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Electronic spectrum and ballistic transport in bent nanotubes

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It is shown that bending of a nanotube leads to splitting the electron energy levels due to breaking the azimuthal symmetry. The bent section of the nanotube acts as a scatterer for ballistic carriers resulting in qualitative changes in the dependence of conductance on the Fermi energy.

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A few past years were marked by growing interest in electro- nanomechanical structures.These are freely suspended objects of a nanoscale size in which it becomes possible to affect the electron motion by making use of mechanical degrees of freedom of the structures: bending, twisting, folding in a roll, etc. In such situations one deals with electronic waves propagating in curvelinear waveguides and electrons are subjected to the action of the so called geometric potential (see, e.g., [1] and references therein).

In a strictly 1D case (curved quantum wire), the geometric potential attracts particles, independent of their charge, to the point of maximal curvature and formation of a bound state is, in principle, possible. A more complicate situation occurs for electrons confined to move upon the surface of a hollow cylinder (nanotube). Just this case is analyzed in the present paper.

1. General relations. Consider a nanotube with the semiconductor type of the electron energy spectrum:

$$\varepsilon_m(k) = Bm^2 + \frac{\hbar^2 k^2}{2\mu}, \tag{1}$$

where $m = 0, \pm 1, \pm 2 \ldots$ is the azimuthal quantum number, k is the longitudinal momentum, B is the rotational constant, $B = \hbar^2/2\mu a^2$, a is the nanotube radius and $/mu$ is the effective mass. All states with $m \neq 0$ are doubly degenerate since energy is independent of the sign of azimuthal moment m. If the nanotube is bent, its cylindrical symmetry breaks down, and this should result in splitting of the states $\pm m$ as well as in a shift of all the energy levels. The reason of such changes in the energy spectrum stems from the geometric potential and, besides, the kinetic energy operator is modified (see [2, 3] and more recent works [4, 5]). Both these factors cause also the electron scattering and, hence, affect the ballistic conductivity of nanotube. In the situation in question we deal with 2D carriers moving on a bent cylinder. The geometric potential has the form [2, 3]:

$$U = -\frac{\hbar^2}{8\mu}\left(\frac{1}{R_1} - \frac{1}{R_2}\right)^2. \tag{2}$$

Here R_1, R_2 are the principal radii of curvature in the point on a surface where electron resides. The operator of kinetic energy is, of course, the Laplacian presented in the proper curvelinear orthogonal coordinates u and v:

$$\hat{T} = -\frac{\hbar^2}{2\mu}\frac{1}{\sqrt{g}}\sum_{\alpha,\beta=1}^{2}\frac{\partial}{\partial u_\alpha}\left(\sqrt{g}g^{\alpha\beta}\frac{\partial}{\partial u_\beta}\right), \tag{3}$$

where g is the determinant of the metric tensor. For the situation in question $R_1 = a$ is the "eigen" radius of nanotube, while $R_2 \equiv R$ is the curvature radius of the bent nanotube.

Suppose the nanotube is bent without twisting, in other words its axis remains a plane curve. Then each small part of the nanotube can be considered as an arc of torus with the local big radius $R(s)$, where s is the length of the nanotube axis counted from an arbitrary origin. As to small radius of the torus it remains constant for any s and equals a. The pair of coordinates u, v can be chosen as $u = a\varphi$, $v = s$, where φ is the azimuthal angle in the torus cross-section. Then the squared element of length on the torus surface takes the form

$$dl^2 = a^2 d\varphi^2 + (1 + a\cos\varphi/R(s))^2 ds^2, \tag{4}$$

while the Laplace operator reads:

$$\hat{\Delta} = \frac{1}{ah}\left(\frac{\partial}{\partial\varphi}\frac{h}{a}\frac{\partial}{\partial\varphi}\right) + \frac{1}{h}\frac{\partial}{\partial s}\frac{1}{h}\frac{\partial}{\partial s}, \tag{5}$$

$$h = h(s,\varphi) \equiv 1 + \frac{a\cos\varphi}{R(s)}.$$

The geometric potential in the coordinates φ, s is

$$U = -\frac{\hbar^2}{8\mu}\left[\frac{1}{a} - \frac{\cos\varphi}{R(s) + a\cos\varphi}\right]^2. \tag{6}$$

By introducing the function $\chi(\varphi, s)$ instead of the wave function ψ in accord with the relation $\psi = \chi/\sqrt{h}$ one can eliminate the first derivative $\partial/\partial\varphi$ and obtain the Schrodinger equation:

$$-B\left[\frac{\partial^2}{\partial\varphi^2} + \frac{a\cos\varphi}{2Rh} + \frac{a^2\sin^2\varphi}{4R^2h^2}\right]\chi - \frac{\hbar^2}{8\mu a^2}\left(1 - \frac{a\cos\phi}{Rh}\right)^2\chi - \frac{\hbar^2}{2\mu\sqrt{h}}\frac{\partial}{\partial s}\frac{1}{h}\frac{\partial}{\partial s}\frac{\chi}{\sqrt{h}} = E\chi. \quad (7)$$

In what follows two effects will be considered in which the bending of nanotube is manifested.

2. Spectrum of a torus arc. Consider the simplest case: $R(s) = \text{const}$ for $0 < s < L$, so we deal with a piece of torus of the lengths L. The boundary conditions are: $\psi(0) = \psi(L) = 0$. Eq. (7) gives immediately $\chi = F(\varphi)\sin\kappa_n s$ with $\kappa_n = n\pi/L$, n is integer and we obtain a 1D Schrodinger equation with a rather complicate effective potential energy $U_{\text{eff}}(\varphi)$. It is reasonable to suppose the condition $a \ll R$ is satisfied and to look for the energy spectrum in the frames of perturbation theory. To do this one has to expand $U_{\text{eff}}(\varphi)$ up to terms of the order of $(a/R)^2$ because these terms contain the factor $\cos 2\varphi$ that gives splitting of the states $m = \pm 1$ in the first order of perturbation approach, while the terms of the type $a\cos\varphi/R$ give the same splitting in the second order[1)]. The splitting is determined by the combined matrix element:

$$V = V^{(2)}_{1,-1} + \frac{V^{(1)}_{1,0}V^{(1)}_{0,-1}}{\varepsilon_1 - \varepsilon_0}, \quad (8)$$

where $V^{(1)}$ and $V^{(2)}$ denote the contributions from $\cos\varphi$ and $\cos 2\varphi$, respectively. The results of calculations give for three lowest subbands of the toroidal segment of nanotube:

$$\varepsilon_{0n} = \frac{\hbar^2\kappa_n^2}{2\mu} - \frac{\hbar^2}{8\mu R^2} + \frac{\hbar^2}{2\mu R^2}\left(\frac{3}{2}\kappa_n^2 a^2 - \kappa_n^4 a^4\right), \quad (9)$$

$$\varepsilon_{\pm n} = B + \varepsilon_{0n} \pm \frac{\hbar^2}{2\mu R^2}\left(\kappa_n^4 a^4 + \frac{3}{4}\kappa_n^2 a^2 - \frac{3}{16}\right). \quad (10)$$

Thus, the absorption line of inter- or intraband transitions in which the subband $m = \pm 1$ is involved splits in accord with Eq. (10) if the nanotube is bent. The splitting rapidly increases with increasing the quantum number of the longitudinal motion n (as n^4). Of course, the perturbative approach should be valid, i.e. $\kappa_n^2 a^2 \ll R/a$.

3. Ballistic transport in bent nanotubes. It is clear from the previous consideration that any bent part of nanotube acts as a scatterer for mobile electrons. In quasi-1D objects scattering simply means nonzero reflection coefficient R and the transmission coefficient T not equalled to 1. Hence, the well known staircase-like dependence of conductance on the Fermi energy should be modified for a bent nanotube.

Suppose the nanotube is asympotically rectilinear, i.e. $R(s) \to \infty$ for $s \to \pm\infty$ and suppose, in addition, that $R(s)$ changes slowly as a function of its argument s: $dR/ds \ll 1$. Then the adiabatic approach to the problem can be developed: at first to omit the term with derivatives $\partial/\partial s$ in Eq. (7) and to find the "momentary" eigenfunctions $\chi_i(\varphi, s)$, where s is treated as a parameter. Then to search for the total wave function as the expansion $\sum c_i(s)\chi_i(\varphi, s)$. An interesting feature of the situation in question is dependence of the coefficient at "slow" part of the Hamiltonian (with derivatives $\partial/\partial s$) on the "fast" variable φ: h depends on φ. Hence, even if one neglects the terms $\partial\chi_i/\partial s$ and $\partial^2\chi_i/\partial s^2$ (the zeroth adiabatic approximation) the system of equations for slow amplitudes $c_i(s)$ will not become decoupled as it usually is the case in other adiabatic problems. Actually, the effective mass in our case is a matrix (depending, of course, on s)

$$-\frac{\hbar^2}{2}\sum_k\left\langle\frac{1}{\mu}\right\rangle\frac{\partial^2 c_k}{\partial s^2} + \varepsilon_i(s)c_i(s) = Ec_i(s), \quad (11)$$

where ε_i are given by Eqs.(9), (10) with $\kappa_n = 0$ and

$$\left\langle\frac{1}{\mu}\right\rangle_{ik} = \frac{1}{\mu}\int\chi_i^*\left(1 + \frac{a\cos\varphi}{R}\right)^{-2}\chi_k d\varphi. \quad (12)$$

In what follows an example is considered when only three states χ_0 and $\chi_\pm$ contribute to the total conductance. In other words the Fermi energy lies below the bottom of the subband $m = \pm 2$: $0 < E_F < 4B$.

If $E_F < B$ only the state $m = 0$ is involved and the bending results merely in arising a potential well of the depth $\hbar^2/8\mu R^2$ (see Eq. (9)). For small Fermi energy $E_F \ll \alpha^2 B$, $\alpha \equiv a/R$, the transmission coefficient in the channel $m = 0$ tends to zero in accord with the well known formula

$$T_{00} = \frac{E}{E + W}, \quad E = E_F, \quad (13)$$

where W depends on the potential shape but is independent of E. Thus, the conductance G of the bent nanotube depends linearly on E_F for very small E_F in the contrast with the ideal (rectilinear) nanotube. In the latter case $G = G_0 = e^2/2\pi\hbar$ (per one spin projection) right from zero Fermi energy, because in nanotubes there exists a nontrivial solution of the Schrodinger equation

[1)] It is easy to see a similarity of the problem in question with Λ-doubling in the spectra of biatomic molecules.

for $E = 0$: $\psi_0 = 1/\sqrt{2\pi}$ (this is not the case for a 1D plane strip due to zero point energy).

Consider now the case $B < E_F < 4B$ (the second step in the conductance), when three channels are involved $m = 0$ and $m = \pm 1$. It is easy to see that all perturbation terms in Eq. (7) contain only $\cos\varphi$ and, hence, preserve the parity of the solutions. That is why it is reasonable to choose three eigenfunctions of the zeroth approximation as[2] $\psi_0 = 1/\sqrt{2\pi}$, $\psi_+ = \cos\varphi/\sqrt{\pi}$, $\psi_- = \sin\varphi/\sqrt{\pi}$. Then the ψ_- state is split off and we come to the following pair of coupled equations for the slow amplitudes c_0, c_+ (only leading terms of the expansion in $\alpha(s)$ are kept):

$$\begin{aligned} c_0'' - \sqrt{2}\alpha c_+'' + \left(k^2 - \frac{\alpha}{2a^2}\right) c_0 = 0, \\ c_+'' - \sqrt{2}\alpha c_0'' + \left(q^2 - \frac{\alpha}{2a^2}\right) c_+ = 0, \end{aligned} \tag{14}$$

where $k^2 = 2\mu E/\hbar^2$, $q^2 = 2\mu(E-B)/\hbar^2 = k^2 - 1/a^2$.

Thus, the nanotube bending causes now both reflection of the electron waves and interchannel transitions. This results in distortion of the rectangular shape of the steps in the dependence $G(E_F)$. In the multichannel situation $G(E_F)$ is given by the sum [6] $T_{00} + T_{++} + T_{--} + T_{0+} + T_{+0}$. The system (14) has been analyzed for $\alpha(s)$ in the form of a rectangular barrier. However it is easy to see that, due to the threshold character of the transitions under consideration, the results have general meaning.

For F_F close to B the transmission coefficient T_{00} may be put to be equalled 1 as the barrier height $\sim \alpha B \ll E_F$. The coefficients T_{++} and T_{--} in the region of onset of the second step ($E_F - B \ll B$) correspond to slow incoming particles and are described by formulae of the type (13) with slightly changed W as it follows from Eqs. (9) and (10). At last, T_{+0} relates to the interchannel scattering in the threshold regime (slow particle in the final state) and depends on energy as $\sqrt{E-B}$ (finite matrix element at $E \to B$ times the ratio of the current densities in subbands ε_+ and ε_0)[3]. The same is true for T_{0+} - all is similar to the transmission of a quantum particle over a potential wall at the energy slightly exceeding the wall height. The latter in our case equals B - the separation between the bottoms of subbands ε_+ and ε_0. So, the leading contribution to the conductance comes from interchannel scattering and the second step in $G(E_F)$ starts as $G_0(1 + \mathrm{const}\sqrt{E_F - B})$. This law holds only for $E_F - B \leq \alpha B$. With energy increasing ($q^2a^2 \gg 1$) the coupling terms in Eqs.(13) become unimportant, T_{++}, T_{--} tend to 1 while T_{+0}, T_{0+} decrease and $G(E_F)$ reaches its second quantized value for the rectilinear nanotube $3G_0$. It is clear that similar behaviour of $G(E_F)$ should be expected at the onsets of all the other steps.

In conclusion, bending of a nanotube results in splitting the energy subbands due to breaking the azimuthal symmetry. Qualitative changes arise at the onset of each step in the staircase-like dependence of ballistic conductance of nanotube on the Fermi energy.

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[2] Here "+" and "-" denote even and odd solutions, correspondingly.

[3] Strictly speaking the density of current in a curvelinear system is changed ($\nabla_s = (1/h)\partial/\partial s$) but asymptotically at $s \to \pm\infty$ we have $h = 1$.