Quantum transport anomalies in DNA containing mispairs

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Abstract

The effect of mispairs on charge transport in DNA of sequence (GC)(TA)\textsuperscript{N}(GC)\textsubscript{3} connected to platinum electrodes is studied using the tight-binding model. With parameters derived from an \textit{ab initio} density functional result, we calculate the current versus bias voltage for DNA with and without a mispair and for different numbers of (TA) basepairs \textit{N} between the single and triple (GC) basepairs. The current decays exponentially with \textit{N} under low bias but reaches a minimum under high bias when a multichannel transport mechanism is established. A (GA) mispair substituting a (TA) basepair near the middle of the (TA)\textit{N} sequence usually enhances the current by one order due to its low ionization energy but may decrease the current significantly when an established multichannel mechanism is broken.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Longitudinal charge transport along DNA has been the subject of extensive study in the last decade \cite{1–3}. Charge transport occurs in the oxidative and reductive DNA damage or repair processes and can happen in the long distance range \cite{1, 4, 5}. Study of the transport properties may lead to a better understanding of the fundamental driving processes in biological evolution. Furthermore, the charge transport process might have been used naturally for basepair mismatch detection during the DNA repairing process. It is already known that, due to chemical reaction and radiative ionization, mispairs or gene mutations happen quite often in the cell. Fortunately, almost all of the mispairs can be detected and repaired during the replication process to keep the material genetically stable. However, some of the mutations may escape from the detecting and repairing processes and result in various genetic diseases including cancer. A recent study indicates a negative correlation between the cancer risk and the sensitivity of the charge transport property of the gene to a mutation \cite{6}. Understanding how mispairs modify the electric properties of DNA then becomes very important \cite{7–9} and, together with the usage of other properties \cite{10, 11}, may improve mutation detecting techniques \cite{12–15}. In addition, thanks to its perfect self-assembling and self-recognition properties found in nature, DNA is also expected to be a potentially functional material for molecular devices. In this case mispairs may be used to obtain unique functions of the devices.

The charge transport through a DNA sequence can be measured by chemical or physical methods \cite{1–3}. In one of the typical chemical experiments, Giese \textit{et al} used DNA of sequence (GC)(TA)\textsuperscript{N}(GC)\textsubscript{3} \cite{16}. They measured the charge transfer rate from the (GC) basepair to the (GC)\textsubscript{3} triple basepair for different numbers \textit{N} of (TA) basepairs, and found a crossover from a rapid decay of the charge transfer rate versus \textit{N} to an almost zero decay around \textit{N} = 3. As an alternative to other explanations \cite{17–22}, we have proposed this as a crossover from one dominant channel transport to a multichannel transport \cite{23}. An example of physical experiments is the one performed by Porath \textit{et al} \cite{24} where a DNA sequence (GC)\textsubscript{m} is located between two platinum electrodes and the current versus voltage is directly measured. This result has also been simulated by simple tight-binding models \cite{25–27}. It is known that the GA mispair in various conformations \cite{11} is the most stable mispair and is often present in DNA \cite{5}. The magnetic properties of DNA were studied earlier and found to be significantly influenced by the presence of the GA mispair \cite{10}. In this paper, we will...
study the effect of mispairs, such as G(anti)-A(anti), indicated in the following as (GaAa), and G(anti)-A(syn), indicated as (GaAs) [28], on charge transport when a Watson–Crick basepair is replaced by a mispair in the DNA sequence (GC)(TA)X(GC)3 connected to platinum electrodes.

### 2. Method

We consider a p-type semiconductor DNA duplex chain of basepairs connected to a circuit via two platinum electrodes suitable for experimental realization [24]. Each platinum electrode is modeled as a semi-infinite one-dimensional (1D) electrode [27] connected to the G base at one end of the first strand as illustrated in figure 1(a). The tight-binding Hamiltonian of the system reads

\[
H = 2 \sum_{\gamma=n}^{\infty} \left[ \epsilon_n c_n^\dagger c_n - t_{n,n+1} \left( c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n \right) \right]
+ 2 \sum_{\gamma=1}^{N} u_n d_n^\dagger d_n - 2 \sum_{\gamma=1}^{N-1} h_{n,n+1} \left( d_n^\dagger d_{n+1} + d_{n+1}^\dagger d_n \right)
- 2 \sum_{\gamma=1}^{N} \lambda_n \left( d_n^\dagger d_n + d_n^\dagger c_n + c_n^\dagger d_n + c_n^\dagger c_n \right). \tag{1}
\]

Here \( c_n^\dagger \) (\( d_n^\dagger \)) is the creation operator of holes in the first (second) strand on site \( n \) of the DNA chain (for \( 1 \leq n \leq N \)), the left electrodes (\( n \leq 0 \)), and the right electrodes (\( n \geq N + 1 \)). The on-site energy of site \( n \) in the first (second) strand is denoted by \( \epsilon_n \) (\( u_n \)), which is equal to the highest occupied molecular orbit (HOMO) energy of the base on this site in the DNA chain and the center of the conduction band in the electrodes. The coupling parameter of the first (second) strand \( t_{n,n+1} \) (\( h_{n,n+1} \)) is equal to the intrastrand coupling parameter between neighboring sites \( n \) and \( n + 1 \) of the DNA for \( 1 \leq n \leq N - 1 \), one-fourth of the conduction band-width in the electrodes \( t_m \) for \( n \leq -1 \) and \( n \geq N + 1 \), and the coupling strength between the electrodes and the DNA strands for \( n = 0 \) and \( N \). The interstrand coupling between sites in the same basepair is described by \( \lambda_n \). The multiplication factor of two in each sum in equation (1) arises from the spin degeneracy.

In transport experiments [24], a high bias voltage can be applied to drive the system far from equilibrium and holes in a wide energy range may contribute to the current. Since the carriers usually come from various energy bands and the profile of band distribution is energy dependent, the effective parameters \( \epsilon_m \) and \( t_m \), which are averages over the profiles, are then energy dependent. We assume that the parameters for the 1D tight-binding model have a similar dependence on energy as in bulk platinum [29] and the dependence is extracted from its 3D band structure. Near the Fermi energy, there are six bands located approximately at \(-5.8, -4.7, -3.7, -2.2, -0.2, \) and \( 2.0 \) eV above the Fermi energy with band-widths of \( 1.9, 1.3, 1.5, 3.1, 1.4, \) and \( 6.0 \) eV respectively. Using Lorentzian broadening, we can mimic the bulk DOS and extract the parameters \( \epsilon_m \) and \( t_m \) as shown in figure 1(b). The parameters are then scaled to match the known values at the Fermi energy as was done in [27]. For electrons at the Fermi energy, the on-site energy is \( \epsilon_m^0 = -0.33 \) eV with a coupling parameter \( \rho_m^0 = 0.55 \) eV. As estimated from the experimental data [25, 27] the equilibrium Fermi energy is 1.73 eV higher than the HOMO on-site energy of the G base when the (GC) basepair makes contact with the platinum electrodes. Here we assume that the first DNA strand is coupled to the electrodes with a contact parameter of \( t_{m,n} = 0.1 \) eV while the second strand does not contact the electrodes directly. Note that our main result is not sensitive to the choice of the electrodes and the contact parameters.

The tight-binding parameters of DNA are estimated based on the HOMO energies of isolated nucleobases and the charge transfer integral between the HOMO orbitals calculated by the \textit{ab initio} density functional method integrated in the ADF (Amsterdam Density Functional) program [10, 11, 30]. The on-site energies for bases G, C, T, and A are \(-9.40, -10.27, -10.46, \) and \(-9.79 \), respectively. The hopping coupling parameters as illustrated in figure 2 are listed in table 1.

The current \( I \) when a voltage bias \( V \) is applied over the two platinum electrodes is then evaluated by the transfer

\[
\begin{array}{c|c|c|c|c|c}
(X_1X_2) & t_{12} & t_{23} & \lambda_2 & h_{12} & h_{23} \\
\hline
5’-G – X_1 – G’ & 0.133 & 0.133 & 0.028 & 0.14 & 0.14 \\
3’-G – X_2 – C’ & 0.164 & 0.400 & 0.070 & 0.154 & 0.099 \\
TA & 0.330 & 0.330 & 0.070 & 0.011 & 0.011 \\
GaAa & 0.400 & 0.164 & 0.029 & 0.055 & 0.002 \\
GaAs & 0.250 & 0.167 & 0.057 & 0.207 & 0.027 \\
\end{array}
\]
The intrastrand coupling parameter between neighboring sites is $t_n$ to those of the sites $\lambda_n$ denoted by ($a$) Current matrix method [2, 23, 31, 32]. For an open system, the secular matrix method is used to obtain the tight-binding parameters. In the first (second) strand, the on-site energy of a HOMO orbital is $\varepsilon_n (u_n)$ and the intrasstrand coupling parameter between neighboring sites is $t_{n,n+1} (h_{n,n+1})$ with $n$ the base index. The interstrand coupling parameter is denoted by $\lambda_n$.

$\varepsilon_n + \lambda_n \Psi_n + t_{n,n+1} \Psi_{n+1} = 0$

$\Psi_n + (u_n - E) \Psi_n + \lambda_n \Psi_{n-1} = 0$

$\Psi_n = (\varepsilon_n - E) \Psi_n + \lambda_n \Psi_{n-1} + t_{n,n+1} \Psi_{n+1}$

$\Psi_{n+1} = (\varepsilon_n - E) \Psi_{n+1} + \lambda_n \Psi_n + t_{n,n+1} \Psi_{n-1}$

with $\Psi_n$ ($\Psi_n$) the wavefunction of the first (second) strand on site $n$. The wavefunctions of the sites $n + 1$ and $n$ are related to those of the sites $n$ and $n - 1$ by a transfer matrix $M$,

$\begin{pmatrix}
\Psi_{n+1} \\
\Psi_{n-1} \\
\Psi_{n} \\
\Psi_{n-1}
\end{pmatrix} = \begin{pmatrix}
\varepsilon_n - E & \lambda_n & 0 & 0 \\
0 & \varepsilon_n - E & \lambda_n & 0 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0
\end{pmatrix}$

$\begin{pmatrix}
\Psi_{n+1} \\
\Psi_{n-1} \\
\Psi_{n} \\
\Psi_{n-1}
\end{pmatrix}$

(2)

The transmission is then calculated by assuming the plane waves propagating in the electrodes for the holes $\Psi_n = A e^{ik_n a} + B e^{-ik_n a}$ for $n \leq 0$ and $\Psi_n = C e^{ik_n a}$ for $n \geq N + 1$ in the left and right electrodes, respectively. Expressing the output wave amplitude $C$ in terms of the input wave amplitude $A$ and the transmission,

$T(E) = \frac{|C|^2 \sin(kR a)}{|A|^2 \sin(kL a)}$

The distance between two neighboring bases along any DNA strand is $a = 3.4 \, \text{Å}$. The net current primarily comes from the hole transmission between the electrodes’ Fermi energies and is calculated as [33]

$I = \frac{e^2}{h} \sum_{\sigma} \int_{-\infty}^{\infty} dE T^\sigma(E)\left[f^\sigma(E) - f^R(E)\right]$

Here the Fermi function is $f^\sigma(E) = 1 / [\exp(E - E_F^\sigma)/k_B T] + 1$ with $X = L$ or $R$ and the room temperature $T = 300$ K. When a bias voltage $V$ is applied between the two electrodes, the left (right) Fermi energy is assumed to be $E_F^L = V/2$ and $E_F^R = -V/2$.

3. Results and discussion

The results for the current ($I$) versus voltage ($V$) for DNA of sequence (GC)(TA)$_N$(GC)$_3$ with $N = 1–11$ are shown in figure 3(a). Each curve except for $N = 1$ has steps at voltages 1.45, 1.64, 1.85, and 2.02 eV indicating that the transport channels are mainly formed at four threshold voltages related to the four kinds of bases. In the $N = 1$ curve, the second step is split into two at $V = 1.62$ and 1.7 V and there is no step at 2.02 V. In a log scale, the two lower-energy steps have almost the same height for all the curves while the height of the two higher-energy steps increases with the number of (TA) basepairs. At a bias voltage lower than the first threshold, the DNA works as an energy barrier for electron transport since the Fermi energy of both electrodes is located between the HOMO and LUMO energies. At a bias near the first and

Figure 2. Illustration of a three-basepair DNA used in the ADF program to obtain the tight-binding parameters. In the first (second) strand, the on-site energy of a HOMO orbital is $\varepsilon_n (u_n)$ and the intrasstrand coupling parameter between neighboring sites is $t_{n,n+1} (h_{n,n+1})$ with $n$ the base index. The interstrand coupling parameter is denoted by $\lambda_n$.

Figure 3. (a) Current $I$ versus bias voltage $V$ of the DNA sequence (GC)(TA)$_N$(GC)$_3$, $N = 1–11$ for curves from the top. (b) Current $I$ versus (TA) basepair number $N$ at fixed bias voltage $V$. The value of $V$ is indicated beside each curve.
I between the two electrodes to obtain the calculations. In addition, a variable bias voltage is applied to the parameters of the DNA and electrode extracted from ab initio as we employ a more realistic model with the tight-binding approach where uniform parameters and virtual electrodes are assumed, only the integer part of the value. (b) Current $I$ versus the number $N$ at several selected bias voltages $V$ indicated by the values beside each curve. The $I–V$ curves and $I–N$ curves for the DNA sequence $(\text{GC})(\text{TA})_{N/2}(\text{GaAa})(\text{TA})_{(N−1)/2}(\text{GC})_3$ are plotted in (c) and (d).

Figure 4. (a) The $I–V$ curves of the DNA sequence $(\text{GC})(\text{TA})_{N/2}(\text{GaAa})(\text{TA})_{(N−1)/2}(\text{GC})_3$ for $N = 3–11$. Here $N/2$ and $(N − 1)/2$ take only the integer part of the value. (b) Current $I$ versus the number $N$ at several selected bias voltages $V$ indicated by the values beside each curve. The $I–V$ curves and $I–N$ curves for the DNA sequence $(\text{GC})(\text{TA})_{N/2}(\text{GaAa})(\text{TA})_{(N−1)/2}(\text{GC})_3$ are plotted in (c) and (d).

The second thresholds ($1.45 < 1.8$ eV), HOMO channels of the (GC) basepairs become available for charge transport but the (TA) basepairs behave as energy barriers for transport. At a bias higher than the third threshold ($V > 1.85$ eV), transport channels of the (TA) basepair also participate in the charge transport across the DNA molecule. Along the curve $N = 1$, we can hardly see the third and the fourth steps. The addition of (TA) basepairs can establish a network of transport channels, as was reported in [23]. Consequently, we observe the height increase of the third and fourth steps in the log scale. The current enhancement due to additional channels may compete with the exponential current decay with the length of the molecule. This results in a current minimum for $N > 5$, as clearly shown in figure 3(b) where the current is plotted versus $N$ at various $V$. At a bias less than 1.8 V, the current decays exponentially with $N$ with almost the same exponent. For a bias higher than 1.8 V, the exponent decreases with $N$ until it is almost zero for $N > 5$ under the bias $V = 2.1$ V or higher. This crossover from a rapid to almost zero decay of the charge transfer versus the (TA) basepair numbers has been observed in [16] with the chemical method and can also be observed in physical experiments as described in [24].

In contrast to our previous simplified model [23] where uniform parameters and virtual electrodes are assumed, we employ a more realistic model with the tight-binding parameters of the DNA and electrode extracted from ab initio calculations. In addition, a variable bias voltage is applied between the two electrodes to obtain the $I–V$ curve. Note that the role of diagonal interstrand hopping is relevant to the electron transport in DNA and its inclusion in the calculation might shift the $I–V$ curve but not the conclusion [34, 35].

To estimate the effect of the mispairs (GaAa) and (GaAs) on the charge transport, we replace one of the (TA) basepairs near the middle of the (TA)$_N$ sequence by a mispair and calculate the corresponding $I–V$ curve. In figures 4(a) and (b), the result for the $(N + 2)/2$th (TA) basepair replaced by a (GaAa) mispair is shown and in (c) and (d) the $(N + 1)/2$th basepair is replaced by a mispair. Here $[R]$ means extracting the integer part of a real number $R$. Note that the curves of odd $N$ are the same in figures 4(a) and (c), corresponding to equal numbers of (TA) basepairs to the left and right of the (GaAa) mispair. For even $N$, there is one more (TA) to the left of the mispair in (a) and one less in (b). With the replacement of the mispair, the current is greatly enhanced after the first threshold voltage (2 eV) as shown in figures 4(a) and (c). This happens because the mispair destroys the resonant transport network formed by the periodic (TA) basepairs series, i.e. the mispair works as an impurity. A weak $N$ dependent current appears only for higher $N$ and at a lower current value, as shown in figures 4(b) and (d) when both the (TA) sequences besides the mispair form a resonant transport network.

In the presence of a mispair, some steps shift and extra steps appear along the $I–V$ curves. For $N = 3$ or DNA of sequence $(\text{GC})(\text{TA})(\text{GaAa})(\text{TA})(\text{GC})_3$, the simplest case with a mispair, three steps at $V = 1.41, 1.55,$ and 1.68 V appear in the $I–V$ curve and the current is enhanced by more than one
order at high voltage with the substitution by a mispair. For $N \geq 5$, however, the first three steps shift to $V = 1.45, 1.53,$ and $1.64$ V with the last one decaying over $N$. Compared to the case without a mispair, one extra step appears at $V = 1.45$ V. In the bias range $1.45 \, V < V < 1.53 \, V$, the curves for $N > 4$ are almost equally separated in the vertical log scale, indicating an exponentially decaying current with $N$ as also shown in figures 4(b) and (d). Furthermore, the mispair location also significantly affects the current. The $N = 4$ curve has steps at the same position as for $N = 3$ in figure 4(a) but as for the $N \geq 5$ curves in figure 4(b). In the range $1.58 \, V < V < 2.2 \, V$, the even $N$ curves are near the curve of $N + 1$ in (a) but near the curve $N - 1$ in (b). The change is also represented by shifted steps along the $V = 1.6 \, V$ curves when comparing figures 4(b)–(d). This observation suggests that the current in this bias range is mainly determined by the length of the (TA)$_n$ sequence between the left single (GC) basepair and the (GaAa) mispair. Under stronger bias, the current at first decays exponentially with $N$ and then fluctuates near a value slightly below 1 nA. This long-DNA current limit is about five times smaller than that observed in the system without a mispair.

When the (GaAa) mispair is replaced by a (GaAs) mispair, the $I$–$V$ curves show fewer steps as illustrated in figure 5. For $N = 3$ there are three steps at $V = 1.45, 1.58,$ and $1.68$ V while for $N \geq 5$ there are only two steps at $V = 1.45$ and $1.61$ V below the bias $2 \, V$. Similar to the case of the (GaAa) mispair shown in figure 4, the $N = 4$ curve also has steps at the position of the $N = 3$ curve in (a) but at the positions of the $N \geq 5$ curves in (b). In addition, the current is mainly limited by the number of (TA) basepairs between the left (GC) basepair and the (GaAs) mispair in the range $1.6 \, V < V < 2.2 \, V$. For $V > 2.2 \, V$, no steps in the curves of $N \leq 7$ suggests again that one transport channel dominates in the short (TA)$_n$ DNA sequence. For large $N$, a series of steps appears in the $I$–$V$ curves and the current does not decrease monotonically with $N$, indicating that the enhancement of current due to the increase of transport channel number with $N$ can compensate the current decay with the length of each channel. The current decays exponentially at $V < 1.6 \, V$ but decays with steps in the range $1.6 \, V < V < 2.2 \, V$. At $V > 2.2 \, V$ the current decays in short DNA and then fluctuates when the multichannel tunneling mechanism dominates in the long (TA)$_n$ sequence. Overall a (GaAs) mispair substitution changes the current less than that of a (GaAa) mispair especially in high bias since the intrastand coupling parameter of a (GaAs) mispair is closer to that of a (TA) basepair.

4. Summary

In summary, we have studied charge transport through DNA connected to two platinum electrodes and containing mispairs within a realistic tight-binding scheme. The energy dependent tight-binding parameters for the electrodes are obtained by fitting the density of states near the Fermi energy of the material. The parameters of DNA are derived from the $ab$ initio density functional calculation of the coupling between HOMO states in neighbor bases. When a (TA) basepair in the (GC)(TA)$_n$(GC)$_3$ sequence is replaced by (GaAa) or (GaAs) mispairs, the current is usually enhanced due to the lower ionization energy of the mispairs. In DNA with a long (TA)$_N$ sequence, the multichannel tunneling mechanism sets a minimal current at a high bias, similar to a previous experimental observation. The substitution of the mispair in this case, however, will break the multichannel tunneling mechanism and decrease the current significantly.
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