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Charge screening in single-walled armchair carbon nanotubes

У рамках методу випадкової фази отримано квазіодновимірний екранований ефективний потенціал взаємодії для заряджених частинок, що локалізовані на стінці одношарової металевої вуглецевої armchair нанотрубки (ВНТ).

В рамках метода случайной фазы получен квазиодномерный экранированный эффективный потенциал взаимодействия для заряженных частиц, локализованных на стенке однослойной металлической углеродной armchair нанотрубки (УНТ).

The screened effective quasione-dimensional interaction potential for charged particles localized on the wall of a single-walled metallic armchair carbon nanotube (CNT) was obtained within the framework of the random phase approximation (RPA).

Introduction. The single-walled CNT is a strip of the 2D graphite plane rolled up into cylinder. Remind that the 2D graphite plane is composed of hexagons, every vertex of which is the carbon atom. The chirality of CNT is defined by two integer numbers (*n, m*) which specify the 2D co-ordinate of the hexagon imposed on the hexagon located at the origin, when the strip of the 2D graphite layer is rolled up. CNTs with (*n, n*) chirality are the "armchair" CNTs. All the previous works [1-5] clearly assert that armchair CNTs with any chirality numbers have metallic conductivity, that is why here we can use approximations that proper to the theories of metals. However, fundamental results of the theory of metals cannot be applied directly to armchair nanotubes for their one-dimensional structure. At the same time their one-dimensional analogues are of the barest necessity for investigation of optical and transport properties of nanotubes. This note is aimed at derivation of one important result of this kind, namely the derivation of explicit expression for the effective quasione-dimensional potential of charged interstitial defect, which would account the collective effect of dielectric screening of the defect by free electrons of nanotube.

Because of its relatively large length (~1-10 μm) and small diameter (~1-10 *nm*) CNT may be considered as a quasione-dimensional system. So we've used here the Lindhard screening theory (so-called RPA approximation) in one dimension. Then in the limiting case of small wavenumber we have got the Thomas-Fermi screened potential for two charges localized on the wall of tube. The further transverse integration of the obtained expression yields the self-consistent one-dimensional charge-charge interaction potential, which can be used for account of multi-particles effects in CNTs.

1.General form of screened potential

Within the framework of the Lindhard screening theory we consider the one-dimensional Fourier transform of the following Poisson equation for screened electrostatic potential $\varphi(\vec{r})$:

$$\left(q^2 - \Delta_{2D}\right)\varphi\left(q,\vec{r}_{2D}\right) = 4\pi\left(\rho^{ext}\left(q,\vec{r}_{2D}\right) + \rho^{ind}\left(q,\vec{r}_{2D}\right)\right), \qquad (1.1)$$

where $\rho^{ext}(q,\vec{r}_{2D})$ is the one-dimensional Fourier transform along the tube axis of the density of extraneous charge, $\rho^{ind}(q,\vec{r}_{2D})$ is that of the charge density induced by the extraneous charge, q is the longitudial component of wave vector, and $\vec{r}_{2D}$ is the transverse component of the radius-vector. For simplicity we will assume that ρ^{ext} is axial symmetric, $\rho^{ext}(q,\vec{r}_{2D}) = \rho^{ext}(q,r_{2D})$, and localized in the small vicinity of the tube wall. As follows $\varphi(q,\vec{r}_{2D})$, $\rho^{ind}(q,\vec{r}_{2D})$ depend on $\vec{r}_{2D}$ only through r_{2D} and besides whatever the case ρ^{ind} is localized in the small vicinity of the tube walls. The ρ^{ind} may be written as follows:

$$\rho^{ind}(q,r_{2D}) = -e\int_0^L \exp(-iqz)\sum_{ks} f(E_s(k))\left|\psi_{sk}(\vec{r})\right|^2 dz - \rho^0(q,r_{2D}), \tag{1.2}$$

where f is the Fermi-Dirac function, $E_s(k)$ and $\psi_{sk}(\vec{r}) = \exp(ikz)u_{sk}(\vec{r})/\sqrt{N}$ are the band energies and the corresponding Bloch wave functions of π-electrons, ρ^0 is the charge density without extraneous charges and L is the length of CNT. Following the Lindhard method we get the linear in φ approximation for the induced charge density:

$$\rho^{ind}(q,r_{2D}) = -e^2\sum_{ks}\sum_{k's'}\frac{f(E_{s'}(k')) - f(E_s(k))}{E_s(k) - E_{s'}(k')}\times$$
$$\times\int_0^L \frac{1}{N^2}\int_{E_3}\overline{u}_{ks}(\vec{r})u_{k's'}(\vec{r})\varphi(\vec{r})\exp(iz(k'-k))d\vec{r}\ \overline{u}_{k's'}(\vec{r})u_{ks}(\vec{r})\exp(iz(k-k'-q))dz, \tag{1.3}$$

where N is the number of unit cells in CNT and s, s' number π-electrons bands crossed by the Fermi level. Further, writing $\varphi(\vec{r})$ in the form

$$\varphi(\vec{r}) = \frac{1}{L}\sum_q e^{iqz}\varphi(q,r_{2D})$$

and taking into account that the sought potential varies slightly inside the unit cell we get from (1.3) that

$$\rho^{ind}(q,r_{2D}) = -\frac{e^2}{L}\sum_{kss'}\frac{f(E_s(k)) - f(E_{s'}(k-q))}{E_{s'}(k-q) - E_s(k)}\varphi(q,R)B_{ss'}(k,k-q,a)\int_0^a \overline{u}_{k-qs}(z,\vec{r}_{2D})u_{ks'}(z,\vec{r}_{2D})dz, \tag{1.4}$$

where a is the longitudial period of nanotube, R - its radius, and

$$B_{ss'}(k,k-q,a) = \int_{E_2}\int_0^a \overline{u}_{ks'}(z,\vec{r}_{2D})\,u_{k-qs}(z,\vec{r}_{2D})\,dz\,d\vec{r}_{2D}. \tag{1.5}$$

By (1.1)

$$\varphi(q,r_{2D}) = 4\pi\int_{E_2} G_0(q,\vec{r}_{2D},\vec{r}'_{2D})\left(\rho^{ext}(q,r'_{2D}) + \rho^{ind}(q,r'_{2D})\right)\,d\vec{r}'_{2D}, \tag{1.6}$$

where $G_0(q,\vec{r}_{2D},\vec{r}'_{2D})$ is the Green's function for 2D Helmholtz equation,

$$G_0(q,\vec{r}_{2D},\vec{r}'_{2D}) = \frac{1}{2\pi}K_0(|q||\vec{r}_{2D} - \vec{r}'_{2D}|), \tag{1.7}$$

where $K_0(|q||\vec{r}_{2D} - \vec{r}'_{2D}|)$ - the modified Bessel function of the second kind. By our assumptions both the $\rho^{ext}(q,r_{2D})$ and $\rho^{ind}(q,r_{2D})$ are actually localized on the tube wall. Hence, for $r_{2D} = R$ from (1.6) and (1.7) we have

$$\varphi(q,R) = \varphi^{ext}(q,R) + 2K_0(|q|R)I_0(|q|R)\int_{E_2}\rho^{ind}(q,r'_{2D})\,d\vec{r}'_{2D}, \tag{1.8}$$

where $\varphi^{ext}(q,R)$ is the contribution to the Fourier transform of the total potential from ρ^{ext}, and $I_0(|q|R)$ is the modified Bessel function of the first kind. We see from (1.4) and (1.8) that

$$\varphi(q,R) = \frac{\varphi^{ext}(q,R)}{\varepsilon_R(q)},$$
$$\varepsilon_R(q) = 1 + \frac{e^2}{\pi}\sum_{s,s'}\int_{-\pi/a}^{\pi/a}\frac{f(E_s(k)) - f(E_{s'}(k-q))}{E_{s'}(k-q) - E_s(k)}\left|B_{s's}(k,k-q,a)\right|^2 dk\,I_0(|q|R)K_0(|q|R). \tag{1.9}$$

For low and room temperatures the main contributions to (1.9) are made by quasi-momenta from the small vicinity of the Fermi quasi-momentum k_F. Due to the orthogonality and normalization condition of the Bloch function for $k \cong k - q \cong k_F$ we have

$$\left|B_{ss'}(k,k-q,a)\right|^2 \cong \begin{cases} 0 \text{ for } s \neq s', \\ 1 \text{ for } s = s' \end{cases}, \tag{1.10}$$

and, besides with account of spin degeneracy

$$\frac{f(E_s(k)) - f(E_{s'}(k-q))}{E_{s'}(k-q) - E_s(k)} \cong 2\delta(E_{s'}(k) - E_F), \tag{1.11}$$

where $\delta(E_{s'}(k) - E_F)$ is the Dirac delta-function. It follows from (1.9) – (1.11) that

$$\varepsilon_R(q) = 1 + \frac{2e^2}{\pi\hbar}\sum_s \frac{1}{V_s} I_0(|q|R)K_0(|q|R), \tag{1.12}$$

where

$$V_s = \frac{1}{\hbar}\left|\frac{\partial E_s(k)}{\partial k}\right|_{k=k_F} \tag{1.13}$$

is the velocity of electrons of the s -th band on the Fermi level.

Actually, according to (1.9) $\varepsilon_R(q)$ is an analogue of the Thomas-Fermi dielectric function for any quasione-dimensional metallic nanotube. The screened quasione-dimensional electrostatic potential produced by a charge e_0, distributed with the density

$$\rho^{ext}(\vec{r}) = \frac{e_0}{2\pi R}\delta(r_{2D} - R)\delta(z),$$

in accordance with (1.12) is given by:

$$\varphi(z,R) = \frac{e_0}{\pi}\int_{-\infty}^{\infty} \frac{I_0(|q|R)K_0(|q|R)\exp(iqz)}{1 + g\, I_0(|q|R)K_0(|q|R)}\, dq \tag{1.14}$$

with the constant

$$g = \frac{2e^2}{\pi\hbar}\sum_s \frac{1}{V_s}. \tag{1.15}$$

Note that the interaction energy E_q of electrons of infinite nanotube with the given external charge due to screening appears to be finite:

$$E_q = \frac{2ee_0}{g} n_e, \tag{1.16}$$

where n_e is the number of electrons per unit length of nanotube.

2.Numerical calculations

Both the velocity of electrons and Fermi energy for the (*n, n*) carbon nanotube can be obtained from any single-electron model (the tight binding method, for example). Band structure of 2D graphite was obtained in [6] within the framework of the tight binding method. It has up to constant shift the following form:

$$E(k_x, k_z) = \pm\gamma_0\sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x b}{2}\right)\cos\left(\frac{k_z b}{2}\right) + 4\cos^2\left(\frac{k_z b}{2}\right)}, \tag{2.1}$$

where $\gamma_0 = 2.79\,eV$ and $b = 0.246\ nm$ are the nearest-neighbour transfer integral and the in-plain lattice constant, respectively. According to [5], when 2D graphite layer is rolled up as cylinder the number of allowed states in the circumferential direction becomes limited. So allowed values for the wavenumber in the circumferential direction for armchair nanotubes can be written as:

$$k_x^{\nu} = \frac{\nu}{n}\frac{2\pi}{b\sqrt{3}}, \tag{2.2}$$

where ν = 1, … , *n*, *n* - chirality number.

Thus one-dimensional dispersion relation for 2*n* energy bands of (*n, n*) single-walled armchair CNT was obtained in [5]. It follows from (2.1) and (2.2) that with respect to (2.1) the Fermi energy $E_F = 0$ and only two bands

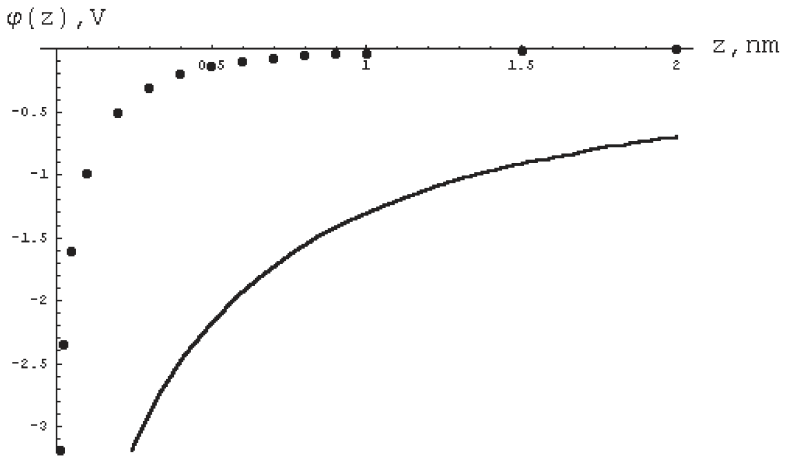

Fig. 1. Screened potential *φ(z)* according to (1.14) for (5,5) nanotube (plotted point by point) in comparison with unscreened averaged Coulomb potential (solid line)

$$E_{\pm}(k) = \pm\gamma_0\left(1 - 2\cos\left(\frac{kb}{2}\right)\right)$$

cross the Fermi level at $k_{\pm} = k_F = \frac{2\pi}{3b}$. As follows,

$$V_{\pm} = \frac{\gamma_0 b\sqrt{3}}{2\hbar}$$

and

$$g = \frac{8e^2}{\pi\sqrt{3}\gamma_0 b} \tag{2.3}$$

is the universal constant for the all armchair tubes within the framework of tight binding approximation. Fig. 1 shows numerically calculated screened potential (1.14) for (5,5) nanotube, with radius $R = 0.339\ nm$, in comparison with unscreened averaged over axial component Coulomb potential.

Thus the dielectric screening of the Coulomb potential by the free π-electrons in armchair nanotubes results in substantial reducing of the effective depth of Coulomb well at the origin and rather faster vanishing of the corresponding potential at infinity.

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