Screening in gated bilayer graphene

L. A. Falkovsky
L.D. Landau Institute for Theoretical Physics, Moscow 117334, Russia
and Institute of the High Pressure Physics, Troitsk 142190, Russia

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The tight-binding model of a graphene bilayer is used to find the gap between the conduction and valence bands, as a function of both the gate voltage and as the doping by donors or acceptors. The total Hartree energy is minimized and the equation for the gap is obtained. This equation for the ratio of the gap to the chemical potential is determined only by the screening constant. Thus the gap is strictly proportional to the gate voltage or the carrier concentration in the absence of donors or acceptors. In the opposite case, where the donors or acceptors are present, the gap demonstrates the asymmetrical behavior on the electron and hole sides of the gate bias.

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Bilayer graphene has attracted much interest partly due to the opening of a tunable gap in its electronic spectrum by an external electrostatic field. Such a phenomenon was predicted by McCann and Fal'ko[1] and can be observed in optical studies controlled by applying a gate bias.[2–7] In Refs. 8 and 9, within the self-consistent Hartree approximation, the gap was derived as a near-linear function of the carrier concentration injected in the bilayer by the gate bias. Recently, this problem was numerically considered[10] using the density-functional theory (DFT) and including the external charge doping involved with impurities. The DFT calculation gives the gap which is roughly half of the gap obtained in the Hartree approximation. This disagreement was explained in Ref. 10 as a result of both the inter- and intralayer correlations.

In this Brief Report, we study this problem within the same Hartree approximation as in Refs. 8 and 9, but including the external doping. We consider the case, where the carrier concentration in the bilayer is less than 10^{13} cm^{-2}, calculating the carrier concentration on both layers. Then, we minimize the total energy of the system and find self-consistently both the chemical potential and the gap induced by the gate bias. Our results completely differ from those obtained in Refs. 8 and 9 even for the range where the external doping is negligible. The dependence of the gap on the carrier concentration, i.e., on the gate voltage, exhibits an asymmetry at the electron and hole sides of the gate bias.

The graphene bilayer lattice is shown in Fig. 1. Atoms in one layer, i.e., a and b in the unit cell, are connected by solid lines and in the other layer, e.g., a_1 and b_1, by the dashed lines. The atom $a(a_1)$ differs from $b(b_1)$ because it has a neighbor just below in the adjacent layer, whereas the atom $b(b_1)$ does not.

Let us recall the main results of the Slonchewski-Weiss-McClure model.[11,12] In the tight-binding model, the Bloch functions of the bilayer are written in the form

$$\psi_a = \frac{1}{\sqrt{N}}\sum_j e^{i\mathbf{k}\mathbf{a}_j}\psi_0(\mathbf{a}_j - \mathbf{r}),$$

$$\psi_b = \frac{1}{\sqrt{N}}\sum_j e^{i\mathbf{k}\mathbf{a}_j}\psi_0(\mathbf{a}_j + \mathbf{a} - \mathbf{r}),$$

$$\psi_{a1} = \frac{1}{\sqrt{N}}\sum_j e^{i\mathbf{k}\mathbf{a}_j}\psi_0(\mathbf{a}_j + \mathbf{c} - \mathbf{r}),$$

$$\psi_{b1} = \frac{1}{\sqrt{N}}\sum_j e^{i\mathbf{k}\mathbf{a}_j}\psi_0(\mathbf{a}_j + \mathbf{c} + \mathbf{a} - \mathbf{r}), \quad (1)$$

where the sums are taken over the lattice vectors $\mathbf{a}_j$ and N is the number of unit cells. Vectors $\mathbf{a}$ and $\mathbf{c}$ connect the nearest atoms in the layer and in the neighbor layers, correspondingly.

For the nearest neighbors, the effective Hamiltonian in the space of the functions (1) contains the hopping integrals $\gamma_0, \gamma_1, \gamma_3, \gamma_4$, and Δ.[13] The largest of them, γ_0, determines the band dispersion near the K point in the Brillouin zone with a velocity parameter v. The parameters γ_3 and γ_4 giving a correction to the dispersion are less than γ_0 by a factor of 10 (see Refs. 4 and 5). The parameters γ_1 and Δ result in the displacements of the levels at K, but Δ is much less than γ_1. Besides, there is the parameter U induced by the gate and describing the asymmetry of two layers in the external electrostatic field. This parameter simply presents the potential energy between two layers, $-edE$, where d is the interlayer distance and E is electric field induced both by the gate voltage and the external charge dopants in the bilayer. In the simplest case, the effective Hamiltonian can be written as

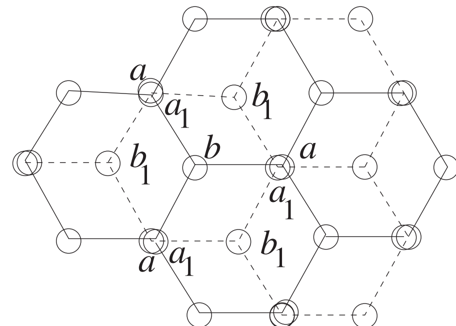

FIG. 1. Bilayer lattice.

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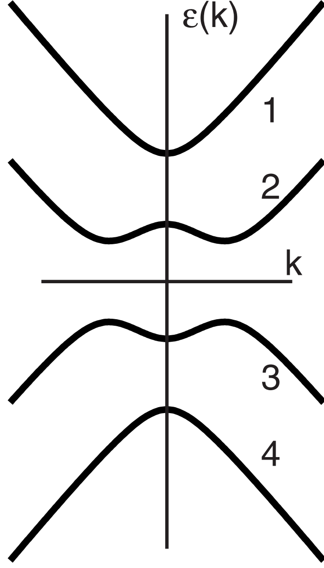

FIG. 2. Band structure of bilayer.

$$H(\mathbf{k}) = \begin{pmatrix} U & vk_+ & \gamma_1 & 0 \\ vk_- & U & 0 & 0 \\ \gamma_1 & 0 & -U & vk_- \\ 0 & 0 & vk_+ & -U \end{pmatrix}, \qquad (2)$$

where the matrix elements are expanded in the momentum $k_\pm = \mp ik_x - k_y$ near the K points.

The Hamiltonian gives four energy bands

$$\varepsilon_{1,4}(q) = \pm\left(\frac{\gamma_1^2}{2} + U^2 + q^2 + W\right)^{1/2},$$

$$\varepsilon_{2,3}(q) = \pm\left(\frac{\gamma_1^2}{2} + U^2 + q^2 - W\right)^{1/2}, \qquad (3)$$

where

$$W = \left(\frac{\gamma_1^4}{4} + (\gamma_1^2 + 4U^2)q^2\right)^{1/2}$$

and we denote $q^2 = (vk)^2$.

The band structure is shown in Fig. 2. The minimal value of the upper energy ε_1 is $\sqrt{U^2+\gamma_1^2}$. The ε_2 band takes the maximal value $|U|$ at $k=0$ and the minimal value $\tilde{U} = \gamma_1|U|/\sqrt{\gamma_1^2+4U^2}$ at $q^2 = 2U^2(\gamma_1^2+2U^2)/(\gamma_1^2+4U^2)$. Because the value of U is much less than γ_1, the distinction between U and $\tilde{U}$ is small and the gap between the bands ε_2 and ε_3 takes the value $2|U|$.

The eigenfunctions $\mathbf{C}$ of the Hamiltonian (2) have the form

$$\mathbf{C} = \frac{1}{C}\begin{pmatrix} (U-\varepsilon_n)[(\varepsilon_n+U)^2 - q^2] \\ -q_-[(\varepsilon_n+U)^2 - q^2] \\ \gamma_1(U^2 - \varepsilon_n^2) \\ \gamma_1 q_+(U-\varepsilon_n) \end{pmatrix}, \qquad (4)$$

where the $\mathbf{C}$ norm squared is

$$C^2 = [(\varepsilon_n+U)^2 - q^2]^2[(\varepsilon_n - U)^2 + q^2] + \gamma_1^2(\varepsilon_n - U)^2[(\varepsilon_n+U)^2 + q^2].$$

The probability to find an electron, for instance, on the first layer is $|C_1|^2+|C_2|^2$, as seen from Eqs. (1).

We assume that carriers occupy only the bands $\varepsilon_{2,3}$, so the chemical potential μ and the gap $2|U|$ are less than the distance between the bands ε_1 and ε_2, i.e., $(|\mu|, 2|U|) < \gamma_1$. The electron dispersion for the $\varepsilon_{2,3}$ bands can be expanded in powers of q^2,

$$\varepsilon_{2,3}^2(q) = U^2 - 4\frac{U^2}{\gamma_1^2}q^2 + \frac{q^4}{\gamma_1^2}. \qquad (5)$$

Then, for $q^2 \gg 4U^2$, we can use the simple relations

$$\varepsilon_{2,3}(q) = \pm\sqrt{U^2 + q^4/\gamma_1^2},$$

$$|C_1|^2 + |C_2|^2 = q^4/[q^4 + \gamma_1^2(\varepsilon_{2,3} - U)^2] = (\varepsilon_{2,3}+U)/2\varepsilon_{2,3}. \qquad (6)$$

Within such the approximation, many observable effects can be analytically evaluated for the intermediate carrier concentration, $4U^2 \ll \gamma_1\sqrt{\mu^2 - U^2} \ll \gamma_1^2$, where we neglect the effect of the "mexican hat."

At zero temperature, for the total carrier concentration n and the carrier concentrations $n_{1,2}$ on the layers, we obtain

$$n = \frac{\gamma_1}{\pi\hbar^2 v^2}\sqrt{\mu^2 - U^2} = \frac{n_0 U}{\gamma_1}\sqrt{x^2-1}, \qquad (7)$$

$$n_{1,2} = \frac{\gamma_1}{2\pi\hbar^2v^2}\int_U^\mu \sqrt{\frac{\varepsilon+U}{\varepsilon-U}}d\varepsilon = \frac{n_0U}{2\gamma_1}[\sqrt{x^2-1} \pm \ln(x+\sqrt{x^2-1})], \qquad (8)$$

where $n_0 = \gamma_1^2/\pi\hbar^2v^2 = 1.2\times10^{13}$ cm^{-2} and $x = \mu/U$.

In order to find the chemical potential μ and the gap $2|U|$ at the given gate voltage, we minimize the total energy containing both the energy V of the carriers and the energy V_f of the electrostatic field. Instead of the chemical potential, it is convenient to use the variable x along with U. Electrons in the ε_2 band or holes in the ε_3 band contribute in the total energy of the system the energy

$$V = \frac{2}{\pi\hbar^2v^2}\int \varepsilon_2(q)qdq = \frac{n_0U^2}{2\gamma_1}[x\sqrt{x^2-1} + \ln(x+\sqrt{x^2-1})]. \qquad (9)$$

The energy of the electrostatic field,

$$V_f = \frac{1}{8\pi}(dE^2 + \epsilon_w d_w E_w^2), \qquad (10)$$

can be written in terms of the carrier concentrations with the help of relations (see Fig. 3)

$$4\pi e(n_1 - n_d/2) = E \text{ and } 4\pi e(n - n_d) = \epsilon_w E_w, \qquad (11)$$

where ϵ_w is the dielectric constant of the wafer, the negative (positive) n_d is the acceptor (donor) concentration, and we

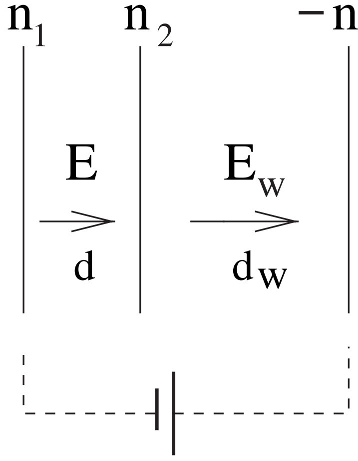

FIG. 3. Electrostatic model; d is the interlayer distance and d_w is the wafer thickness.

suppose that the donors and acceptors are equally divided between two layers.

We seek the minimum of the total energy as a function of two variables, U and x, under the gate bias constraint

$$eV_g = -edE - ed_w E_w. \tag{12}$$

Excluding the Lagrange multiplier and assuming the interlayer distance to be much less than the thickness d_w of the dielectric wafer, we obtain the following equation:

$$4\pi e^2 d\left(n_2 - \frac{n_d}{2}\right)\left(\frac{n_{1x}}{n_x} - \frac{n_{1u}}{n_u}\right) = \frac{V_x}{n_x} - \frac{V_u}{n_u}. \tag{13}$$

Let us emphasize that this equation is invariant only with respect to the simultaneous sign change in $n_{1,2}$ and n_d that expresses the charge invariance of the problem. At the fixed sign of the external doping n_d, the gap on the electron and hole sides of the gate bias is not symmetrical.

The derivatives in Eq. (13) are calculated with the help of Eqs. (7)–(11). As a result, Eq. (13) becomes

$$\frac{\gamma_1 n_d}{U n_0} = \sqrt{x^2-1} \pm \left\{ f(x) + \frac{x f(x)}{\Lambda[x f(x) - \sqrt{x^2-1}]} \right\}, \tag{14}$$

with the function $f(x)=\ln(x+\sqrt{x^2-1})$ and the dimensionless screening constant

$$\Lambda = \frac{e^2 \gamma_1 d}{(\hbar v)^2}.$$

For the parameters of graphene $d=3.35$ Å, $\gamma_1=0.4$ eV, and $v=10^8$ cm/s, we get $\Lambda=0.447$.

First, consider an ideal undoped bilayer with $n_d=0$, namely, $|\gamma_1 n_d/Un_0| \ll 1$. We obtain a solution, as $x_0=6.2784$, only for one sign in Eq. (14) determining the polarity of the layers [see Eq. (8)]. This value gives $2|U/\mu| = 2/x_0 = 0.3186$ for the ratio of the gap to the chemical potential. According to Eq. (7), the gap as a function of the carrier concentration (see Fig. 4) takes a very simple form

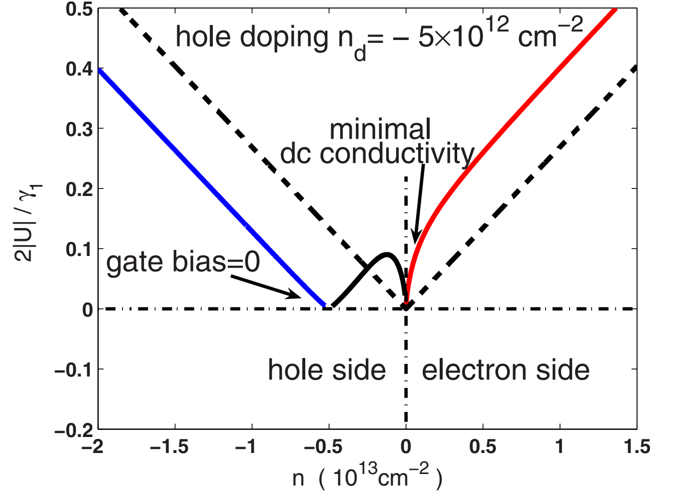

FIG. 4. (Color online) The gap in units of $\gamma_1=0.4$ eV vs the carrier concentration for the hole doping with concentration $n_d=-5\times10^{12}$ cm^{-2} (solid line) and in the absence of doping, $n_d=0$ (dashed line); the positive (negative) values of n correspond to the electron (hole) conductivity.

$$2|U/n| = \frac{2\gamma_1}{n_0\sqrt{x_0^2-1}} = 1.08 \times 10^{-11} \text{ meV cm}^2, \tag{15}$$

where the right-hand side does not depend on the gate bias at all, but only on the screening constant Λ.

We can compare Eq. (15) to the corresponding result of Ref. 8

$$2|U/n| = \frac{e^2 d}{2\epsilon_0}\left[1 + 2\Lambda\frac{|n|}{n_0} + \Lambda \ln\frac{n_0}{|n|}\right]^{-1}. \tag{16}$$

Both equations are in the numerical agreement at $|n|=0.1n_0 \simeq 10^{12}$ cm^{-2}. However, contrary to Eq. (15), Eq. (16) contains the carrier concentration in the right-hand side, giving rise to the more rapid increase in the gap with $|n| \ll n_0$. This increase also contradicts to the DFT calculations.[10]

For the bilayer with acceptors or donors, $n_d \neq 0$, Eq. (14) presents a solution $w=\gamma_1 n_d/Un_0$ as a function of x. We obtain, evidently, the small values of w for x close to $x_0=6.28$. In this region of the relatively large $|U|$, we find again with the help of Eqs. (7) and (14) the linear dependence

$$2|U| = 2\gamma_1\frac{|n-n_d|}{n_0 x_0} = 1.08|n-n_d| \times 10^{-11} \text{ meV cm}^2.$$

For the small gap, $|Un_0/\gamma_1 n_d| < 1$, we obtain different results for the electron and hole types of conductivity. For instance, if the bilayer contains acceptors (Fig. 4) with concentration n_d, the gap decreases linearly with the hole concentration and vanishes when the gate bias is not applied and the hole concentration equals n_d. Starting from this point, the gap increases and, thereafter, becomes again small (equal to zero in Fig. 4) at the carrier concentration corresponding to the minimal value of the dc conductivity. Therefore, the difference observed in Ref. 15 between these two values of carrier concentrations, at the zero bias and at the minimal conductivity, gives directly the donor or acceptor concentra-

tion in the bilayer. Then, for the gate bias applied in order to increase the electron concentration, the gap is rapidly opening with the electron appearance.

We see that the asymmetry arises between the electron and hole sides of the gate bias. This asymmetry can simulate a result of the hopping integral Δ in the electron spectrum.[14] In order to obtain the gap dependence for the case of electron doping, $n_d > 0$, the reflection transformation $n \to -n$ has to be made in Fig. 4.

The gap in the vicinity of the minimal conductivity point reaches indeed a finite value due to several reasons. One of them is the form of the mexican hat shown in Fig. 2. Second, the trigonal warping is substantial at low carrier concentrations. Finally, the graphene electron spectrum is unstable with respect to the Coulomb interaction at the low-momentum values. For the graphene monolayer as shown in Ref. 16, the logarithmic corrections appear at the small momentum. In the case of the bilayer, the electron self-energy contains the linear corrections, as can be found using the perturbation theory. The similar linear terms resulting in a nematic order were also obtained in the framework of the renormalization group.[17]

In conclusions, the gap $2U$ opening in the gated graphene bilayer has an intriguing behavior as a function of carrier concentration. In the presence of the external doping charge, i.e., donors or acceptors, this function is asymmetric on the hole and electron sides of the gate bias and it is linear only for the large gate bias.

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