Contact phenomena in carbon nanotubes

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Abstract

Poor screening of the long-range Coulomb interaction in one-dimensional carbon nanotubes results in a peculiar picture of contact phenomena. Being brought to a contact with a metal, conducting nanotube accumulates electric charge whose density decays slowly with the distance from the contact. This should be contrasted to a conventional metal-metal contact where the charge density decreases exponentially at atomic distances. Implications for experiments are discussed.

Key words: Carbon nanotubes; metal-metal contacts; screening of the Coulomb interaction

The contacts to metallic electrodes play a major role in the study of electron transport in carbon nanotubes. The difference in the work functions of a metal (Au,Pt) and graphite results in the charge transfer between the nanotube and electrodes, which shifts the Fermi level of the nanotube downward from half-filling. Corresponding shift of the Fermi vector $k_F$ away from the band-crossing point $K = 2\pi/3a$ has been detected experimentally in the pattern of standing electron waves in SWNTs on a gold substrate [1].

In conventional metal-metal contacts the charge density induced by a mismatch of the work functions decays within the Thomas-Fermi screening distance ($\sim 0.5$ Å) away from the interface. Despite conducting SWNTs have metallic electronic spectrum, the Coulomb screening is expected to be substantially less effective due to reduced dimensionality of the system. The analysis of contact phenomena in this case is the goal of our work.

For simplicity we assume that conducting electrons in SWNT are confined to the surface of a cylinder of radius $R$. The electrostatic potential $\Phi(R, z) \sim \Phi_q e^{iqz}$ at the surface can be found from the solution of the Poisson equation,

\begin{equation}
\Phi_q = u_q \rho_q, \quad (1)
\end{equation}

where $\rho_q e^{iqz}$ is a linear density of charge, $u_q = 2I_0(qR)K_0(qR)/\kappa$ is a bare Coulomb interaction and $\kappa$ is an effective dielectric constant of the medium. The charge density

\begin{equation}
\rho_q = -e\nu_q W_q \quad (2)
\end{equation}

is related to the total potential $W_q = V_q + e\Phi_q (e > 0)$ induced by the external potential $V_q$ [2].

In the long wave length limit ($q \ll K$) $\nu_q$ is given

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by the single-particle density of states in SWNT, $\nu_q = \nu = 4/(\pi \hbar v_F)$. In this case the total potential $W(z) = -\rho(z)/e\nu$ corresponds to the deviation of the local Fermi level from half-filling. Eqs. 1, 2 determine the response of the system $W_q = V_q/\varepsilon_q$, $\varepsilon_q = 1 + e^2 \nu_q u_q$ to the external potential $V_q$, which will be studied for three situations.

(i) Edge contact. Consider SWNT aligned along $z$ axis ($z > 0$) and contacting the plane $xy$ of a metallic electrode ($z < 0$) at $z = 0$. The difference $V = \varphi_M - \varphi_N$ of the work functions of a metal ($\varphi_M$) and a nanotube ($\varphi_N$) plays a role of the external potential which induces charge at the nanotube. In order to take the image charges into account we introduce $\rho(-z) = -\rho(z)$ ($z > 0$) and modify the external potential accordingly, $V(z) = -V \text{sign}(z)$. As a result we obtain,

$$W(z) = -\frac{V}{\ln(z/R)}, \quad (3)$$

for $z \gg R$ and $g = 2e^2 \nu/\kappa \gg 1$ ($2e^2 \nu \approx 7.4$). Numerical results for moderate values of the interaction are presented in Fig. 1.

(ii) Lateral point contact. We consider SWNT contacted by a small metallic electrode at $z = 0$. The external potential can be approximated by a delta function $V(z) = V_0 \delta(z)$ whose amplitude depends on the microscopic details of the contact ($V_0 \propto V$). The position of the Fermi level at $|z| \gg R$ is given by,

$$W(z) = -\frac{V_0}{2g |z| \ln^2(|z|/R)}, \quad (4)$$

for $g \gg 1$. The same relation with $-V_0/2g \rightarrow e^2/\kappa g^2$ describes screened Coulomb interaction in isolated nanotube. Despite the screened interaction is by a factor $g^2 \gg 1$ weaker than unscreened one, it decays only marginally faster.

(iii) Lateral long contact. Finally we treat SWNT on the surface of a metal. Assuming that the charge is distributed uniformly around the circumference of the cylinder (SWNT) and that the distance $d$ between the cylinder and the metal surface is small $d \ll R$, we modify Eq. 1 as follows, $\Phi = 2\rho d/R$. The "external potential" of the nanotube is fixed at $-V$ (cf. (i)). Using Eq. 2 we obtain $W = V/\varepsilon_l$ with $\varepsilon_l = 1 + 2e^2 \nu d/R$. For a nanotube on gold $V \approx 0.8$ eV [1]. Loosely estimating $d = a \approx 2.46$ Å we obtain the deviation of the Fermi level from half-filling, $W \approx 0.22$ eV for (10,10) SWNT. The agreement with the experimental value $W_{\text{exp}} \approx 0.3$ eV [1] is reasonable, taking into account simplicity of our model.

We conjecture that the shift of the Fermi level from half-filling can be detected in the pattern of Friedel oscillations from impurities or ends of a nanotube.

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References

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