Interchain versus intrachain hole transmission through desoxyribonucleic acid molecular wires

Eric R. Bittner

Department of Chemistry and Center for Materials Chemistry
University of Houston
Houston, TX 77204

(Dated: November 21, 2018)

We present a methodology for computing the current-voltage response of a molecular wire within the Landauer-Buttiker formalism based upon transforming the cumulative transmission probability into an eigenvalue problem. The method is extremely simple to apply since does not involve construction of the molecular Greens function, and hence avoids the use of complex integration contours to avoid poles. We use this method to study the effect of base-pair sequence on the conductivity of holes in DNA chains containing A-T bridges between guanine chains. Our results indicate that sequence plays a substantial role in ballistic transport via tunneling resonances tuned by sequence and interchain interactions. We also find that ballistic transport is dominated by intrachain transport and that hole transmission is insensitive to interchain fluctuations.

I. INTRODUCTION

Advances in synthetic technique and nano-scale device fabrication have facilitated the creation of prototypical electronic logic components in which the length scale of the device is on the order of the de Broglie wavelength of an electron. The prospect of using such “molecular electronic” components in technological applications is a strong driving force in the emerging science and engineering of nanotechnology. The real promise of nanotechnology relies upon our ability to predictably manipulate matter on the molecular length scale. In particular, for molecular electronic materials, the goal is to be able to fine tune the quantum mechanical energy states so that the properties of the individual quantum states is expressed whatever macroscopic device we are trying to engineer. The challenge here is then to build the interconnects between the individual molecules and the “outside world” so that one can reliably address and access the molecular-scale components.

The sequence dependence of charge transport in DNA is a topic of considerable interest from both experimental and theoretical viewpoints. From a design standpoint, DNA has a number of desirable properties. It possess a high degree of of site specific binding between single strands of DNA and its related self-assembly properties. Furthermore, one can synthesize essentially any sequence desired and hence potentially tune its properties in a controllable way. Such characteristics have made DNA an ideal candidate for incorporation into molecular scale electronic devices. With such motivation, a number of studies have been performed and there is an emerging consensus regarding the mechanism for single-electron transport in DNA chains. However, the DNA’s intrinsic conductivity remains highly controversial. Depending upon the experiment, DNA is a) an insulator at room temperature, b) a wide-band gap semiconductor at all temperatures, c) Ohmic at room temperature and an insulator at low temperatures, or d) metallic down to low temperatures with induced superconductivity. A recent review by Endres, Cox, and Singh nicely summarizes these varied experiments.

A number of studies have been performed at various levels of theory with the aim of computing the current-voltage (IV) response of a molecular wire. The studies differ widely in terms of the level of treatment of the electronic structure, the coupling between the molecule and the semi-infinite leads, and the change of electrostatic potential due to bias across the system. Both first principles and semi-empirical treatments have been used, with the former being restricted to smaller scale systems.

We consider the case where the terminal G’s and C-C pairs are anchored to opposing semi-infinite continua corresponding to the metal contacts. Similar models have been considered by Jortner and Bixon considering the canonical transfer rate from $G_i$ to $G_f$ separated by $(T - A)_n$ bridges. Here, we consider the microcanonical transmission probability at a given scattering energy, $T(E)$. From this we can compute the transmission current as a function of applied voltage bias via:

$$I(V) = \frac{2e}{h} \int T(E, V)(f_L(E - V/2) + f_R(E + V/2))dE(1)$$

where $f_L, f_R$ are the Fermi distribution functions for the left and right hand electrodes and $T(E, V)$ is the transmission probability at a given energy $E$ and applied voltage bias $V$. We examine how permuting base-pairs changes the transmission probabilities and hence the current-voltage response. Aside from differences in parameterization of the models, the results presented herein parallel those of Roche et al. who considered the same problem.

Here we compare intra- vs. interchain hole transport whereas the work by Roche et al considered considered the DNA strand as a single quasi-one dimensional strand.
As the hole propagates along the chain, sites containing A-T pairs act as potential barrier between guanine sites that must be overcome by quantum mechanical tunneling. Between guanine sites, hole transfer is taken to be effectively barrierless with no net change in free energy as the hole hops from \( \text{G}_n \) to \( \text{G}_{n+1} \). Since scattering dynamics is dominated entirely by what happens when the particle encounters a potential change, the terminal G units can be considered to be effective sites linking a short segment containing \( (T-A) \) bridges to the asymptotic region.

When there is a single barrier in for the hole, the hole can tunnel through the barrier and be transmitted. If there are multiple barriers, there is the possibility of resonant tunneling through quasi-bound hole-states on the chain. These resonant states will appear as discrete peaks in the transmission probability as a function of energy. Loosely speaking, each quasi-bound state corresponds to a particular single-particle eigenstate delocalized over the entire chain.

For this consider a simple Hückel chain connected to left and right electrodes at the left and right most sites:

\[
H_m = \sum_j \epsilon_j c_j \dagger c_j + \sum_{i \neq j} t_{ij}^{(m)} (c_i \dagger c_j + c_j \dagger c_i)
\]

where \( t_{ij}^{(m)} \) is the hopping integral, \( c_j \) and \( c_j \dagger \) are fermion operators which create or remove a hole from the \( j \)th site, and \( \epsilon_j^{(m)} \) the site energy. For metal contacts, we constructed two \( 5 \times 5 \times 5 \) simple cubic lattices each located at the ends of the molecular chain. This we do to insure that the density of states of the contacts is properly accounted for. The DNA sequence itself was connect to the center of the opposing faces of the left and right clusters. The cluster Hamiltonians were taken to be tight-binding

\[
H_m = \sum_j \epsilon_j b_j \dagger b_j + \sum_{i \neq j} t_{ij}^{(c)} (b_i \dagger b_j + b_j \dagger b_i)
\]

where the hopping integral couples nearest neighbor sites. Finally, the clusters and DNA strands were connected via

\[
V_{Lmc} = t_{mc}^{(c)} (b_i \dagger c_j + c_j \dagger b_i)
\]

\[
V_{Rmc} = t_{mc}^{(c)} (b_i \dagger c_k + c_k \dagger b_k)
\]

where the subscripts indicate the connected sites between the bridging DNA strand and the contact.

The various 4-base-pair chains considered here are depicted in Fig. 1. The dashed lines between chains the indicate non-zero off-diagonal transfer integrals between sites on opposing chains. Each nucleotide site has associated with it a hole-wavefunction \(|i\rangle\), a site energy, \( \epsilon_i \) and a transfer integral \( t_{ij}^{(m)} \) to the other sites in the sequence.

Since we are dealing with a tight-binding model, connectivity between sites plays a central role in determining the energetics of the system. We consider the following general scheme: For intrachain transport, hopping occurs between nearest neighboring pairs. For interchain hopping, we assume that the hole on the \( n \)th unit can hop
to an unit on the other chain one site removed, $n \pm 1$. Furthermore, we assume that interchain hops can occur between units of the same type,

$$
\begin{align*}
T_n \leftrightarrow T'_{n \pm 1} & \quad (0.0032 \text{eV}) \\
G_n \leftrightarrow G'_{n \pm 1} & \quad (0.019 \text{eV}) \\
C_n \leftrightarrow C'_{n \pm 1} & \quad (0.0007 \text{eV}) \\
A_n \leftrightarrow A'_{n \pm 1} & \quad (0.035 \text{eV})
\end{align*}
$$

or between $G - A'$ and $A - T'$ interchain neighbors

$$
\begin{align*}
T_n \leftrightarrow T'_n & \quad (0.021 \text{eV}) \\
A_n \leftrightarrow A'_n & \quad (0.016 \text{eV})
\end{align*}
$$

The logic behind this scheme is that there is better $\pi$ overlap between interchain neighbors displaced by one step than those directly adjacent. This allows relatively facile hopping to occur between neighboring interchain pairs. This scheme has been verified via quantum chemical calculations by Voityuk and the parameters for our model we take from a recent study by Lakhno, Sultanov, and Pettitt who considered a combined hopping/super-exchange model for computing hole-transfer rates through such model chains. The values of the interchain hopping terms and remaining parameters are available as supplementary material. Since all of hopping terms are positive, these can be considered as barriers for the delocalization of the hole over connected units.

**B. Embedding system in continuum**

To connect the cluster-DNA-cluster system to a continuum, we consider the system as if it were embedded in between two semi-infinite continua acting as reservoirs. Once we assume this, we can partition the state space of the total system into three domains, $Q_{Lo}$ and $Q_{Ro}$ which span the states of the left and right electrodes and $P$ which spans the electronic states of the bridging DNA molecule. Thus, the full Hamiltonian has the structure

$$
H = \begin{pmatrix}
H_L & V_{mL} & 0 \\
V_{mL} & H_m & V_{mR} \\
0 & V_{mR} & H_R
\end{pmatrix}
$$

where the diagonal terms are the Hamiltonians for the uncoupled subsystems and $V_{mL}$ and $V_{mR}$ are the couplings between the DNA and the left and right electrodes. There is considerable ambiguity in how this partitioning can be constructed since the metal contacts and the DNA bridge are in intimate contact. Here, we take a somewhat middle ground and define our partition between system and reservoir by including the inner three layers of atoms in the contacts in the “molecular” subspace in order to properly include the surface density of states and the electronic interaction between the DNA and surface in our calculations. Once we have made this partitioning, we can use the Schwinger-Keldysh formalism to derive the self-energy operators, $\Sigma_L$ and $\Sigma_R$, which embed the molecular sub-space into the continuum. As a result, the Greens function for quantum particle moving through the molecular subspace is

$$
G(E) = (E - H + \Sigma_L + \Sigma_R)^{-1}.
$$

Note that in general $\Sigma_L$ and $\Sigma_R$ are complex non-local operators which depend upon the scattering energy, $E$,

$$
\Sigma_{mm'} = \sum_k \frac{V_{mk}V_{km'}}{E - \epsilon_k + i\eta}.
$$

Here, $V_{mk}$ is the coupling between the chain and the contact and the sum is over the energy eigenvalues $\epsilon_k$ of the contacts. The $i\eta$ in the denominator insures that the proper retarded scattering boundary conditions are enforced.

Written in tight-binding site-representation, they can be written in a local form

$$
\Sigma_{L,n} = i\Delta_n(E) + \Lambda_n(E)
$$

where $\Lambda(E)$ shifts the site energy of the $n$th site. $\Delta_n(E)$ has the effect of acting as an absorbing potential for the scattering wave function. This insures that the scattering wave function obeys the proper asymptotic boundary conditions as we move away from the scattering region.

We assume that the absorbing boundary conditions can be constructed as local self-energy terms within the subspace of the clusters by setting the site energy of any atom located beyond a given cut-off radius from the point of contact between the bridge and the cluster to be complex

$$
\epsilon_{c,n} = \epsilon + i\Gamma
$$
with $\Gamma = 0.2eV$. In the examples that follow, we set the cut-off radius such that at least two atomic layers of the contact cluster were inside the cut-off radius and two layers were outside the cut-off. This provided a reasonable compromise between having enough atoms in the cluster to represent the density of states of a simple cubic continuum, and provide a reasonable absorbing boundary condition region for the scattering wave functions.

C. Computing Transmission and Current

To compute transmission and current through the DNA strand, we use the Landauer-Büttiker formula for relating the current, $I(V)$ to the transmission probability, $T(E,V)$, which may depend upon the applied bias, $V$,

$$I(V) = \frac{2e}{h} \int T(E,V)(f_L(E - V/2) + f_R(E + V/2))dE$$

where $f_{L,R}$ are the Fermi distribution functions for the left and right hand electrodes. The transmission probability is microcanonical rate for an electron injected on one end of the chain to leave on the other end as given by the Caroli equation.

$$T(E) = 4Tr \left( \Gamma_L G^\dagger_R (E) \Gamma_R G^\dagger_R (E) \right),$$ (12)

where $\Gamma_{L,R}$ are the imaginary parts of the left and right self-energies describing the coupling of the molecular wire to the left and right hand continua. Finally, $G_r$ is the reduced Greens function describing hole propagation through the bridging region

$$G_r(E) = (E - H + \Sigma)^{-1},$$ (13)

where $H$ is the molecular Hamiltonian with $\Sigma = \Sigma_L + \Sigma_R$ being the self-energy operator of the hole on in the bridge.

We can also consider $I(V)$ in terms of the number of modes contributing to the current

$$I = \frac{2e}{h} M (F^+ - F^-)$$ (14)

where $F^\pm$ are the potentials for the incoming and outgoing holes and $M$ is the number of modes. We can generalize this by letting the trace in $T(E)$ be the sum over the probability that a given mode will contribute to the current at a given energy,

$$T(E) = \sum_n p_n(E) = Tr(P).$$ (15)

Since the trace of a matrix is invariant to representation, we can construct the probability matrix

$$P(E) = 4\Gamma_L^{1/2}G^\dagger (E) \Gamma_R G(E) \Gamma_R^{1/2},$$ (16)

and $p_n(E)$ are then the eigenvalues of $P(E)$ which are bound by $p_n(E) \in [0,1]$. If we invert $P$, we have

$$P^{-1} = \frac{1}{4} \Gamma_L^{-1/2}(E - H + \Sigma^*) \Gamma_R^{-1}(E - H + \Sigma) \Gamma_L^{-1/2}.$$ (17)

and the eigenvalues of $P^{-1}$ are $\rho_n^{-1}$. Consequently, we can compute the transmission and hence current by summing the eigenvalues of the $P$-matrix which we can construct directly from $H$. Any singularity which may be present in the Greens function no longer presents a problem when performing the energy integration in the Landauer-Büttiker equation.

In practice, there is usually only one low-lying eigenvalue of the $P^{-1}$ matrix and this eigenvalue is typically on the order of unity. The remaining eigenvalues are typically on the order of $10^7$ greater than the lowest eigenvalue. Consequently, we can use matrix diagonalization techniques optimized for finding isolated eigenvalues. Since only the lowest eigenvalue of $P^{-1}$ contributes to $Tr[P]$ to any significant extent, once this eigenvalue has been determined, we do not need to compute the remaining eigenvalues. Furthermore, for determining $N(E)$, we do not need to compute the eigenvectors of $P^{-1}$. Since computing $P^{-1}$ and its lowest eigenvalue involves simple matrix-vector manipulations, these tasks can be efficiently performed on a parallel computer. Also, the method is universal and can be used to compute transmission through any model system given model Hamiltonian and a self-energy representing the coupling of the model system to a continuum.

One final comment regarding implementation of the Manthe-Miller algorithm is that as expressed $P$ is a singular matrix if $\Gamma_L$ and $\Gamma_R$ are localized to finite region and cannot be formally inverted. To remedy this, we allow the absorbing potential to be very small in regions outside the absorbing region $\Gamma_{L,R} = \eta$. Typically, we set $\eta$ to be between $10^{-7}$ to $10^{-10}eV$.

D. Transmission through peptide chains

We considered transmission through four model sequences as shown in Fig. [1]. Furthermore, to explore the effect of intra- vs. interchain transmission we considered three possible contact scenarios between the chain and the electrode surfaces. In the first case, the terminal sites on both chains are connected directly to the cluster surfaces. In this case, hole injection and extraction occurs through both chains and can lead to destructive and constructive interferences as in a two-slit experiment. Secondly, we considered the case where only one chain, the one with the terminal G sites, is directly connected to the clusters. Here, the second chain acts as a hole acceptor and one expects to see only resonances coming from the intra-chain scattering pathways. Lastly, we consider the case where one chain is connected to each cluster and the chains are connected by their complementary base pairs. This scenario has a potential technological ramifications in designing current probes which bind only to specific complementary sequences on the opposite cluster surface. In this case, current through the DNA must occur via interchain hops. This we expect to be quite weak, given that the interchain hopping matrix elements are roughly
an order of magnitude less than the intrachain hopping matrix elements.

The corresponding transmissions through each sequence is shown in Fig. 3. In the black curves plotted in Fig. 3A through D, both terminal G-C units are “connected” to the left and right metal clusters through transfer integral terms. In this case, current can result via transfer through both opposing chains. The interchain hopping leads to constructive and destructive interferences between the two current pathways. In the red curves plotted in Fig. 3A through D we consider the case in which only the terminal G sites are capable of transferring holes between the contacts and the chain. Here, loosely speaking, scattering interferences can occur when the hole hops from the initial chain to the second and back to the first. Since this process is also present in the dual contact cases, we can distinguish purely intrachain processes from multi-chain scattering processes by identifying peaks present in both spectra.

In cases A and B we compare a $-A-A-$ bridge to a $-T-T-$ bridge. In both cases, there is a weak broad resonance at $E = 0$. However, the primary effect is to switch the order of the single resonance at $E = 0.8\,eV$ with the cluster of three resonances at $E = 0.5\,eV$. It is also interesting to note that the gap between the single resonance and the cluster is almost unchanged by the switch. Comparing the dual contact transmission to the single contact transmission, we note that the single resonance peak is present in both in the single and dual contact cases and that two of the three resonances in the cluster about $E = 0.5\,eV$ are present in the single contact case. For B the resonance at $E \approx 0.4\,eV$ is present in both cases; however, in the single contact case, only one of the three corresponding resonances peaks from the dual contact case is present. In both A and B, the weak resonance at $E = 0\,eV$ disappears when there is only a single contact.

In case C we have a $-T-A-$ linkage and we can see clearly three resonance peaks, a doublet centered at 0.4 eV and a single peak at 0.7 eV. In each of these cases, the corresponding eigenstate of the isolated molecular Hamiltonian is a delocalized interchain state. The other eigenstates are more or less localized to one chain or the other and do not extend fully across the bridge. Changing the DNA-metal contact so that only the terminal G’s are connected profoundly diminishes the intensity of each transmission resonance. Consequently, for the case of $-T-A-$ linkages, interchain pathways appear to play an important role. In case D, we transpose the linkage in case C to $-A-T-$, here, we observe the same resonance peaks as in case C, except with uniformly greater intensity even when we change the nature of the DNA-metal contact.

Next, we consider the sensitivity of the transmission to interchain fluctuations. Within our model, the interchain hopping terms represent the tunneling splitting between two neighboring interchain sites. Since tunneling is highly sensitive to distance of separation, structural fluctuations should have a profound effect on the ability of a hole to tunnel between the chains. Such fluctuations can be included in the present model by sampling the interchain hopping matrix elements from a normal distribution centered about some average value. For the blue curves, we allowed each off-diagonal interchain term to fluctuate about its average value by $\sigma = 0.01\,eV$ and then sampled over an ensemble of 100 configurations. Comparing the blue and red curves in Fig. 3A, the narrow resonance at $0.4\,eV$ is more or less washed out entirely by the interchain fluctuations. On the other hand, the two other resonances are clearly present in both the static case and in the fluctuating case indicating that at least some of the resonance features are insensitive to interchain fluctuations. These surviving resonances are certainly due to intrachain transmission. For the other three cases, the main resonance features are more or less unaffected by the interchain fluctuations.

In the last case, we connect one strand to the left contact and the complimentary strand on the other such that current can only pass through the sequence through interchain hopping. Such a scenario could be useful in developing a sequence specific probe since current can only flow if the complementary strands match. Unfortunately, however, our calculations indicate essentially zero
transmission through any of the strand combinations considered above. This is somewhat surprising considering that in each case at least one eigenstate of the isolated chain Hamiltonians are delocalized over the entire chain and have some appreciable amplitude on both of the terminal contact sites.

III. DISCUSSION

These results are both encouraging and discouraging for the potential utility of using current/voltage probes to assay sequence. They are encouraging since clearly sequence has a very profound impact on the hole transmission probability. If one assumes that a given chain can be decomposed into a series of A-T potential barriers separated by a series of G’s and that net transmission probability through the chain can computes as the product as a series of incoherent transition probabilities at a given energy, one could effectively engineer a DNA wire with specific voltage turn-on characteristics. For instance, having paired -A-A- or -T-T- sections as in

\[
5' - G - A - A - G - \cdots - G - T - T - G - 3' \]

would lead to a turn-on voltage of about 0.4 eV since both chain segments A and B have a series of resonances starting at this energy. Placing a -G-T-A-G- segment on the chain as in

\[
5' - G - A - A - G - G - T - A - G - G - T - T - G - 3' \]

would lead to a slightly higher turn-on voltage since the transmission probability for the -G-T-A-G- (sequence D) has a series of resonance peaks at \( \approx 0.45 \) eV and this is in the middle of the cluster of resonances for sequences A and B. Moreover, transposing the A and T to -G-A-T-G- (sequence C) as in

\[
5' - G - A - A - G - G - A - T - G - G - T - T - G - 3' \]

will result in a similar turn-on voltage for the current, however, the current will be roughly half that of when we have -G-T-A-G-.

What is also surprising is that the transmission is dominated by intrachain transport rather than a combination of intra- and interchain hopping. This is surprising given that the interchain hopping terms generally less positive then the intra-chain hopping matrix elements. A positive hopping term between sites implies that the lower energy eigenstates will be the more localized than the higher energy states. The greater the hopping term, the more localized the lower energy states become. This is the opposite case from conjugated polyenes where the hopping term is negative leading delocalized low energy states and resonance stabilization. Consequently, the delocalized interchain states should be lower in energy than the delocalized intrachain states. The problem then is that they are insufficiently delocalized over the chain to provide a conduit from one end of the bridging molecule to the other.

Finally, we note that the transmission only occurs above a certain threshold energy determined by the scattering resonances of the bridging system. Equally important is density of available states in the regions on ether side of DNA bridge. Here, we took the contacts to be three-dimensional simple-cubic solids with a fairly high density of states in the energies considered. However, in a real DNA molecular wire, the bridging region is more like

\[
5' - G - \cdots - G - (\text{bridge}) - G - \cdots - G - 3' \]

and one should use a sequence of G’s in building the density of states and the self-energies. If we consider a sequence of \( 5' - G - \cdots - G - \) to be a quasi-one dimensional chain with hopping integral \( \gamma \) between neighboring sites, then the dispersion relation for the chain is simply

\[
\epsilon_k = 2\gamma \cos(k) \]

with \( k \) in units of \( h/2a \) and \( a \) being the lattice spacing. Consequently, if the bandwidth \( 2\gamma \) is less than the resonance energy of the bridge, the transmission through the bridge will not occur since the density of incoming states at that energy is zero. On the other hand, if \( \gamma \) is large, and one has a wide band for the holes in the guanine chains, then transmission through the bridge can occur. This suggests that the conductivity properties of a DNA chain are highly dependent upon both the base-pair sequence of the DNA chain and the mobility of holes between neighboring G sites.

Acknowledgments

This work was supported by the National Science Foundation and the Robert Welch Foundation. I also wish to acknowledge conversations with Prof. B. M. Pettitt concerning electronic transport in DNA sequences.

[1] V. D. Lakhno, V. B. Sultanov, and B. M. Pettitt, (preprint)
[2] V. D. Lakhno and N. S. Fialko, JETP Lett. 78 336 (2003).
[3] M. Bixon and J. Jortner, J. Phys. Chem. B 104, 3906 (2000).
[4] M. Bixon, B. Giese, S. Wessely, T. Langenbacher, M. E. Michel-Beyerle, and J. Jortner, Proc. Nat. Acad. Sci.
USA 96, 61 (1999).

[5] A. A. Voityuk, J. Jortner, M. Bixon, and N Rösch. J. Chem. Phys. 114, 5614 (2001).

[6] F. C. Grozema, Y. A. Berin, and L. D. A. Siebbeles, Int. J. Quant. Chem. 75, 1009 (1999)

[7] F. C. Grozema, Y. A. Berin, and L. D. A. Siebbeles, J. Am. Chem. Soc. 112, 10903 (2000).

[8] J. Jortner, M. Bixon, A. A. Voityuk, and N Rösch. J. Chem. Phys. 114, 5614 (2001).

[9] F. C. Grozema, Y. A. Berin, and L. D. A. Siebbeles, J. Am. Chem. Soc. 112, 10903 (2000).

[10] J. Jortner, M. Bixon, A. A. Voityuk, and N Rösch, J. Phys. Chem. B 106, 7599 (2002).

[11] C. Dekker and M. A. Ratner, Phys. World, 14, 29 (2001).

[12] E. Braun, Y. Eichen, U. Sivan, and G. Ben-Yoseph, Nature (London) 391, 775 (1998).

[13] P. J. de Pablo, F. Moreno-Herrero, J. Colchero, J. Gómez Herrero, A. M. Bar, P. Prdjón, J. M. Soler, and E. Artacho, Phys. Rev. Lett. 85, 4992 (2000).

[14] A. J. Storm, J. van Noort, S. de Vries, and C. Dekker, Appl. Phys. Lett. 79, 3881 (2001).

[15] Y. Zhang, R. H. Austin, J. Kraeft, E. C. Cox, and N. P. Ong, Phys. Rev. Lett. 89, 198102 (2002).

[16] D. Porath, A. Bezryadin, S. De Vries, and C. Decker, Nature (London) 403, 635 (2000).

[17] A. Rakitin, P. Aich, C. Papadopoulos, Y. Kobzar, A. S. Vedeneev, J. S. Lee, and J. M. Xu, Phys. Rev. Lett. 86, 3670 (2001).

[18] H. W. Fink and C. Schönenberger, Nature (London), 398, 407 (1999)

[19] L. Cai, H. Tabata, and T. Kawai, Appl. Phys. Lett. 77, 3105 (2000).

[20] P. Tran, B. Alavi, and G. Grüner, Phys. Rev. Lett. 85, 1564 (2000).

[21] K.-H. Yoo, D. H. Ha, J.-O. Lee, J. W. Park, J. Kim, J. J. Kim, H.-Y. Lee, T. Kawai, and H. Y. Choi, Phys. Rev. Lett. 87, 198102 (2001).

[22] B. Hartzel, B. McCord, D. Asare, H. Chen, J. J. Heremans, and V. Sogomonian, Appl. Phys. Lett. 82, 4800 (2003).

[23] B. Hartzel, B. McCord, D. Asare, H. Chen, J. J. Heremans, and V. Sogomonian, J. Appl. Phys. 94, 2764 (2003).

[24] Y. A. Kasumov, M. Kociak, S. Gueron, B. Ruelet, and V. T. Volkov, Science 291, 280 (2001).

[25] R. G. Endres, D. L. Cox, and R. R. P. Singh, Rev. Mod. Phys. 76, 195 (2004).

[26] M. Ernzerhof and M. Zhuang, J. Chem. Phys. 119, 4134 (2003).

[27] E. G. Emberly and G. Kirczenow, Phys. Rev B 64, 235412 (2001).

[28] X. G. Zhang, P. S. Krstic, and W. H. Butler, Int. J. Quant. Chem. 95, 394 (2003).

[29] A. Nitzan, Annual Reviews of Phys. Chem. 52, 681 (2001).

[30] A. Nitzan and M. A. Ratner, Science 300, 1384 (2003).

[31] V. Mujica, M. Kemp, and M. Ratner, J. Chem. Phys. 101, 6849 (1994).

[32] V. Mujica, M. Kemp, A. Roitberg and M. Ratner, J. Chem. Phys. 104, 7296 (1996).

[33] Electronic transport in mesoscopic systems, S. Datta (Cambridge Univ. Press, New York, 1995).

[34] Electrical transport through individual DNA molecules. Xin-Qi Li and YiJing Yan Appl. Phys. Lett. 79, 2190 (2001).

[35] P. A. Derosa and J. M. Seminario, J. Phys. Chem. B 105, 471 (2001).

[36] P. Damle, A. W. Ghosh, and S. Datta, J. Phys. Chem. B 106, 7599 (2002).

[37] M. Brandbyge, J. L. Mozos, P. Prdejon, and K. Stockbro, Phys. Rev. B 65, 165401 (2002).

[38] P. S. Krstic, X. G. Zhang, and W. H. Butler, Phys. Rev. B 66, 205319 (2002).

[39] S. Datta, W. Tian, S. Hong, R. Reifenberger, J. I. Henderson, and C. P. Kubiak, Phys. Rev. Lett. 79, 2530 (1997).

[40] R. Landauer, IMB J. Res. Dev. 1, 233 (1957); R. Philos. Mag. 21, 863 (1970).

[41] M. Buttiker Phys. Rev. Lett. 57, 1761 (1986).

[42] S. Roche, Phys. Rev. Lett. 91, 108101 (2003)

[43] S. Roche, D. Bicout, E. Maciá and E. Kats, Phys. Rev. Lett. 91, 228101 (2003).

[44] U. Manthe and W. H. Miller, J. Chem. Phys. 99, 3411 (1993).

[45] Quantum Collision Theory, C. J. Joachain (North-Holland, Amsterdam, 1975).

[46] C. Caroli, R. Combescot, P. Nozieres, D. Saint-James, J. Phys. C 4, 916 (1971).

[47] T. Seideman and W. H. Miller, J. Chem. Phys. 96, 4412 (1992).