Transport in nanotubes: Effect of remote impurity scattering

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The theory of the remote Coulomb impurity scattering in single-wall carbon nanotubes is developed within a one-electron approximation. The Boltzmann equation is solved within the drift-diffusion model to obtain the tube conductivity. The conductivity depends on the type of the nanotube band structure (metal or semiconductor) and on the electron Fermi energy. We found that the exponential dependence of the conductivity on the Fermi energy is due to the Coulomb scattering rate having a strong dependence on the momentum transfer. We calculate intrasubband and intersubband scattering rates and present general expressions for the conductivity. Numerical results, as well as obtained analytical expressions, show that the degenerately doped semiconductor tubes may have very high mobility unless the doping level becomes too high and the intersubband transitions impede the electron transport.

I. INTRODUCTION

Carbon nanotubes, discovered in the last decade,[1] attract the attention of physicists not only due to their beautiful symmetry, extreme quantum scale, and quasi-one-dimensional (1D) structure, but also due to numerous applications, already existing[2–4] and foreseen in the future. Among those, the applications, which will use transport properties of nanotubes,[3,5] are sensitive to details of a charge carrier scattering. It was shown that the scattering in an ideal *metallic* single-wall nanotube (SWNT) is greatly diminished as in a full symmetry of an armchair nanotube the back-scattering between states at a Fermi level (in a thin shell near an electrochemical potential at $T \neq 0$) is forbidden.[6] In contrast, an electron in a doped *semiconductor* SWNT, which has different symmetry (zigzag or other chiral symmetry), can be backscattered. In field effect devices the semiconductor nanotubes are used. To obtain high conductivity the doping level is controlled, thus, our study of the transport mechanisms and the semiconductor SWNT conductivity[7] and their dependence on the doping level becomes very timely.

Among most important mechanisms of elastic[8] scattering, responsible for the low-temperature resistivity of nanoscale systems, one may encounter a defect scattering, a Coulomb center scattering, and an electron-electron interaction; the latter is beyond the scope of one-electron theory and will be studied elsewhere. The first two are distinct as a scattering potential is long ranged for the Coulomb center, and it is short ranged for a neutral (mechanical) defect, which may be a substitutional (not charged) impurity or another type of lattice defect. The charge carrier scattering by the Coulomb center, charged impurity, and/or ionized dopant is the focus of our paper. At low temperatures this mechanism is comparable or even stronger than other scattering mechanisms. Modern high mobility semiconductor devices have so small a size scale that the device channel may contain no substitutional impurity/dopant atom. The remote impurity scattering may still limit the transport in this case. Recent experiments[9,10] showed that even long channel semiconduc-tor SWNT devices may have very high mobility at the high doping level. Our theory addresses this case, taking into account Coulomb scattering at the remote impurities and including effects of intersubband scattering at the high (doping) Fermi energy.

Specifics of the Coulomb interaction in nanotubes is that the effective potential, seen by the delocalized electrons, has a cutoff at the radius of the tube R. Thus, even if the Coulomb impurity is at the closest (atomic) distance from the tube surface,[11] the effective Coulomb potential is the potential of a remote scatterer. The situation is similar to what is known for HEMT devices. We propose that the remote impurity scattering mechanism is responsible for a residual resistance of the semiconductor nanotube at low temperature. It may define a limit for an electron mobility (on current) in the nanotube field effect transistor if other scattering mechanisms are less effective. The same theory is applicable to the scattering in metallic nanotubes which are proposed for use as interconnects and ballistic wires[12] and especially in metallic field effect transistors.[13]

We develop a theory of the remote impurity scattering for the SWNT device, calculate a scattering rate at one surface impurity, scattering by a dilute distribution of random impurities (in a Born approximation), a zero and finite temperature conductivity in a drift-diffusion (DD) model. It is known that in pure (mesoscopic) systems, a quantum interference correction to the DD conductivity depends on the system dimension and it is of the order of the conductivity itself in the 1D case. This manifests as a 1D localization. However, for a quasi-1D system of the nanotube it may not hold due to fast phase breaking. It may explain why considerably simple classical one-electron theory describes the nanotube experiment fairly well.[14–16] Among possible mechanisms responsible for the fast phase breaking we notice *e-e* and *e*-phonon interactions. The latter mechanism was shown to be very fast in SWNT's in optical studies.[17] We will discuss the role of *e-e* interaction later on.

We calculate the dependence of the SWNT conductivity on the Fermi energy. The strong degeneracy of carriers in the semiconductor tubes is required to obtain the high mobility.[18]

We show that this is consistent with calculated scattering rates. The same condition of the large Fermi energy allows one to apply the Boltzmann equation for transport calculations.

It is commonly used that the conduction in SWNT's happens via states of one subband (of orbital quantization). We note that at the high doping level the new conduction channel (through the next subband) must appear. Then, an interesting question arises: how the scattering between *different subbands* may change the conductivity. In semiconductors, the role of intervalley scattering is not very important. The difference in the transport at high fields consists mainly of the renormalization of an effective mass of the electron of the conduction band. We will show that for the quasi-1D band structure of the SWNT, where a phase space of scattering is very restricted, the opening of a new scattering channel may change the conductivity qualitatively, especially for metallic armchair nanotubes and for high mobility semiconducting nanotubes. We found that for the Coulomb scattering mechanism it results in a giant drop of the conductivity at low temperature. We present a general expression for the concentration dependence of the conductivity and study its analytical limits that clearly demonstrates the physics of this effect.

1D conductivity σ_{1D} is known to have a dimension of a diffusion coefficient $\langle \text{length} \rangle^2 / \langle \text{time} \rangle$ (see, for example, Ref. 19). Thus, the conductance of the 1D system is σ_{1D}/L where L is the system length. We demonstrate below that a simple expression is valid for the DD conductivity of the SWNT: $\sigma_{1D} \sim G_0 \Lambda$, where $G_0 = e^2/2\pi\hbar$ is the quantum of conductance and $\Lambda \sim v\tau$ is a mean free path of the electron (v and τ are the electron velocity and lifetime). We calculated Λ as a function of the Fermi energy and a strength of the random impurity potential. Within the model discussed, the conductance can be written as

$$ G \sim \sigma_{1D} \frac{1}{L} \sim G_0 \frac{R}{L} f_1 \left(\frac{E_F}{U_s} \right) f_2 \left(\frac{E_F}{E_g} \right) g \left(\frac{E_F}{E_g} \right), \qquad (1) $$

where R is the SWNT radius (characteristic transverse length of the 1D channel), E_F is the electron Fermi energy, $U_s = (ee^*)\sqrt{n_s}$ is a strength of the 1D potential of the Coulomb impurities with an effective charge e^* and a surface density n_s, E_g is the SWNT gap, f_1 and f_2 are some power law functions, and $g(x)$ is an exponential function of its argument. The conductivity (and conductance) is so sensitive to the change of the Fermi energy (exponential function of E_F) because of the exponential dependence of $g(x)$ that reflects a strong dependence of the Coulomb matrix element on a transferred momentum. Allowed backscattering transitions within a single subband have a large momentum transfer at large E_F, while the transition between subbands may have smaller momentum transfer. Thus, the appearance of the new scattering channel drastically decreases the mean free path of the electron Λ, which becomes small, and G drops several orders of magnitude. We notice that the power law function $f_1(x) \gg 1$ because its argument is large: $E_F \gg U_s$. This inequality is also a necessary condition for applicability of the Boltzmann equation.

Below we consider charged impurities which are likely present on the surface of any substrate. The deposition methods which are currently used in fabrication of the nanotube devices may produce such impurities in large quantities. Charged impurities are known to exist at the surface of SiO_2 substrate, commonly used for nanotube devices. Use of high-ϵ dielectrics may even increase the role of this scattering mechanism.

We assume that the impurities are (single) ionized and uniformly distributed on the insulating surface with a 2D density n_s. Both assumptions are not vital for the model and make no qualitative change in the final results. However, the derivation of the Eq. (1), for example, is more clear in this geometry. The generalization of our theory to the case of 3D distribution of the Coulomb centers is straightforward. It gives a description for the SWNT embedded in an insulating matrix and will be published elsewhere.[20] For the Coulomb substitutional impurities located directly in the lattice of the SWNT and for the charged impurities encapsulated inside the tube, an order of magnitude estimate for the DD conductivity can be obtained by substituting U_s^2 by $W_s E_c$, where W_s is the strength of a random potential of 1D impurities and $E_c \sim e^2/C$ is a Coulomb charging energy of the tube. We note the logarithmic divergence of the latter with L as well as the same logarithmic divergence of the 1D Coulomb matrix element.[21]

II. REMOTE IMPURITY SCATTERING RATE

A. Model assumptions

The nanotube is situated at the van der Waals distance from the surface of the substrate. This distance is about 3.4 Å, and the Coulomb centers are removed from the device channel. The Born approximation, which implies independent scattering events, is used in what follows to calculate the elastic scattering rate. We consider scattering of the electrons in different subbands and between subbands. One can apply this theory to the transport in multiwall nanotubes, which are believed to conduct by the outermost shell. Here, we restrict ourselves to the case of single-wall tubes and consider armchair and zigzag SWNT's, though, the final result is more general and can possibly be used for an arbitrary tube.

The Coulomb scattering manifests itself in low-dimensional systems. The long-range Coulomb potential is known to be underscreened in a 1D case,[21,22] in nanowires[14] and nanotubes,[23,24] which means that the screened potential diverges as a logarithm of the distance. Thus, the Coulomb scattering becomes the most important scattering mechanism in certain conditions. It is well known that the random potential results in a localization of carriers in an infinite 1D system.[25] We assume that an effective phase breaking mechanism exists in the SWNT's, which destroys the interference. It is known that the e-e scattering time is very short for these systems, even though the e-e interaction in *a single 1D band* cannot suppress the localization, because the total momentum of the electronic subsystem is conserved. However, in the nanotubes there is a number of different e channels which may be not coherent. It is clear that the e-e scat-

tering between the electrons that belong to *the different bands* breaks the phase of the wave function and, thus, destroys the interference. What are these different e bands? The transport in nanotubes occurs via the band formed by highest valence electrons, so called, π-electron band. The rest of the valence electrons are localized and form low-lying σ bands. The e-e scattering between these two different bands does not preserve the electron phase. Also, in a real experimental situation, in the SWNT rope or in the multiwall nanotube, the scattering between π electrons at the different walls/tubes destroys the interference as well. For what follows we accept that the phase breaking time is short enough to neglect the interference correction and use the Boltzmann equation approach for the calculation of the DD conductivity of the SWNT.

B. Envelope wave functions

We use SWNT envelope wave functions[26] for the electronic structure calculation, which are obtained as a solution of a tight-binding (TB) Hamiltonian for π electrons.[27] Our approach is very close to what was presented in Ref. 26 and then widely used in the nanotube literature, so we skip details and give only the final wave functions for the two-band scheme (π electrons only):

$$|\psi_{m,k,\zeta}\rangle = \frac{1}{\sqrt{2}}(|A\rangle + \zeta c_{mk}|B\rangle)e^{ikz}e^{im\alpha}, \quad (2)$$

where an orbital momentum m labels orbital subbands of the SWNT electronic structure, k labels states with a longitudinal momentum, both m and k are good quantum numbers (discrete and continuum, respectively) for an ideal, long enough nanotube. $\zeta = \pm 1$ is a pseudospin. A pseudospinor vector is formed by a two-component amplitude of the wave function defined for two atoms in a graphite unit cell (A and B). Coordinate along the tube is z, and α is an angle along the nanotube circumference (by this we explicitly assume the electron to be confined to a surface of a cylinder of fixed radius R). The components of the pseudospinor are c-numbers, in general, defined up to an arbitrary phase. It is taken such that the coefficient for the A component is purely real and equal to $1/\sqrt{2}$, then a matrix element of the dimensionless TB Hamiltonian gives the second component of the pseudospinor.[28] This determines a dependence of c_{mk} on the subband index m and the 1D momentum k. The pseudospin ζ distinguishes between states of valence and conduction band.[29]

So far, we considered an equilibrium (nonperturbed) electronic wave functions. We assume, as usual, that the scattering can be modeled perturbatively if the interference terms are negligible as it was discussed in the last section. The perturbation operator is the Coulomb potential

$$V_i(\mathbf{r}) = \frac{ee^*}{\sqrt{(z - Z_i)^2 + (x - X_i)^2 + (y - Y_i)^2}}, \quad (3)$$

where $e < 0$ is an electron charge. x, y, and z are the coordinates of the electron. These three coordinates are not independent as the electron motion is restricted to the surface of

the cylinder. e^* is an effective charge of an impurity, its position is given in a Cartesian coordinate system as $[X_i, Y_i, Z_i]$. For the scattering at a single impurity, a relative position of the Coulomb center along the (infinite) nanotube Z_i may be chosen arbitrary. The coordinate X_i (normal to the substrate surface) approximately equals h, a negative height of the nanotube, which assumes that the impurity size is negligible and that the impurity is not buried in the substrate (both assumptions are reasonable but the model works without this simplification as well). We will define an effective charge of the impurity, e^*, in the last section, when discussing the screening.

C. Matrix element of the impurity potential

One needs to know matrix elements of the Coulomb potential between the TB wave functions of the electron to calculate the scattering. The potential of the remote impurity is smooth at the surface of the nanotube and, therefore, it is almost constant within the unit cell. Hence, the matrix elements of the potential with the envelope wave functions (2) can be approximated by the 1D Fourier components of Eq. (3):

$$\langle km|\frac{ee^*}{|\mathbf{r}|}|k'n\rangle = \frac{2ee^*}{L}e^{-i\varphi(m-n)}e^{-iZ(k-k')}$$

$$\times I_{|m-n|}(|k-k'|R)K_{|m-n|}(|k-k'|\rho), \quad (4)$$

where $I_\mu(x)$ and $K_\mu(x)$ are the modified Bessel functions[30] (of imaginary argument) of the order μ, $\mathbf{r}$ is the vector between the impurity center and the point on the surface of the nanotube, and R is the nanotube radius. In a cylindrical coordinate system, φ is the angle of the impurity position, ρ is the distance from the axis of the nanotube to the impurity and Z is its longitudinal coordinate.

These matrix elements of the potential are needed for calculating the remote scattering rates. In addition to that, the analytical expression for the remote potential (4) is interesting by itself. We are not aware of a calculation of the Coulomb potential for the charge center *removed from the nanotube*. This formula gives a generalization of an expression for the 1D Fourier transformation of the Coulomb interaction between charges which are *both on the nanotube surface* (which may be found, for example, in Ref. 31). Let us present analytical limits of our result at large and small transferred momentum and demonstrate how the dimension of the nanotube system shows up.

The interaction strength decreases rapidly with the transferred momentum $q = |k - k'|$, which is well known property of the Coulomb potential at any dimensions. Using the asymptote of the Bessel function at $q \gg \rho^{-1}, R^{-1}$, we reduce Eq. (4) to

$$\frac{2ee^*}{L}e^{-i\varphi(m-n)}e^{-iZ(k-k')}\frac{e^{-|k-k'|(\rho-R)}}{|k-k'|\sqrt{\rho - R}} \quad (5)$$

and recover formula e^{-qa}/q, the expression for the Fourier component of the Coulomb potential in 2D.[32] This is not surprising, because in the short-wavelength limit one restores
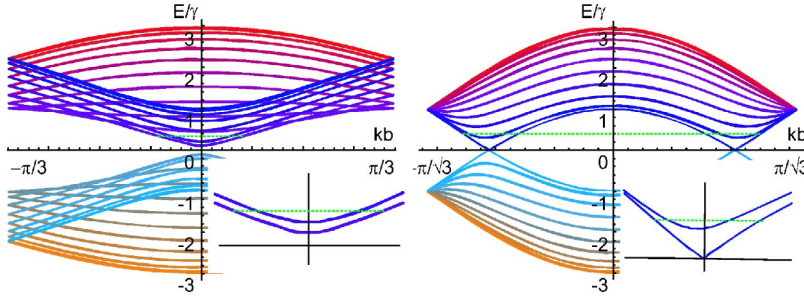
FIG. 1. (Color online) Electron energy dispersion for armchair [10,10] and zigzag [17,0] SWNT's. Inset: Zoom out of the lowest subbands and the electrochemical potential (green dashed line).

the planar geometry when the curvature of the graphite sheet becomes unimportant.

On the other hand, at small q and $m=n$ the matrix element (4) logarithmically diverges as $\sim\ln(q\rho/2)$, which is according to 1D electrostatics.[21] In contrast, at $m \neq n$ and small q, the limit of the matrix element has no dependence on q. Instead it is proportional to $(R/\rho)^{|m-m'|}$, and decays exponentially with the transferred angular momentum $|m-m'|$ as in the multipole expansion series. It is consistent with understanding of R^{-1} as a minimum cutoff momentum in the Coulomb matrix element.

D. Averaging of the random potential

In the Born approximation each scattering event is statistically independent and the electron wave function is not coherent between events. Thus, one has to sum probabilities of the scattering over the realization of impurities (to be averaged later). Let us write the partial probability of the single scattering event using the Fermi golden rule

$$W_{mn}(k) = \frac{2\pi}{\hbar}\sum_q \left(\frac{2ee^*}{L}\right)^2 I_{|m-n|}^2(qR)$$
$$\times K_{|m-n|}^2(q\sqrt{h^2+Y^2})\delta(E_{n,k+q}-E_{m,k}), \quad (6)$$

where q is the transferred momentum, and for the SWNT the sum has only several terms (less than four) if any, which depends on m, n, and k quantum numbers. Here, h and Y are the Cartesian coordinates of the impurity (without loss of generality, we chose the coordinate origin such that $Z=0$). We remind the reader that the axis of the nanotube is at the distance $X=h$ from the substrate. L is the tube length.

The Coulomb centers are distributed on the surface of the substrate randomly. One has to perform averaging in the plane to obtain a statistical description of the scattering. We assume that the impurity positions are not correlated. Then for the electron with the momentum k in the subband $|m\rangle$, an elastic lifetime due to the remote impurity scattering is written as

$$\tau^{-1}(m,k) = \frac{8}{\hbar}(ee^*)^2 n_s \sum_n \sum_{q_k} \left(\frac{\partial E_n}{\partial k}\right)^{-1}_{k=q_k} \frac{\mathcal{G}(q_k)}{q_k}, \quad (7)$$

where n_s is a 2D density of the surface impurities and q_k are the solutions of the equation $E_{n,k+q}=E_{m,k}$. As we noticed before, this equation may have up to four solutions within the first Brillouin zone (see Fig. 1). For example, for the $[N,N]$ armchair nanotube we have

$$q_k = -k \pm \frac{2}{b}\arccos\left[-\frac{1}{2}\cos\frac{m\pi}{N} \pm \frac{1}{2}\right.$$
$$\left.\times\sqrt{\cos^2\frac{m\pi}{N} + 4\cos\frac{kb}{2}\left(\cos\frac{kb}{2}+\cos\frac{n\pi}{N}\right)}\right],$$
$$(8a)$$

and for the $[N,0]$ zigzag SWNT

$$q_k = -k \pm \frac{2}{\sqrt{3}b}\arccos\left[\frac{1}{2\cos\frac{m\pi}{N}}\left(-\cos\frac{2m\pi}{N}+\cos\frac{2n\pi}{N}\right.\right.$$
$$\left.\left.+\cos\frac{\sqrt{3}kb}{2}\cos\frac{n\pi}{N}\right)\right], \quad (8b)$$

where $b \simeq 0.14$ nm is the bond length and N is the SWNT index.

We use the notation $\mathcal{G}(q_k)=I_{|m-n|}^2(q_kR)\mathcal{F}_{|m-n|}(q_kh)$ for a reduced Coulomb matrix element in Eq. (7). Here the factor $\mathcal{F}$ comes after averaging in the plane and equals

$$\mathcal{F}_n(x) = \int_{-\infty}^{\infty} dt K_n^2(\sqrt{x^2+t^2})$$
$$= \frac{\pi}{2}\int_{4x}^{\infty} dt K_{2n}(t)$$
$$= \frac{\pi^2}{4}\left\{(-1)^n\{1-4x[K_0(4x)\mathbf{L}_{-1}(4x)+K_1(4x)\mathbf{L}_0(4x)]\}\right.$$
$$\left.+\frac{4}{\pi}\sum_{j=1}^n (-1)^{j+1}K_{2(n-j)+1}(4x)\right\}, \quad (9)$$

where $\mathbf{L}$ are the modified Struve functions[30] (of imaginary argument).

Now we analyze these expressions in the limit of small and large q_k. For small q_kh one can write

$q_k^{-1}\mathcal{G}(q_k)$

$= q_k^{-1} I_{|m-n|}^2(q_k R)\mathcal{F}_{|m-n|}(q_k h)$

$$\approx \begin{cases} \pi^2/4q_k & \text{if } n=m, \\ \dfrac{\pi R}{16}\dfrac{R}{h} & \text{if } |n-m|=1, \\ \dfrac{\pi h(2|n-m|-3)!!}{2^{3|m-n|+1}|n-m||n-m|!}\left(\dfrac{R}{h}\right)^{2|m-n|} & \text{if } |n-m|>1. \end{cases}$$

(10)

The numerical factor is rather small in case of intersubband transitions $n \neq m$ and decreases with the separation between subbands $|m-n|$ rapidly. Thus, the scattering into the same subband (transition with the orbital quantum number conservation) is the most effective scattering channel for small q_k.

For large $q_k R$ the scattering rate exponentially decreases with the transferred momentum $\sim\exp[-2(2h-R)q_k]$, due to the exponential decay of the modified Bessel function. The main term of a Poisson series of the matrix element does not depend on $|m-n|$:

$$q_k^{-1}\mathcal{G}(q_k) \approx \sqrt{\frac{\pi}{128hR^2 q_k^5}}e^{-2(2h-R)q_k}$$

$$\times\left(1 + \frac{\left(h/R-\frac14\right)\left(|m-n|^2-\frac14\right)+\frac{1}{64}}{qh}+\cdots\right).$$

(11)

We will use these analytical expressions (10) and (11) for the calculation of the scattering rates in what follows.

III. CONDUCTIVITY: DRIFT-DIFFUSION APPROACH

In this section we calculate the conductivity in a drift-diffusion (DD) model which is widely used for description of the transport in multiwall nanotubes. It is also applicable for very long SWNT's if the phase breaking and/or inelastic scattering lifetime is short as discussed in the Introduction.

It is known that a Schottky barrier forms near the metal contact.[15,33] For the short channel SWNT device this Schottky barrier almost determines important transport characteristics. The theory of the nanotube transport, taking into account phenomena in the contact regions, is presented in Refs. 15 and 33 and we do not address this subject in our paper. Instead we focus on the scattering in the rest of the tube. The contact region has a finite length which is about a typical screening length, e.g., a distance to the backgate.[34,35] If this distance is much smaller than the length of the nanotube, one may define the device channel conductivity.[36,37] For the sake of clarity, we restrict ourselves to the case of the armchair or zigzag SWNT. The generalization of our model to the case of any chiral SWNT is straightforward.

The conductivity in a single channel is as follows:

$$\sigma_i = \frac{g}{2\pi}\int\frac{e^2\tau(E)}{\hbar^2}\frac{\partial E}{\partial k_i}\frac{\partial f}{\partial E}dE.$$

(12)

Here g is the degeneracy of the current channel. By the channel of conductivity we understand here any fixed subband of

the orbital quantization which can carry the current. $\tau(E)$ is the transport lifetime and $f(E)$ is an equilibrium distribution function. The derivative of the distribution function $\partial f/\partial E$ is peaked at the electrochemical potential (delta function of the Fermi energy $E=E_F$ for $T=0$). However, we keep the integral sign even at $T=0$ because of several channels corresponding to several non-zero terms in the conductivity, as given by Eqs. (8a) and (8b). σ has nontrivial temperature dependence due to the strong dependence of the lifetime on the electron energy.

It is important to include the intersubband scattering terms (if corresponding transition is allowed) because the Coulomb scattering rate decreases with the transferred momentum (see also Fig. 3). With increasing E_F the scattering into the same subband may become less effective than the scattering into the other subband. We demonstrate below that this is the case for the semiconductor SWNT at the high doping levels.

Equation (7) can be conveniently rewritten as

$$\tau^{-1}(m,k) = \frac{8U_s^2}{\hbar^2}\sum_{n,q_k}' v_{n,q_k}^{-1} q_k^{-1}\mathcal{G}_{|m-n|}(q_k),$$

(13)

with use of notations $U_s = (ee^*)\sqrt{n_s}$ for a characteristic energy of the Coulomb disorder and $v_m = \hbar^{-1}\partial E/\partial k$ for the electron velocity. The prime sign reminds us that the summation is over the roots of Eqs. (8a) and (8b).

Let us first consider the scattering of the electron in the same subband $|m,k\rangle \rightarrow |m,k+q\rangle$.

A. Armchair nanotubes: Intrasubband scattering

The expression for the scattering roots for the armchair SWNT, (8a) in the limit of intrasubband scattering ($m=n$) reduces to

$$q_k = -k \pm \frac{2}{b}\arccos\left[\cos\frac{m\pi}{N}+\cos\frac{kb}{2}\right],-2k,0. \quad (14)$$

We remind the reader that N is the $[N,N]$ SWNT index.

The last root means no scattering because all quantum numbers are conserved and has to be discarded. The first root is, in fact, the intersubband backscattering near the same Fermi point (see Fig. 1, right inset), which is forbidden for the two crossing subbands of the armchair SWNT by the pseudospin conservation rule.[38] The root $q=-2k$ is the backscattering of the electron within the same subband to other Fermi point (see Fig. 1, right). Only this transition between two Fermi points with a large transferred momentum ($q_k \approx 4\pi/3\sqrt{3}b$ for small E_F) is allowed by the symmetry of the armchair SWNT. Thus, the analytical limit (11) can be used for calculating $\tau(E)$. The transport lifetime of the electron contains a large exponential factor $\propto\exp[4\pi(2h-R)/3\sqrt{3}b]$ and, hence, this mechanism gives the negligible scattering rate.

Because of the exponential dependence of the matrix element on the transferred momentum, the conductivity of the armchair nanotube increases dramatically, when the Fermi energy reaches the next subband. This subband has a different symmetry[29] and the intersubband scattering near the same Fermi point (see Fig. 1, right inset) is not forbidden.

Then, the intersubband scattering rate of the armchair nanotube is high and given by an expression which is similar to the case of zigzag nanotube. We will consider these two mechanisms together in Sec. III C.

B. Zigzag nanotubes: Intrasubband scattering

In the last section we show that the remote impurity scattering is negligible in the armchair SWNT's. The scattering due to any other long range potential, except for torsional phonon modes,[39] was shown to be ineffective as well.[16] The case of the zigzag nanotube is less trivial. We substitute Eq. (7) into Eq. (12) and obtain the conductivity at zero temperature

$$\sigma = \frac{e^2 g}{2\pi\hbar 8 U_s^2} \sum_{m,k_{Fm}} \left[\sum_{n,k_{Fn}} \frac{\mathcal{G}_{|m-n|}(|\vec{k}_{Fm} - \vec{k}_{Fn}|)}{v_m v_n |\vec{k}_{Fm} - \vec{k}_{Fn}|} \right]^{-1}, \quad (15)$$

where $g=4$ is the current channel degeneracy (for the spin and orbital momentum); v_m is the electron velocity at the Fermi energy (near the Γ point), $v_m = \hbar^{-1}\partial E/\partial k$. Taking into account the nonparabolicity of the energy dispersion of the mth subband $E_{k,m}$ we obtain

$$v_m = \frac{6b\gamma}{4\hbar E_F}\sqrt{E_F^2 - E_m^2} = V_F \sqrt{1 - \frac{E_m^2}{E_F^2}}, \quad (16)$$

where $V_F = 3b\gamma/(2\hbar)$ is the Fermi velocity in the (metallic) massless subband. The Fermi momentum of the electron in the mth subband is

$$k_m(E_F) = \frac{2}{3b\gamma}\sqrt{E_F^2 - E_m^2}, \quad (17)$$

where the bottom of the mth subband is

$$E_m = \gamma \left| 1 + 2\cos\frac{\pi m}{N} \right| \simeq \frac{\hbar V_F m}{3R}. \quad (18)$$

These expressions are essentially similar but not equivalent to the ones obtained with the kp method because of the nonparabolicity of the energy dispersion in the tight-binding model.

For the Fermi energy located within the lowest subband $E_m < E_F < E_{m\pm1}$, the only level of orbital quantization is populated at $T=0$, which has $m=(N+\text{Mod}_3[N])/3$. We use the standard notation $\text{Mod}_3[N]$ for N modulo 3, (the remainder on division of N by 3) here and below. Because the intersubband transitions become allowed only at $E_F > E_{m\pm1}$ the single backscattering term with $m=n$ has to be substituted in Eq. (15) which gives

$$\sigma_z^{(1)} = G_0 g v_m \tau(m, k_F) = \frac{G_0 g \hbar^2}{8 U_s^2} 2 k_F v_m^2 \mathcal{G}^{-1}(2k_F), \quad (19)$$

where $G_0 = e^2/2\pi\hbar$ is the conductance quantum and the electron velocity is

$$v_m^2(E_F) = V_F^2 \times \begin{cases} 1 - \dfrac{E_m^2}{E_F^2} & \text{if } \eta = \text{Mod}_3(N) \neq 0, \\ 1 & \text{if } \eta = \text{Mod}_3(N) = 0, \end{cases} \quad (20)$$

where the index $\eta = \text{Mod}_3(N)$ distinguishes between the zigzag metallic $[\eta = \text{Mod}_3(N) = 0]$ and semiconductor SWNT's $[\eta = \text{Mod}_3(N) \neq 0]$.

Let us now apply the expression (10) for analysis of the conductivity at small E_F. Because at small k_F the function $\mathcal{G}^{-1}(2k_F)$ does not depend on k_F in the leading term, we find the DD conductivity of the zigzag tube at the low doping level depends on the concentration as

$$\sigma_z^{(1)} = \frac{G_0 g E_F \hbar V_F}{4 U_s^2} \mathcal{G}^{-1} \times \begin{cases} \left(1 - \dfrac{E_m^2}{E_F^2}\right)^{3/2} & \text{if } \eta \neq 0, \\ 1 & \text{if } \eta = 0. \end{cases} \quad (21)$$

We drop the argument of $\mathcal{G}^{-1}$ in the expression above because its limit is $4/\pi^2$ at small k_F. The DD conductivity is different for the metallic and semiconductor tubes: it is linear in E_F for the metallic (zigzag, $\eta = 0$) SWNT and it depends on the Fermi energy as

$$E_F \left(1 - \frac{E_m^2}{E_F^2}\right)^{3/2}$$

for the degenerately doped semiconductor SWNT (zigzag, $\eta \neq 0$).

The conductivity at small E_F depends linearly on E_F owing to the matrix element of the Coulomb potential of the 2D remote centers. The square of the matrix element is $\sim q^{-1}$, because in our model the centers are distributed on the (2D) surface of the substrate (the generalization to the 3D case is obvious). The linear dependence of the square of the matrix element in q^{-1} results in the linear dependence of the conductivity on E_F.

At larger E_F the energy dependence of the transport lifetime (of the matrix element of the transition) is different. In this case, Eq. (11) has to be used, which results in a fast exponential growth of the conductivity because of the large suppression of the transitions with increasing momentum transfer. Then, Eq. (21) transforms into

$$\sigma_z^{(1)} \simeq \frac{8 R G_0 g E_F^2}{U_s^2} \sqrt{\frac{h E_F}{\pi\hbar V_F}} \sqrt{1 - \frac{E_m^2}{E_F^2}} \left(1 - \frac{E_m^2}{E_F^2}\right)^2$$

$$\times \exp\left[4(2h-R)\frac{E_F}{\hbar V_F}\sqrt{1 - \frac{E_m^2}{E_F^2}}\right]$$

$$\overset{\epsilon_F \to 1}{\sim} \frac{2^{21/4} R G_0 g E_F^2}{U_s^2} \sqrt{\frac{hm}{3\pi R}}(\epsilon_F - 1)^{9/4}$$

$$\times \exp[8(2h-R)(\epsilon_F - 1)], \quad (22)$$

where $\epsilon_F = E_F/E_m$ is the dimensionless Fermi energy of the semiconductor tube: $\epsilon_F \to 1$ and $\epsilon_F < 1$ in expression (22). This equation gives the conductivity of the zigzag nanotube for the transport through only one channel (of the lowest subband). The result of our calculation [Eqs. (21) and (22)] is presented in Fig. 2, where the drift-diffusion conductivity of
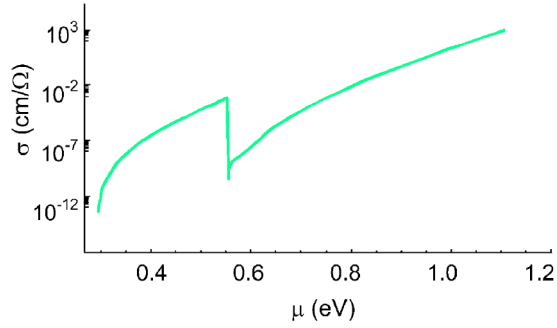
FIG. 2. (Color online) Conductivity of a zigzag [17,0] SWNT vs the electrochemical potential (the doping level).
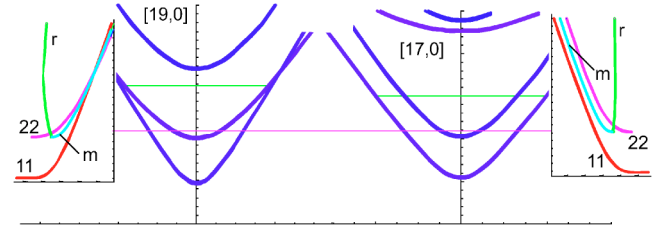

FIG. 3. (Color online) Bandstructures for zigzag SWNT's of two types. Left: $[3q+1,0]$ SWNT; Right: $[3q-1,0]$ SWNT. Doping level is shown as horizontal lines: pink/green (lower/upper) line is for low/high doping level. Insets show the scattering rates for different scattering mechanisms as a function of energy as in left and right diagrams, respectively.

the zigzag SWNT is plotted as a function of the Fermi energy (doping level). With increasing doping level the conductivity grows exponentially. This is not because more carriers are available for transport but due to the energy-dependent transport lifetime that grows exponentially with the increase of the momentum transfer between initial and final states. This momentum transfer is $2k_F \propto E_F$ when the linearization of the TB Hamiltonian is possible. The momentum transfer increases until the Fermi energy reaches the next subband. Then, suddenly, the new backscattering channel opens. The momentum transfer between the next subband and the lowest subband is small at this critical doping level. Thus, the remote impurity scattering becomes very efficient and the conductivity drops several orders of magnitude.

The maximum conductivity may be reached when the Fermi energy is close to the edge of the second subband but lower than it. We note that the phonon scattering may limit the transport, at least, at high temperatures.[40] Therefore, for not very low temperature and high enough doping level, it may be possible to observe switching from the remote scattering to the phonon scattering mechanism.

Also at $T \neq 0$, the finite temperature distribution function makes the $\sigma(E_F)$ dependence smooth near the step at $\epsilon_F \sim 1$, as it will be shown next.

C. Intersubband scattering

The remote impurity scattering between the subbands may happen only when the doping level is high enough to essentially populate the second subband $E_F \gtrsim E_{m \pm 1}$. Then, the scattering rate becomes high and the mean free path becomes short. The expressions for the DD conductivity of armchair metallic, zigzag quasimetallic, and zigzag semiconductor nanotubes are essentially the same in this region. This is because the density of state (DOS) in the vicinity of the Fermi point is a universal function[41] of the energy (doping level), and because there is no special selection rule for the transitions *between different subbands* of the orbital quantization. Let us consider the single Fermi point and find which scattering channel defines the conductivity at $E_F \gtrsim E_{m \pm 1}$. As before, because of the large momentum transfer, we neglect transitions between different Fermi points, which are possible for the armchair SWNT. As shown in Fig. 3, we have two left-going and two right-going (current) states/channels (to be multiplied with the spin and orbital momentum degen-

eracy $g=4$). We introduce four scattering rates τ_{ij}^{-1} and calculate it with the Eq. (13).

Let us assign the index $i=1$ to the subband with the largest momentum at the Fermi energy k_{Fi} (which may change with changing the Fermi energy if the subbands cross). The intrasubband lifetimes $\tau_{11/22}$ are given by the terms in Eq. (7) with $n=m$. There are two intersubband lifetimes $\tau_r^{(12)}$ and $\tau_m^{(12)}$ for the transition with the same/opposite sign of the electron velocity in the initial and final states $|n\rangle$ and $|m\rangle = |n \pm 1\rangle$.

For certain tube symmetry the subband crossing may happen with increasing E_F. When the Fermi energy is above the crossing point the subbands 1 and 2 are interchanged in the equations given below. The case of the metallic (armchair or zigzag) SWNT is similar to the case of noncrossing subbands and will not be considered separately. There is only one difference for the armchair SWNT as compared with the zigzag SWNT case: the dispersion in the subband 1 is massless. Thus, $v_1 = V_F$ is the constant and, by symmetry, $\tau_{11} = \infty$ ("intrasubband" scattering in the lowest subband is not allowed).

We recalculate the distribution functions in all four channels using the Boltzmann equation and taking into account the interchannel transitions. When the scattering is weak one can neglect it and use the equilibrium distribution function. This is not the case for the SWNT at $\epsilon_F \gtrsim 1$, where the scattering rates at the edge of the second subband are very high.

General expression for the DD conductivity with nonzero intersubband scattering is rather cumbersome even in the approximation of the two closest subbands:

$$\sigma = G_0 g \frac{v_1 \tau_r + \dfrac{(v_1+v_2)^2}{2v_1}\tau_{22} - \dfrac{(v_1-v_2)^2}{2v_1}\dfrac{\tau_r}{\tau_m}\tau_{22} + v_2\dfrac{\tau_r}{\tau_{11}}\tau_{22}}{1 + \dfrac{\tau_r}{\tau_m} + \dfrac{2v_2}{v_1}\dfrac{\tau_{22}}{\tau_m} + \dfrac{2\tau_r}{\tau_{11}} + \dfrac{v_2}{v_1}\dfrac{\tau_{22}}{\tau_{11}}\left(1+\dfrac{\tau_r}{\tau_m}\right)}$$

$$\simeq \frac{G_0 g \hbar^2}{8U_s^2}\left\{ v_1 v_2 |k_1-k_2|\mathcal{G}^{-1}(|k_1-k_2|)\right.$$

$$\times\left(1 - \frac{|k_1-k_2|\mathcal{G}^{-1}(|k_1-k_2|)}{|k_1+k_2|\mathcal{G}^{-1}(|k_1+k_2|)}\right) + \frac{(v_1+v_2)^2 v_2}{2v_1}2k_2\mathcal{G}^{-1}(2k_2)$$

$$\left.\times\left[1 - \left(1+\frac{(v_1-v_2)^2}{(v_1+v_2)^2}\right)\frac{|k_1-k_2|\mathcal{G}^{-1}(|k_1-k_2|)}{|k_1+k_2|\mathcal{G}^{-1}(|k_1+k_2|)}\right] + \cdots\right\},$$

$$(23)$$

and we study below the limiting cases where simpler analytical expressions are available.

At small k_{F2}, at the second subband edge (see Fig. 3, the Fermi energy is at lower/pink line), the momentum transfer of the intersubband scattering $(1 \rightleftarrows 2)$ is larger than of the intrasubband scattering $(2 \rightleftarrows 2)$ (see Fig. 3, inset) and the last scattering channel is more effective. The corresponding contribution to the σ is $\propto v_2 \tau_{22}$, where the velocity at the Fermi energy is given by Eq. (16) (the lowest subband $i=1$ has the larger velocity).

According to the inequality

$$\tau_r^{-1} > \tau_{22}^{-1} > \tau_m^{-1} > \tau_{11}^{-1} \qquad (24)$$

the most important term in the σ is $\propto v_1 \tau_r$, if the shortest time is τ_{22}. Thus the DD conductivity reads

$$\sigma = G_0 g v_1 \tau_r + \cdots \simeq \frac{G_0 g \hbar^2}{8 U_s^2} v_1 v_2 |k_1 - k_2| \mathcal{G}^{-1}(|k_1 - k_2|), \qquad (25)$$

where $v_1 = V_F \sqrt{1 - (\hbar V_F)^2/(3RE_F)^2}$ and $v_2 = V_F \sqrt{1 - (2\hbar V_F)^2/(3RE_F)^2}$.

With increasing E_F (see Fig. 3, Fermi energy at upper/green line), since $q_{22} > q_{12}$, then, $\tau_{22} < \tau_r$ (see inset of Fig. 3), and the leading term of Eq. (23) is due to the intrasubband transition $(2 \rightleftarrows 2)$. Then, for the armchair and zigzag $(\eta \neq +1)$ nanotubes, the main term in the DD conductivity is

$$\sigma = G_0 g \frac{(v_1 + v_2)^2}{2 v_1} \tau_{22} + \cdots$$

$$\simeq \frac{G_0 g \hbar^2}{8 U_s^2} \frac{(v_1 + v_2)^2 v_2}{2 v_1} 2 k_2 \mathcal{G}^{-1}(2k_2). \qquad (26)$$

In the zigzag $\eta = +1$ SWNT, the crossing of the lowest subbands occurs in the studied region (shown in Fig. 3, left). In that case $k_{F1} > k_{F2}$ for the E_F is lower than the crossing point, and $k_{F1} < k_{F2}$ for the E_F is higher than the crossing point. So the greatest scattering rate is due to $(2 \rightleftarrows 2)$ intrasubband transition below the crossing point and $(1 \rightleftarrows 1)$ intrasubband transition above the crossing point (see left inset of Fig. 3). Thus, the indices 1 and 2 must be exchanged in Eqs. (23) and (26). By considering these two cases we cover all possible situations and present possible analytical expressions for the DD conductivity within the remote center scattering model.

IV. CONDUCTIVITY AT FINITE TEMPERATURE AND IMPURITY POTENTIAL FLUCTUATION

In the last section we studied the conductivity of the nanotube in the zero temperature limit. The temperature dependence adds to the above result via substituting Fermi-Dirac distribution functions in Eq. (12) instead of step functions as we implicitly used before. We present the numerical result on the temperature dependence of the conductivity in Fig. 4.

We already discussed an important assumption of our model: the phase breaking time has to be short enough which seems to fulfill for the nanotubes due to the e-e interaction
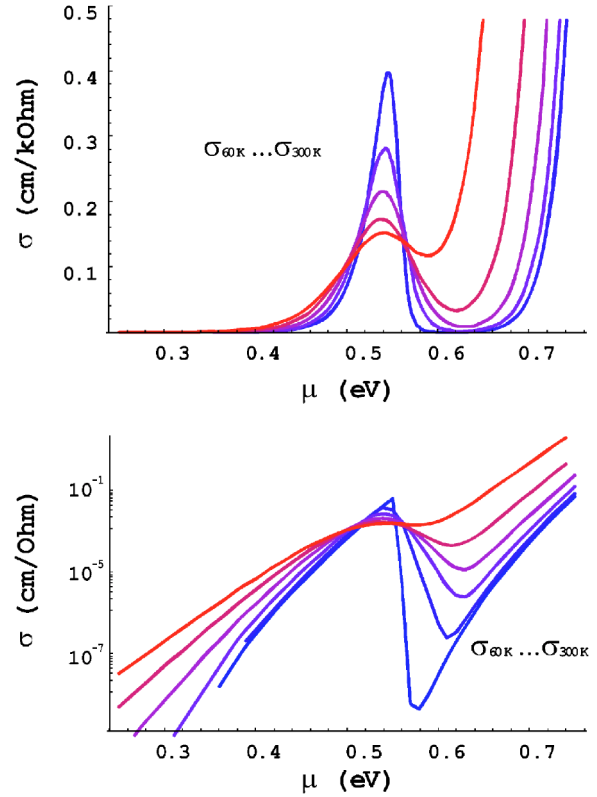

FIG. 4. (Color online) Temperature dependence of the conductivity of a zigzag [17,0] SWNT vs the electrochemical potential in a vicinity of the second subband edge.

and scattering of the electron into the channels/bands which are different from the transport channel/band. This allows one to neglect the interference correction which is normally dominating in pure 1D systems. However, the bare 1D Coulomb potential may still localize the carriers in a nanowire for the infinite channel length. We remind the reader that the *quasi-one-dimensional* potential created at the nanotube channel by the random distribution of remote impurities on the substrate surface has the cutoff length and, thus, a maximum amplitude of the potential. The localization length in a finite system is defined by the average fluctuation of the random potential. Our theory is applicable only in the limit of the electrochemical potential which is much higher than the average fluctuation of the random potential of the remote scatterers.

Since the Coulomb centers are located on the substrate and the 1D electron is on the nanotube, there are two different types of averaging for the 2D distribution of impurities and for the 1D random potential for the electron. The operator of the Coulomb potential is given by Eq. (3). It creates the 1D potential along the nanotube, which reads

$$U_{1D}(z) = \sum_i V(Y_i, Z_i), \qquad (27)$$

where the sum is over impurities that have random positions.

To calculate the average fluctuation of this potential along the nanotube we average it over the impurity positions

$$\delta U = \sqrt{\langle U_{1D}^2 \rangle - \langle U_{1D} \rangle^2} = 2\sqrt{2 + 2\ln 2 + \ln^2 2} \, ee * \sqrt{n_s}. \tag{28}$$

At low temperature, for random impurity distribution, this average fluctuation gives an estimate for a lower bound of the electrochemical potential at which the Born approximation for the scattering is applicable:

$$\mu, E_F \gg U_s. \tag{29}$$

V. EFFECTIVE IMPURITY CHARGE AND SWNT DEPOLARIZATION

Though the actual charge of impurity is not known, we assume it to be an elementary charge e. However, the substrate polarization results in a reduction of this value. As long as the distance between the charge center and the substrate surface is much smaller than all other lengths of the problem: R, h, etc., one may use an effective dielectric function of the substrate to define the effective charge as $e* \rightarrow 2e/(\varepsilon+1)$ where ε is the dielectric function of the substrate and unity stays for the permittivity of the vacuum. It is the leading term of expansion series of the image charge potential, which has to be kept in the remote scattering calculation.

One must take into consideration an effect of depolarization of the Coulomb potential due to the screening by carriers in the nanotube. This changes the remote scattering potential essentially. We calculate this effect using a continuum model for SWNT electrostatics.[35,42] Within the model, the depolarization of the SWNT at a distance D_g from a conducting gate is given by the following expression:

$$V_{\text{eff}} = \frac{1}{1+\alpha}V = \frac{C_Q^{-1}}{C_g^{-1} + C_Q^{-1}}V, \tag{30}$$

where the depolarization α is written in terms of the geometric capacitance per unit length of the SWNT $C_g^{-1} = 2\ln(2D_g/R)$ and the quantum capacitance per unit length, which equals $C_Q^{-1} = 1/(e^2\nu_M)$ for the metallic and degenerately doped semiconductor tube. The depolarization can be taken into account together with the substrate image charge effect simultaneously:

$$e* = e\frac{2}{\varepsilon+1}\frac{C_Q^{-1}}{C_g^{-1} + C_Q^{-1}}. \tag{31}$$

VI. CONCLUSION

In summary, we have developed a microscopic quantum-mechanical model of an electron scattering by remote Coulomb impurities lying on the substrate surface. We consider a uniform 2D distribution of the charged impurities. The theory is readily generalized for the three-dimensional distri-

bution of the impurities whose case is applicable to the modeling of an insulator surrounding the nanotube channel (to be published elsewhere). A general expression for a Fourier transform of the Coulomb potential of a charge which is removed from the nanotube surface is given. The matrix element for calculating the remote impurity scattering in the nanotubes is derived. We obtain a zero and finite temperature conductivity within a drift-diffusion transport model. We assume that the e-phonon and e-e scattering between the electrons in the π-electron band (transport band) and the electrons in other bands (or/and other tubes in the rope, or/and other walls in a multiwall nanotube) presents a fast mechanism of the phase breaking. It allows us to use the Boltzmann equation and neglect interference corrections for the classical conductivity. Self-consistent calculation of the SWNT depolarization factor, taking into account image charges in the substrate, is performed and yields an effective charge of the impurity, used for computing the scattering rate.

The remote impurity scattering is almost negligible for the armchair SWNT's if the Fermi energy is below the edge of the second subband, which is consistent with other calculations for other scattering mechanisms with long range potentials. In contrast, the scattering rate for the zigzag SWNT is high enough. In general, the DD conductivity of the SWNT is $\sim G_0\Lambda$, where the mean free path $\Lambda \sim v\tau$. Analytical expressions for the conductivity are obtained in the limit of small and large momentum transfer. We numerically studied the dependence of the conductivity on the Fermi energy position and found that the highest conductivity (of a semiconductor SWNT) may be observed for the degenerately doped SWNT when the Fermi energy is close to (but lower than) the second subband edge. The dependence $\sigma(E_F)$ is not monotonic. At even higher doping level, the conductivity is low when we take into account the intersubband scattering. This is because Λ becomes short with opening a new scattering channel, when the Fermi energy is higher than the second subband edge. Thus, overdoping of a semiconducting nanotube does not improve its transport properties. Our theory may be applicable for multiwall nanotubes, although, an additional analysis will be required, especially because of different screening.

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