Spin-polarized scattering of 2D Dirac fermion on a region of arbitrary shape

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Abstract

Spin-dependent scattering of 2D Dirac fermions on a single-connected region of an arbitrary shape has been developed.

Introduction

The use of nanostructured systems as elements of nanoelectronics requires a qualitatively new level of modeling of their electronic and transport properties with a ground on a full quantum-mechanical description of the systems. For most problems, this leads to the problems of nonrelativistic quantum mechanics, the approaches to the solution of which are well developed. For a number of low dimensional systems, in particular for graphene and graphene-like materials, the correct description is the description in the framework of relativistic quantum mechanics or quantum field theory in two dimensional space.

Simulation of quantum coherent transport in two-dimensional systems necessarily involves calculation of both bound states and scattering states of the system. The known approaches rely mainly on simplest analytically solvable problems corresponding to rectangular and radial potential wells of a finite depth. A systematic analysis of the problems with a general type of the boundary is practically absent for scalar scattering models, and almost completely absent for the case of spin dependent scattering.

Here we consider an approach to numerical analysis of the 2D quantum scattering problem of Dirac particles on a two-dimensional, simply connected object of an arbitrary shape.

1 Model

Let our scattering quantum system be in a simply connected two-dimensional domain D with boundary Γ. Two-dimensional Dirac equation can be represented in the form [1]

$$\left(\sigma \cdot (i\hbar \nabla - \frac{e}{c}\vec{A}) + \sigma_z mc^2 + V(\vec{r})\right) \Psi(\vec{r}) = E\Psi(\vec{r}) \tag{1}$$

where, c is the speed of light, m is the mass term, $\vec{A}\,(\vec{r})$ is the vector potential of an external electromagnetic field, $V(\vec{r})$ is the scalar potential, $\sigma = (\sigma_x, \sigma_y)$ is two-dimensional vector of Pauli matrices, σ_z is the third Pauli matrix. In what follows, we use a system of units with the speed of light and the Planck constant to be equal to unity.

For the problems we consider a macroscopic external electromagnetic field can be omitted, and the scalar potential will be not an electromagnetic, but only determined by properties of the scattering region. Then, in the region external to the scatterer, this scalar potential is set to zero, and inside the scatterer, it is to a constant positive potential

$$V(\vec{r}) = \begin{cases} 0, & \vec{r} \notin D \\ V_0, & \vec{r} \in D \end{cases} \tag{2}$$

The scattering problem is stated as follows. The wave function of an initial state is an incident plane wave of the form $\Psi_i(\,\vec{r}\,) = A\exp(i\vec{k}\cdot\vec{r})$ with the energy $E = \sqrt{\vec{k}^2 + m^2}$, the final state is represented as a superposition of the incident Ψ_i and scattered waves Ψ_s

$$\Psi(\,\vec{r}\,) = \Psi_i(\,\vec{r}\,) + \Psi_s(\,\vec{r}\,) \tag{3}$$

As usual, one represents the Hamilton operator in the form of a free particle operator $\hat{H}_0$ and a perturbation operator $\hat{V}$. Then introducing the Green's function into consideration by the relation $\hat{G}(E) = \left(E - \hat{H}\right)^{-1}$, one can obtain the connection between an unperturbed and the full Green's functions in the form of the so-called Dyson equation [2]

$$\hat{G} = \hat{G}_0 + \hat{G}\hat{V}\hat{G}_0 \tag{4}$$

The formal solution to the scattering problem can be represented in the form of the integral equation - the Dyson equation [2, 3]

$$|\Psi\rangle = |\Psi_i\rangle + \hat{G}_0\hat{V}\,|\Psi\rangle\,. \tag{5}$$

In the coordinate representation, it has the form

$$\Psi(\vec{r}) = \Psi_i(\vec{r}) + \int d\vec{r}' \, \langle \vec{r}| \, \hat{G}_0 \, |\vec{r}'\rangle \, \hat{V}(\vec{r}')\Psi(\vec{r}') \tag{6}$$

integration in (6) is carried out over all space.

The only approximate solution of equation (6) is usually possible and the methods essentially depend on the dimension of the space [3]. In one-dimensional case, it is important to take into account multiple scattering; in spaces of dimensions three and higher, the so-called Born approximation is almost always excellent, when the initial state function is substituted for the full wave function in the right-hand side of (6)

$$\Psi^{(1)}(\vec{r}) = \Psi_i(\vec{r}) + \int d\vec{r}' \, \langle \vec{r}| \, \hat{G}_0 \, |\vec{r}'\rangle \, \hat{V}(\vec{r}')\Psi_i(\vec{r}') \tag{7}$$

For two-dimensional problems, the sufficiency of this Born approximation is still open. In what follows we restrict ourselves to this approximation only, taking into account additional difficulties caused by the spinor nature of the wave functions of our problem.

The Green function for the two-dimensional free field Dirac equation can be obtained as follows. Since the anticommutation relations for the Pauli and Dirac matrices are of the same, and their square is identity matrix, in momentum representation one should simply replace one matrix with another one in the Feynman propagator for the fermion field [4] and obtain

$$\hat{G}_0(\vec{k}) = \frac{-i(\vec{k}\cdot\vec{\sigma} + m)}{k^2 - m^2} \tag{8}$$

Then, for the matrix element of the Green's function of a free two-dimensional fermion field in the coordinate representation, we have

$$\langle \vec{r}| \, \hat{G}_0 \, |\vec{r}'\rangle = \int d\vec{k}' \exp\left(i\vec{k}'\cdot(\vec{r} - \vec{r}')\right) \frac{-i(\vec{k}'\cdot\vec{\sigma} + m)}{k'^2 - m^2} \tag{9}$$

After substitution of the explicit expressions for the spinor function of the plane incident wave $\Psi_i = \begin{pmatrix}\alpha\\ \beta\end{pmatrix} \exp\left(i\vec{k}\cdot\vec{r}\right)$, the scatterer potential (2) and (9), changing the order of integration, one obtains

$$\Psi^{(1)}(\vec{r}) = \left(Id\, e^{i\vec{k}\cdot\vec{r}} + \int d\vec{k}' e^{i\vec{k}'\cdot\vec{r}} \frac{-i(\vec{k}'\cdot\vec{\sigma} + m)}{k'^2 - m^2} \; V_0 \iint\limits_D e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} d\vec{r}' \right) \begin{pmatrix}\alpha\\ \beta\end{pmatrix} \tag{10}$$

where Id is the operator unit.

The last double integral in brackets is the Fourier transform of the potential V shifted by the value of the initial wave vector $\vec{k}$. Denote it by the scalar function of the vector argument $F(\vec{k})$. Obviously $F(\vec{0})$ gives the full area of the scatterer region, for large k the function quickly tends to zero due to the fast oscillations of the complex exponent. Due to its dependence only on the difference of wave vectors, this function can be easily tabulated once for a given region of the scatterer and leads no computational difficulties. The first integral representing the two-dimensional inverse Fourier transform, but with the operator included in it (a 2x2 matrix acting in the space of spinors), is more complicated. Let us consider it separately.

The action of the operator in the numerator of the fraction in (10) on the spinor explicitly gives

$$\vec{k'} \cdot \vec{\sigma} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta(k_x - ik_y) \\ \alpha(k_x + ik_y) \end{pmatrix} \tag{11}$$

so that the amplitude of scattering wave can be expressed as

$$\Psi_s(\vec{r}) = -i \int d\vec{k'} e^{i\vec{k'}\cdot\vec{r}} \frac{F(\vec{k} - \vec{k'})}{k'^2 - m^2} \begin{pmatrix} \beta(k'_x - \imath k'_y) + m\alpha \\ \alpha(k'_x - \imath k'_y) + m\beta \end{pmatrix} \tag{12}$$

and there is the necessity to calculate three independent integrals of the form

$$\int d\vec{k'} e^{i\vec{k'}\cdot\vec{r}} \frac{F(\vec{k} - \vec{k'})}{k'^2 - m^2}, \quad \int d\vec{k'} e^{i\vec{k'}\cdot\vec{r}} \frac{k_x F(\vec{k} - \vec{k'})}{k'^2 - m^2}, \quad \int d\vec{k'} e^{i\vec{k'}\cdot\vec{r}} \frac{k_y F(\vec{k} - \vec{k'})}{k'^2 - m^2} \tag{13}$$

Two-dimensional integrals include scalar products of vectors $\vec{k}, \vec{r}$, the latter being a constant. We choose a coordinate system in u-space so that the x axis is along the vector $\vec{r}$ and introduce polar coordinates. Then, for example, for the first integral in (12) we have

$$I_1 = \int d\vec{k'} e^{i\vec{k'}\cdot\vec{r}} \frac{F(\vec{k} - \vec{k'})}{k'^2 - m^2} = \int_0^{2\pi} d\varphi \int_0^{\infty} \frac{k'}{k'^2 - m^2} dk' e^{ik'r\cos\varphi} F(\vec{k}, k', \varphi) \tag{14}$$

In the last formula, we explicitly indicated that the vector $\vec{k'}$ should be represented through variables k', φ. The integral over the module of the

wave vector (along k ') is calculated using the residue theorem after taking the residue at the point $k' = m$ and leads to the formula

$$I_1 == \frac{1}{2}\int\limits_0^{2\pi} d\varphi e^{imr\cos\varphi} F(\vec{k}, m, \varphi) \tag{15}$$

Similarly, the second and third integrals are transform to the form

$$I_x = \int d\vec{k'} e^{i\vec{k'}\cdot\vec{r}} \frac{k_x F(\vec{k}-\vec{k'})}{k'^2 - m^2} = \frac{m}{2}\int\limits_0^{2\pi} d\varphi cos\varphi e^{imr\cos\varphi} F(\vec{k}, m, \varphi) \tag{16}$$

$$I_y = \int d\vec{k'} e^{i\vec{k'}\cdot\vec{r}} \frac{k_y F(\vec{k}-\vec{k'})}{k'^2 - m^2} = \frac{m}{2}\int\limits_0^{2\pi} d\varphi \sin\varphi e^{imr\cos\varphi} F(\vec{k}, m, \varphi) \tag{17}$$

Conclusion

The proposed approach allows to simulate spin dependent scattering of 2D fermions on a scatterers of arbitrary shape.

References

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