

A qualitative investigation of electrical conductivity in three-layer graphene structures

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Received 30 September 2024; Accepted for publication 17 June 2025; Published 11 July 2025

Abstract. We study the interlayer distance d effect on the electrical conductivity $\sigma_1, \sigma_2, \sigma_3$ of a three-layer monolayer graphene system (3MLG) made of parallel-placed monolayer graphene layers at $T=0$ K by two methods: the first based on the relation between the impurity - electron effective interactions $W_{11}(d), W_{22}(d), W_{33}(d)$ and $\sigma_1(d), \sigma_2(d), \sigma_3(d)$; the second being traditional calculations. We pay attention to the first method consisting of three steps. In the first step, we calculate W_{11}, W_{22}, W_{33} by using the multi-component random phase approximation (M-RPA). In the second step, we define the dependence of W_{11}, W_{22}, W_{33} on interlayer distance d , dielectric constant $\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4$, and temperature T in the case of a 3MLG system. In the third step, we identify the proportional relations between $W_{11}(d), W_{22}(d), W_{33}(d)$ and $\sigma_1(d), \sigma_2(d), \sigma_3(d)$ which were done in the framework of the semiclassical Boltzmann theory and the relaxation time approximation. Based on the obtained results, we deduce the rules of change of $\sigma_1, \sigma_2, \sigma_3$ when d varies which after that, are checked by the second method.

Keywords: correlated impurities; monolayer graphene (MLG); double-layer systems; multi random phase approximation.

Classification numbers: 73.20.Hb; 73.21.Ac; 73.22.Pr.

This is an extended version of the talk presented at the 49th Vietnam Conference on Theoretical Physics, Hue, Vietnam (2024).

1. Introduction

After monolayer graphene was isolated in 2004 by Andre Geim and Kostya Novoselov [1, 2], many authors have investigated multilayer [3–6] and N-layer [7–23] graphene structures. Among these studies, transport properties such as electrical conductivity, thermopower, ... have attracted considerable theoretical and experimental attention [7–17]. In theoretical studies of transport, the semiclassical Boltzmann transport framework combined with the relaxation-time approximation (RTA) is a widely used approach. Within this formalism, the evaluation of transport coefficients typically reduces to integrals of the form [24]

$$I_\alpha(T) = e^2 g \int \frac{d\vec{k}}{(2\pi)^2} (\hat{e}\vec{v}_{\vec{k}})^2 \tau(E_{\vec{k}}, T) (E_{\vec{k}} - \mu(T))^\alpha \left(\frac{-\partial f}{\partial E} \right), \quad (1)$$

where e is the elementary charge, g is the spin–valley degeneracy factor, $\vec{k}$ is the two-dimensional (2D) wave vector, $\vec{v}_{\vec{k}}$ is the group velocity of carriers, $\hat{e}$ is the unit vector along the applied electric field, $\tau(E_{\vec{k}}, T)$ denotes the energy- and temperature-dependent relaxation time, $E_{\vec{k}}$ is the carrier energy, $\mu(T)$ is the temperature-dependent chemical potential, α is an integer index characterizing the transport moment, and f is the Fermi–Dirac distribution function. The derivative $\frac{-\partial f}{\partial E}$ acts as a thermal broadening function, sharply peaked at the Fermi level for low temperatures.

The direct numerical computation of $I_\alpha(T)$ can be challenging, especially for multilayer and N-layer graphene systems. While monolayer, bilayer, and double-layer graphene systems have been studied extensively within this framework, there is, to the best of our knowledge, no prior work addressing the electrical conductivity of three-layer monolayer graphene (3MLG) structures.

Motivated by these considerations, in this paper we propose a three-step method to qualitatively study the electrical conductivity, which we apply to a three-layer monolayer graphene system. In particular, we investigate the dependence of the conductivities of the first, second, and third layers, σ_1 , σ_2 and σ_3 on the interlayer distance d at $T = 0$ K.

2. Methodology

We consider 3MLG structures, shown in Fig.1, composed of three doped MLG. Three layers are electrically isolated via two isolating spacers of thickness d [6]. We also assume that charged impurities are located only in the first (or the second, or the third) layer. In these systems, the qualitative study of electrical conductivity is carried out in three steps.

2.1. Step 1: Calculate impurity-electron effective interactions W_{11}, W_{22}, W_{33} using the multi-component random phase approximation (M-RPA)

Random phase approximation is an approximation for microscopic quantum mechanical interactions between electrons in matter. It accounts for the screening effect on the impurity-electron Coulomb potential, which is expressed as

$$W = (1 - V_{bare}\Pi_0)^{-1}V_{bare}^{imp} = \epsilon^{-1}V_{bare}^{imp}, \quad (2)$$

where $W(V_{bare}^{imp})$ is the screened (unscreened) impurity-electron interaction, V_{bare} is the unscreened electron-electron interaction, Π_0 is the irreducible polarization function, and ϵ is the dielectric function. W is referred to as the effective interaction between impurity-electron. In the case of the

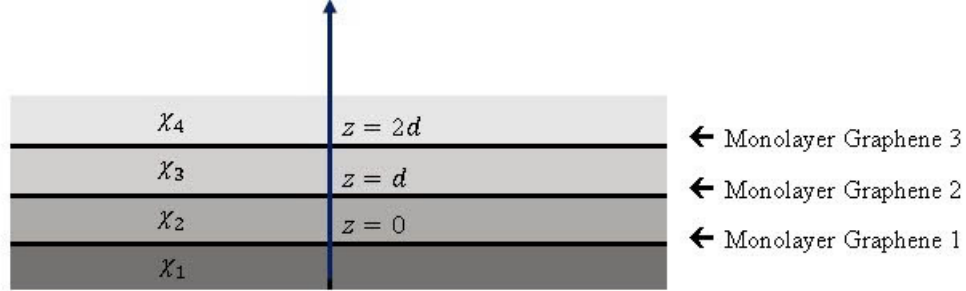


Fig. 1. A three-layer monolayer graphene immersed in an inhomogeneous dielectric environment

multi-component random phase approximation, Eq. (2) is still correct; however, $W, V_{bare}^{imp}, V_{bare}, \Pi_0$ are four matrices.

For three-layer monolayer systems, $W, V_{bare}^{imp}, V_{bare}$ and Π_0 are square matrices of order 3. As considering charged impurities located only in the studied layer, the effective interaction in this layer takes the form

$$W_{11} = \frac{V_{11} - \Pi_2^0(V_{11}V_{22} - V_{12}^2) - \Pi_3^0(V_{11}V_{33} - V_{31}^2) + \Pi_2^0\Pi_3^0\det(V_{bare})}{\det(1 - V_{bare}\Pi^0)}, \quad (3)$$

$$W_{22} = \frac{V_{22} - \Pi_1^0(V_{11}V_{22} - V_{12}^2) - \Pi_3^0(V_{22}V_{33} - V_{23}^2) + \Pi_1^0\Pi_3^0\det(V_{bare})}{\det(1 - V_{bare}\Pi^0)}, \quad (4)$$

$$W_{33} = \frac{V_{33} - \Pi_1^0(V_{11}V_{33} - V_{13}^2) - \Pi_2^0(V_{22}V_{33} - V_{23}^2) + \Pi_1^0\Pi_2^0\det(V_{bare})}{\det(1 - V_{bare}\Pi^0)}. \quad (5)$$

Here Π_1^0 (Π_2^0 or Π_3^0) is the irreducible polarization function of the first (second or third) monolayer graphene, V_{11}, V_{22} and V_{33} are intralayer unscreened electron-electron interactions on the first, second and third monolayer graphene, V_{ij} ($i, j = 1, \dots, 3$ and $i \neq j$) is the interlayer unscreened electron-electron interaction, and

$$\det V_{bare} = V_{11}V_{22}V_{33} + 2V_{12}V_{23}V_{31} - V_{22}V_{13}^2 - V_{11}V_{23}^2 - V_{33}V_{12}^2, \quad (6)$$

$$\begin{aligned} \det(1 - V_{bare}\Pi^0) = & 1 - \Pi_1^0\Pi_2^0\Pi_3^0\det V_{bare} + \Pi_1^0(\Pi_3^0(V_{11}V_{33} - V_{13}^2) - V_{11}) \\ & + \Pi_2^0(\Pi_1^0(V_{11}V_{22} - V_{12}^2) - V_{22}) + \Pi_3^0(\Pi_2^0(V_{22}V_{33} - V_{23}^2) - V_{33}). \end{aligned} \quad (7)$$

2.2. Step 2: Study how W_{11}, W_{22} and W_{33} depend on the interlayer distance d in a three-layer monolayer graphene

The relationship between $W_{11}/W_{22}/W_{33}$ and d is determined by form of the V_{bare} matrix. In the case of inhomogeneous 3MLG structures, nine elements of this matrix can be derived from Poisson equation and expressed as [6]

$$V_{ij} = \frac{2\pi e^2}{q} f_{ij}, \quad (8)$$

where

$$f_{11}(q) = \frac{2[(\chi_2 + \chi_3)(\chi_3 - \chi_4) + 2\chi_3(\chi_2 - \chi_3)e^{2dq} + (\chi_2 + \chi_3)(\chi_3 + \chi_4)e^{4qd}]}{M(qd)}, \quad (9)$$

$$f_{22}(q) = \frac{8e^{2qd}[\chi_1 \cosh(qd) + \chi_2 \sinh(qd)][\chi_3 \cosh(qd) + \chi_4 \sinh(qd)]}{M(qd)}, \quad (10)$$

$$f_{33}(q) = \frac{2[(\chi_2 + \chi_3)(\chi_2 - \chi_1) + 2\chi_2(\chi_3 - \chi_2)e^{2dq} + (\chi_1 + \chi_2)(\chi_2 + \chi_3)e^{4qd}]}{M(qd)}, \quad (11)$$

$$f_{12}(q) = f_{21}(q) = \frac{8\chi_2 e^{2qd}[\chi_3 \cosh(qd) + \chi_4 \sinh(qd)]}{M(qd)}, \quad (12)$$

$$f_{13}(q) = f_{31}(q) = \frac{8\chi_2 \chi_3 e^{2qd}}{M(qd)}, \quad (13)$$

$$f_{32}(q) = f_{23}(q) = \frac{8\chi_3 e^{2qd}[\chi_2 \cosh(qd) + \chi_1 \sinh(qd)]}{M(qd)}, \quad (14)$$

with

$$M(x) = (x_1 - x_2)(x_2 + x_3)(x_3 - x_4) + 2e^{2x}(x_2 - x_3)(x_1 x_3 - x_2 x_4) + e^{4x}(x_1 + x_2)(x_2 + x_3)(x_3 + x_4). \quad (15)$$

For a monolayer graphene, $\Pi(q, T = 0 \text{ K})$ is given as [6, 9]

$$\Pi(q, T = 0 \text{ K}) = -D_0 \begin{cases} 1 & q \leq 2k_F \\ 1 + \frac{\pi q}{8k_F} - \frac{1}{2} \sqrt{1 - \frac{4k_F^2}{q^2}} - \frac{q}{4k_F} \sin^{-1}\left(\frac{2k_F}{q}\right) & q \geq 2k_F. \end{cases} \quad (16)$$

Here, $D_0 = \frac{2E_F}{\pi(\hbar v_F)^2}$, $E_F = \hbar v_F k_F$, $k_F = \sqrt{\pi n}$ and n are the density of states at the Fermi energy, Fermi energy, Fermi wave-vector, and electron density, respectively.

2.3. Step 3: Identify proportional relations between $W_{11}(d)$ ($W_{22}(d)$ or $W_{33}(d)$) and $\sigma_1(d)$ ($\sigma_2(d)$ or $\sigma_3(d)$) using the semiclassical Boltzmann theory and the relaxation time approximation

The conductivity of the i th MLG within the semiclassical Boltzmann approach and the relaxation time approximation is given by [24]

$$\sigma = \frac{e^2 v_{F,i}^2}{2} \int_0^\infty dE D_i(E) \tau_i(E, T) \left(-\frac{\partial f}{\partial t}\right). \quad (18)$$

Here, $D_i(E)$, $v_{F,i}$, τ_i are the density of states, the Fermi velocity, the relaxation time of the monolayer graphene i .

When $T = 0 \text{ K}$:

$$\sigma_i = \frac{e^2}{h} \frac{2E_{F,i} \tau_i(E_F, T = 0 \text{ K})}{\hbar}, \quad (19)$$

where $\tau_i(E_F, T = 0 \text{ K})$ is given as

$$\frac{1}{\tau_i(E_F, T = 0 \text{ K})} = \frac{n_{I,i} D_{0,i}}{4\hbar} \int_0^{2k_F} \frac{dq}{k_{F,i}} \frac{q^2}{k_{F,i}^2} \sqrt{1 - \left(\frac{q}{2k_{F,i}}\right)^2} |W_{ii}(q, T = 0 \text{ K})|^2 \quad (20)$$

From (19) and (20), we see that

$$\sigma_i \sim \tau_i(E_F, T = 0 \text{ K}) \sim |W_{ii}(q, T = 0 \text{ K})|^{-2} \quad (21)$$

Therefore, the dependence of $|W_{ii}|^2$ on the interlayer distance d will deduce the information of the d dependence electrical conductivity σ_i .

3. Result and Discussion

Firstly, we present numerical results for $W_{11}^2(q)$, $W_{22}^2(q)$, $W_{33}^2(q)$ at $T = 0 \text{ K}$ with $n_{i1}/n_{i2}/n_{i3} = 10^{11} \text{ cm}^{-2}$, and $d = 1 \text{ nm}$, $d = 3 \text{ nm}$, $d = 10 \text{ nm}$, $d = 20 \text{ nm}$ for some values of $(\chi_1, \chi_2, \chi_3, \chi_4)$. After that, we derive the dependence of $\sigma_1, \sigma_2, \sigma_3$ on d . Finally, we confirm the obtained results by showing the d –dependent conductivity values table.

3.1. The results of the dependence of $W_{11}^2(q)$, $W_{22}^2(q)$, and $W_{33}^2(q)$ on d

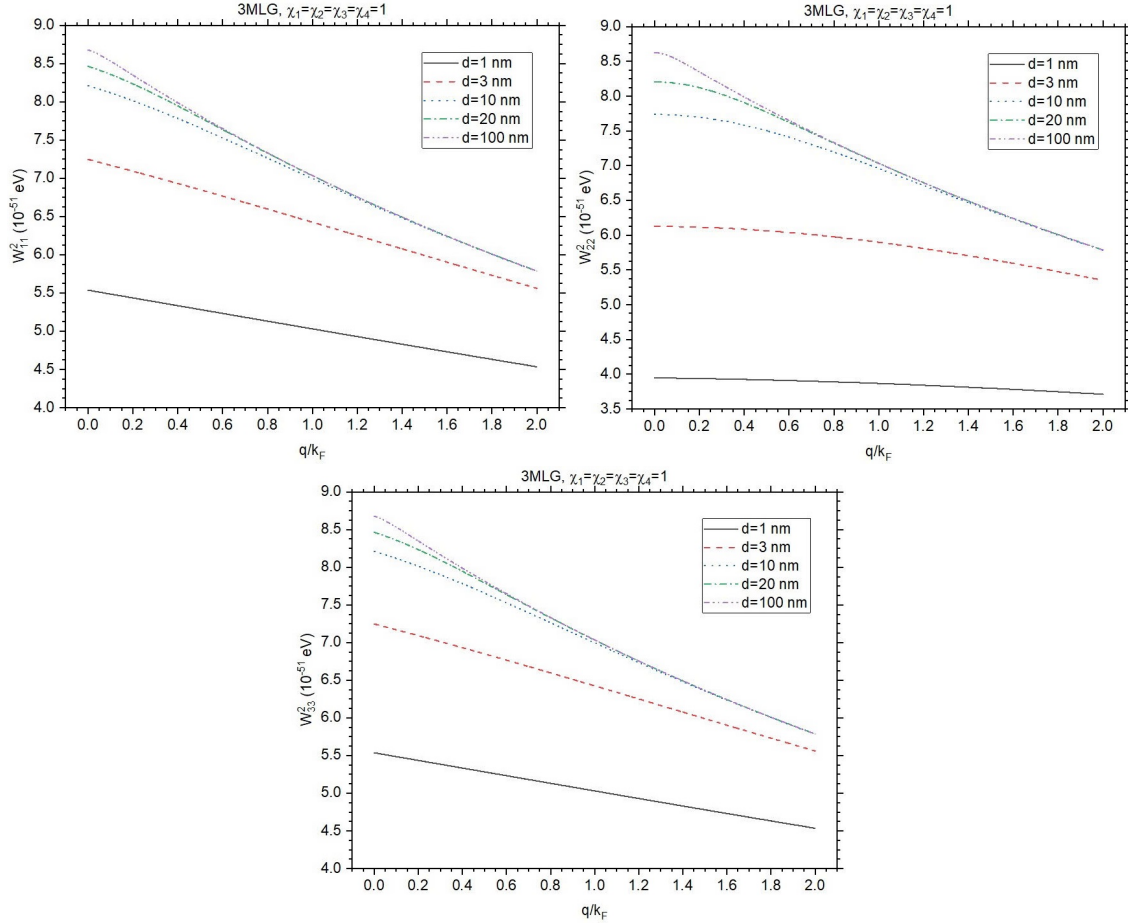


Fig. 2. The electron-impurity interaction potential is a function of q at $T = 0 \text{ K}$ when $\chi_1 = \chi_2 = \chi_3 = \chi_4 = 1$.

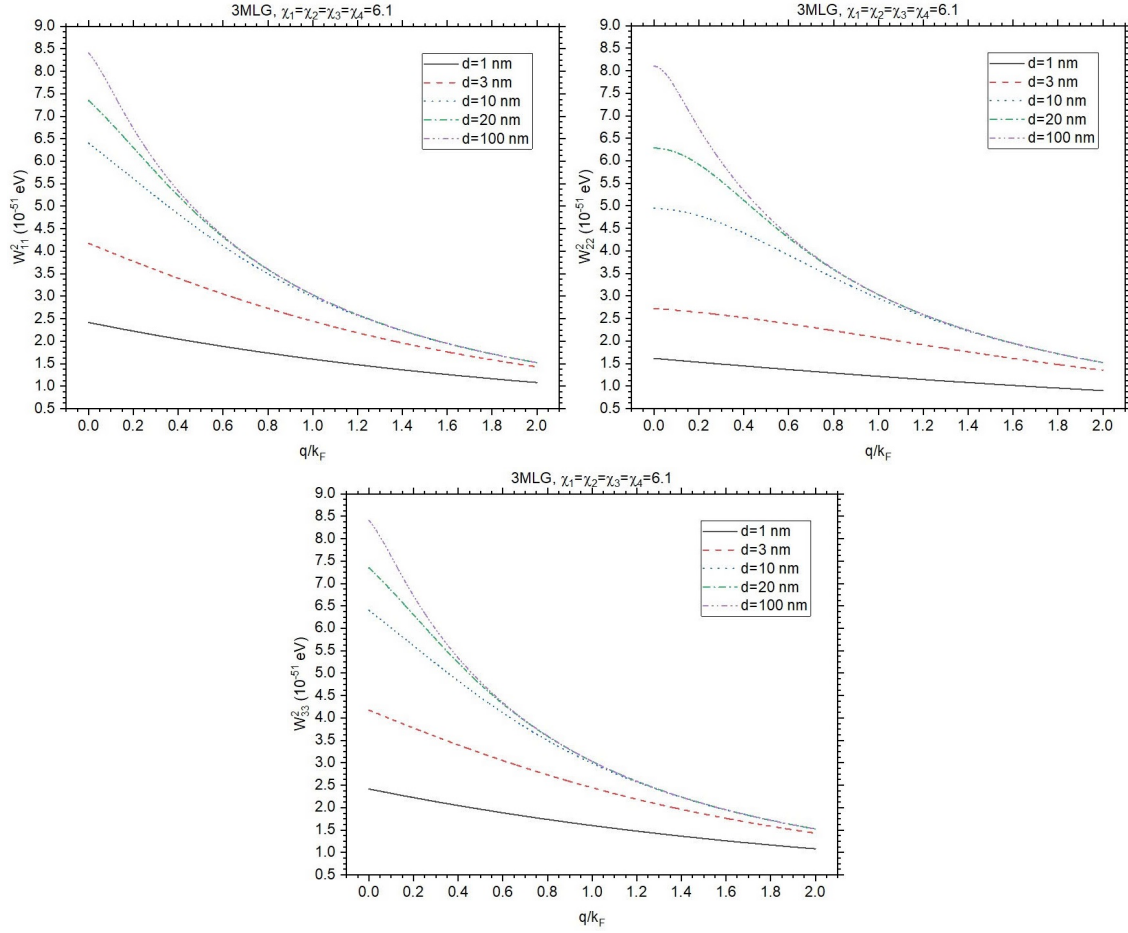


Fig. 3. The electron-impurity interaction potential is a function of q at $T = 0$ K when $\chi_1 = \chi_2 = \chi_3 = \chi_4 = 6.1$.

The dependence of W_{11}^2 , W_{22}^2 , and W_{33}^2 on (q/k_F) for four values of d are shown in Figs. 2, 3 and 4. The first two figures are cases of homogeneous dielectric environments and the last is for nonhomogeneous. In Fig. 2 (Fig. 3), we observe that $W_{11}^2(q)$, $W_{22}^2(q)$, and $W_{33}^2(q)$ increase with increasing d . Based on these quantities, we predict that σ_1 , σ_2 and σ_3 will decrease when d increase. Besides, the value of W_{11}^2 is similar to W_{33}^2 (hence, σ_1 is equal to σ_3). We also find that when W_{11}^2 is greater than W_{22}^2 , σ_2 is smaller than σ_1 . In Figs. 2 and 3, we see that W_{11}^2 , W_{22}^2 and W_{33}^2 decrease with increasing $(\chi_1, \chi_2, \chi_3, \chi_4)$. Therefore, we predict that when dielectric constants of the homogeneous environment increase, the electrical conductivity of the first, second and third layers shall increase too. Finally, in Fig. 4, we see that W_{11}^2 , W_{22}^2 , and W_{33}^2 decrease with decreasing d for $(\chi_1 > \chi_2 > \chi_3 > \chi_4)$. Consequently, these results deduce that $\sigma_1(d)$, $\sigma_2(d)$ and $\sigma_3(d)$ are three decreasing functions. Moreover, when d is very large, $W_{33}^2 > W_{22}^2 > W_{11}^2$ deduce to $\sigma_3 < \sigma_2 < \sigma_1$. However, the value of $W_{22}^2(W_{11}^2)$ is the largest(smallest) for $d = 1$ nm.

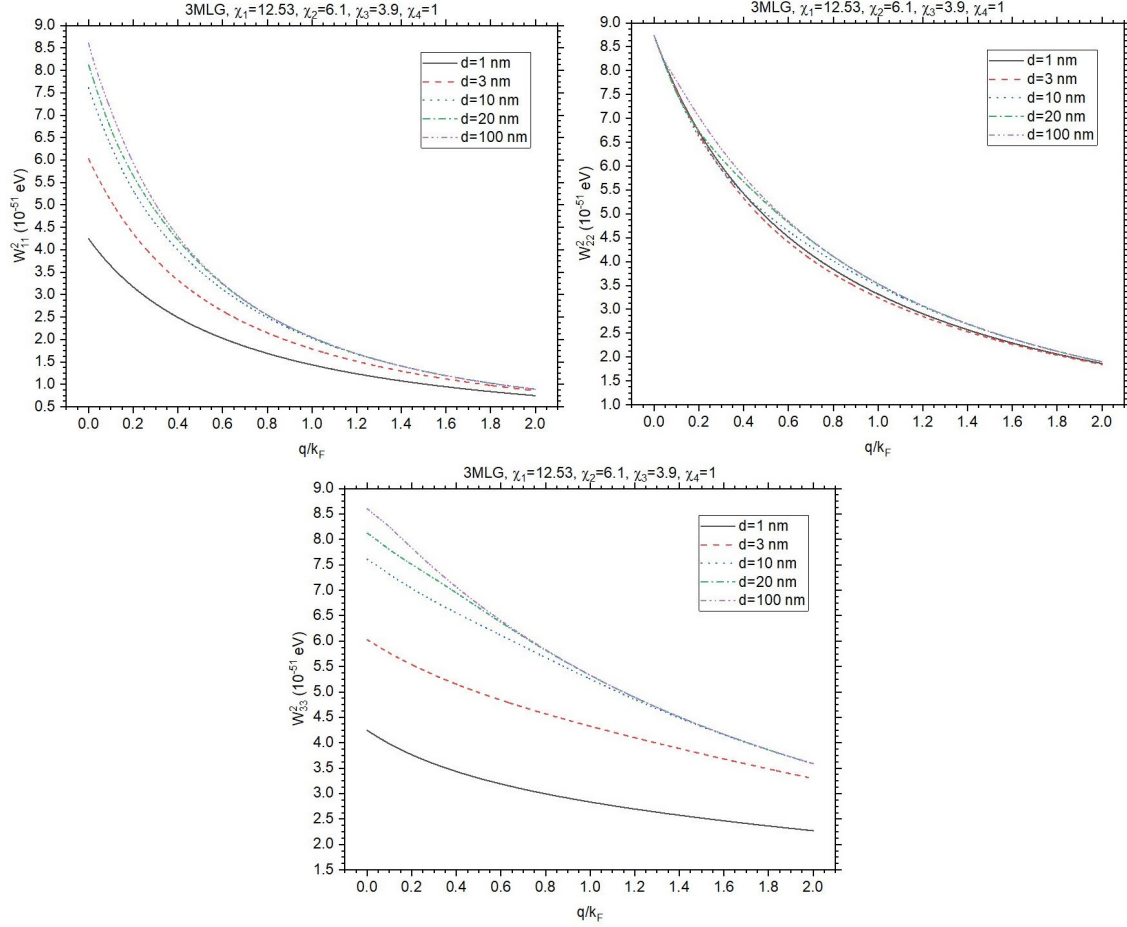


Fig. 4. The electron-impurity interaction potential is a function of q at $T = 0$ K when $\chi_1 = 12.53, \chi_2 = 6.1, \chi_3 = 3.9, \chi_4 = 1$.

3.2. Verification with value of $\sigma_1(d), \sigma_2(d), \sigma_3(d)$

In Table 1, we show the dependence of electrical conductivity σ on the distance d between the layers with different values of $(\chi_1, \chi_2, \chi_3, \chi_4)$. We show that $\sigma_1, \sigma_2, \sigma_3$ decrease with increasing $d(\chi_1, \chi_2, \chi_3, \chi_4)$. These results are consistent with the subsection 3.1.

4. Conclusion

In conclusion, we have presented M-RPA and the proportional relation method applied to the three-layer graphene system. We find that the W_{ii}^2 is dependent on the interlayer distance d that shows the influence of d on the 3MLG electrical conductivity. For a homogeneous dielectric environment W_{11}^2 is equal to W_{33}^2 (hence, σ_1 is equal to σ_3) and $W_{11}^2 > W_{22}^2$ (therefore, $\sigma_1 < \sigma_2$). Besides, $W_{ii}^2(\sigma_i)$ increases (decreases) enormously with increasing environment dielectric constant. Finally, in the case of a nonhomogeneous dielectric environment, when $\chi_1 > \chi_2 > \chi_3 > \chi_4$, $W_{ii}^2(\sigma)$ is the increasing(decreasing) function of d . Therefore, we have also calculated the conductivity

Table 1. The dependence of electrical conductivities σ_1 , σ_2 , and σ_3 on the distance d between the layers for three different dielectric configurations: ($\chi_1 = \chi_2 = \chi_3 = \chi_4 = 1$), ($\chi_1 = \chi_2 = \chi_3 = \chi_4 = 6.1$), and ($\chi_1 = 12.53$, $\chi_2 = 6.1$, $\chi_3 = 3.9$, $\chi_4 = 1$)

$T = 0\text{ K}$	$\sigma_1 (e^2/\hbar)$	$\sigma_2 (e^2/\hbar)$	$\sigma_3 (e^2/\hbar)$
$d = 1\text{ nm}$	29.2 (100.6, 119.6)	37.1 (128.8, 50.9)	29.2 (100.6, 53.9)
$d = 3\text{ nm}$	23.16 (68.71, 97.65)	24.81 (78.58, 51.76)	23.16 (68.71, 35.81)
$d = 10\text{ nm}$	21.62 (58.24, 88.02)	21.71 (59.18, 48.96)	21.62 (58.24, 30.63)
$d = 20\text{ nm}$	21.54 (57.37, 86.94)	21.55 (57.51, 48.45)	21.54 (57.37, 30.29)
$d = 100\text{ nm}$	21.53 (57.23, 86.73)	21.53 (57.23, 48.36)	21.53 (57.23, 30.25)

qualitatively without using the formula in [18], the information of the effective interaction potential $W_{11}^2, W_{22}^2, W_{33}^2$ between impurities and electrons. The rules for changing W_{11}^2, W_{22}^2 and W_{33}^2 allow us to predict how σ_1, σ_2 and σ_3 depend on $d, \chi_1, \chi_2, \chi_3$ and χ_4 .

Acknowledgments

Khanh-Linh Dang was funded by the Program of Fundamental Research of the Ministry of Education and Training (Vietnam) under Grant No. B2023-SPS-08-VL.

Conflict of interest

The authors have no conflicts of interest to declare.

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