

Electron transport through SWNT/*trans*-PA/ SWNT structure (the role of solitons): A t-matrix technique

S A KETABI¹, H MILANI MOGHADDAM^{2,3} and N SHAHTAHMASEBI²

¹School of Physics, Damghan University of Basic Sciences, Damghan, Iran

²Department of Physics and Center for Nanotechnology Researches, Ferdowsi University of Mashhad, Mashhad, Iran

³Department of Physics, University of Mazandaran, Babolsar, Iran

E-mail: saketabi@dubs.ac.ir; saketabi@yahoo.com

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Abstract. Using a tight-binding model and a transfer-matrix technique, we numerically investigate the effects of the coupling strength and the role of solitons on the electronic transmission through a system in which *trans*-polyacetylene (*trans*-PA) molecule is sandwiched between two semi-infinite single-walled carbon nanotubes (SWNT). We rely on Landauer formalism as the basis for studying the conductance properties of this system. Our calculations show that the solitons play an important role in the response of this system causing a large enhancement in the conductance. Also our results suggest that the conductance is sensitive to the CNT/molecule coupling strength.

Keywords. *Trans*-polyacetylene; t-matrix; carbon nanotube; electronic transmission; soliton.

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1. Introduction

Substantial progress has been made on the rapidly developing field of molecular scale electronics [1–4]. The study of electron transport in nanoscale molecular devices has become the center of attraction of the theoretical and experimental researches in recent years [5–8]. This is due to the wide applications of these systems in the nano and molecular electronics and also fundamental importance of the electronic structure in the low-dimensional structures [9,10]. The typical systems considered are usually organic or polymer molecules sandwiched between two electrodes. The current flowing through this molecular device is mainly affected by (i) the quantum nature of molecular states in these systems, (ii) electronic properties of the electrodes near the Fermi energy level, (iii) the strength of the molecule/electrode coupling and (iv) the geometrical structure of the molecule and

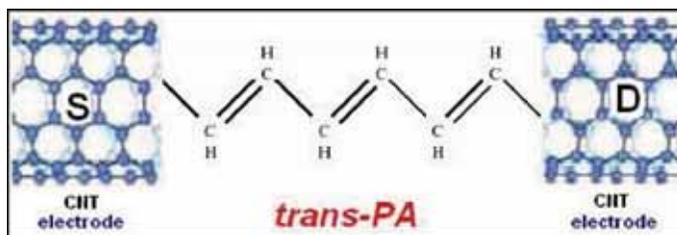


Figure 1. A schematic representation of the CNT/*trans*-PA/CNT structure as described in the text.

electrodes. Doping of conjugated polymers give rise to geometrical defects in their structure. In *trans*-PA these defects are ‘solitons’ and may effectively affect the electronic conduction through the polymer [11]. As a model, we numerically investigate the conductance properties of *trans*-PA molecule in the CNT/*trans*-PA/CNT structure, where the nanocontact is considered as the armchair (l, l) single-walled carbon nanotubes (SWNT). In general, there are M atomic positions over the interfacial end-atoms of the tubes. For an armchair (l, l) SWNT topology imposed, the number of carbon sites at the interface is $M = 2l$. In our model (figure 1) the number of hybridization contacts between a tube and the molecule is set 1 (single contact case). Also it is shown that SWNT may be used as quasi-one-dimensional electrodes to construct CNT/(single)molecule/CNT structure with molecular scale width and channel length, such as single electron molecular transistors [12–14]. Our results suggest that the solitons in *trans*-PA play an important role in enhancing the conductance of the CNT/*trans*-PA/CNT structure. The procedures we have used in this work are based on two powerful numerical methods particularly suitable to treat the electron transmission through the large systems, the Landauer formalism and transfer-matrix (t-matrix) technique, where the solution of the Schrödinger equation is obtained by means of a product of 2×2 matrices. The outline of the paper is as follows: In §2 the methodology to calculate the t-matrices and the transmission coefficient are described. The results and discussion are presented in §3 followed by a summary in §4.

2. Methodology

We use the following generalized Hamiltonian for the description of the CNT/molecule/CNT structure:

$$H = H_{\text{CNT}} + H_{\text{SSH}} + H_{\text{C}}, \quad (1)$$

where H_{CNT} , H_{SSH} and H_{C} describe the semi-infinite CNT nanocontacts, the well-known SSH Hamiltonian [11] for the *trans*-PA molecule and the couplings of the contacts to the molecule, respectively. The SWNT is modeled within the tight-binding Hamiltonian with only one π -orbital per atom [15,16]. This Hamiltonian can describe reasonably well the band structure of a nanotube especially near the Fermi level which is zero in this case since the on-site energy is assumed to be zero and each orbital is half-filled,

$$H_{\text{CNT}} = \sum_j \varepsilon_j c_j^\dagger c_j - \sum_j t_{j+1,j} (c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}), \quad (2)$$

where $c_j (c_j^\dagger)$ is the annihilation(creation) operator of an electron at the j th site. For the semi-infinite CNT contacts we set $\varepsilon_j = \varepsilon_0$ for all j and $t_{j,j\pm 1} = t_{\text{CNT}}$ between all j and $j \pm 1$ for the nearest-neighbor hoppings. The electronic part of H_{SSH} is given as follows [17]:

$$H_{\text{SSH}} = - \sum_n t_{n+1,n} (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}), \quad (3)$$

in which $t_{n+1,n}$ is the nearest-neighbor transfer integral and is given as

$$t_{n+1,n} = t_0 + \alpha(u_n - u_{n+1}), \quad (4)$$

where t_0 is the hopping integral of an undimerized chain, α is the electron-phonon coupling constant and u_n is the displacement of the n th carbon atom from its equilibrium position. The reference energy is chosen such that the carbon atom on-site energy is zero. For perfectly dimerized *trans*-PA, u_n and bandgap are given as $u_n = (-1)^n u_0$ and $2\Delta_0 = 8\alpha u_0$, respectively. Throughout this study for $2\Delta_0 = 1.4$ eV, we shall use the parameters of ref. [11], so $\alpha = 4.1$ eV/Å and $t_0 = 2.5$ eV. These correspond to an equilibrium dimerization amplitude $u_0 \approx 0.04$ Å.

In *trans*-polyacetylene a soliton corresponds to a phonon field configuration that minimizes the total energy. In the presence of solitons the displacements of carbon atoms are determined in such a way to minimize the total energy and to give optimum shape for the soliton. Accordingly, the displacements of the carbon atoms are modeled as [18,19]

$$u_n = (-1)^n u_0 \prod_m \tanh \left[\frac{(n-m)a}{\xi} \right], \quad (5)$$

where $2\xi \cong 14a$, with $a = 1.22$ Å (lattice constant), is the width of a soliton, ma is the location of the m th soliton center on the chain. Finally H_C is given as

$$H_C = -t_C (c_L^\dagger c_1 + c_1^\dagger c_L + c_R^\dagger c_N + c_N^\dagger c_R). \quad (6)$$

We consider a *trans*-PA molecule with $N = 56$ carbon atoms and with one state per site. In eq. (6), t_C denotes the interaction between single electron state $1(N)$ in *trans*-PA molecule and the electron state in the left (L) and right (R) electrodes, respectively. Here we present a short description of the t-matrix technique and Landauer formalism which we have applied to calculate the electronic transmission through the CNT/*trans*-PA/CNT structure. Let us start by considering a general Hamiltonian as

$$H = \sum_i (|i\rangle \varepsilon_i \langle i| + t_{i,i+1} |i\rangle \langle i+1| + t_{i,i-1} |i\rangle \langle i-1|), \quad (7)$$

where ε_i is the on-site energy of the site i and $t_{i,i\pm 1}$ are the nearest-neighbor hopping integrals between the sites i and $i \pm 1$. The electronic properties of this system is then studied through the following Schrödinger equation:

$$t_{i,i-1}\psi_{i-1} + (\varepsilon_i - E)\psi_i + t_{i,i+1}\psi_{i+1} = 0, \quad (8)$$

where ψ_i is the probability amplitude at site i . Solving for ψ_{i+1} we find the t-matrix formulation as

$$\begin{pmatrix} \psi_{i+1} \\ \psi_i \end{pmatrix} = \begin{pmatrix} \frac{E-\varepsilon_i}{t_{i,i+1}} & -\frac{t_{i,i-1}}{t_{i,i+1}} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_i \\ \psi_{i-1} \end{pmatrix} = M_i(E) \begin{pmatrix} \psi_i \\ \psi_{i-1} \end{pmatrix}, \quad (9)$$

where $M_i(E)$ is the local t-matrix associated with site i . Defining $U_i = \begin{pmatrix} \psi_i \\ \psi_{i-1} \end{pmatrix}$ and $M(E) = \prod_{i=1}^N M_i(E)$ as the global t-matrix of the system, eq. (9) is generalized as follows:

$$\begin{pmatrix} \psi_{N+1} \\ \psi_N \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = \prod_{i=1}^N M_i(E) \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}, \quad (10)$$

where

$$M(E) = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}. \quad (11)$$

We see that t-matrices depend on energy E . If the eigenenergies and U_1 are known, then all the eigenfunctions will easily be calculated from the t-matrices. Now, we proceed to calculate the transmission coefficient $T(E)$, whose magnitude is directly related to the conductance through the Büttiker–Landauer formula [20],

$$G = \frac{2e^2}{h} T(E). \quad (12)$$

In the absence of non-coherent elastic transport [21], inelastic scattering and electron–electron correlations, Landauer theory provides a general framework for calculations of the electronic current through mesoscopic conductors coupled to single or multi-channel quasi-one-dimensional leads. It relates the electronic current to the transmission probability for an electron incident from the source lead scattered elastically through the conductor into the drain. By connecting the *trans*-PA molecule to two semi-infinite carbon nanotubes, then $T(E)$ is identical to the probability that an incident electron with energy E in the left-hand CNT emerges in the right-hand one. Using eq. (10), the transmission coefficient is given by [22–24]

$$T(q) = \frac{4(1 - q^2)}{(Z + qY)^2 + (1 - q^2)X^2}, \quad (13)$$

where the dimensionless parameters q , X , Y and Z are given as follows:

$$\begin{aligned} q &= 1 - \frac{E}{2t_{\text{CNT}}}; \quad X = m_{22} + m_{11}; \\ Y &= m_{22} - m_{11}; \quad Z = m_{21} - m_{12}. \end{aligned} \quad (14)$$

$t_{\text{CNT}} = 3 \text{ eV}$ is the hopping integral of semi-infinite CNTs and $m_{ij}(i, j = 1, 2)$ are the matrix elements of the global t-matrix, $M(E)$ of the system.

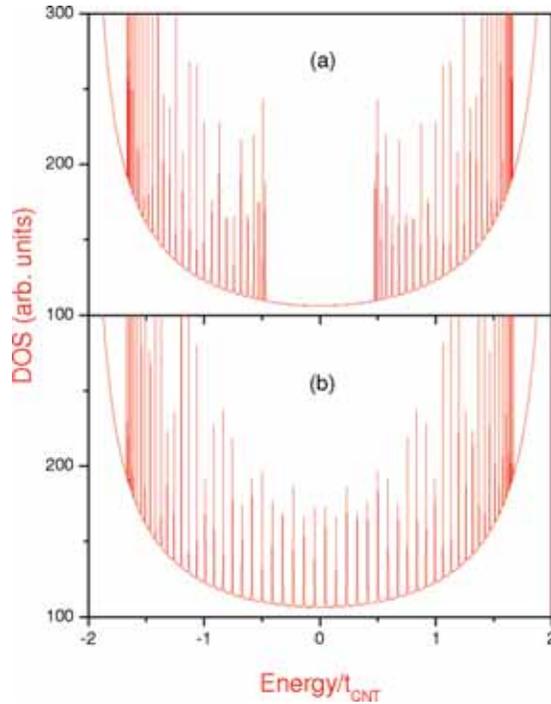


Figure 2. A plot of the electronic DOS vs. the dimensionless parameter $\text{Energy}/t_{\text{CNT}}$ for the CNT/*trans*-PA/CNT system with the parameters of $t_{\text{CNT}} = 3$ eV and $t_C = 0.3$ eV as described in the text. Plots (a) and (b) show the results for the *trans*-PA molecule with $N = 56$ carbon atoms without soliton and with three solitons, respectively.

3. Results and discussion

Based on the formalism described in §2, we have investigated the electronic conduction properties of CNT/*trans*-PA/CNT structure in the presence of solitons. Figure 2 illustrates the electronic density of states (DOS) of the CNT/*trans*-PA/CNT system in the absence and in the presence of solitons (see panels (a) and (b), respectively). The plots show that the presence of solitons induces electronic states within the bandgap and causes a large enhancement in the conductance of the system. In figure 3 the conductance of the system is shown which corresponds to figure 2. In these figures the strength of CNT/*trans*-PA coupling is fixed. Similar calculations were performed for the system with different values of t_C , and the results are shown in figure 4. This plot suggests that any increase in t_C considerably enhances the conductance of the system. Also the order parameter $\varphi_n = -(-1)^n u_0$ for three solitons in *trans*-PA molecule is shown in figure 5. For a fully dimerized chain $u_n = (-1)^n u_0$, with $u_0 \approx 0.04$ Å and for doped samples, in the presence of solitons, u_n is given by eq. (5). The order parameter is an easy way to observe different soliton distributions along the *trans*-PA chains, since $\varphi_n = 0$ means a soliton has been located at the n th site.

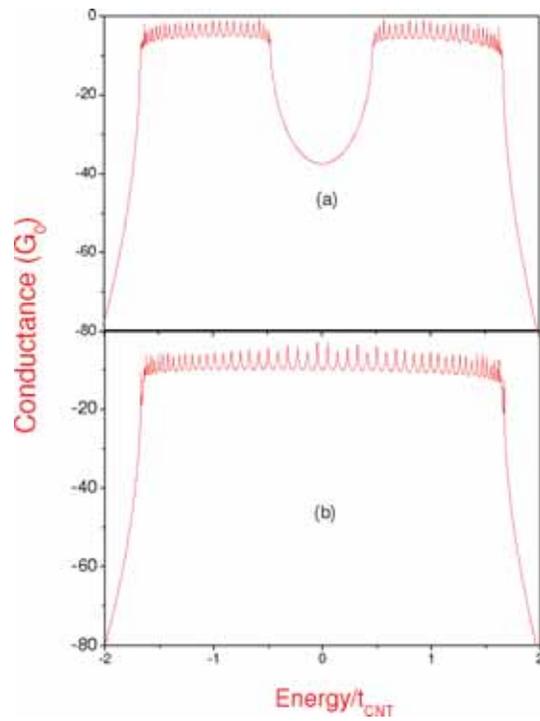


Figure 3. The logarithm of conductance in units of G_0 vs. the dimensionless parameter $\text{Energy}/t_{\text{CNT}}$ for the CNT/*trans*-PA/CNT structure with $t_{\text{CNT}} = 3$ eV and $t_C = 0.3$ eV. Plots (a) and (b) show the results for the *trans*-PA molecule with $N = 56$ carbon atoms without soliton and with three solitons, respectively.

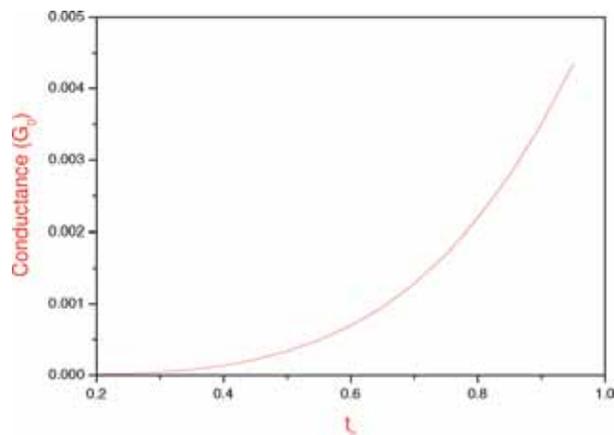


Figure 4. Conductance in units of G_0 vs. t_C , the CNT/molecule coupling strength for the CNT/*trans*-PA/CNT structure with $t_{\text{CNT}} = 3$ eV, $N = 56$ carbon atoms and three solitons.

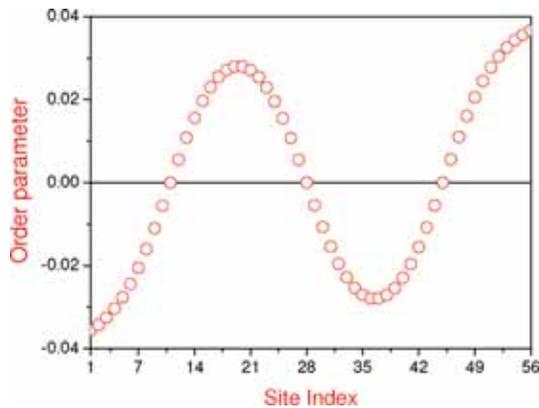


Figure 5. Order parameter, φ_n , for *trans*-PA molecule with $N = 56$ carbon atoms and three solitons.

4. Summary

In brief, we have studied in details the role of solitons and the CNT/molecule coupling strength on the conductance in the CNT/*trans*-PA/CNT structure. We have applied some well-known numerical procedures and models such as transfer-matrix technique, Landauer formalism as well as SSH Hamiltonian model to investigate the electron conduction through the CNT/*trans*-PA/CNT structure. Our results show that (i) the presence of solitons induces electronic states within the bandgap which give rise to large enhancement in the conductance and (ii) the conductance is sensitive to the CNT/*trans*-PA coupling, i.e., any increase in t_C considerably increases the conductance of the system.

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