# NUMERICAL CALCULATION OF 1D ZRP CHAIN ELECTRICAL CONDUCTIVITY

STEPAN BOTMAN

*School of Life Sciences, Immanuel Kant Baltic Federal University*
*Nevskogo 14, 236004 Kaliningrad, Russia*

(received: 14 February 2017; revised: 10 March 2017;
accepted: 20 March 2017; published online: 12 April 2017)

**Abstract:** In this paper we present a numerical procedure for calculation of electrical conductivity in a periodic lattice of one-dimensional zero range potentials with a case of dominant impurity scattering. The conductivity was previously obtained in an integral form via an approximate solution of the kinetic Kolmogorov equation. The proposed approach is based on the quadrature formula for certain type of integrals. The results are compared with the low temperature limit approximation.

**Keywords:** conductivity, kinetic equation, numerical computation

**DOI:** https://doi.org/10.17466/tq2017/21.2/g

## 1. Introduction

It is known that the properties of dimensional structures exhibit a considerable difference from their bulk analogs [1, 2]. These features allow such structures to be utilized in practical applications as the core part of different electronic devices.

We start from the statement that the electric charge transport process is a non-equilibrium process, hence, it implies a kinetic description. One of the ways to approach this problem is to use the Kolmogorov equation for distribution functions [3]. A scattering integral of the system should be provided to solve it.

In some cases a one-dimensional model can be a good approximation for real systems [4]. However, even for this simplified problem, an explicit analytical solution can be found only assuming the number of approximations.

The idea of this work is to exclude the low-temperature approximation from the previously obtained expression for the point impurity induced resistivity in the Dirac comb potential [5]. For this purpose an integration technique was proposed.

In section 2 we start from providing some known electron properties in the Dirac comb potential and the previously obtained expression for conductivity

in an explicit form. Next, in Section 3 a quadrature formula and details of the numerical integration procedure for a certain type of integrals are proposed. Then, the calculation results for different parameters are presented and compared with the low temperature approximation in Section 4. Finally, Section 5 contains conclusions.

## 2. 1D conductivity calculation

Let us start from a model electron moving in the Dirac comb potential:

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

where $\beta$ – the parameter of the potential, $a$ – the period of the cell.

For this model, expressions for the band structure and other relevant physical quantities can be obtained in an analytical form [5]:

$$K(E) = \frac{1}{a}\arccos\left[\cos\left(\frac{\sqrt{2mE}}{\hbar}a\right) + \frac{m\beta}{\hbar\sqrt{2mE}}\sin\left(\frac{\sqrt{2mE}}{\hbar}a\right)\right] \tag{2}$$

$$\rho(E) = \frac{2}{\pi}\left(\frac{dE}{dK}\right)^{-1} = \frac{2}{\pi}K'(E) \tag{3}$$

$$v(E) = \frac{1}{\hbar}\frac{dE}{dK} = \frac{1}{\hbar}\frac{1}{K'(E)} \tag{4}$$

$$m^* = \frac{1}{\hbar^2}\frac{d^2K}{dE^2} \tag{5}$$

where $\rho$ – the density of states, $v$ – the electron velocity, $m^*$ – the effective mass.

An analytical form of (3), (4) and (5) can be trivially obtained. One may notice that (3) can be easily integrated over $E$ which allows straightforward calculation of the Fermi energy.

Let us introduce the Bloch wave basis set for system (1) and use it for the scattering probability calculation.

Assuming point impurity with potential $\gamma\delta(x - x_0)$, the scattering probability can be expressed as follows:

$$W = \left(1 - |b_-|^2\right)\left|\frac{(b_+e^{ikx_0} + e^{-ikx_0})^2\gamma m}{(b_- - b_+)(i\hbar^2k + \gamma m) + \gamma m(b_-b_+e^{2ikx_0} + e^{-2ikx_0})}\right|^2 \tag{6}$$

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

$$b_\pm = \frac{e^{\pm iKa}e^{-ika} - 1}{e^{\pm iKa}e^{ika} - 1} \tag{7}$$

One can see that expression (6) for Bloch waves differs a lot from plain wave scattering:

$$W_{\text{pw}} = \frac{1}{1 + (\frac{k}{\gamma})^2\frac{\hbar^4}{4m^2}} \tag{8}$$

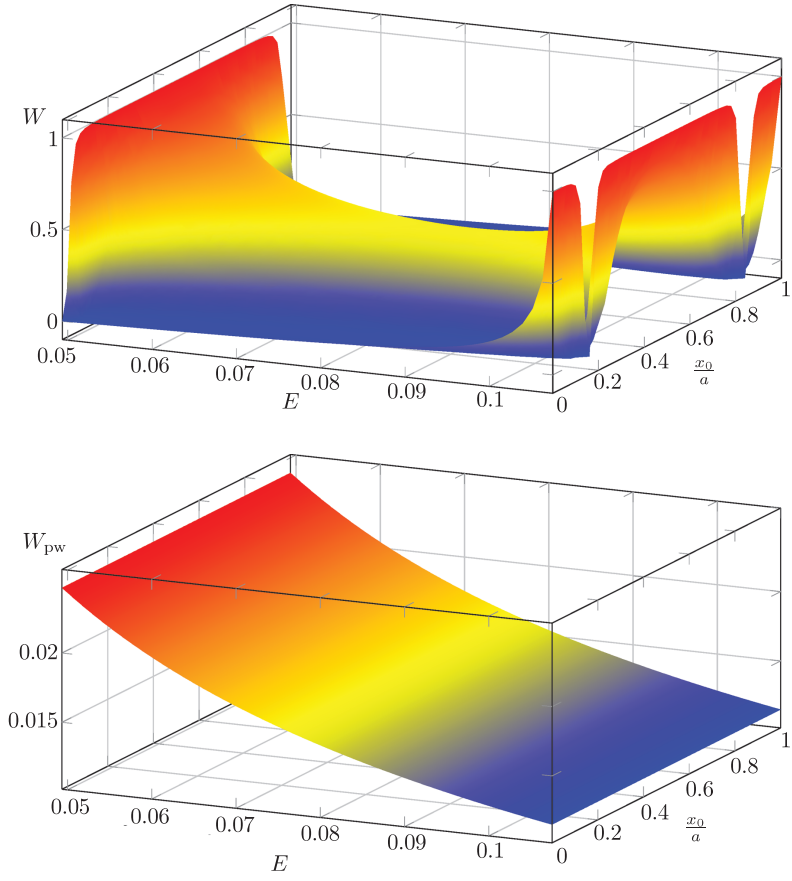


**Figure 1.** Scattering probability for Bloch waves (top) and plain waves (bottom)

For a static conductivity problem with a purely electrostatic field applied, assuming that current is homogeneous and small, one can find conductivity of the system:

$$\sigma = -\frac{e^2}{\pi\hbar}\int \frac{1}{W}\frac{\partial f_0}{\partial k}dE \tag{9}$$

where $f_0$ – the Fermi-Dirac distribution function:

$$f_0(E,T) = \frac{1}{e^{\frac{E-\mu}{k_B T}}+1}$$

## 3. Numerical integration

### *3.1. Quadrature*

Consider the following integral:

$$\int_0^{\infty} F(E)n'_f(E,\mu,T)dE \approx \int_{E_{\min}}^{E_{\max}} F(E)n'_f(E,T,\mu)dE \tag{10}$$

The Fermi-Dirac distribution function:

$$n_f(E,T) = \frac{1}{e^{\frac{E-\mu(T)}{k_B T}} + 1}, \tag{11}$$

where $k_B$ – the Boltzman constant, $\mu$ – the chemical potential ($\mu(T=0) = E_f$, $E_f$ – Fermi energy), $T$ – the temperature.

The behavior of functions $K(E)$ and $n'_F(E,\mu,T)$ makes it impossible to calculate an integral with the classical numerical integrations techniques. Thus, one should create an appropriate quadrature formula.

In order to construct proper numerical procedure let us note that $n'_f$ – a rapidly changing function, and $F(E)$ (which is $K(E)$ or another function) – a slowly changing function.

$$\begin{aligned}\int_{E_{\min}}^{E_{\max}} n'_f(E,T,\mu)F(E)dE &= \sum_{i=1}^{N-1} \int_{E_i}^{E_{i+1}} n'_f(E,T,\mu)F(E)dE \approx \\ &\approx \sum_{i=1}^{N-1} F(\bar{E}_i) \int_{E_i}^{E_{i+1}} n'_f(E,T,\mu)dE = \sum_{i=1}^{N-1} F(\bar{E}_i)\left[n_f(E_{i+1},T,\mu) - n_f(E_i,T,\mu)\right]\end{aligned} \tag{12}$$

In equation (12) we used the fact that function $F(E)$ can be replaced for every small interval $[E_i, E_{i+1}]$ with its value $F(\bar{E}_i)$ at point $\bar{E}_i \in [E_i, E_{i+1}]$, and taken outside the integral sign.

As has been shown before, a derivative of function $K(E)$ equals infinity at the band edge points. In this case, procedure (12) will not suit and one should use the trapezoidal method as a fallback.

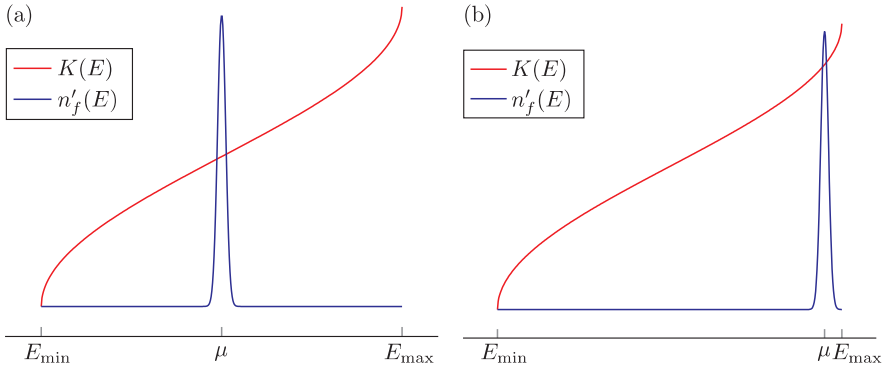


**Figure 2.** Mutual position of $n'_f(E,\mu)$ (blue) and $K(E)$ (red) functions

### *3.2. Grid*

The fact that $n'_f(E)$ decays exponentially to zero on both sides of point $E = \mu$ allows us to shrink the integration area to a relatively small interval around the peak. The integration interval was set in terms of the peak width $2k_BT$. It is natural to set a grid centered on the peak of $n'_F(E,\mu,T)$ functions.

In the case if $\mu$ is far from the band edges, the integration interval is $[\mu - mk_BT, \mu + mk_BT]$, where $m$ – some positive number. In the case if $\mu$ is near the band edge, the grid is chosen in the way that both $\mu$ and the nearest band edge are points of the grid.

### 3.3. Error estimation

The absolute error for (12) can be estimated as follows:

$$\int_{E_{\min}}^{E_{\max}} n'_f(E,T,\mu)F(E)dE = \sum_{i=1}^{N-1} F(\bar{E}_i) \int_{E_i}^{E_{i+1}} n'_f(E,T,\mu)dE + Q$$

where

$$Q = \sum_{i=1}^{N-1} R_i(E) \int_{E_i}^{E_{i+1}} n'_f(E,T,\mu)dE \le \frac{Mh}{2} \int_{E_1}^{E_2} n'_f(E,\mu,T)dE \le \frac{Mh}{2}$$

Next,

$$\left|R_i(E)\right| = \left| \left.\frac{dF}{dE}\right|_{E=\xi} (E - \bar{E}_i) \right| \le \frac{h}{2} \max_{[E_{\min}, E_{\max}]} \left|\frac{dF}{dE}\right| = \frac{Mh}{2}$$

where $\xi \in [E_i, E_{i+1}]$.

In order to estimate the error associated with the integration interval reduction, let us consider the following integral:

$$\int_{E_1}^{E_2} n'_f(E,\mu,T)dE = n_f(E,\mu,T)\Big|_{E_1}^{E_2} = \left. \frac{1}{\frac{E-\mu}{k_BT}+1} \right|_{E_1}^{E_2} \tag{13}$$

Let $E_1 = \mu - mk_BT$ and $E_2 = \mu + mk_BT$, where $m$ – some positive number. Let us substitute $E_1$ and $E_2$ to (13) and set it equal to the full integral $-1$ plus error associated with truncating $\Delta$:

$$\left. \frac{1}{\frac{E-\mu}{k_BT}+1} \right|_{\mu - mk_BT}^{\mu + mk_BT} = \frac{1-e^m}{e^m+1} = -1 + \Delta$$

which means that if the integral of the remainder parts equals $\Delta$ and for a given $\Delta$ one can write:

$$m = \ln\left(\frac{2}{\Delta} - 1\right) \approx -\ln\left(\frac{\Delta}{2}\right)$$

which means that:

$$\int_{\mu - mk_BT}^{\mu + mk_BT} n'_f(E,\mu,T)dE = -1 + \Delta$$

## 4. Results and discussion

The results of numerical experiments compared with a direct evaluation based on low temperature approximation [6] are shown in Figure 3 (original

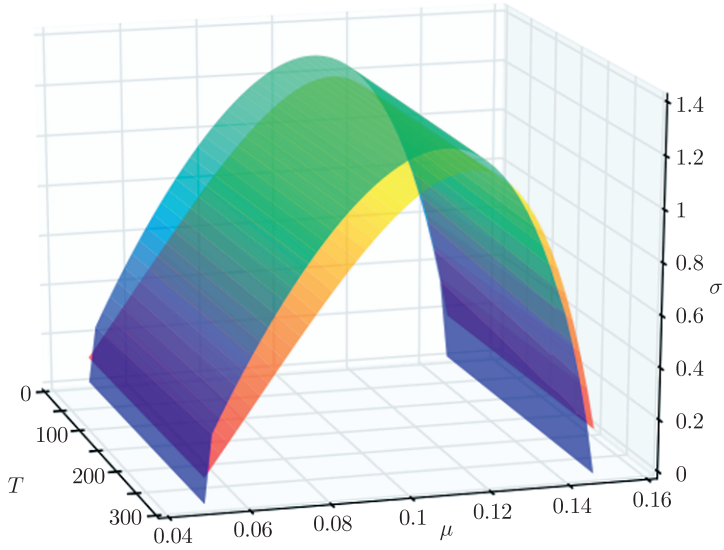


**Figure 3.** Conductivity results obtained within numerical procedure (blue-green surface) and within low temperature approximation (red-yellow surface)

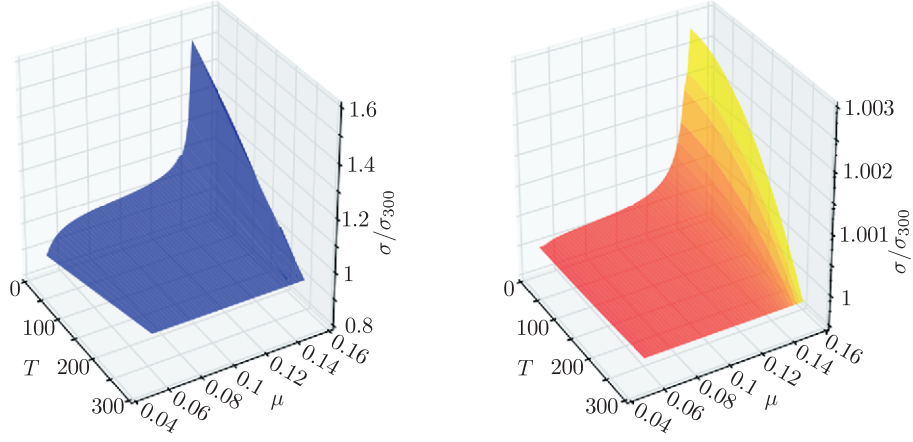


**Figure 4.** Normalized conductivity results obtained within numerical procedure (left) and within low temperature approximation (right)

plots) and Figure 4 (normalised to 300 K plots). Both approaches have shown a tolerable consistency, which supports the validity of the proposed integration method.

It is known that for low temperatures (up to room temperatures) the main contribution to the resistivity is made by defect scattering. For a regular structure of a quasi 1D nanoobject, the surface can be treated as a defect. Considering this, the basic model parameters depend on radius $r$ as follows: $\beta = \text{const}$, $\gamma = \gamma(r) \sim 2\pi r l$. Another parameter which depends on $r$ and $l$ is a full number of electrons (which is essential for the Fermi energy and the chemical potential

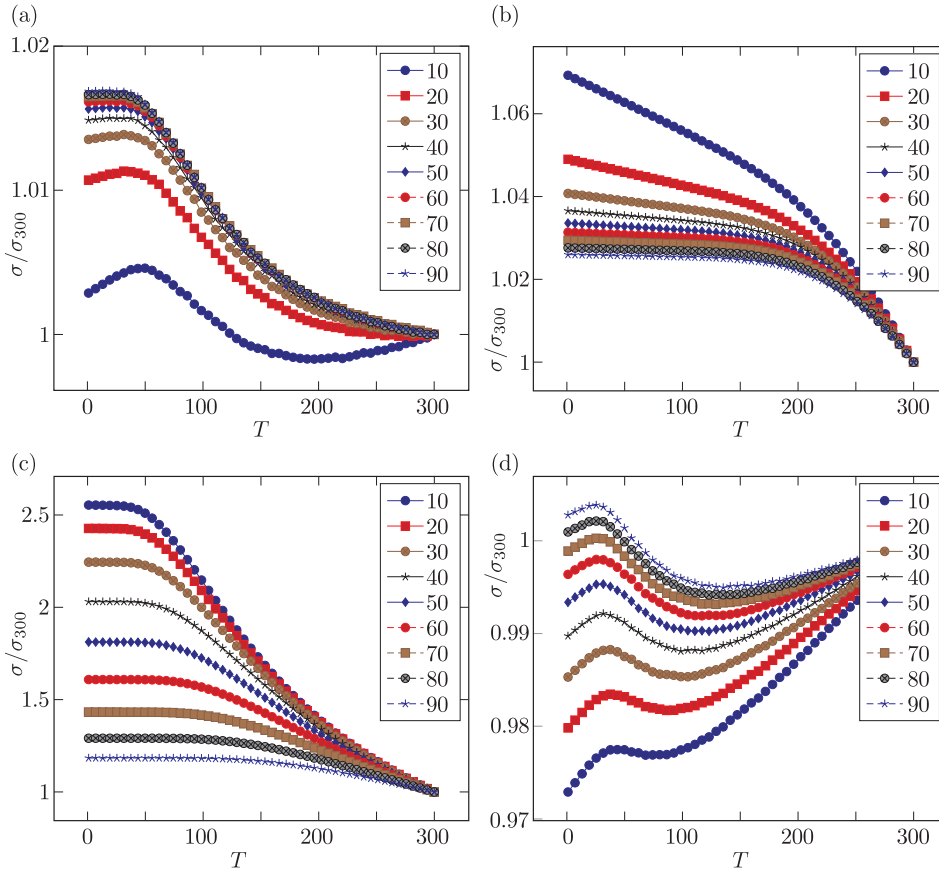


**Figure 5.** Numerical experiments for radius dependence:
(a) $\beta=-1$, $a=10$, $x_0=a/2$, $\gamma=-0.1-0.01r$, $N=1.75+(0.001r)^2$;
(b) $\beta=-0.5$, $a=10$, $x_0=a/2$, $\gamma=-0.1-0.01r$, $N=0.25+(0.001r)^2$;
(c) $\beta=-1.5$, $a=10$, $x_0=a/2$, $\gamma=-0.1-0.01r$, $N=0.25+(0.005r)^2$;
(d) $\beta=-1.0$, $a=10$, $x_0=a/2$, $\gamma=-0.1-0.001r$, $N=1.8+(0.001r)^2$

calculation): $N_e=N_e(d)\sim\pi r^2 l$. Next, the following model for radius dependence of parameters was considered: $a=const$, $\beta=const$, $\gamma=\gamma_0+\gamma_1 r$, $N=N_0+(N_1 r)^2$. The results are shown in Figure 5.

The model approbation has shown promising results with a vast variety of dependency types observed. However, there is no way at the moment to confidently link the parameters of the model to a real system. The next step of the research will be a three-dimensional model with a cylindrical symmetry assumed.

## 5. Conclusions

In order to calculate the impurity induced electrical conductivity a quadrature formula for integration was proposed. The obtained results showed agreement with the known low temperature approximation formula. The variety of conductivity temperature dependences encourage optimism towards future development

of this model, including linking it to the experimental results. The proposed integration method can be also used in other problems, where the integrand consists of an integrable quick changing function and a slow changing function.

## *Acknowledgements*

I would like to express my great appreciation to Sergey Leble, PhD for his guidance, encouragement and continuous support during the planning and development of this research work. His willingness to give his time so generously is very much appreciated.

## *References*

[1] Dresselhaus M, Lin Y-M, Rabin O, Black M, Kong J, and Dresselhaus G 2007 *Nanowires*, in *Springer Handbook of Nanotechnology*, Springer 113
[2] Lin Y-M, Sun X, and Dresselhaus M S 2000 *Physical Review B* **62** (7) 4610
[3] Kolmogoroff A 1931 *Mathematische Annalen* **104** (1) 415
[4] Demkov Yu and Ostrovskii V 2013 *Zero-range potentials and their applications in atomic physics*, *Springer Science & Business Media*
[5] Botman S and Leble S 2016 *TASK Quarterly* **20** (2) 197
[6] Botman S and Leble S 2017 *Nanosystems: Physics, Chemistry, Mathematics* **8** (2) 231