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Electrical conductivity model for quasi-one-dimensional structures

S. A. Botman, S. B. Leble

Immanuel Kant Baltic Federal University,
ul. Aleksandra Nevskogo, 14, Kaliningrad, 236016, Russia
sbotman@innopark.kantiana.ru, sleble@kantiana.ru

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The electron-impurity scattering coefficient of Bloch waves for one dimensional Dirac comb potential is used for calculating the temperature dependence of conductivity within kinetic theory. We restrict ourselves by scattering on impurities that is also modelled by zero-range potential. The conductivity is obtained by standard averaging in momentum space, it is expressed by integral that is evaluated within temperature expansion.

Keywords: Dirac comb, resistivity, kinetic equation, Bloch wave scattering.

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1. Introduction

Quasi one-dimensional structures such as nanowires, nanorods and nanoribbons are important due to wide range of applications, particularly as photodetectors, logic devices, thermoelectric coolers, chemical and biological sensors etc. Knowledge of the electronic properties for this class of materials is essential for practical application.

The latest theoretical and experimental results in the field of transport in low-dimensional structures have demonstrated that by changing particular conditions and parameters of such objects, the conductivity properties in low-dimensional materials can be drastically changed from highly conductive to that of the insulator regime. The transport properties of low dimensional systems is of intense interest for the physics of condensed matter and has been the subject of investigation by many physicists and mathematicians for more than 50 years [1, 2]. Recent progress raises both general academic questions and technological demands in the understanding of transport phenomena through low-dimensional and nanosystems.

In order to elaborate an understanding in the challenging problem of transport in low-dimensional and nanosystems, a theoretical model should be created. Although various methods of calculation may give reasonable results for conductivity in some cases, they do not provide insight into the basic concepts of transport properties in these types of systems.

There are nanoobjects, whose transport properties non-trivially depend on the temperature and diameter of samples [3–6]. These phenomena still need more general theoretical consideration. In pure single crystal nanowires, boundary scattering processes are believed to be dominant. Thus, at low temperatures (up to 300 K) phonon contribution to resistivity is not crucial. One may conclude that scattering on defects determine general resistivity properties of the system.

The aim of this work is to create and verify general model for quasi 1D systems, based on zero range potential (ZRP) model for atomic network and its irregularities, revealing conduction dependence on temperature and structure parameters of real quasi 1D nanoobject. As the nodal element of our model, we take the electron-surface impurity scattering coefficient of Bloch waves.

2. Conductivity calculation

2.1. 1D model

If one of the crystal lattice axis is aligned with nanowire direction, one can treat it as a series of homogeneous atom layers. In order to investigate properties of electrons moving longitudinally though such a nanowire, let us use Dirac comb potential — i.e. potential of equidistant Dirac delta functions:

$$\hat{V} = \beta\delta(x - na), \quad n = 0, \pm 1, \ldots \tag{1}$$

where β — parameter of potential, a — period of cell, x — longitudinal axis coordinate, n — number of transversal layer of atoms.

To enhance the 1D model, we propose to use the fact that defects of a wire are primarily concentrated in the vicinity of the surface. The origin of such phenomenon is due to "contradiction" between the crystal-like net of atoms inside and the cylindrical geometry of the surface. So, going to the 1D model, we transfer all action of such surface deformation to the plane of the wire and model it by 1D ZRP posed at x_0. Next, we introduce total number of electrons also considering 3D wire geometry. Translational symmetry of the model allows us to introduce Bloch wave basis set [9] and corresponding set up quantum scattering problem within this basis. It was shown [7] that scattering probability for a Bloch wave for (1) on point impurity with potential $\gamma\delta(x-x_0)$ can be expressed as follows:

$$W = \left(1-|b_-|^2\right)\left|\frac{\left(b_+e^{ikx_0}+e^{-ikx_0}\right)^2\gamma m}{(b_--b_+)(i\hbar^2k+\gamma m)+\gamma m\left(b_-b_+e^{2ikx_0}+e^{-2ikx_0}\right)}\right|^2, \tag{2}$$

where $k=\sqrt{2mE}/\hbar$ — electron wave number, m — electron rest mass, $\hbar$ — Planck constant, γ — impurity strength, x_0 — impurity position and $b_\pm$ stands for:

$$b_\pm = \frac{e^{\pm iKa}e^{-ika}-1}{e^{\pm iKa}e^{ika}-1}. \tag{3}$$

Here, $K=K(E)$ is momentum energy dispersion relation.

2.2. Kolmogorov equation

Thus, in order to study conductivity of nanostructures It's more convenient to use Kolmogorov equation as defects scattering process prevalent for them. The Kolmogorov [8] equation is a kinetic equation which describes evolution of a distribution function $f(\boldsymbol{k},\boldsymbol{r},t)$ in phase space. Generally, It can be written as:

$$\frac{\partial f}{\partial t}+\dot{\boldsymbol{k}}\frac{\partial f}{\partial \boldsymbol{k}}+\dot{\boldsymbol{r}}\frac{\partial f}{\partial \boldsymbol{r}} = \left.\frac{\partial f}{\partial t}\right|_{coll}, \tag{4}$$

where $\boldsymbol{r}$ — particle position vector, $\boldsymbol{k}$ — particle momentum vector.

There are two factors which cause f to evolve: scattering which causes discontinuous changing of $\boldsymbol{k}$ (right side of equation) and acceleration of the particles (left side of equation). Taking into account semi-classical equations of motions: $\dot{\boldsymbol{r}}=\boldsymbol{v}$ and $\hbar\dot{\boldsymbol{k}}=\boldsymbol{F}$, and assuming electro-magnetic field with components $\boldsymbol{E}$ and $\boldsymbol{H}$ applied to a system, equation (4) for electron moving in this field can be written as:

$$\frac{\partial f}{\partial t}+\boldsymbol{v}\frac{\partial}{\partial \boldsymbol{r}}f-e\left(\boldsymbol{E}+\frac{1}{c}[\boldsymbol{v}\times\boldsymbol{H}]\right)\frac{\partial}{\partial \boldsymbol{k}}f = I_{coll}(f), \tag{5}$$

where $f=f(\boldsymbol{k},\boldsymbol{r})$ is ensemble average nonequilibrium distribution function, $I_{coll}(f)$ is a collision integral. For scattering on static potential one may use:

$$I_{coll}(f) = \sum_{\boldsymbol{k}'} W\left(\boldsymbol{k},\boldsymbol{k}'\right)\left[f\left(\boldsymbol{k}'\right)-f(\boldsymbol{k})\right], \tag{6}$$

where $W\left(\boldsymbol{k},\boldsymbol{k}'\right)$ is a collision probability.

Let's rewrite equation (5) for electrons in solid making several simplifications. First, we will assume that the applied filed is electrostatic ($\boldsymbol{H}=\boldsymbol{0}$). Second, we will focus on the static conductivity problem $\left(\frac{\partial f}{\partial t}=0\right)$. Third, we will adopt homogeneous current hypothesis $\left(\frac{\partial f}{\partial r}=0\right)$. Fourth, we will assume that the deviation of the distribution function from its equilibrium is small ($f=f_0+f_1$, $|f_1|\ll f_0$). Because the equilibrium distribution function f_0 is $\boldsymbol{k}$-symmetric, it has no impact on the collision integral.

Applying all aforementioned simplifications, one can rewrite (5) as follows:

$$-e\boldsymbol{E}\frac{\partial f_0}{\partial \boldsymbol{k}} = \sum_{\boldsymbol{k}'} W\left(\boldsymbol{k},\boldsymbol{k}'\right)\left[f_1\left(\boldsymbol{k}'\right)-f_1(\boldsymbol{k})\right]. \tag{7}$$

For the one dimensional case ($W\left(\boldsymbol{k},\boldsymbol{k}'\right)=W(k,-k)=W$, $f_1(-k)=-f_1(k)$), further simplification is possible:

$$f_1 = \frac{1}{2W}e\boldsymbol{E}\frac{\partial f_0}{\partial \boldsymbol{k}}. \tag{8}$$

Solution of this equation gives us the non-equilibrium distribution function for a given external field $\boldsymbol{E}$ and collision mechanism $I(f)$, which in turn can be used to determine electric current (in form of electron quasiparticle propagation studied by Drude, Sommerfeld, Bloch, Landau):

$$\boldsymbol{j} = -\frac{e}{V}\sum_k \boldsymbol{v}_k f, \tag{9}$$

where summation is performed over qusiparticle states k, $\boldsymbol{v}_k$ is group velocity $\boldsymbol{v}_k = \frac{1}{\hbar}\frac{\partial \varepsilon_k}{\partial \boldsymbol{k}}$, V is sample volume. For real systems, it is useful to transform sum in (9) into integral. Thus, one can find conductivity of the system using (8), (9) and classical definition of conductivity $\boldsymbol{j} = \sigma \boldsymbol{E}$:

$$\sigma = -\frac{e^2}{\pi\hbar}\int \frac{1}{W}\frac{\partial f_0}{\partial k}dE. \tag{10}$$

The equilibrium distribution function is the Fermi-Dirac distribution function.

2.3. Evaluation of integral for low temperatures

Let's consider integral in the following form:

$$I = \int\limits_0^\infty F(E)n'_f(E,T)dE, \tag{11}$$

where $F(E)$ — some function of energy, $n'_f(E,T)$ — first derivative of the Fermi-Dirac distribution function:

$$n_f(E,T) = \left(e^{\frac{E-\mu}{k_B T}} + 1\right)^{-1}, \tag{12}$$

where μ — chemical potential, k_B — Boltzmann constant. The chemical potential can be found from the normalization condition for total numbers of electrons: $N_e = \int n_f(E,T)\rho(E)dE$, where $\rho(E)$ is density of states.

It's known, that at low temperatures $n'_f(E,T)$ has a sharp peak at $E = \mu$. Taking this into consideration, we replace the lower integration limit with $-\infty$ and expand $F(E)$ to a Taylor series at μ point. Thus, for the integral, we have:

$$I = \int\limits_0^\infty F(E)n'_f(E,T)dE = \sum_0^\infty \frac{F^{(n)}(\mu)}{n!}\int\limits_{-\infty}^\infty n'_f(E,T)(E-\mu)^n dE. \tag{13}$$

Next, we introduce new variable: $z = \dfrac{E-\mu}{k_B T}$:

$$I = -\sum_0^\infty \frac{F^{(n)}(\mu)}{n!}\int\limits_{-\infty}^\infty \frac{e^z}{(e^z+1)^2}(zk_BT)^n dz. \tag{14}$$

Obviously, $e^z/(e^z+1)^2 = 1/2(\cosh(z)+1)$ is an even function and $(zk_BT)^n$ is either odd or even depending on number n. Thus, integral can be transformed into:

$$I = -F(\mu) - \sum_1^\infty \frac{F^{(2n)}(\mu)(k_BT)^{2n}}{2n!}\int\limits_0^\infty \frac{e^z}{(e^z+1)^2}z^{2n}dz. \tag{15}$$

Equation (15) describes how integral (11) behaves at low temperatures. The first order approximation gives us a quadratic temperature dependence.

It can be shown using integration by parts that:

$$\int\limits_0^\infty \frac{e^z}{(e^z+1)^2}z^{2n}dz = \left(\frac{2^{2n}-2}{2^{2n}}\right)\zeta(2n)\Gamma(2n), \tag{16}$$

where $\Gamma(n)$ — Gamma function, $\zeta(n)$ — Riemann zeta function:

$$\Gamma(n) = \int_0^\infty z^{n-1} e^{-z} dz = (n-1)!, \tag{17}$$

$$\zeta(n) = \sum_{m=1}^{\infty} \frac{1}{m^n}. \tag{18}$$

Further, one can rewrite (16) in terms of Bernoulli numbers. It can be shown, that for integer n:

$$\zeta(2n) = (-1)^{n+1} (2\pi)^{2n} \frac{B_{2n}}{2(2n)!}, \tag{19}$$

where B_n — n-th Bernoulli number.

Thus, combining (16), (18) and (19) one may obtain first order approximation of integral (11) for low temperatures:

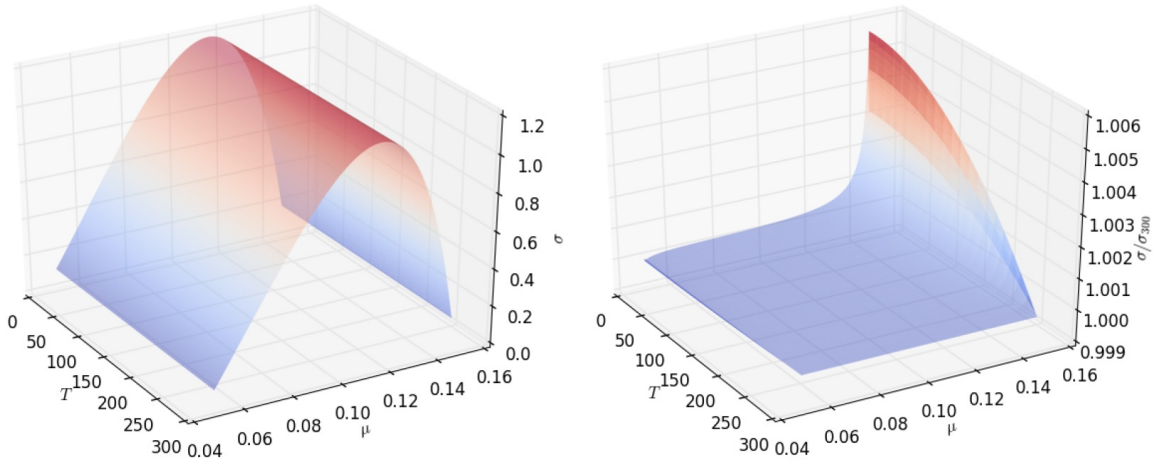
$$I = \int_0^\infty F(E) n_f'(E,T) dE \approx -F(\mu) - \frac{F''(\mu)(k_B T)^2}{8} \pi^2 B_2. \tag{20}$$

Applying obtained expression (20) to conductivity calculation one may obtain the following expression:

$$\sigma = -\frac{e^2}{\pi\hbar} \int \frac{1}{W(E)} \frac{\partial n_f}{\partial k} dE \approx \frac{e^2}{\pi} \sqrt{\frac{2}{m}} \left[\frac{\sqrt{\mu}}{W(\mu)} + \left(\frac{\sqrt{E}}{W(E)} \right)'' \Big|_{E=\mu} \frac{\pi^2 B_2}{8} (k_B T)^2 \right]. \tag{21}$$

3. Results and discussion

In order to test the model, one has to substitute parameters according to Bi nanowire experimental data [3] and calculate conductivity plots. Within the given model, conductivity plots were obtained (Fig. 1). For certain model parameters σ/σ_0 peak can be clearly seen. Thus, the model can exhibit behavior similar to that of real systems. There are two different ways of model implementation: a) choose model parameters in the way that certain basic physical quantities of real systems agrees with ones of model, b) fit model parameters to resemble experimental resistance behavior.



a) b)

FIG. 1. Results of numerical experiments for a) conductivity and b) conductivity normalized by values at $T = 300$. Model parameters for both pictures are: $a = 10$, $\beta = -0.25$, $x_0 = a/2$, $\gamma = -0.1$

The main features of this work are as follows: obtained temperature dependence of conductivity, impurity scattering was implied as main source of electron scattering, result was obtained for Bloch waves. In previous work [11], the expression for d. c. conductivity was obtained for Umklapp processes within memory matrix approach. The first non-constant term of conductivity temperature expansion (21) is quadratic which agrees

with [11]. Depending on the parameters of the model conductivity can either increase or decrease, but there is not enough data to compare results quantitatively [13].

It's known that for low temperatures (up to room temperatures) main contribution to resistivity is made by defect scattering. There is the possibility to choose the 1D model parameters on base of 3D picture, linking its values with cylindrical geometry of a wire. For a regular structure of quasi 1D nanoobject, surface irregularities can be treated as defect which has had its position shifted with respect to the net. Considering nanoobject has length l and diameter d, the parameters diameter dependence is as follows: $\beta = \text{const}, \quad \gamma = \gamma(d) \sim \pi d\, l$. One other parameter, which depends on d and l is the full number of electrons (which is essential for Fermi energy and chemical potential calculation): $N_e = N_e(d) \sim \pi d^2\, l/4$.

The model approbation showed promising results. The next step of the research will be two-dimensional model with cylindrical symmetry assumed. For one of important direction of a development of the theory we would mention [10] where a model of point-like interaction between electrons with spin account and bosons was considered.

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