Role of the Trigonal Warping on the Minimal Conductivity of Bilayer Graphene

József Cserti,[1] András Csordás,[2] and Gyula Dávid[3]

[1]*Department of Physics of Complex Systems, Eötvös University, H-1117 Budapest, Pázmány Péter sétány 1/A, Hungary*
[2]*Statistical and Biological Physics Research Group, HAS-ELTE, H-1117 Budapest, Pázmány Péter sétány 1/A, Hungary*
[3]*Department of Atomic Physics, Eötvös University, H-1117 Budapest, Pázmány Péter sétány 1/A, Hungary*

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Using a reformulated Kubo formula we calculate the zero-energy minimal conductivity of bilayer graphene taking into account the small but finite trigonal warping. We find that the conductivity is independent of the strength of the trigonal warping and it is 3 times as large as that without trigonal warping and 6 times larger than that in single layer graphene. Although the trigonal warping of the dispersion relation around the valleys in the Brillouin zone is effective only for low-energy excitations, our result shows that its role cannot be neglected in the zero-energy minimal conductivity.

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Recent experiments have proved that the charge carriers in graphene (single or stacks of atomic layer of graphite) are massless Dirac fermions [1–3]. For recent reviews on graphene, see Refs. [4–6]. Besides the unusual transport properties observed and reviewed in the above works, another important experimental feature is the minimal conductivity of the graphene systems which was considered theoretically [7] long before the experimental evidence. After the above-mentioned experimental works on graphene, a number of theoretical studies [8–18] have predicted the conductivity of the order of e^2/h. Very recently, Miao *et al.* have experimentally confirmed [19] most theoretical predictions [11,13–18], namely, the minimum conductivity in wide and short strips approaches the universal value $\sigma_{xx}^{\min} = (4/\pi)e^2/h$ in single layer graphene.

The bilayer graphene was studied first experimentally [3] by Novoselov *et al.* and theoretically [20] by McCann and Fal'ko. McCann has calculated the asymmetry gap in the electronic band structure of bilayer graphene [21]. In biased bilayer graphene it was demonstrated that the gap can be tuned by electric field effect [22]. In bilayer graphene the semiconductor gap has recently been controlled experimentally by Ohta *et al.* [23]. The optical and magneto-optical far infrared properties of bilayer graphene has been studied by Abergel and Fal'ko [24]. The role of the impurities in biased bilayer graphene has been studied by Nilsson and Castro Neto [25]. The realization of quantum dots in bilayer graphene has theoretically been demonstrated recently by Pereiera *et al.* [26]. Ludwig has considered the conductance of a normal-superconductor junction in bilayer graphene [27]. Recently, Koshino and Ando have investigated the transport in bilayer graphene in self-consistent Born approximation [28] and they found that in the strong-disorder regime $\sigma_{xx}^{\min} = (8/\pi)e^2/h$, while in the weak-disorder regime $\sigma_{xx}^{\min} = (24/\pi)e^2/h$, which is 6 times larger than in single layer graphene. Similarly, Katsnelson has also calculated the minimal conductivity in bilayers using the Landauer approach [29] and he obtained a different value $\sigma_{xx}^{\min} = 2e^2/h$. In Ref. [17] we found $\sigma_{xx}^{\min} = (8/\pi)e^2/h$ which was confirmed later by Snyman and Beenakker [30] using the Landauer approach.

However, much fewer theoretical works paid attention to the role of the trigonal warping in bilayer graphene. The influence of the trigonal warping on the weak localization effect has been investigated by Kechedzhi *et al.* [31], while on the minimal conductivity only by Koshino and Ando [28] using an effective 2×2 Hamiltonian. Our aim in this work is to calculate the minimal conductivity using the Hamiltonian suggested originally by McCann and Fal'ko [20]. This Hamiltonian allows us to find the zero-energy minimal conductivity as a function of the strength of the trigonal warping in bilayer graphene. We use the Kubo formula rewritten in a form suitable for obtaining the zero-energy minimal conductivity in graphene systems. Surprisingly, we find that the conductivity is *independent* of the strength of the trigonal warping and *six* times as large as that for single layer graphene.

The bilayer graphene consists of two coupled honeycomb lattices with basis atoms A_1, B_1 and A_2, B_2 in the bottom and the top layers, respectively. The two layers are arranged in Bernal stacking ($A_2 - B_1$). The intralayer coupling between A_1 and B_1 and A_2 and B_2 is γ_0. The strongest interlayer coupling is between A_2 and B_1 with coupling constant γ_1. A direct hopping between A_1 and B_2 is taken into account by the coupling constant $\gamma_3 \ll \gamma_1$. This coupling is responsible for the trigonal warping. The above coupling constants are estimated as $\gamma_0 = 3.16$ eV [32], $\gamma_1 = 0.39$ eV [33], and $\gamma_3 = 0.315$ eV [34].

To model the bilayer graphene we use the same gapless Hamiltonian as that in Refs. [20,35] which takes into account the trigonal warping. The Hamiltonian in the basis A_1, B_1, A_2, B_2 in the valley $\mathbf{K}$ and in the basis B_1, A_1, B_2, A_2 in the valley $\mathbf{K}'$ reads

$$H_{b1} = \xi \begin{pmatrix} 0 & vp_- & 0 & v_3 p_+ \\ vp_+ & 0 & \xi\gamma_1 & 0 \\ 0 & \xi\gamma_1 & 0 & vp_- \\ v_3 p_- & 0 & vp_+ & 0 \end{pmatrix}, \qquad (1)$$

where $p_\pm = p_x \pm ip_y$, $v = \sqrt{3}a\gamma_0/(2\hbar)$, and $v_3 = \sqrt{3}a\gamma_3/(2\hbar)$, while $\xi = +1$ for the valley $\mathbf{K}$ and $\xi = -1$ for the valley $\mathbf{K}'$ ($a = 0.246$ nm is the lattice constant in the honeycomb lattice). The strength of the trigonal warping is described by the parameter $\beta = v_3/v = \gamma_3/\gamma_0$. According to previous studies [20,32,34] $\beta \approx 0.1$.

The four eigenvalues of (1) as functions of the wave number $\mathbf{k} = k(\cos\varphi, \sin\varphi)$ are given by

$$E_n^2(k, \varphi) = \frac{\gamma_1^2}{2}[1 + \tilde{k}^2(\beta^2 + 2) + (-1)^n\Gamma], \quad \text{where } \Gamma = \sqrt{1 - 2\tilde{k}^2(\beta^2 - 2) + \tilde{k}^4\beta^2(\beta^2 + 4) + 8\tilde{k}^3\beta\cos 3\varphi}, \tag{2}$$

where $n = 1, 2$, while the rescaled wave number is $\tilde{k} = k\hbar v/\gamma_1$.

Owing to the $\cos 3\varphi$ term the eigenvalues are threefold rotational invariant for finite β. The eigenvalues $\pm E_1$ become zero at the $\mathbf{K}$ point of the Brillouin zone, i.e., at $\tilde{k} = 0$, and at the center of the three pockets located at $\tilde{k} = \beta$ and $\varphi = 0, 2\pi/3, 4\pi/3$. Around these zeros the constant energy lines are distorted as shown in Fig. 1. This is called trigonal warping. At moderate energy, direct hopping between A_1 and B_2 leads to trigonal warping of the constant energy lines about each valley, but at an energy E less than the Lifshitz energy $E_L = \gamma_1\beta^2/(4 + \beta^2) \approx 1$ meV, the effect of trigonal warping is dramatic. It leads to a Lifshitz transition [36]: the constant energy line is broken into four pockets, which can be referred to as one central and three leg parts. For $v_3 \ll v$, i.e., $\beta \ll 1$, we find that the separation of the 2D Fermi line into four pockets would take place for very small carrier densities $n < n_L \sim 1 \times 10^{11}$ cm^{-2} (here n_L is the Lifshitz density). For $n < n_L$, the central part of the Fermi surface at energy E is approximately circular with area $\mathcal{A}_c \approx \pi E^2/(\hbar v_3)^2$, and each leg part is elliptical with area $\mathcal{A}_\ell \approx \frac{1}{3}\mathcal{A}_c$. For $E \ll E_L$ the dispersion relation is linear in k. The constant energy lines are similar around the $\mathbf{K}'$ point. For $\beta = 0$ there is no trigonal warping; i.e., the eigenvalues are rotational symmetric and the Dirac cones are only at the $\mathbf{K}$ and $\mathbf{K}'$ points.

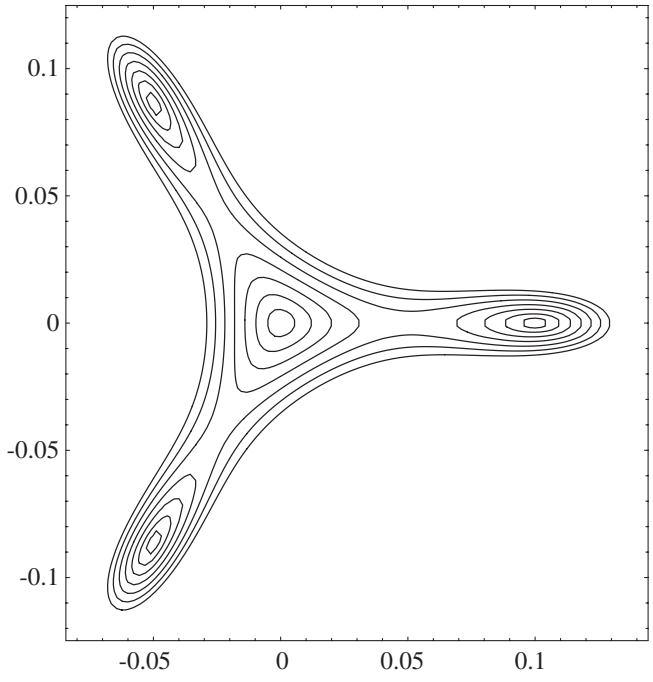

FIG. 1. Constant energy lines (in units of γ_1) of the dispersion relation of the positive eigenvalue E_1 in the $(\tilde{k}_x, \tilde{k}_y)$ plane around the $\mathbf{K}$ point of the Brillouin zone (at the origin in this figure). Here $\beta = 0.1$ and the contour lines are plotted equidistantly with the most outer contour line corresponding to energy $2E_L$.

Recently, in self-consistent Born approximation Koshino and Ando [28] have investigated the minimal conductivity for bilayer graphene using an approximated 2×2 Hamiltonian which mimics the trigonal warping and is given by

$$H_{b2} = g_2\begin{pmatrix} 0 & \tilde{p}_-^2 - \tilde{p}_+ \\ \tilde{p}_+^2 - \tilde{p}_- & 0 \end{pmatrix}, \tag{3}$$

where the effective coupling constant is $g_2 = \gamma_1\gamma_3^2/\gamma_0^2$, and the rescaled momentums are $\tilde{p}_\pm = (p_x \pm ip_y)/p_0$ and $p_0 = 2\hbar\gamma_1\gamma_3/(\sqrt{3}a\gamma_0^2)$.

The simplest effective Hamiltonian valid for $E \ll \gamma_1$ and first introduced by McCann and Fal'ko [20] to study the Hall conductivity of bilayer graphene is given by

$$H_{b3} = -g_3\begin{pmatrix} 0 & p_+^2 \\ p_-^2 & 0 \end{pmatrix}, \tag{4}$$

where $g_3 = v^2/\gamma_1$ is the effective coupling constant. In this case the trigonal warping is absent. In this work, we calculate the minimal conductivity for all three Hamiltonians, H_{b1}, H_{b2}, and H_{b3}.

To find the minimal conductivity for graphene systems we start from the Kubo formula used by Ryu *et al.* in Ref. [18] which at zero temperature and for dc conductivity (at zero frequency ω) is given by

$$\sigma_{\mu\nu}^{\min} = n_s n_v \lim_{\eta\to 0}\sigma_{\mu\nu}(\eta), \tag{5a}$$

where

$$\sigma_{\mu\nu}(\eta) = -\delta_{\mu\nu}\frac{\hbar}{4\pi}\int\frac{d^2\mathbf{r}}{S}\int d^2\mathbf{r}'\Sigma_{\mu\nu}(\mathbf{r}, \mathbf{r}'; E = 0, \eta), \tag{5b}$$

$$\Sigma_{\mu\nu}(\mathbf{r}, \mathbf{r}'; E, \eta) = \mathrm{Tr}[G^{\mathrm{AR}}(\mathbf{r}, \mathbf{r}'; E, \eta)j_\mu G^{\mathrm{AR}}(\mathbf{r}, \mathbf{r}'; E, \eta)j_\nu]. \tag{5c}$$

Here $(\mu, \nu) = x, y$, the spin degeneracy is $n_s = 2$, the valley degeneracy corresponding to the valley $\mathbf{K}$ and $\mathbf{K}'$ is $n_v = 2$, the area of the sample is S, while

$$G^{\mathrm{AR}}(\mathbf{r}, \mathbf{r}'; E, \eta) = G^-(\mathbf{r}, \mathbf{r}'; E, \eta) - G^+(\mathbf{r}, \mathbf{r}'; E, \eta) \tag{5d}$$

is the difference between the advanced (A) and the retarded (R) Green's functions. The trace is taken over the spinor indices and for systems with translation invariance, the single-particle Green's functions are given by

$$G^{\pm}(\mathbf{r}_1, \mathbf{r}_2; E, \eta) = \int \frac{d^2\mathbf{k}}{(2\pi)^2} e^{i\mathbf{k}(\mathbf{r}_2-\mathbf{r}_1)} G^{\pm}(\mathbf{k}; E, \eta), \quad (5e)$$

$$G^{\pm}(\mathbf{k}; E, \eta) = [E \pm i\eta - H(\mathbf{k})]^{-1}, \quad (5f)$$

$$H(\mathbf{k}) = H(\mathbf{p} = \hbar\mathbf{k}), \quad (5g)$$

and the current operator is

$$j_\mu = i\frac{e}{\hbar}[H, r_\mu] = \frac{e}{\hbar}\frac{\partial H(\mathbf{k})}{\partial k_\mu}. \quad (5h)$$

The above expression (5b) for the conductivity can be simplified using the identity

$$(-z - H)^{-1} - (z - H)^{-1} = -2z(z^2 - H^2)^{-1}.$$

Then with $z = i\eta$ and for translational invariant systems $\sigma_{\mu\nu}(\eta)$ in Eq. (5b) has a form

$$\sigma_{\mu\nu}(\eta) = \delta_{\mu\nu}\frac{2e^2}{h}\eta^2 I(\eta), \quad (6a)$$

where

$$I(\eta) = \int \frac{d^2\mathbf{k}}{(2\pi)^2} \mathrm{Tr}\Big[[\eta^2 + H^2(\mathbf{k})]^{-1}\frac{\partial H(\mathbf{k})}{\partial k_\mu} \times [\eta^2 + H^2(\mathbf{k})]^{-1}\frac{\partial H(\mathbf{k})}{\partial k_\nu}\Big]. \quad (6b)$$

Before we turn to the case of the bilayer it is instructive to see how the expression (6b) works for single layer graphene. In this case the Hamiltonian is given by $H_s(\mathbf{k}) = g_s(\tau_x k_x + \tau_y k_y)$, where $g_s = \hbar v$, and τ_x and τ_y are the Pauli matrices acting on the isospin space. The integrand in Eq. (6b) can easily be calculated using polar coordinates for $\mathbf{k}$, and one finds $I(\eta) \equiv I_s(\eta) = 1/(2\pi\eta^2)$, which is independent of the coupling constant g_s. Note that the main contribution in the integral $I(\eta)$ comes from the vicinity of $k = 0$; therefore, the integral over k can be extended to infinity [15]. Then from Eqs. (6a) and (5a) we obtain the well-known universal value of the minimal conductivity for single layer graphene: $\sigma_{xx}^{\min} = (4/\pi)(e^2/h)$ [11,13–18].

We now consider the bilayer graphene taking into account the effect of the trigonal warping. For bilayer with Hamiltonian (1) the current operator j_x is

$$j_x = \xi\frac{ev}{\hbar}\begin{pmatrix} 0 & 1 & 0 & \beta \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ \beta & 0 & 1 & 0 \end{pmatrix}. \quad (7)$$

Similarly, j_y can easily be calculated. The integral $I(\eta) \equiv I_{b1}(\beta, \eta)$ in Eq. (6b) will depend on β. It can be shown that $\sigma_{xx} = \sigma_{yy}$ and $\sigma_{xy} = \sigma_{yx} = 0$. Using polar coordinates for $\mathbf{k}$, and rescaling the variables k and η as $k \to k\hbar v/\gamma_1$ and $\eta \to \eta/\gamma_1$, a straightforward algebra yields for the case of $\xi = +1$ (valley $\mathbf{K}$)

$$I_{b1}(\beta, \eta) = \int_0^\infty \int_0^{2\pi} k\frac{A + B\cos 3\varphi}{(C + D\cos 3\varphi)^2}\frac{d\varphi}{2\pi}\frac{dk}{2\pi}, \quad (8a)$$

$$A = k^4(2 + 5\beta^2) + (1 + \eta^2)[4k^2(1 + \beta^2) + 2\eta^2 + \beta^2(1 + \eta^2)], \quad (8b)$$

$$B = 4k^3\beta, \qquad D = -2k^3\beta, \quad (8c)$$

$$C = k^4 + \eta^4 + \eta^2 + k^2[2\eta^2 + \beta^2(1 + \eta^2)]. \quad (8d)$$

The integrand has a threefold rotational symmetry as should be for trigonally warped bilayer graphene. It can be shown that for $\xi = -1$ (valley $\mathbf{K}'$) we have the same results. The conductivity is twofold degenerate according to the valleys, i.e., $n_v = 2$. The integral over φ can be performed analytically and $I_{b1}(\beta, \eta)$ becomes

$$I_{b1}(\beta, \eta) = 2\int_0^\infty k\frac{AC - BD}{(C^2 - D^2)^{3/2}}\frac{dk}{2\pi}. \quad (9)$$

Without trigonal warping, i.e., for $\beta = 0$, one finds

$$I_{b1}(\beta = 0, \eta) = \int_0^\infty \frac{dk}{2\pi}\frac{4k(k^4 + \eta^4 + \eta^2 + 2k^2 + 2k^2\eta^2)}{(k^4 + \eta^4 + \eta^2 + 2k^2\eta^2)^2} = \frac{1}{\pi\eta^2}. \quad (10)$$

Thus, using Eqs. (6a) and (5a) the minimal conductivity for bilayer graphene without trigonal warping is $\sigma_{xx}^{\min}(\beta = 0) = (8/\pi)(e^2/h)$. This result has been derived first in Ref. [17] in a different way, and subsequently by Snyman and Beenakker in Ref. [30] using the Landauer approach.

After a tedious calculation the integral in Eq. (9) for finite value of β can be performed yielding

$$I_{b1}(\beta, \eta) = \frac{1}{4\pi\eta^2}\left(12 - \frac{127 + 145\beta^2 + 38\beta^4}{\beta^6 + \beta^4}\eta^2\right), \quad (11)$$

plus terms of the order of $O(\ln\eta)$ and $O(\eta^2)$. Again, using Eqs. (6a) and (5a) we find a remarkable result; namely, the minimal conductivity for bilayer graphene with trigonal warping takes a universal value $\sigma_{xx}^{\min}(\beta) = (24/\pi)(e^2/h)$ independent of the strength β of the warping. This is our central result in this Letter. This value is 6 times as large as the conductivity in single layer graphene. It is surprising that $\sigma_{xx}^{\min}(\beta)$ is not a continuous function around $\beta = 0$. Indeed, as we have seen $\sigma_{xx}^{\min}(\beta = 0) = (8/\pi)(e^2/h)$, while for *any finite* values of β it is 3 times larger. This nonanalytic behavior of $\sigma_{xx}^{\min}(\beta)$ at $\beta = 0$ is a consequence of the fact that the minimal conductivity results from the electronic dynamics in the limit of zero density $n \to 0$. For any nonzero β, such density is *always* below the Lifshitz density $n < n_L$ where the 2D Fermi line around each valley forms four separate pockets, whereas for $\beta = 0$, the

Lifshitz transition does not occur and there is always a single Fermi line at each valley.

In the framework of self-consistent Born approximation, the same result was predicted by Koshino and Ando [28] using the Hamiltonian H_{b2} given by Eq. (3). Note that in this Hamiltonian there is no adjustable parameter for the strength of the trigonal warping like β for Hamiltonian (1). The effective coupling constant g_2 drops out in Eq. (6b); therefore, in this model the trigonal warping is built in without the possibility to change its strength. Using Eq. (6) we repeat the calculation with the Hamiltonian (3) and find

$$I(\eta) \equiv I_{b2}(\eta) = \frac{1}{4\pi\eta^2}(12 - 127\eta^2), \qquad (12)$$

plus terms of the order of $O(\ln\eta)$ and $O(\eta^2)$. Thus, the minimal conductivity takes the same universal value $\sigma_{xx}^{\min}(\beta) = (24/\pi)(e^2/h)$ as that for H_{b1} in Eq. (1).

Finally, we calculate the minimal conductivity using the simplest Hamiltonian H_{b3} given by Eq. (4). Then the integral in (6b) can exactly be calculated: $I(\eta) \equiv I_{b3}(\eta) = 1/(\pi\eta^2)$. Thus, the minimal conductivity takes the same universal value $\sigma_{xx}^{\min} = (8/\pi)(e^2/h)$ as that for Hamiltonian (1) with $\beta = 0$.

In summary, we compared the minimal conductivity in bilayer graphene obtained from three different effective Hamiltonians used in the literature. We found that for the case when the trigonal warping is absent, the conductivity is *always* 2 times larger, while in the presence of trigonal warping it is *6 times* larger than that for single layer graphene and is independent of the strength of the warping. Our universal results suggest that the conductivity has a topological origin, which can be a further research topic in the future.

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