Resonant Tunneling In Graphene-DNA Base-Graphene Junctions

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Abstract. The current-voltage characteristics in electrode-DNA-electrode system are calculated for three types of graphene electrodes: a monolayer, AA and AB bilayers. We found that AA bilayer electrodes provide higher currents in comparison with both graphene monolayer and AB bilayer thus making this material more favourable for fabrication of DNA base sequencing devices.

The electronic circuit consisting of two electrodes with molecule (quantum dot) accommodated between them (see figure 1) is the simplest object of molecular electronics which allows one to design such important devices as rectifiers [1], switches, transistors [2], and sensors [3]. Moreover, similar systems lie in the base of a new rapid and low-cost methods for whole-genome analysis where specific physical and electronic properties of DNA nucleotides are monitored. Recently, such DNA sequencing approach has been proposed by Zwolak and DiVentra [4]. According to this method gold electrodes are embedded within solid-state nanopore to measure the transverse current through single-strand DNA-molecule as it pulls through the pore by a voltage applied in parallel to DNA backbone axis. It has been suggested that the use of atomically thin graphene electrodes with planar geometry is able to essentially boost productivity of both DNA sequencing device [5] and an elementary device of molecular electronics [6] in comparison with the metallic ones. In both types of devices the productivity is defined by effectiveness of electron transport which in turn depends on electronic properties of junctions [7].

In this paper, we compare the transport properties of electrode-quantum dot-electrode device for three types of graphene electrodes: monolayer, AA bilayer, and AB bilayer. To this end, current-voltage characteristics of these devices are studied. A quantum dot in our system acts as an object with electronic properties similar to a certain DNA nucleotide. The current-voltage characteristics are calculated within the extended method of independent channels which was earlier used for description of field emission from AAA graphite, nanotubes, and few-layer (AB and ABC) graphene [8, 9, 10].

We assume that contacts have macroscopic sizes while a quantum dot is an atomic scale object. The total current is defined as the difference between the tunneling currents from the left and right electrodes in the form

\[ I = I_L - I_R = \frac{2e}{h} \int_{-\infty}^{+\infty} [f_L(\varepsilon) - f_R(\varepsilon)]D^{LR}(\varepsilon)d\varepsilon, \]

(1)
where \( I_{L,R} = \int d\varepsilon f_{L,R}(\varepsilon)D^{LR}_{\varepsilon} \) are currents from the left and right electrodes, respectively, \( f_{L,R} = f(\varepsilon \mp V/2) \), \( V \) is a bias voltage, \( f(\varepsilon) \) is the Fermi-Dirac distribution function, and \( D^{LR}_{\varepsilon} \) is the transmission probability of an electron through a potential barrier.

The transmission probability is written as [11]

\[
D^{LR}_{\varepsilon} = \frac{D_{L,R} D_{R}}{1 - 2 \sqrt{R_{L,R}} \cos \theta + R_{L,R}}
\]

with \( \theta \) being a phase shift acquired in one round-trip between the scatterers, and \( R_{L,R} = 1 - D_{L,R} \). \( D^{LR}_{\varepsilon} \) can be expressed as a sum over modes (channels) at given energy \( n_{L,R}(\varepsilon) \) normalized by the total number of channels \( N_{L,R} \). Such normalization condition follows from the sum rule [11]. One gets

\[
D_{L,R}(\varepsilon) = P(\varepsilon)D_{L,R}(\varepsilon),
\]

where \( D_{L,R} \) is the transmission probability for one channel and \( P(\varepsilon) = n_{L,R}(\varepsilon)/N_{L,R} \). Here we assume that \( D_{L,R} \) does not depend on a type of the channel. Indeed, within the framework of the WKB approximation \( D_{L,R} \) depends only on a shape of the barrier and a distance between the vacuum energy level and given energy.

Let us consider a case of a single resonant level. This approximation can be used for low bias voltage (less than 0.5 V) because a distance between nearest levels in noninteracting DNA base is of an order of 1 eV (see [12]). Assuming that \( R_{L,R} \approx 1 \), one can rewrite (2) via the Breit-Wigner formula

\[
D^{LR}_{\varepsilon} = \frac{\Gamma_{L}\Gamma_{R}}{(\varepsilon - \varepsilon_{r})^{2} + \left(\frac{\Gamma_{L} + \Gamma_{R}}{2}\right)^{2}},
\]

where \( \Gamma_{L,R}/h = \nu D_{L,R} \) and \( \nu \) is an attempt frequency [11]. Finally, the tunneling current through a single resonant level is written as

\[
I = \frac{2e}{h} \int_{-\infty}^{\infty} \frac{\Gamma_{L}(\varepsilon - \varepsilon_{r} - V/2)\Gamma_{R}(\varepsilon - \varepsilon_{r} + V/2)}{(\varepsilon - \varepsilon_{r})^{2} + (\Gamma(\varepsilon)/2)^{2}}(f_{L}(\varepsilon) - f_{R}(\varepsilon))d\varepsilon,
\]

where \( \Gamma(\varepsilon) = \Gamma_{L}(\varepsilon - \varepsilon_{r} - V/2) + \Gamma_{R}(\varepsilon - \varepsilon_{r} + V/2) \). Notice that the same result can be obtained by using of either the sequential model or non-equilibrium Green function formalism [7, 13, 14].
Let the dot be located near the armchair edge. In this case, the localised edge states do not appear\ [15] and the channel density can be written as $P(\varepsilon) = 2a_0\Delta p_y(\varepsilon)/\hbar$ with $2\Delta p_y(\varepsilon)$ being a “shadow” of the constant energy line on a plane normal to the tunneling direction in the momentum space\ [9, 16], and $a_0$ the interatomic distance. One has

$$\Gamma_{L,R} = \frac{a_0\Delta p_y(\varepsilon)}{\pi} \nu D_{L,R}. \quad (6)$$

Our numerical calculations are based on (5) and (6). The difference between the resonant level and the Fermi energy of contacts is estimated as $\varepsilon_F - \varepsilon_r = \phi - A \equiv \Delta$, where $A$ is an electron affinity of the DNA base. Thus, we have equated vacuum levels of DNA and the contact. In accordance with\ [12] $|\Delta| \approx 0.1$ eV for all DNA bases. We apply the WKB-type approximation for the transmission probability

$$D = \exp[-\lambda(d - d_0)], \quad \lambda = -\frac{2\sqrt{2m\phi}}{\hbar} \quad (7)$$

with the work function $\phi = 4.7$ eV, $\lambda = 0.22$ nm$^{-1}$, and $d_0 = 0.135$ nm being a typical covalent bond length. One has $\hbar \nu \approx \hbar^2/(2md_0^2N)$ where $N$ is a number of atoms in a DNA base having $p_z$ electrons ($N$ is taken to be equal to ten in average), so that $\nu \sim 10^{14}$ s$^{-1}$.

The ”shadows” for graphene can be calculated as

$$\Delta p_y^A(\varepsilon) = 2\varepsilon/\nu_F, \quad (8)$$

$$\Delta p_y^{AB}(\varepsilon) = \frac{\sqrt{|\varepsilon|(|\varepsilon| + \gamma_1)} + \theta(|\varepsilon| - \gamma_1)\sqrt{|\varepsilon|(|\varepsilon| - \gamma_1)}}{\nu_F}, \quad (9)$$

$$\Delta p_y^{AA}(\varepsilon) = \frac{|\varepsilon - \alpha_1| + |\varepsilon + \alpha_1|}{\nu_F}. \quad (10)$$

We assume that $\gamma_1 = \alpha_1 = 0.4$ eV, $d_L = d_R = 2d_0$, and $a_0 = 0.142$ nm. The results are shown in figures 2-5.

The current-voltage (I-V) characteristics for three types of electrodes are presented in figure 2. Figure 4 illustrates a smoothing role of the temperature factor. Notice that all curves are symmetric, nonlinear and have a step-like behaviour. As is seen from figure 3, at low voltage ($V < 2|\Delta|$) the current for AA bilayer grows more intensively in contrast to other electrodes. This finding can be explained by the energy dependence of the ratios $\Gamma$ for different electrodes (see figure 5). Indeed, both $\Gamma^A$ and $\Gamma^{AB}$ grow with energy and have a similar behaviour while $\Gamma^{AA}$ remains a constant up to the point $\gamma_1 = 0.4$ eV and has a bigger. This can be also directly seen from the approximate expression for conductivity in the small voltage limit

$$\sigma = \frac{2e^2}{\hbar} \frac{1}{1 + \Delta^2/\Gamma^2}. \quad (11)$$

At $V > 2|\Delta|$ the curves for the monolayer and AB bilayer increase with the voltage while for AA bilayer the current tends to a saturation value (see figures 2 and 4). The behaviour of tunneling rates in figure 5 clarifies the saturation of the current at $V > 2|\Delta|$ for AA bilayer as well as its absence for graphene monolayer and AB bilayer.

In conclusion, we have calculated the current-voltage characteristics in electrode-quantum dot-electrode system for three types of electrodes: graphene monolayer, AA and AB bilayers. Our analysis shows that at the same bias voltage AA graphene bilayer electrodes provide a higher current in comparison with both graphene monolayer and AB bilayer. This finding can
be explained by the fact that at the Fermi level the density of channels takes a nonzero value for AA bilayers while in AB bilayers and monolayers it tends to zero. Thus, the use of electrodes on the base of AA graphene bilayer is expected to be much more productive in such devices.

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