BLOCH WAVE – ZRP SCATTERING AS A KEY ELEMENT OF SOLID STATE PHYSICS COMPUTATION: 1D EXAMPLE

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Abstract: This paper presents calculation of the electron-impurity scattering coefficient of Bloch waves for one dimensional Dirac comb potential. The impurity is also modeled as delta function pseudopotential that allows explicit solution of the Schrodinger equation and scattering problem for Bloch waves.

Keywords: Dirac comb, resistivity, Boltzmann equation, scattering

1. Introduction

There are many processes in solid state physics in which the electron mean velocity is small in the sense that its de Broglie wavelength is large compared to the effective potential characteristic scales. For example, it relates to such important processes as transport phenomena. In such circumstances the behavior of electrons is effectively described by the so-called Zero Range Potentials (ZRP) [1], which use an essentially simplified theoretical description.

Important ingredients of the transport theory contain a basic notion of the electron state description in terms of Bloch functions and their derivatives such as the spectrum description, density of states and Fermi energy level. The mechanism of low temperature conductivity includes scattering on impurities the contribution of which essentially increases in case of mesoscopic and nano- problems, for which the surface atom contribution is relatively large.

The scattering theory provides powerful direct ways for treatment of quantum systems and enables obtaining essential information about these systems. In Solid State Physics the scattering theory has been used to describe various transport phenomena. The main feature in this case is the presence of a periodic potential due to the lattice structure which results in the basis of Bloch functions.

Scattering in terms of Bloch functions has been studied in a number of works. The works of Morgan [2] and Newton [3] are based on the Korringa-Kohn-Rostoker equations [4, 5] and give rather a general description of Bloch electron scattering on impurities in crystals.

Unfortunately, the resulting expressions for the scattering amplitudes are complicated, their direct use in evaluation of transport properties is difficult. In this paper we propose, perhaps, the simplest model formulation and realization of the scattering problem on the basis of the Dirac comb potential and the ZRP model for an impurity. We will repeat that the mean velocity of conductivity electrons is low in the above mentioned sense [1]. It justifies applications of zero-range potentials (ZRP).

The Dirac Comb model is a special case of the Kronig-Penney model [6], which ranks among the small number of exact solvable problems in quantum mechanics. It is interesting to investigate aspects of electron Bloch scattering within a simple model which allows an insight into basic properties of the Bloch electron scattering in systems with periodic potentials.

In this work we construct flux normalized Bloch wavefunctions and use them for determining the impurity scattering probability. In section 2.1 we start from reproducing some classical results of electron properties in the Dirac comb potential. Next, in section 2.3 flux normalization for a Bloch wave basis set is provided. Then, in section 3.2 we use the obtained expression for energy dispersion to study the chemical potential temperature dependence for the considered system. Finally, in section 4 the ZRP impurity scattering probability is derived in explicit form. Section 5 contains summary and discussion.

2. Dirac comb potential Bloch wave functions

2.1. Statement of problem

Let us reformulate the classical calculation (see, *e.g.* [7]) of electron properties in a lattice under the influence of an attractive Dirac Comb potential presented for the reader's convenience in notations, specified for scattering problem applications. By definition the Bloch wavefunction must be an eigenfunction of both Hamilton and translation operators [7].

Consider a problem of stationary states of an electron in the potential of equidistant Dirac delta functions:

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

where β is a parameter of the potential, the lattice constant is denoted as a. Generally, the parameter β can be both negative (attractive zero range potential (ZRP)) and positive.

Each delta function in (1) represents the simplest ZRP. For such a case, the Shrodinger equation with the potential (1) can be replaced by the following set of the boundary conditions for the Hamiltonian eigenfunction (see *e.g.* [1]):

$$\psi'\Big|_{x=na-0}^{x=na+0} - \frac{2m}{\hbar^2}\beta\psi\Big|_{x=na} = 0, \quad n = 0, \pm 1, ... \tag{2}$$

where ψ is the wavefunction. Obviously, the first term of the expression (2) is non zero and the wavefunction ψ has a finite discontinuity of the first derivative at the points of potential location.

The wave function for the domain between two point potentials located at $x = 0$ and $x = a$ (*i.e.* for $x \in [0, a)$) should be a linear combination of two plain waves:

$$\psi_{[0,a)} = A\ e^{ikx} + Be^{-ikx} \tag{3}$$

where A, B – two complex constants, the wave vector $k = \sqrt{2mE}/\hbar$ is proportional to an electron momentum.

According to the definition, the shift operator acts as

$$\hat{T}_a\psi(x) = \psi(x + a) \tag{4}$$

A corresponding spectral problem for (4) introduces the parameter μ:

$$\hat{T}_a\psi(x) = \psi(x + a) = \mu\psi \tag{5}$$

It is known that the Hamiltonian spectral problem with the condition (5) has only a continuous spectrum. The condition of the Bloch wavefunction ψ boundedness at both infinities is guaranteed by the restriction

$$|\mu| = 1 \rightarrow \mu = e^{iKa} \tag{6}$$

where K is a real constant, its link with the Hamiltonian eigenvalue E defines the structure of the continuous spectrum. The finite solid is often modeled by the Born-von Karman condition that leads to the discrete spectrum. In our 1D case for K:

$$K = \frac{2\pi n}{Na}, \quad n = 0, \pm 1, ... \tag{7}$$

2.2. Solutions of the problem: left/right Bloch functions

Applying the shift operator (5) to $\psi_{[0,a)}$ wavefunction (3) and taking into account (6) one can obtain the wavefunction for the domain $[-a, 0)$:

$$\psi_{[-a,0)} = \hat{T}_a\psi_{[0,a)} = e^{iKa}\left(A\ e^{ik(x+a)} + Be^{-ik(x+a)}\right) \tag{8}$$

Substitution of (3) and (8) into the continuity condition for ψ at point $x = 0$ and (2) gives the system:

$$A\left(e^{iKa}e^{ika} - 1\right) + B\left(e^{iKa}e^{-ika} - 1\right) = 0 \tag{9}$$

$$A\left(ik - ike^{iKa}e^{ika} - \frac{2m}{\hbar^2}\beta\right) + B\left(-ik + ike^{iKa}e^{-ika} - \frac{2m}{\hbar^2}\beta\right) = 0 \tag{10}$$

The system of equations (9)) and (10)) is system of linear homogeneous equations for A and B. The condition of a nonzero solution (zero determinant of the matrix of coefficients) gives:

$$\cos(Ka) = \cos(ka) + \frac{m\beta}{\hbar^2}\frac{\sin(ka)}{k} \tag{11}$$

Equation (11) is well known and in fact gives a band structure – the dependence between energy $E = (\hbar k)^2/2m$ and the quasi wave vector K. A typical band structure of the Dirac comb is shown in Figure 2. The tuning of β and a parameters allows setting the arbitrary zone/bandgap ratio (as shown in Figure 3) which can be useful for building real systems approximations.

It is essential to note that for every allowed energy we will have two Bloch functions: for $|K|$ and $-|K|$, which are associated with left and right Bloch waves.

The solution of system (9), (10) gives the dependence between coefficients $A_\pm = f_\pm(k,K,\beta)B_\pm$ and furthermore several equivalent forms of the solution can be obtained:

$$A_\pm = B_\pm\left[1 + i\frac{4m}{\hbar^2}\frac{k}{\beta}\left(e^{\pm iKa}e^{-ika}\right)\right] \tag{12}$$

or

$$B_\pm = A_\pm\frac{e^{\pm iKa}e^{ika} - 1}{e^{\pm iKa}e^{-ika} - 1} \tag{13}$$

From now on we will use (13), as its form is more convenient.

Let us introduce the following coefficients b_+ and b_- for shortening:

$$A_\pm = B_\pm b_\pm, \quad b_\pm = \frac{e^{\pm iKa}e^{-ika} - 1}{e^{\pm iKa}e^{ika} - 1} \tag{14}$$

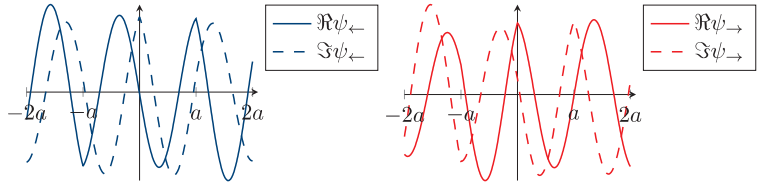

Figure 1. Left and right Bloch functions (real and imaginary parts are labeled with continuous and dashed lines respectively)

Thus, the physical meaning of such classification of Bloch waves is related to the corresponding fluxes defined in the forthcoming section. Moreover, the free choice of constants allows the left and right waves to be independently normalized. Namely the equations (18), (17) and (13) are used to determine coefficients $A_\pm$ and $B_\pm$ consequently.

2.3. Flux normalization

It is essential to note that K in (11) is in the cosine, so for every allowed energy we will have two Bloch functions: for K and $-K$. The Bloch functions for K and $-K$ will give us the appropriate flux in opposite directions.

For one dimension the flux can be calculated as follows:

$$j(\psi) = -i\frac{\hbar}{2m}\left(\psi^* \frac{d}{dx}\psi - \psi\frac{d}{dx}\psi^*\right) \tag{15}$$

Direct substitution (3) into (15) yields:

$$j(\psi) = \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right) \tag{16}$$

Equation (16) is true for any x. The substitution of (13) into (16) gives:

$$j(\psi_{\rightleftarrows}) = \frac{\hbar k}{m}|A_{\pm}|^2 \frac{\pm\sin(Ka)\sin(ka)}{1-\cos(\pm Ka+ka)} \tag{17}$$

Next, equation (17) is used for flux normalization:

$$j(\psi_{\rightleftarrows}) = \pm 1 \tag{18}$$

3. Solid state physics ingredients

3.1. Density of states

Moreover, (11) allows deriving analytical expressions for several solid state physics quantities such as density of states and electron velocity (see [7]):

$$\rho(E) = \pm\frac{2}{\pi}\left(\frac{dE}{dK}\right)^{-1} = \frac{2}{\pi}K'(E) \tag{19}$$

$$v(E) = \frac{1}{\hbar}\frac{dE}{dK} = \frac{1}{\hbar}\frac{1}{K'(E)} \tag{20}$$

Expressing $K(E)$ from (11):

$$K(E) = \frac{1}{a}\arccos\left[\cos\left(\frac{\sqrt{2mE}}{\hbar}a\right) + \frac{m\beta}{\hbar\sqrt{2mE}}\sin\left(\frac{\sqrt{2mE}}{\hbar}a\right)\right] \tag{21}$$

evaluating the derivate of (21) one may obtain an analytical form of (19) and (20).

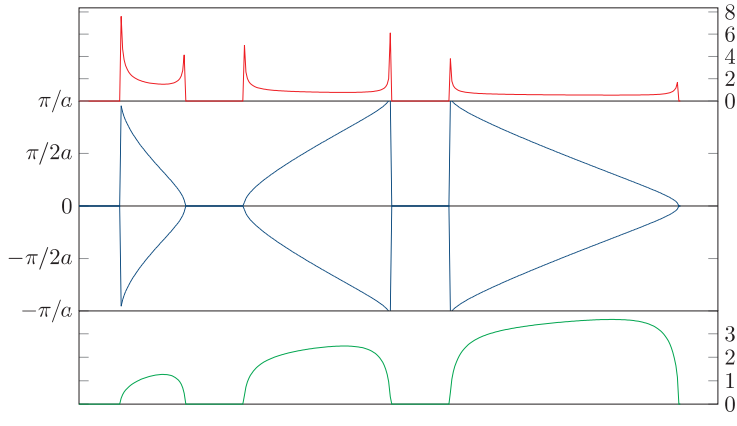

Figure 2. Density of states (top, red), energy dispersion (middle, blue), electron velocity (bottom, green)

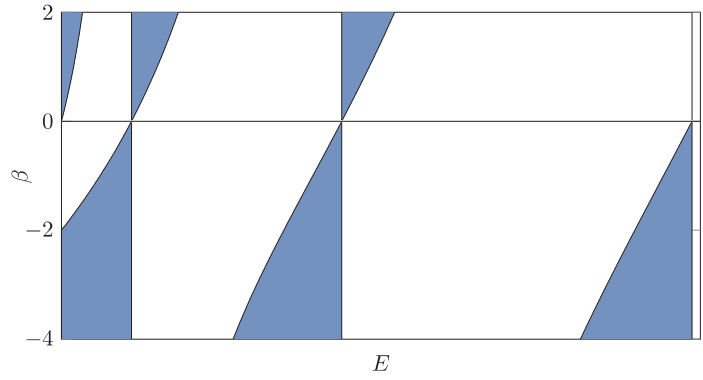

Figure 3. Zone edges depending on β parameter (parameter $a=1$)

3.2. Fermi energy

The obtained expression (19) for the density of states allows us to calculate the Fermi energy and chemical potential for the electron in the Dirac comb potential. We start from the Fermi-Dirac distribution:

$$n_f(E,T) = \frac{1}{e^{\frac{E-\mu(T)}{k_B T}} + 1} \tag{22}$$

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

Obviously, (22) must satisfy the normalization condition for a total number of electrons. We will take into account that at zero temperature the Fermi distribution function reduces to a step function:

$$\begin{aligned} N_e = \int_0^\infty n_f(E,T=0)\rho(E)dE = \int_0^{E_f} \rho(E)dE = \\ \sum_{\text{valence bands}} \frac{2a}{\pi} K(E)\Big|_{E_{\text{band min}}}^{E_{\text{band max}}} + \frac{2a}{\pi} K(E)\Big|_{E_{\text{band min}}}^{E_f} = \\ \sum_{\text{valence bands}} 2N + \frac{2a}{\pi} K(E)\Big|_{E_{\text{band min}}}^{E_f} \end{aligned} \tag{23}$$

where $\rho(E)$ – the density of states, N_e – the total number of electrons, N – the number of cells in wire (assuming each atom in wire has only one electron). Thus, E_f can be calculated within this model using (23) and (21).

3.3. Chemical potential

The chemical potential can be obtained in a similar way:

$$N_e = \int_0^\infty n_f(E,T,\mu)\rho(E)dE = \int_0^\infty n_f(E,T,\mu)\frac{2a}{\pi}K'(E)dE \tag{24}$$

In some cases it may be more convenient to use the following form (here only the valence band is taken into account):

$$N_e = \int_0^{\infty} n_f(E,T,\mu)\frac{2}{\pi}K'(E)dE = \frac{2a}{\pi}\underbrace{n'_f(E,T,\mu)}_{0 \text{ or } 1}\underbrace{K(E)}_{0 \text{ or } \pi/a}\Big|_{E_{\text{band min}}}^{E_{\text{band max}}} - \frac{2a}{\pi}\int_{E_{\text{band min}}}^{E_{\text{band max}}} n'_f(E,T,\mu)K(E)dE = \tag{25}$$
$$2 - \int_{E_{\text{band min}}}^{E_{\text{band max}}} n'_f(E,T,\mu)K(E)dE$$

The chemical potential temperature dependence calculated within the numerical procedure showed negligible shifts for points within the band except for the k_BT neighborhood of the upper bandedge, where the local maximum is formed.

4. Impurity scattering

Generally the Bloch wavefunction for the Dirac comb potential (1) has the following form:

$$\psi_{\rightleftarrows} = e^{\pm iKna}\left(A_{\pm}e^{ikx} + B_{\pm}e^{-ikx}\right) \quad \text{for } x \in [na,(n+1)a) \tag{26}$$

Let us assume that electron Bloch wave propagates from $-\infty$ to ∞ and scatters at the potential center $\gamma\delta(x-x_0)$ located at point $x_0 \in (ma,(m+1)a)$. Thus, the scattering ansatz appears as follows:

$$\begin{aligned}\Psi_{(ma,x_0]} &= C_i\psi_{B+} + C_s\psi_{B-}\\ \Psi_{[x_0,(m+1)a)} &= C_t\psi_{B+}\end{aligned} \tag{27}$$

where index i stands for incident, s stands for scattered, t stands for transmitted waves.

Now a boundary condition (analogue to (2)) should be applied at point x_0 that gives:

$$\begin{aligned}&C_te^{iKma}ik\left(A_+e^{ikx_0} - B_+e^{-ikx_0}\right) -\\ &C_ie^{iKma}ik\left(A_+e^{ikx_0} - B_+e^{-ikx_0}\right) -\\ &C_se^{-iKma}ik\left(A_-e^{ikx_0} - B_-e^{-ikx_0}\right) =\\ &\frac{2m\gamma}{\hbar^2}C_te^{iKma}\left(A_+e^{ikx_0} + B_+e^{-ikx_0}\right)\end{aligned} \tag{28}$$

We should add one more condition for continuity at point x_0).

$$\begin{aligned}&C_ie^{iKma}\left(A_+e^{ikx_0} + B_+e^{-ikx_0}\right) +\\ &C_se^{-iKma}\left(A_-e^{ikx_0} + B_-e^{-ikx_0}\right) =\\ &C_te^{iKma}\left(A_+e^{ikx_0} + B_+e^{-ikx_0}\right)\end{aligned} \tag{29}$$

Both (28) and (29) form a system. We state $C_i = 1$ (it corresponds to the incident flux normalized to one) and solve the system for C_s and C_t:

$$C_s = -\gamma m\left(A_+ e^{ikx_0} + B_+ e^{-ikx_0}\right)^2 \left[i\hbar^2 k\left(A_- B_+ - A_+ B_-\right) + \gamma m\left(A_- B_+ + A_+ B_-\right) + A_- A_+ \gamma e^{2ikx_0} m + B_- B_+ \gamma e^{-2ikx_0} m\right]^{-1} \tag{30}$$

$$C_t = -i\hbar^2 k\left(A_- B_+ - A_+ B_-\right)\left[i\hbar^2 k\left(A_- B_+ - A_+ B_-\right) + \gamma m\left(A_- B_+ + A_+ B_-\right) + A_- A_+ \gamma e^{2ikx_0} m + B_- B_+ \gamma e^{-2ikx_0} m\right]^{-1} \tag{31}$$

And one in shorter form, using (14):

$$C_s = -\frac{1}{B_-}\frac{\left(b_+ e^{ikx_0} + e^{-ikx_0}\right)^2 \gamma m}{(b_- - b_+)(i\hbar^2 k + \gamma m) + \gamma m\left(b_- b_+ e^{2ikx_0} + e^{-2ikx_0}\right)}$$
$$C_t = \frac{i\hbar^2 k\left(b_- - b_+\right)}{(b_- - b_+)(i\hbar^2 k + \gamma m) + \gamma m\left(b_- b_+ e^{2ikx_0} + e^{-2ikx_0}\right)} \tag{32}$$

$W = |C_s|^2$ gives the scattering probability. $T = |C_t|^2$ gives the transmission probability. In order to calculate the scattering probability one should replace $A_\pm$ and $B_\pm$ with (13) and (17) taking into account flux normalization (18).

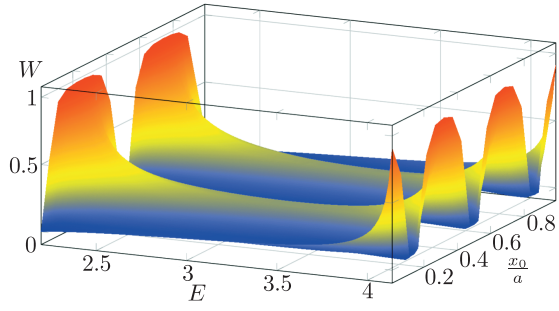

Figure 4. Scattering probability W depending on scatterer position x_0

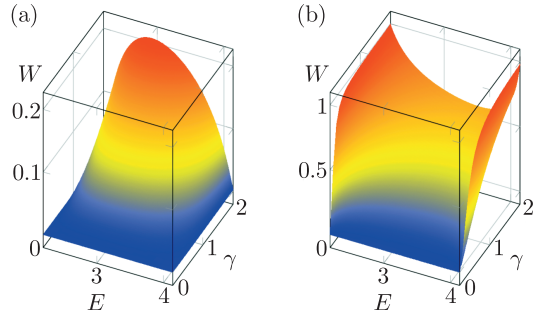

Figure 5. Scattering probability W depending on scatterer strength γ, where (a) – scatterer located at $x_0 = \frac{a}{2}$ and (b) – scatterer located at $x_0 = \frac{a}{4}$

5. Summary and discussion

The scattering probability of a Bloch electron on impurity depending on the scatterer parameters and energy was obtained. The data showed nontrivial behavior of the scattering probability. It is planned to apply the results in the transport phenomena theory.

One dimensional scattering problem gives us a good "toy" model that has a very interesting application in the inverse scattering method of the soliton theory (nonlinear equation of Korteweg-de Vries type) [8]. The results of scattering from the ZRP theory may be applied in the context of the integrable potentials theory as well [9], its Bloch functions version could give an impulse to develop the theory.

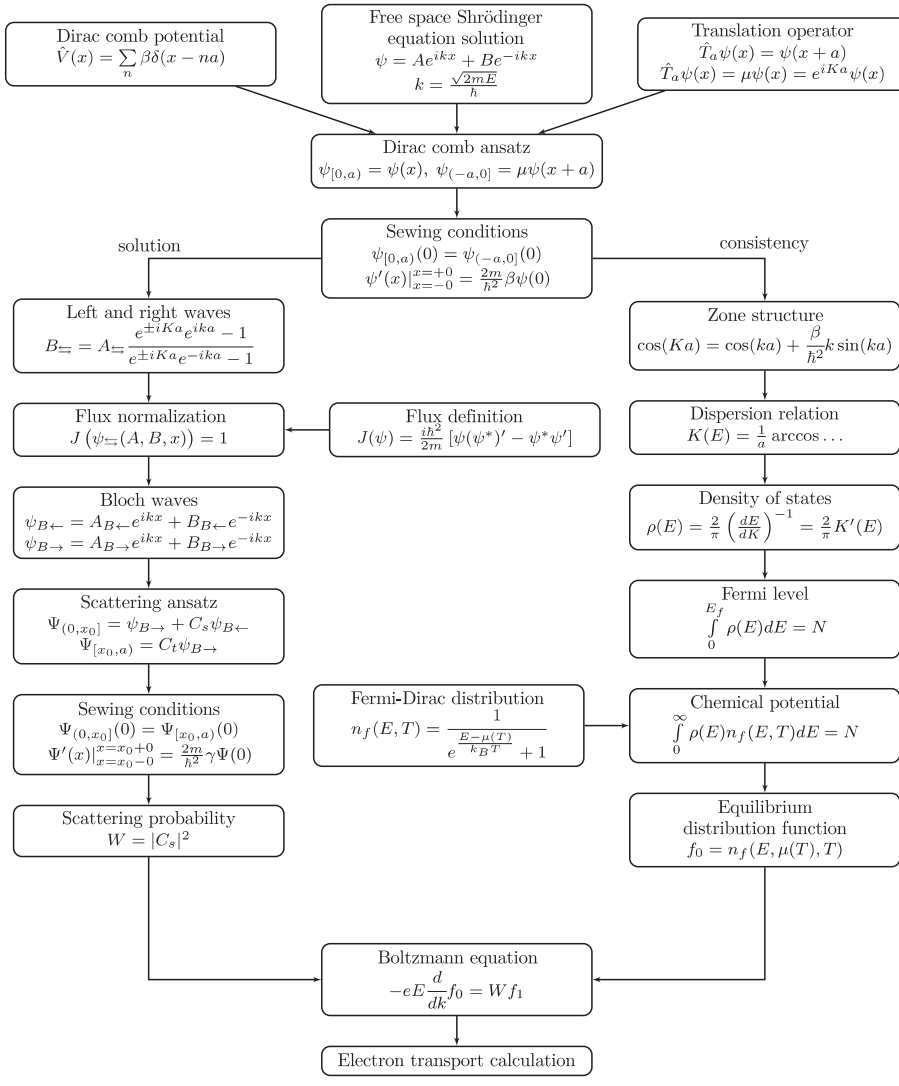

Figure 6. Resistivity calculation workflow

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