in the parameters due to the limited accuracy in experimental measurements or theoretical calculations. Moreover, there are some real factors which may change these parameters. For example, it is known that stretching changes the distance and relative angles between adjacent BPs, resulting in changes to the transfer integrals between the BPs [36]. Similarly, in the so-called *M*-DNA, the hopping rate between nearby BPs can also be very different due to suitable doping of metallic atoms [37]. Thus, in our studies, we choose parameters similar to those obtained from experimental data or first-principles calculations. We also change some of these parameters (to mimic some experiments) to study how the results may change under different experimental conditions.

The ionization energies for the four types of bases are $\varepsilon_G = 7.77$ eV, $\varepsilon_C = 8.87$ eV, $\varepsilon_A = 8.25$ eV, and $\varepsilon_T = 9.13$ eV. We use the on-site energy for BPs *CG* and *AT* as $\varepsilon_{CG} = (\varepsilon_C + \varepsilon_G)/2 = 8.32$ eV and $\varepsilon_{AT} = (\varepsilon_A + \varepsilon_T)/2 = 8.69$ eV. The on-site energy for BB is $\varepsilon_0 = 12.27$ eV [15]. In the calculation, we have made an overall energy shift such that $\varepsilon_{CG} = -\varepsilon_{AT} = -W$ ($W = 0.19$ eV for most cases, except for the inset in Fig. 4). After the shift, the on-site BB energy is $\varepsilon_0 = 3.76$ eV. The hopping constants are $\simeq 1$ eV (see captions for details). The transport properties depend on the specific DNA molecular structure. We use random BP sequences such as those for λ-DNA. The BPs *AT* and *CG* are distributed randomly with p being the concentration of *CG* BPs. In this model, W and p are the two quantities describing the degree of disorder of the system. In the calculations, we have carried out averages over 400 disordered configurations and the statistical error is around 0.5%.

In Fig. 1, we show the normalized localization length (NLL) $\Lambda = \lambda/N$ versus energy for the BP (a) and BB (b)

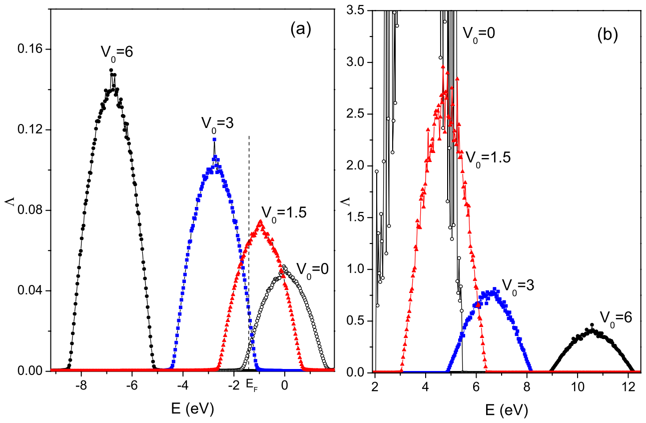

FIG. 1. (Color online) Normalized localization length vs energy for different interchannel couplings (V_0 in units of eV). (a) Base pair channel; (b) backbone channel. Parameters used are $W=0.19$ eV, $\varepsilon_0=3.76$ eV, $t_c=0.8$ eV, $t=0.85$ eV, $p=0.5$, and $N=3000$.

channels. In Fig. 1(a), we see that the NLL increases with increasing interchannel coupling V_0. The maximum localization length at $E=-1$ eV for $V_0=1.5$ eV is about 1.5 times the maximum localization length at $E=0$ for the case without interchannel coupling. A rough estimate of the conductance is provided by $G=\frac{2e^2}{h}\exp\{-2N/\lambda\}=\frac{2e^2}{h}\exp\{-2/\Lambda\}$; this expression is accurate for very low temperatures such that the coherence length $l_c > L=Nb$, where $b=3.4$ Å is the separation between BPs. N should be replaced by l_c/b when $l_c < L$. This would suggest that the conductance for $V_0=1.5$ eV increases by 5 orders of magnitude compared to that without interchannel coupling (Λ_0). Larger V_0 results in even larger enhancements, as clear from Fig. 1(a). A similar picture remains for other values of t_c, although both Λ and Λ_0 become smaller (larger) for smaller (larger) values of t_c.

We can obtain a quantitative description of the overall degree of wave-function extension or localization by calculating the channel participation ratio (PR). PR is defined as $\text{PR}=1/\Sigma_{i\in I,m}|a_m^{(i)}|^4$, where $a_m^{(i)}$ is the probability amplitude of a particle at site m of the ith eigenstate in channel I (=BP,BB, or all channels). The PR is a constant for a system with extended states and tends to zero as $\sim 1/N$ for systems with localized states. The values of PR for our system are listed in Table I. It is clear that the overall degree of extension of the eigenfunction in the BP channel (BB channel) increases (decreases) with increasing interchannel coupling. The total PR increases with increasing interchannel coupling, as somewhat of a precursor of more extended behavior in two-dimensional systems. Thus, despite the localization due to disorder in the BP sequence, carrier transport can be improved by coupling to the ordered BB channel. As also shown in the perturbative analysis, the basic physical picture of this BB-assisted transport is that the charge (mainly holes in the HOMO) has certain probability (which increases with increasing interchannel coupling) to hop to the BB, move along the ordered BB, and then come back to BP. Another noteworthy feature is that the transport properties depend strongly on the position of the Fermi level. For instance, if the system's Fermi energy is at $E_F=-1.4$ eV (many factors may affect the position of Fermi level; for more discussions on the position of Fermi level, see [38]), the localization length changes nonmonotonically. The localization length for $V_0=1.5$ eV is larger than those for $V_0=6$ eV and $V_0=0$ [see Fig. 1(a)].

TABLE I. PR for various interchain couplings. The parameters are the same as those for Fig. 1.

V_0	BP channel	BB channel	Total
0.0	0.074	0.668	0.067
1.5	0.131	0.568	0.106
3.0	0.201	0.467	0.141
6.0	0.252	0.393	0.154

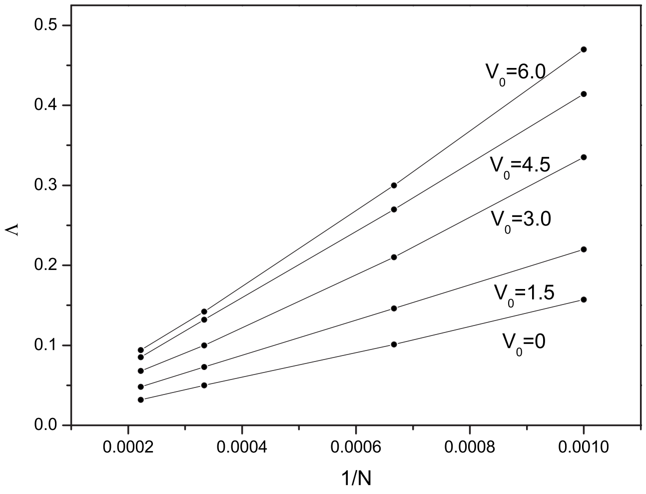

FIG. 2. The dependence of the BP normalized localization length Λ on system size. $N=1000, 1500, 3000, 4500$. Same parameters as in Fig. 1, with $p=0.5$.

The impact of the disorder in the BP channel back on the BB channel is shown in Fig. 1(b). It is clear that the NLL decreases with increasing interchannel coupling. Here, we want to point out that there are extended states with NLL larger than unity for finite systems (i.e., $\lambda > N$), even for $V_0=1.5$ eV. These states are not truly extended in the thermodynamical limit, which is consistent with the one-parameter scaling theory for low dimensional noncorrelated disordered systems [32,39].

The length dependence is one of the important issues in charge transport in DNA molecules. Figure 2 shows the dependence of NLL on the size of the system N for various interchannel couplings. One can see that the NLL is inversely proportional to N, so that the system size has great impact on the charge transport. For instance, for the case with $N=1500$ and interchannel coupling $V_0=1.5$ eV, the conductance (for $E_F=-1$ eV) is approximately 10^6 times that for a system size $N=3000$. The NLL Λ versus Λ_0 (for the case without interchannel coupling) for different system size is shown in the inset of Fig. 3. Each line is for the same interchannel coupling, but with different N. One can see from that figure that the enhancement of NLL Λ/Λ_0 is nearly independent of N, although both Λ and Λ_0 increase with

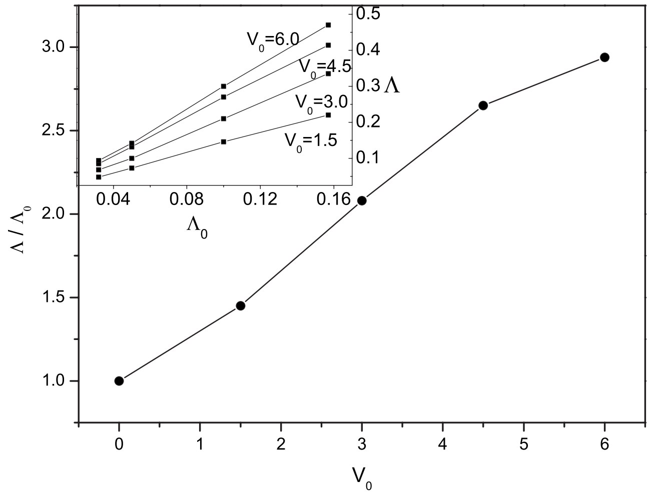

FIG. 3. Enhancement of localization length in the BP channel, Λ/Λ_0 (averaged over N values), vs interchannel hopping constant V_0. Inset: Λ vs Λ_0 for various interchannel couplings and system sizes. Same parameters as in Fig. 2.

decreasing system size. With increasing interchannel coupling, the NLL enhancement in the BP channel indicates that the ordered BB has a profound impact on the charge transport in the BP channel.

Having explored the effects from the ordered BB channel, we take a look at the dependence on the degree of disorder, which is determined by W and p. Figure 4 shows the normalized localization length for different W and p values. As shown in the main panel and the left insert of Fig. 4, the NLL in the BP channel decreases with increasing degree of disorder, i.e., increasing W and/or p, as one would expect.

In the right insert, we show Λ for the BB channel for a set of particular parameters and different W values. Clearly, the dependence of Λ on W is not monotonic. With increasing W, Λ first decreases and then increases for larger W. This is due to the fact that the distribution of the on-site energy in the BB channel is so large that there is only a small number of states with energies close to the energies of the states in the BP channel. Therefore, the ordered channel has a weaker effective coupling to the disordered channel [40] and has less impact on that channel, leading to a smaller localization length.

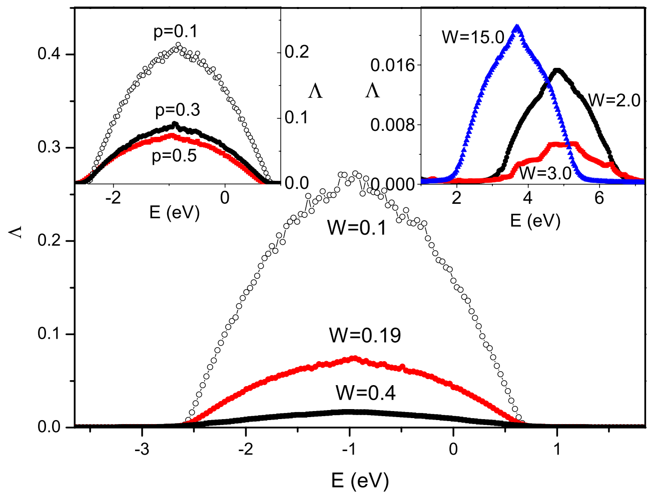

FIG. 4. (Color online) Dependence of normalized localization length Λ on the degree of disorder. Main panel shows Λ vs W for the BP channel (concentration of CG pairs is $p=0.5$). The left inset is Λ vs p (with $W=0.19$). Right inset is for Λ vs W in the BB channel ($p=0.5$). Other parameters are $\varepsilon_0=3.76$ eV, $t_c=0.8$ eV, $t=0.85$ eV, $V_0=1.5$ eV, and $N=3000$.

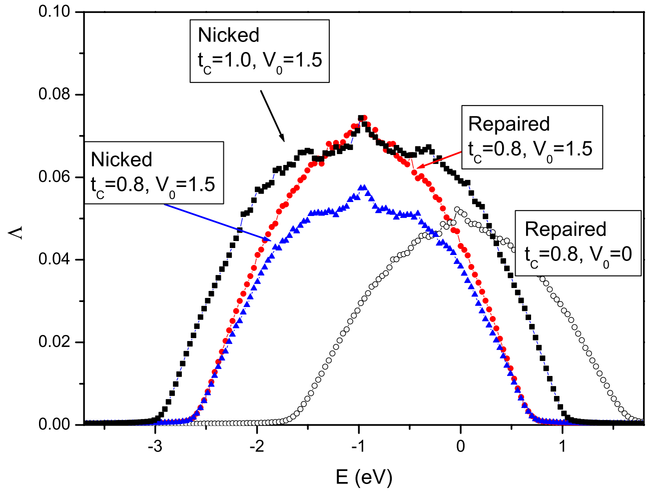

FIG. 5. (Color online) Normalized localization length vs energy for nicked and repaired DNA molecules in the BP channel. Parameters used are $W=0.19$ eV, $\varepsilon_0=3.76$ eV, $t=0.85$ eV, $V_0=1.5$ eV, and $p=0.5$.

Our model and results can help us understand qualitatively several experiments. Hartzell *et al.* found that the transport properties for repaired DNA molecules were better than for "nicked" DNA molecules with defects in the BB. This experimental observation can be understood within our theory. For repaired DNA, the ordered BB channel can assist the charge transport in the disordered BP channel, as shown above. However, in nicked DNA molecules, there are defects in the BB, such that the charge has to overcome energy barriers to propagate in the BB channel. Thus the assistance from the BB channel is limited and the conducting behavior is poor due the disorder in the BP sequences. One should mention that it is possible that the "nick" in the BB may induce additional structural deterioration of the BP channel, which would produce additional contrast between the two situations (nicked vs. repaired). These authors also studied DNA molecules doped with metallic atoms (the so-called M-DNA) and found Ohmic behavior even for nicked DNA molecules [41]. One can understand this observation as follows. Although the BB may have less of an enhancement effect on the transport in the BP channel, due to the presence of the nick, the doping of metallic atoms may increase the hopping between the nearby BPs and enhance the charge transport. In Fig. 5, we compare the NLL for different situations to demonstrate the interplay between the BB channel and BP channel. The curve with white dots is for the situation without interchannel coupling, which shows poor transport due to Anderson localization. The curve with (red) dots is for the case with nonzero interchannel hopping, which shows relative better transport properties because of the assistance from the ordered BB channel. The curve with (blue) triangle is for the nicked DNA molecule. We consider two nicks lying in the position 12 from both ends of the DNA molecules as in the experiments. In our calculation, we used hopping amplitudes at the nicked position of only 0.005 eV in the BB and 0.05 eV in the BP. In this situation, the transport is poor and has the same order of magnitude values as without the coupling to the BB. The curve with (black) squares is for the sample as that for the nicked DNA, except that the hopping constant between BPs is 1.0 eV (instead of 0.8 eV, except at the nicked positions). This curve mimics the system with doped metal atoms (thus larger inter-BP hopping) and nicks. The transport is better than for the nicked structure. All these results are consistent with experimental observations, even as our model only allows a qualitative comparison. For a quantitative analysis between experiments and theory, efforts in both experiment and theory are needed. Measurements of the charge transport on a single molecule would be very helpful in helping one determine the appropriate model and various parameter values appropriate for the experimental situation. Real experimental systems are rather complex and dependent on detailed experimental conditions. We have neglected several other factors such as the influence of water molecules and ions, the possible correlation in the DNA sequences, polaron effects, and others. The formation of polarons may lead to a decreasing effective bandwidth or even localization (for small polaron) of charge carriers. This effect may be less important for low temperatures if the coupling is weak. Nevertheless, our theory points out the important roles of the ordered BB and provides a possible mechanism for the experimental observation of Ohmic conducting behavior in DNA with random sequences of BPs.

Before concluding, we would like to make a few comments on the comparison to other models involving the BB and its states. Cuniberti *et al.* [10] considered the effect of the BB as the source of dissipation. In the fishbone model [13] or the model with disordered on-site energy for BB [42], there is no hopping between nearby sugar phosphates and thus no conducting band in the BB channel. In those models, the effects of the BB channel are mainly to suppress the transport, resulting for instance in the appearance of antiresonances [42].

IV. CONCLUSION

Motivated by experimental observations, we have proposed and studied a simple model of coupled *ordered* BB and disordered BP sequences, analyzing the interplay between the BB and the BP channel on charge (hole) transport in DNA. We find that the presence of BB may enhance the transport greatly and lead to good conducting behavior, despite the disorder in the BP channel, which otherwise leads to poor conduction according to localization theory in low dimensions. We find that the conductance is very sensitive on the system size, as one would anticipate, although the presence of interchannel coupling greatly enhances conductance. Our theory can qualitatively explain important features of several experiments. One of the key results of our model is that an ordered BB channel can change transport significantly, depending on the temperature (thus l_c) or the position of Fermi energy, despite the fact that the BB assisted transport is essentially a second-order process and the BB levels are far from the BP channel and the Fermi level.

A final remark is that our model is not limited to applications in DNA systems. It generally sheds light on the interesting physics of coupled ordered and disordered systems, which may be fabricated or implemented in a variety of different experimental situations.

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