Absence of zero-temperature transmission rate of a double-chain tight-binding model for DNA with random sequence of nucleotides in thermodynamic limit

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The zero-temperature transmission rate spectrum of a double-chain tight-binding model for real DNA is calculated. It is shown that a band of extended-like states exists only for finite chain length with strong inter-chain coupling. While the whole spectrum tends to zero in thermodynamic limit, regardless of the strength of inter-chain coupling. It is also shown that a more faithful model for real DNA with periodic sugar-phosphate chains in backbone structures can be mapped into the above simple double-chain tight-binding model. Combined with above results, the transmission rate of real DNA with long random sequence of nucleotides is expected to be poor.

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DNA is the biological molecule which keeps and propagates the secrets of life for all the creatures on the earth, and it has many interesting properties. It consists of two chains of nucleotides. The nucleotides are of four types, usually denoted as A, T, C and G. Electrons are occupied on the nucleotides and can hop from one nucleotide to its intra-chain and inter-chain neighbors. Each pair of inter-chain nearest-neighbor nucleotides can only belong to one of the four ‘base-pairs’ A − T, T − A, C − G and G − C while other kinds of combinations are forbidden. Therefore, when the sequence of nucleotides in one chain of a DNA is determined, the sequence in the other chain is determined, too. Fig. 1(a) shows schematically a part of a DNA sequence.

The electronic transportation properties of DNA has attracted much attention since Elley et al. suggested that DNA may become one-dimensional conductor. Different conclusions are obtained by different experiments. Some experiments suggested that DNAs are conductors. Later, other experiment groups claimed that DNAs are insulators. Direct measurement on single molecule showed that they seem to be semiconductors. Some hints of superconduction behavior have even been reported. Further experiments show that the conduction behavior of DNA molecules of different base-pair sequences, say, identical base-pair sequence and disordered base-pair sequence, seems different.

In the aspect of theoretical studies, a simple one-electron model was originally proposed by Iguchi. In this simple model, each nucleotide is represented by a site and different types of nucleotides have different on-site energies. Since the coupling between nucleotides is short-range, it is assumed that electron hopping occurs only between nearest-neighbor nucleotides and the possible randomness in hopping constants is neglected. Thus the electron behavior in a DNA is represented by a double-chain tight-binding model (TBM). Many studies on electronic properties of DNA are based on this model or its modified versions. In this short paper, we shall show that this simple model may not be appropriate for real DNAs if they do have conductor behavior. A system should have extended states to provide conductor behavior. It is well known by the famous Bloch theorem that a periodic TBM has bands of extended states. However, the sequence of base-pairs in each chain of real DNAs are disordered rather than periodic, and this leads to random on-site energies in the corresponding TBM. According to the scaling theory of localization, uncorrelated random on-site disorders in a one-dimensional TBM will drive all electronic states to exponentially localized states. At a first glance, the double-chain TBM for DNAs seems different from a common TBM with uncorrelated random on-site energies since the restriction of the combination of inter-chain base-pairs in DNA will induce local correlations between the two chains. However, by calculating the zero-temperature transmission rate spectrum directly we shall show that this double-chain TBM for real DNAs cannot have conductor behavior, either. There have already been some theoretical studies on similar problems, and we shall also discuss and compare our results with them.

![Figure 1](image_url)

**FIG. 1:** (a) Schematic illustration of a part of DNA sequence; (b) the corresponding double-chain TBM of the sequence in (a). $\epsilon_A$, $\epsilon_T$, $\epsilon_C$, $\epsilon_G$ denote the different on-site energies for the corresponding nucleotides. $t$ denotes intra-chain coupling and $t_{inter}$ inter-chain coupling.

The Hamiltonian of the double-chain TBM for disordered DNAs is as following

$$\hat{H}_2 = \hat{H}_{intra} + \hat{H}_{inter}$$

(1)
where
\[ \hat{H}_{\text{intra}} = \sum_n [\epsilon_{n,1} \hat{C}^\dagger_{n,1} \hat{C}_{n,1} + \epsilon_{n,2} \hat{C}^\dagger_{n,2} \hat{C}_{n,2} + t(\hat{C}^\dagger_{n+1,1} \hat{C}_{n,1} + \hat{C}^\dagger_{n+1,2} \hat{C}_{n,2})] \] (2)
and
\[ \hat{H}_{\text{inter}} = t_{\text{inter}} \sum_n \hat{C}^\dagger_{n,1} \hat{C}_{n,2}. \] (3)

\( \epsilon_{n,1} \) and \( \epsilon_{n,2} \) are the on-site energies of nucleotides in the two chains which can take four possible values \( \epsilon_A, \epsilon_T, \epsilon_C, \epsilon_G \). \( t \) and \( t_{\text{inter}} \) are the intra-chain and inter-chain couplings, respectively. Fig.1(b) shows the corresponding double-chain TBM for the part of DNA sequence in Fig.1(a).

In order to introduce the effect of disorder in on-site energies, we consider the simplest case that only two types of nucleotides, say, \( A \) and \( T \), exist in the two chains while the sequence of \( A \) and \( T \) in each chain is random. This may be considered as a minimum model to include on-site disorder effect because in a general sequence in DNA all four possible base-pairs exist randomly which will only enhance the effect of disorders. For this special case, without loss of generality we can take the average on-site energy of nucleotides \( A \) and \( T \) as the energy reference point i.e., \( (\epsilon_A + \epsilon_T)/2 = 0 \), and set the intra-chain coupling \( t \) as the energy unit, i.e., \( t = 1 \). Then, we need only consider the case that \( \epsilon_A = +\epsilon \) and \( \epsilon_T = -\epsilon \), and \( \epsilon \) can be considered as the disorder strength in on-site energies. Fig.2(a) shows a part of such a DNA sequence, and Fig.2(b) is the corresponding double-chain tight-binding model.

**FIG. 2:** The double-chain random tight-binding model for DNA. (a) Schematic illustration of a part of the double-strand DNA with only \( A \) and \( T \) as we consider; (b) the corresponding double-chain tight-binding model.

The zero-temperature transmission rate of an eigenstate of energy \( E \) in unit of \( G_0 = 2e^2/h \) is given by
\[ g(E) = \frac{G(E)}{G_0} = \frac{1}{1 + \cosh \lambda_n(E)} \] (4)
where \( \lambda_n(E) \) are eigenvalues of the operator \( \hat{T}(E) \hat{T}(E) \) and \( \hat{T}(E) \) is the transfer matrix of the system. The eigenvalues \( \lambda_n(E) \) and the transmission rate spectrum can be calculated by standard transfer matrix algorithm. This mathematical framework is essentially the same as the one Roche et. al. have used in their study. We shall show that the transmission rate spectrum of the double-chain TBM for disordered DNAs is strongly suppressed and all electronic states are localized in the thermodynamic limit.

**FIG. 3:** The transmission rate spectrum \( g(E) \) for a double-chain tight-binding model with random on-site energies. (a) \( t_{\text{inter}} = 1 \) with \( L = 10000 \), (b) \( t_{\text{inter}} = 3 \) with \( L = 10000 \), (c) \( t_{\text{inter}} = 5 \) with \( L = 10000 \), (d) \( t_{\text{inter}} = 9 \) with \( L = 10000 \), (e) \( t_{\text{inter}} = 9 \) with \( L = 50000 \), (f) \( t_{\text{inter}} = 9 \) with \( L = 100000 \).

Let us look at the numerical results. Since all results are symmetric with \( E=0 \), we only provide the part of \( E > 0 \). Fig.3 is for \( L = 10000 \) with (a) \( t_{\text{inter}} = 1 \), (b) \( t_{\text{inter}} = 3 \), (c) \( t_{\text{inter}} = 5 \), (d) \( t_{\text{inter}} = 9 \). The parameter for the disorder strength of on-site energies is taken as \( \epsilon = 1 \), and the probabilities of the occurrence of both \( A \) and \( T \) in each chain are set as 1/2. Essentially the same results are obtained for other non-zero value of \( \epsilon \) and non-zero occurrence probabilities of \( A \) and \( T \).

For weak inter-chain coupling \( t_{\text{inter}} = 1 \), the transmission rate is zero everywhere, which means that all states are localized. When inter-chain coupling increases, say, \( t_{\text{inter}} = 3 \), peaks begin to exist in the spectrum, similar to the behavior of a random single-chain TBM of finite length. For further strong inter-chain coupling, say, \( t_{\text{inter}} = 5 \), the curve begins to form a band with sharp peaks. With further increase of \( t_{\text{inter}} \), say, \( t_{\text{inter}} = 9 \), a band of finite transmission rate emerges. However,
as shown in Fig 3(d), (e) and (f) for $t_{inter} = 9$ with $L = 10000, 50000$ and $100000$, respectively, it is clear that this band tends to vanish at large $L$. Thus the existence of a band of finite transmission rate in the case of strong inter-chain coupling does not mean the existence of truly extended states. It is only a finite-size effect which is expected to disappear when the chain length $L$ tends to infinity.

According to the above results, we may come to the following conclusions. A disordered double-chain TBM for real DNAs with weak inter-chain couplings does not have conducting electronic states. When inter-chain couplings become strong, the model with finite chain length forms an energy band of finite transmission rate, similar to that of a periodic single-chain TBM. However, this is due to finite-size effect and does not mean the existence of true conducting states. In the thermodynamic limit, the band tends to disappear and all electronic states are localized. Therefore, the conductor behavior of real DNAs, if exists, cannot be explained by the simple one-electron double-chain TBM with random on-site energies.

FIG. 5: (a) Schematic illustration of the faithful model of a part of a single-chain DNA with only $A$ and $T$ nucleotides; (b) the corresponding single-chain TBM of the sequence in (a). $S$ and $P$ denote sugar and phosphate sites. $\epsilon_S$ and $\epsilon_P$ denote on-site energies of sugar and phosphate sites, respectively. $\epsilon_A$ and $\epsilon_T$ denote on-site energies for $A$ and $T$ nucleotides, respectively. $t_{SP}$ denotes intra-chain coupling between a sugar and its neighboring phosphate. $t_{PA}$ and $t_{PT}$ the coupling between a phosphate and $A$ and $T$ nucleotides, respectively.

$E$ is the eigen-energy we consider, $\epsilon_S$ and $\epsilon_P$ are on-site energies of sugar and phosphate sites, and $t_{SP}$ is the coupling between neighboring sugar and phosphate sites in the original model of Fig 5. (Both $\epsilon'_{P}$ and $t_{PP}$ diverge at $E = \epsilon_S$ which should be treated by considering directly the original stationary Schrodinger equations.) For each given $E$, the above decimation only gives a global shift for the on-site energies of each phosphate site and does not introduce any disorder because $\epsilon_S$, $\epsilon_P$ and $t_{SP}$ are constant values in the original model.

However, it is well-known that there is a periodic sugar-phosphate chain in each backbone structure of real DNA. Therefore, a faithful model for a real double-chain DNA should be as shown in Fig 4. (b) and (b), where $S$ and $P$ denote sugar and phosphate and $A, T$ denote the nucleotides. Thus there comes a question on whether the simple model in Fig 4 can be renormalized into the model in Fig 5 by the real-space decimation renormalization technique. We shall still restrict to the simplest case that only $A$ and $T$ exist in the two chains.

Let us first look at a single-chain DNA with series of random nucleotides as shown in Fig 5(a). We shall show that it can be mapped into a single chain Anderson TBM with random on-site energies. As a first step, let us renormalize a local phosphate-sugar-phosphate structure into a phosphate-phosphate structure by decimation of the sugar site, as shown in Fig 6. Perform this decimation process on all local phosphate-sugar-phosphate structures, one can decimate all sugar sites. The decimation process renormalizes the on-site energy of all phosphate sites into $\epsilon'_{P}$

$$\epsilon'_{P} = \epsilon_{P} + \frac{2t_{SP}^{2}}{E - \epsilon_{S}}$$

and introduces a direct coupling $t_{PP}$ between nearest-neighboring phosphates

$$t_{PP} = \frac{t_{SP}^{2}}{E - \epsilon_{S}}.$$  

FIG. 6: A local phosphate-sugar-phosphate structure (a) is renormalized into a phosphate-phosphate structure (b) by decimation of the sugar site $S$.

The second step is to renormalize a local phosphate-phosphate-phosphate structure by decimation of the nucleotide coupled with the middle phosphate as shown in Fig 7. This decimation process only renormalizes the on-site energy of the middle phosphate $\epsilon_{P}$ into

$$\epsilon'_{P} = \epsilon_{P} + \frac{t_{PA}^{2}}{E - \epsilon_{A}}.$$
where $\epsilon_A$ is the on-site energy of the nucleotide coupled with the middle phosphate. ($\epsilon'_P$ diverges at $E = \epsilon_A$, which means that the electron wave of energy $E = \epsilon_A$ is totally reflected at this point, similar to the ‘anti-resonance’ phenomenon in diatomic molecules. Since the series of $A$ and $T$ nucleotide are random for the case we consider, this decimation process introduces effectively randomness into renormalized on-site energies of phosphate sites. Perform this decimation step for all local phosphate-phosphate-phosphate structures, one finally obtain a single chain of phosphate sites with uncorrelated random on-site energies. According to the scaling theorem, the on-site disorder localizes states of all eigen-energies.

$\mathcal{E}$

FIG. 7: A local phosphate-phosphate-phosphate structure with the middle phosphate coupled with a nucleotide is renormalized into a phosphate-phosphate-phosphate structure by decimation of the nucleotide coupled with the middle phosphate site.

$\mathcal{E}$

FIG. 8: A local structure (a) is renormalized into a local structure (b) by decimation of the nucleotide pair.

Now let us consider the double-chain model as shown in Fig. 11(b). Perform the same process as shown in Fig. 10 one can decimate all sugar sites. In order to map into the model of Fig. 2, one needs to decimate all the nucleotide pairs. This can be done by considering the decimation process shown in Fig. 9 where a pair of coupled nucleotides connecting two phosphates in each chain are decimated. This will renormalize the on-site energies of the two phosphates as

$$
\epsilon'_A = \epsilon'_P + \frac{(E - \epsilon_T)t^2_{PA}}{(E - \epsilon_A)(E - \epsilon_T) - t^2_{AT}}
$$

$$
\epsilon'_T = \epsilon'_P + \frac{(E - \epsilon_A)t^2_{PT}}{(E - \epsilon_A)(E - \epsilon_T) - t^2_{AT}}
$$

(8)

($\epsilon'_P$ is as in Eq. (5) and introduce a direct inter-chain coupling between the two phosphates as

$$
\epsilon'_P = \frac{t_{PA}t_{PT}t_{AT}}{(E - \epsilon_A)(E - \epsilon_T) - t^2_{AT}}.
$$

(9)

$\epsilon'_A$, $\epsilon'_T$ and $\epsilon'_{AT}$ diverge at $(E - \epsilon_A)(E - \epsilon_T) - t^2_{AT} = 0$ which should be treated by considering directly the original stationary Schrodinger equations. It is easy to see that this decimation process introduces correlated randomness into on-site energies of each pair of inter-chain-coupled phosphate sites. Therefore, the model in Fig. 11 is mapped into essentially the same model as shown in Fig. 2. According to numerical results for the model in Fig. 2, we may conclude that no extended states exist in thermodynamic limit for both models.

FIG. 9: A double-chain TBM model for DNA with couplings between nucleotide and its neighboring sugar sites (a) is renormalized into a double-chain TBM (b) by decimation of the sugar sites and nucleotide pairs.

It should be noted that extended states may emerge when other kinds of couplings are included in the above model. For example, let us take into account the couplings between a nucleotide and its nearest-neighboring sugar sites as shown in Fig. 11(a). Then, by decimation of both the sugar sites and nucleotide pairs, one can obtain a model of Fig. 11(b) where both random on-site energies and random couplings in each group of four nearest-neighboring sites are correlated. Such a model may have extended states because it looks similar to generalized dimer models which have been shown to have extended states in recent studies.

Before making the summary, we would like to make some discussions about our results and recent theoretical and experimental results on similar problems. Iguchi has studied a single chain of DNA with periodic nucleotide series, which always has extended states due to Bloch’s theorem. Roch et al. have studied both periodic approximations of aperiodic DNA series and series extracted from real DNAs. Their results for series of real DNAs are similar with our results. Yamada and Yamada et al. have studied the influence of correlated on-site disorder in the model and found similar localization behaviors as our results suggest. In the aspect of experiments, Yoo et al. have found that the conduction behavior of DNA with identical base-pairs may be well explained by bands of extended states separated by localized states which is possible for a periodic TBM model. While Tran et al.’s studies on $\lambda-$DNA with disordered sequence of base-pairs seem to suggest that no truly extended states exist, which agrees with our results.

In summary, we have studied the disordered double-chain TBM with and without periodic sugar-phosphate...
chain in the backbone structure for real DNAs. Numerical results combined with real-space decimation renormalization technique show that in both cases no truly extended states exist in the thermodynamic limit, regardless of how strong the inter-chain couplings are. Therefore, the double-chain TBM for real DNAs considered in this paper always has zero transmission rate in thermodynamic limit, and bad conduction is expected for real DNAs with long random series of nucleotides.

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