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Electronic Transmission Wave Function of Disordered Graphene by Direct Method and Green's Function Method

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Abstract: We describe how to obtain electronic transport properties of disordered graphene, including the tight binding model and nearest neighbor hopping. We present a new method for computing, electronic transport wave function and Greens function of the disordered Graphene. In this method, based on the small rectangular approximation, break up the potential barriers in to small parts. Then using the finite difference method, the Dirac equations of disordered graphene, reduce to the discrete matrix equation. The discrete matrix equation is solved by direct and Green's function methods. In this method, geometry of disorder plays an important role. This method allows for an amenable inclusion of several disorder mechanisms at the microscopic level. The effect of impurity on the transmission probability and conductivity are obtained, using the electronic transport wave function. The results show that, for the conductance, geometry plays an important role. In addition, by transmission probability and using Landau formula, the Fano factor is investigated.

Keywords: Disordered graphene, Finite difference method, Graphene, Green's function.

1. Introduction

Due to graphene unusual and remarkable properties and its potential to basis for a new generation of electronic devices, has attracted the attention of many scientists since the first experiments in 2004. Since it was first produced, several synthesis methods have been proposed. All efforts have been based on produce better quality sample to improve the transmission properties. Although Klein-Gordon paradox in graphene which makes the transmission probability of the vertical electron one [1]. The scientists have not achieved to the perfect ballistic regime and disorders always play an important role in electron transport. The overcoming source of disorder which influence transport and optical properties

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of graphene is uncertain. The disorder appears in different forms, such as charge impurities, surface adsorbents, resonant scattering [2, 3].

Many theoretical methods have been proposed to describe electron transport in disordered graphene [4–6]. One of the best methods is the Greens function method [7–10]. Graphene with one and two impurities are studied in different ways, such as: a graphene with two coulomb impurities [11], a gapped graphene with two oppositely charged impurities [12] and a graphene with single impurity which is considered by Greens function and wave function of the system [13].

The goal of this paper is to show how to calculate electronic transport properties of disordered graphene, with tight-binding method and nearest-neighbor hopping, using the direct method and green's function method. In our method, geometry of disorder plays an important role. We present an efficient discretization scheme to implement our method for disordered graphene. To this end, we use the small rectangular approximation and break up the potential barrier, caused by impurities, to small rectangles. Then, the equation of each part in graphene by finite different method reduces to a discrete matrix equation which is solved by Greens function and direct methods. Eventually, as applications of transmission electron wave function, transmission probability [14] and conductivity and Fano factor are calculated [15–19].

This paper is organized as follows: In Sec. II, we briefly describe the small rectangular approximation and calculate the wave function of the graphene with arbitrary impurities

In Sec. III, we derive transmission probability, conductivity and Fano factor. Finally, the conclusion is given in Sec. VI.

2. Small Rectangular Approximation

In this section, a rectangle graphene sheet with length L and width W, which is fixed by leads in two sides, is considered. Hamiltonian of the disordered graphene based on Dirac Hamiltonian is:

$$H = \vartheta_f \, \vec{p}.\vec{\sigma} - V(x, y) \tag{1}$$

In which ϑf = 3at/2 ≈ 106m/s is fermi velocity, σi are Pauli matrices and $\vec{p} = -i\hbar\vec{\nabla}$ is momentum operator of graphene in two dimension and V (x, y) stands for a local potential due to disordered which is added to the tight binding Hamiltonian.

The implementation scheme presented in this paper is recommended when the system is translational invariance at the vertical direction and its translational invariance at the transverse direction is broken up by disorders. So the potential is as follows:

$$V(x,y) = V_0 F(x) \tag{2}$$

The component of wave function is considered to be

$$\begin{cases} \psi(x,\ y)\ = \psi(x)\ exp(ik_y y) \\ \varphi(x,\ y)\ = \varphi(x)\ exp(ik_y y) \end{cases} \tag{3}$$

Substitute the wave function in Hamiltonian, which became

$$H\begin{bmatrix} \psi(x,y) \\ \varphi(x,y) \end{bmatrix} = E\begin{bmatrix} \psi(x,y) \\ \varphi(x,y) \end{bmatrix} \tag{4}$$

The basic idea is to break up potential barriers in X direction of the graphene sheet into N + 1 small equal parts with length $\Delta = L/n$. The parts with numbers lower than 1 and larger than N +1 represent the left and right leads, respectively. So, here Vi denotes the potential of isolated ith part which is constant approximately. Therefore, each part has a constant potential. Neighboring parts in sample are connected to each other because of nearest-neighbor hopping. The first and last parts are connected to the leads. By choosing an input electron wave function in the left lead, and using Eq. (4) for each part, we can obtain the output electron wave function in right lead. Using the finite difference method [20], Eqs. (4), (3) for each part is converted to a recursive relation in term of wave functions of that part and its neighbors, as follows,

$$\frac{\psi_{i-1}(x) - 2\psi_i(x)\ + \psi_{i+1}(x)}{\Delta^2} - k_y^2\,\psi_i(x) = \left(\frac{E - V_i}{\hbar \vartheta_f}\right)^2 \psi_i(x) \tag{5}$$

In this manner, second component of the total wave function became:

$$\varphi_i(x) = \frac{-i\hbar \vartheta_f}{E - V_i}\left[\frac{\psi_{i+1}(x) - \psi_{i-1}(x)}{2\Delta} - k_y\,\psi_i(x)\right] \tag{6}$$

This kind of operation is repeated throughout the method. For i = 0, equation (5) gives a relation between input and output wave functions of first potential barrier which is given by,

$$\frac{\psi_{-1}(x) - 2\psi_0(x)\ + \psi_{+1}(x)}{\Delta^2} - k_y^2\,\psi_0(x) = \left(\frac{E}{\hbar \vartheta_f}\right)^2 \psi_0(x) \tag{7}$$

$\psi_{-1}(x)$ represents the unperturbed wave function where electrons are found in part n = 0 or left lead, so the input wave function can be written as

$$\psi_{-1}(x)\ = Ae^{ik_x x} + \ (\psi_0 - A)e^{-ik_x x} \tag{8}$$

By substituting Eq. (8) in (7), is obtained

$$\frac{\psi_0(x)e^{ik_l\Delta}-2\psi_0(x)+\psi_{+1}(x)}{\Delta^2}-k_y^2\psi_0(x) \\ -\left(\frac{E-V_0}{\hbar\vartheta_f}\right)^2\psi_0(x)=\frac{A}{\Delta^2}(e^{ik_l\Delta}-e^{-ik_l\Delta}) \tag{9}$$

We proceed analogously in order to obtain last part's relation. So for i = N + 1 we have

$$\frac{\psi_N(x)-2\psi_{N+1}(x)+\psi_{N+2}(x)}{\Delta^2}-k_y^2\psi_{N+1}(x)=\left(\frac{E}{\hbar\vartheta_f}\right)^2\psi_{N+1}(x) \tag{10}$$

$\psi_{N+2}(x)$ represents the wave function where electrons are found in part i = N +2 or right lead

$$\psi_{N+2}(x)=\psi_{N+1}(x)e^{ik_R\Delta} \tag{11}$$

As we see above, Eqs.(5),(7) and (10), can be used to process a matrix equation for wave functions of potential barriers. As a result, we find

$$(E'I-H')\psi(x)=q \tag{12}$$

Where I is the identity matrix and H′ is a matrix, whose dimension is defined by the number of parts N + 2, which it's elements are as follows:

$$\begin{cases} E'=\left(\dfrac{E-V_i}{\hbar\vartheta_f}\right)^2, \quad H'=-\dfrac{2}{\Delta^2}-k_y^2, \quad H'_{i,i+1}=H'_{i+1,i}=\dfrac{2}{\Delta} \\ q_0=\dfrac{A}{\Delta^2}(e^{ik_y\Delta}-e^{-ik_y\Delta}), \qquad q_{i\neq 0}=0, \\ H'_{00}=-\dfrac{2}{\Delta^2}-k_y^2+\dfrac{e^{ik_l\Delta}}{\Delta^2}, \qquad H'_{N+1,N+1}=-\dfrac{2}{\Delta^2}-k_y^2+\dfrac{e^{ik_R\Delta}}{\Delta^2} \end{cases} \tag{13}$$

In this part, we consider Eq.(12) by the Green's function and direct methods.

A. Green's function method

In the following we show how to obtain electron wave function from Green's function method. To calculate the Green's function of the disordered graphene, equation (12) is written in the form of a matrix, as follows

$$\begin{bmatrix} -H_1+E_1 & t_1 & 0 \\ t_1^+ & -H_d+E_d & t_2^+ \\ 0 & t_2 & -H_2+E_2 \end{bmatrix}\begin{bmatrix} |\psi_1\rangle \\ |\psi_d\rangle \\ |\psi_2\rangle \end{bmatrix}=\begin{bmatrix} |q_0\rangle \\ 0 \\ 0 \end{bmatrix} \tag{14}$$

In the above relation, $|\psi_d\rangle$ represents an electron wave function of the graphene and $|\psi_1\rangle$ and $|\psi_1\rangle$ represents electron wave function of the left and right leads, respectively. t_1 and t_2 are hoping matrix elements connecting parts together. H_1 and H_2 are the Hamiltonians of leads which connect to graphene and H_d is Hamiltonian of the graphene. Solving Eq. (14) by Green's function method gives

$$(E-H)\mathrm{G(E)}=\mathrm{I} \tag{15}$$

Therefore the matrix equation becomes

$$\begin{bmatrix} -H_1+E_1 & t_1 & 0 \\ t_1^+ & -H_d+E_d & t_2^+ \\ 0 & t_2 & -H_2+E_2 \end{bmatrix}\begin{bmatrix} G_1 & G_{1d} & G_{12} \\ G_{d1} & G_d & G_{d2} \\ G_{21} & G_{2d} & G_2 \end{bmatrix}=\begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix} \tag{16}$$

G_d is Green's function's matrix element which is related to graphene sample without leads effects. As follows

$$G_d = (E_d - H_d - \Xi_1 - \Xi_2)^{-1} \tag{17}$$

in which

$$\Xi_i = t_i^+ g_i t_i \tag{18}$$

Where, $g_i = 1/(E_i - H_i)$.

In eq.(12), $|q_0\rangle$ is like a perturbation, then the wave function in term of operator G(E) is

$$|\psi\rangle = -G(E)|q_0\rangle \tag{19}$$

Based on the third row of the matrix equation, the electron wave function on the right lead in term of electron wave function over graphene is given

$$|\psi_2\rangle = g_2(E)t_2|\psi_d\rangle \tag{20}$$

The electronic wave function in left lead is the sum of two terms, incident and reflection wave function. So, we have,

$$\begin{bmatrix} H_1+t_1 \\ H_d+t_1^++t_2^+ \\ H_2+t_2 \end{bmatrix}(|\psi_{1,n}\rangle+|\psi_R\rangle)=\begin{bmatrix} E_1 \\ E_d \\ E_2 \end{bmatrix}(|\psi_{1,n}\rangle+|\psi_R\rangle) \tag{21}$$

According Eq.(21), graphene's wave function is obtained

$$|\psi_d\rangle = G_d\, t_1^+ |\psi_{1,n}\rangle \tag{22}$$

Respect to Eq.(20), right lead's wave function is obtained

$$|\psi_2\rangle = g_2 t_2 |\psi_d\rangle = g_2 t_2 G_d\, t_1^+ |\psi_{1,n}\rangle \tag{23}$$

Therefore, the total wave function in left lead become

$$|\psi_1\rangle = (1 + g_1 t_1 G_d t_1^+)|\psi_{1,n}\rangle \tag{24}$$

Following the second component of wave function is achieved:

$$H\psi(x) = \varphi(x) + q'. \tag{25}$$

So, the electronic wave function in each part of the system is obtained.

B. Direct method

In this section we show how to obtain the electron wave function of disordered graphene directly. We begin by Eq. (12) and rewrite it as follows

$$(A + B + \varepsilon)|\psi\rangle = \Delta^2 |q\rangle \tag{26}$$

In Eq.(26), matrix (EI − H′) is break up into three matrix, A, B and ε. So, we have,

$$A = \begin{bmatrix} 2+k_y^2\Delta^2 & 0 & \dots & \dots & 0 \\ 0 & 2+k_y^2\Delta^2 & 0 & \dots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \dots & 0 & 2+k_y^2\Delta^2 & 0 \\ 0 & \dots & \dots & 0 & 2+k_y^2\Delta^2 \end{bmatrix}_{N,N} = (2+k_y^2\Delta^2)I \tag{27}$$

Where matrix A is a diagonal matrix with (N +2)(N +2) dimension and this elements refer to Hamiltonian of the isolated rectangle parts without connection with nearest-neighbors and effect of left and right leads.

Matrix B is a three diagonal matrix with (N+2)(N+2) dimension and its diagonal elements are zero. The off diagonal non-zero elements refer to nearst-neighbor hopping, each part is in connection with its neighbor. This matrix is like the matrix representation of the creation and annihilation operators of the quantum harmonic oscillator in orthonormal number basis.

So, the eigen-values and the eigen-vectors of the annihilation and creation operators are useful to analyze the matrix B. The matrix B become:

$$B = \begin{bmatrix} 0 & 2 & \dots & \dots & 0 \\ 2 & 0 & 2 & \dots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \dots & 2 & 0 & 2 \\ 0 & \dots & \dots & 2 & 0 \end{bmatrix}_{N,N} \tag{28}$$

Matrix ε is a diagonal matrix with energy elements like matrix A, the difference is that the leads have contributed in. We have,

$$\varepsilon = \begin{bmatrix} E_1\Delta^2 - e^{ik_x\Delta} & 0 & ... & ... & 0 \\ 0 & E_2\Delta^2 & 0 & ... & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & ... & 0 & E_{N+1}\Delta^2 & 0 \\ 0 & ... & ... & 0 & E_N\Delta^2 - e^{ik_x\Delta} \end{bmatrix}_{N,N} \tag{29}$$

The state vectors $|\psi\rangle$ and $|q\rangle$ in number basis become

$$|\psi\rangle = \begin{bmatrix} \psi_0 \\ . \\ . \\ . \\ \psi_N \end{bmatrix}, \quad |q\rangle = \begin{bmatrix} q_0 \\ 0 \\ . \\ . \\ 0 \end{bmatrix} \tag{30}$$

The eigen values of B matrix are achieved

$$B|m\rangle = \lambda_m |m\rangle, \quad \lambda_m = 2Cos(\frac{m\pi}{N+1}) \tag{31}$$

Where we use $\langle m|m\rangle = 1$.

Then eigen vectors of B matrix become

$$|m\rangle = C_m \sum_{n=1}^{N} Sin\left(\frac{nm\pi}{N+1}\right)|n\rangle, \quad m = 1,2,3,...,N \tag{32}$$

In which, $C_m = 1\Big/\sqrt{\sum_{n=1}^{N} Sin^2(\frac{nm\pi}{N+1})}$.

According to A matrix is diagonal, eigen values and eigen vectors of B matrix, can be considered as the eigen values and eigen vectors of A matrix, Therefore, the wave function can be defined in terms of eigen vectors of matrix A and B , as follows

$$|\psi\rangle = \sum_{m=1}^{N} D_m |m\rangle \tag{33}$$

Substitute Eq.(33) in Eq.(26) gives

$$(2 + k_y^2\Delta^2)D_m + \lambda_m D_m + \sum_{m'=1}^{N} \langle m|\varepsilon|m\rangle D_{m'} = \Delta^2 \langle m|q_0\rangle \tag{34}$$

Where

$$\langle m|\varepsilon|m'\rangle = C_m C_m^{'} \sum_{n=1}^{N}\sum_{n'=1}^{N} Sin\left(\frac{mn\pi}{N+1}\right) Sin\left(\frac{m'n'\pi}{N+1}\right)\langle n|\varepsilon|n'\rangle \tag{35}$$

Where

$$\langle n|\varepsilon|n'\rangle = \delta_{n,n'}\Delta^2 E_n + \delta_{n,n'}(\delta_{n,1}+\delta_{n,N})e^{ik_x\Delta}, \tag{36}$$

So we obtain

$$\langle m|\varepsilon|m'\rangle = C_m C_m^{'}[\sum_{n=1}^{N} Sin\left(\frac{mn\pi}{N+1}\right) Sin\left(\frac{m'n\pi}{N+1}\right)\Delta^2 E_n + Sin\left(\frac{m\pi}{N+1}\right) Sin\left(\frac{m'\pi}{N+1}\right)e^{ik_x\Delta}] \tag{37}$$

Respect to Eq.(37) and (34) we achieve

$$MD_m = \Delta^2\langle m|q\rangle - \sum_{m'=1}^{N}\varepsilon_{m,m'}D_{m'} \tag{38}$$

where

$$M = (2 + k_y^2\Delta^2 + \lambda_m) \tag{39}$$

Above equation in matrix form is

$$D = M^{-1}\Delta^2\langle m|q\rangle - M^{-1}\varepsilon D \tag{40}$$

This equation is solved by perturbation method. The solution of equation to the second order is,

$$\begin{cases} D^{(0)} = \Delta^2 M^{-1}|q\rangle \\ D^{(1)} = \Delta^2 M^{-1}|q\rangle - \Delta^2 M^{-1}\varepsilon M^{-1}|q\rangle \\ D^{(2)} = \Delta^2 M^{-1}|q\rangle - \Delta^2 M^{-1}\varepsilon M^{-1}|q\rangle + \Delta^2 M^{-1}\varepsilon M^{-1}\varepsilon M^{-1}|q\rangle \end{cases} \tag{41}$$

According to this relations, the electronic wave function in the number basis becomes

$$\psi_n = \langle n|\psi\rangle = \sum_{m=1}^{N} D_m\langle n|m\rangle = \sum_{m=1}^{N}\sum_{n'=1}^{N} D_m C_m Sin\left(\frac{n'm\pi}{N+1}\right)\langle n|n'\rangle \tag{42}$$

By using the wave function, transmission probability of the system is achieved.

3. Transmission Probability and Conductivity

The electron transmission wave function can be used to describe many of the physics of transport. In this section we want to study the effect of disorder on the electronic transmission by electronic transmission wave function. So, the electronic transmission probability become

$$T = \left| t\, t^{*} \right| \tag{43}$$

Here t is the transmission matrix across the system which is the ratio of output to input current density, like this

$$t = j_{out} / j_{in}, \tag{44}$$

The current density in relative quantum mechanics is

$$j_i = \psi^{+} \alpha_i \psi, \tag{45}$$

Using the output and input wave functions, transmission coefficient is achieved

$$t = \frac{1}{K_R \Delta} \frac{\left|\psi_{N+1}(x)\right|^2}{\left|\psi_0 - A\right|^2 - \left|A\right|^2} \frac{\mathrm{Im}\, e^{ik_R \Delta}}{\mathrm{Re}\, e^{i\theta}}, \tag{46}$$

Where

$$\tan\theta = k_x / k_y, \quad \left|K_R\right| = \sqrt{k_x^2 + k_y^2} \tag{47}$$

Thus transmission probability become

$$T = \left(\frac{\left|\psi_{N+1}(x)\right|^2}{\left|\psi_0 - A\right|^2 - \left|A\right|^2} \right)^2 \frac{Sin^2(K_R \Delta)}{Cos^2\theta} \frac{1}{(K_R \Delta)^2} \tag{48}$$

If it is assumed that in y direction, periodic boundary conditions are satisfied, the wave number is $k_y = m\pi / W$ and the number of published modes in y direction is

$$M = Int\left[\frac{W}{\lambda_f} \right], \tag{49}$$

That λ_f is fermi wave length.

The zero temperature linear conductance is given by the Landaure formula [21],

$$G = g_0 \sum_{m=0}^{M-1} T_m, \quad g_0 = 4e^2 / \hbar, \tag{50}$$

Hence with respect to Eq.(48), conductivity is obtained,

$$G = g_0 \sum_{m=0}^{M-1} \left(\frac{\left|\psi_{N+1}(x)\right|^2}{\left|\psi_0 - A\right|^2 - \left|A\right|^2} \right)^2 \frac{Sin^2(K_{Rm} \Delta)}{(K_{Rm} \Delta)^2} \tag{51}$$

The Fano factor is another quantity which can be evaluated by transmission coefficient. It is given by the expression

$$F = 1 - \frac{Tr(tt^{+}tt^{+})}{Tr(tt^{+})} \tag{52}$$

Where,

$$F = 1 - \frac{\sum_{m=0}^{M-1} \left(\frac{|\psi_{N+1}(x)|^2}{|\psi_0 - A|^2 - |A|^2} \right)^4 \frac{Sin^4(K_{Rm}\Delta)}{(K_{Rm}\Delta)^4}}{\sum_{m=0}^{M-1} \left(\frac{|\psi_{N+1}(x)|^2}{|\psi_0 - A|^2 - |A|^2} \right)^2 \frac{Sin^2(K_{Rm}\Delta)}{(K_{Rm}\Delta)^2}}. \tag{53}$$

4. Conclusion

We have studied the effect of disorders on the transmission electron wave function by using a new method based on small rectangular approximation and obtained the wave function of the system by Green's function and direct methods. The transmission probability of the disordered graphene is calculated. Conductivity and Fano factor using Landau formula is obtained. This method can be used for different type of disorders.

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