Electron energy spectrum and the Berry phase in a graphite bilayer

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We emphasize that there exist four Dirac-type points in the electron energy spectrum of a graphite bilayer near the point K of its Brillouin zone. One of the Dirac points is at the point K, and three Dirac points lie nearby. Each of these three points generates the Berry phase π, while the Dirac point at K gives the phase $-\pi$. It is these four points that determine the Berry phase in the bilayer. If an electron orbit surrounds all these points, the Berry phase is equal to 2π.

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In the recent Letter[1] McCann and Fal'ko considered the electron energy spectrum of a graphite bilayer in the vicinity of the point K of its Brillouin zone and stated that in this bilayer the low-energy electronic excitations correspond to chiral quasiparticles with a parabolic dispersion exhibiting Berry phase 2π. This value of the Berry phase explains the unconventional Hall effect observed in the bilayer.[2] Here we refine some details of the spectrum and show that in reality this Berry phase in the bilayer is generated by four Dirac points of its spectrum.

First of all we point out that the electron spectrum of the bilayer[1] can be easily obtained from the well-known Slonzewski-Weiss-McClure spectrum[3] of bulk graphite if one puts $\cos\xi=0.5$ and $\gamma_2=\gamma_5=0$ (the parameters γ_2 and γ_5 describe the interaction of the atoms in the next-nearest-neighbor layers of graphite that are absent in the bilayer; ξ is the dimensionless wave vector perpendicular to the graphite layers). The Slonzewski-Weiss-McClure model[3] describes the wave-vector dependence of four electron energy bands of graphite $E(\mathbf{k})$ in the vicinity of the vertical edge HKH of its Brillouin zone. These bands can be found from the fourth-order secular equation

$$\det|\hat{H}-E|=0, \tag{1}$$

where the Hamiltonian matrix $\hat{H}$ has the form

$$\hat{H}=\begin{pmatrix} E_1 & 0 & H_{13} & H_{13}^* \\ 0 & E_2 & H_{23} & -H_{23}^* \\ H_{13}^* & H_{23}^* & E_3 & H_{33} \\ H_{13} & -H_{23} & H_{33}^* & E_3 \end{pmatrix}. \tag{2}$$

Here the following notations have been used:

$$\begin{aligned} E_1&=\Delta+\gamma_1\Gamma+\tfrac{1}{2}\gamma_5\Gamma^2, \\ E_2&=\Delta-\gamma_1\Gamma+\tfrac{1}{2}\gamma_5\Gamma^2, \\ E_3&=\tfrac{1}{2}\gamma_2\Gamma^2, \\ H_{13}&=\tfrac{1}{\sqrt{2}}(-\gamma_0+\gamma_4\Gamma)e^{i\alpha}\zeta, \\ H_{23}&=\tfrac{1}{\sqrt{2}}(\gamma_0+\gamma_4\Gamma)e^{i\alpha}\zeta, \\ H_{33}&=\gamma_3\Gamma e^{i\alpha}\zeta, \end{aligned} \tag{3}$$

where α is the angle between the direction of the vector $\mathbf{k}$ and the ΓK direction in the Brillouin zone, $\Gamma=2\cos\xi$, ξ and ζ are dimensionless wave vectors in the direction of the z axis (i.e., HKH axis) and in the basal plane, respectively, $\xi=(\pi/2)(k_z/|KH|)$ and $\zeta=(2\pi/\sqrt{3})(k_\perp/|\Gamma K|)$, $k_\perp=\sqrt{k_x^2+k_y^2}$, and $\mathbf{k}$ is measured from the point K. The parameter γ_0 which describes the interaction between neighbor atoms in a graphite layer is sufficiently large as compared to the other parameters γ_i and Δ which describe relatively weak interactions between atoms in different graphite layers.[4] As it was mentioned above, the spectrum of the bilayer is obtained if one puts $\Gamma=1$ and $\gamma_2=\gamma_5=0$. Note that in this way one can allow for the small parameter γ_4 that was neglected in Ref. 1.

In the interval $E_c\ll|E|\ll\gamma_1$ Eqs. (1)–(3) lead to the approximate formula for the two low-energy bands of electrons (e) and holes (h) in the bilayer

$$E^{e,h}(k_x,k_y)\approx\pm\frac{\gamma_0^2}{\gamma_1}\zeta^2, \tag{4}$$

which exhibits a quadratic dependence on $k_\perp$ discussed in Ref. 1. Here $E_c=(\gamma_1/4)(\gamma_3/\gamma_0)^2\approx 2$ meV, and the signs plus and minus correspond to the electrons and holes, respectively.

At energies $|E|<E_c$ the role of the so-called trigonal warping[5] increases, and this warping breaks the line $E=$const in the k_x-k_y plane into one central and three side pockets,[1] see Fig. 2 in Ref. 1. We emphasize here that each of these pockets contains a point at which the electron and the hole bands contact, and near all these points the spectrum is *linear* in $\mathbf{k}$, Fig. 1, see also Refs. 6–8. Thus, similarly to bulk graphite[9] and in contrast with graphene, in the graphite bilayer near the point K there are *four* points of the Dirac type. The central contact point coincides with K, while the three side contact points are at a distance of $(\sqrt{3}/2\pi)(\gamma_3\gamma_1/\gamma_0^2)|\Gamma K|\approx 0.005|\Gamma K|$ from K where $|\Gamma K|$ is the distance between the point K and the center Γ of the Brillouin zone.

Before analyzing the Berry phase in the bilayer, we point out a general property of this phase for closed semiclassical electron orbits in crystals with inversion symmetry in the magnetic field $\mathbf{H}$. The Berry phase Φ_B for such an orbit Γ lying in the Brillouin zone and belonging to a band 0 is given by[10,11]

$$\Phi_B=\oint_\Gamma \mathbf{\Omega}d\mathbf{k}, \tag{5}$$

where the direction of the integration is determined by the vector $[\mathbf{H}\times\partial E^0/\partial\mathbf{k}]$, $\mathbf{\Omega}$ is the intraband matrix element of

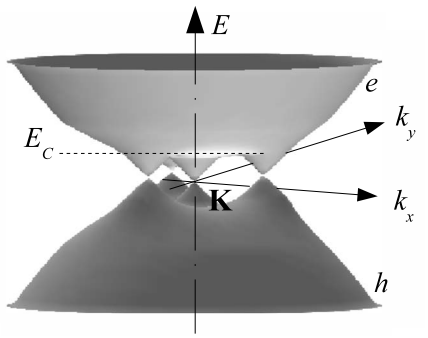

FIG. 1. Shown is the dispersion law $E(k_x,k_y)$ of the electrons (e) and holes (h) in the graphite bilayer near the point K. The spectrum contains four Dirac points. At the energy $E_c \sim 2$ meV all the electron cones merge. Note that without neglecting the parameter $\gamma_4 \approx 0.044$ eV, the spectrum $E(k_x,k_y)$ is slightly asymmetric relative to the plane $E=0$: The Dirac points in the central and side cones are at energies $E=0$ and $E=2\gamma_4\gamma_1\gamma_3^2/\gamma_0^3 \approx 0.15E_c$, respectively. Thus, in contrast with graphene, the graphite bilayer is a semimetal, and changing the Fermi level in it, one cannot obtain the concentration of the charge carriers less than $\sim 10^8$ cm^{-2}. Scales of the plot are distorted for clarity.

the periodic (in $\mathbf{k}$) part of the coordinate operator in the crystal momentum representation,[12]

$$\mathbf{\Omega}(\mathbf{k}) = \imath \int d\mathbf{r} u_{\mathbf{k}0}^*(\mathbf{r}) \nabla_{\mathbf{k}} u_{\mathbf{k}0}(\mathbf{r}), \tag{6}$$

and $u_{\mathbf{k}0}(\mathbf{r})$ is the periodic factor in the electron Bloch wave function of the band 0, $\psi_{\mathbf{k}0}(\mathbf{r}) = \exp(\imath \mathbf{kr}) u_{\mathbf{k}0}(\mathbf{r})$. This Berry phase manifests itself in the Onzager-Lifshitz-Kosevich quantization condition[13,14] for energy levels ε of an electron in the magnetic field,

$$S(\varepsilon, k_H) = \frac{2\pi eH}{\hbar c}(n+\gamma), \tag{7}$$

where S is the cross-sectional area of the closed orbit in the $\mathbf{k}$ space, k_H is the component of $\mathbf{k}$ along the magnetic field $\mathbf{H}$, n is a large integer ($n>0$), e is the absolute value of the electron charge, and the constant γ is given by the formula[11]

$$\gamma = \frac{1}{2} - \frac{\Phi_B}{2\pi}. \tag{8}$$

If one reverses the direction of the magnetic field, the direction of the integration in Eq. (5) is also reversed, and the Berry phase changes its sign, while γ changes by Φ_B/π. However, the electron spectrum in the magnetic field has to be invariant under this transformation. Since in the semiclassical approximation the quantity γ is defined up to an integer, we conclude that the Berry phases for such the orbits are always multiple of π.[15] This property of the Berry phase agrees with the results of Ref. 11. It was shown in that paper that if the electron orbit Γ surrounds band-contact lines (Dirac points in the two dimensional case), each of the lines (the Dirac points) contributes $\pm\pi$ to Φ_B. If the orbit does not surround the band-contact line (the Dirac points), the Berry phase is equal to zero. This property of the Berry phase also means that Φ_B can change only abruptly when the crystal potential is perturbed, and a small variation of this potential can, in principle, lead to an essential change of the Berry phase.

McCann and Fal'ko derived the Berry phase for the electron orbits in the bilayer from an effective Hamiltonian that leads to the parabolic spectrum (4). However, it is clear that parabolic spectra are idealization, and they never occur in crystals, and at least a small warping of these spectra always exists. As it was mentioned above, this small warping may essentially change the Berry phase, and in principle, different symmetries of the small warping may lead to different values of the Berry phase since the number of the Dirac points depends on symmetry of a crystal. In the case of the bilayer the trigonal warping generates the three additional side Dirac points and changes the type of the central band-contact point. Thus, for the derivation of the Berry-phase value to be justified, it is necessary to consider the real symmetry of the spectrum in the bilayer and to take into account all the band-contact points of this spectrum.

Although each of the four Dirac point in the bilayer generates the Berry phase $\pm\pi$, it is necessary to find the signs of these phases. This can be done using the approach of Ref. 15 in which the effect of a small spin-orbit interaction on the Berry phase was investigated. It is important that if this interaction is weak, it does not change the Berry phase. However, the interaction enables one to fix the sign of the phase.[16] This is clear from the following considerations: Without the spin-orbit interaction the quantity $[\nabla_{\mathbf{k}} \times \mathbf{\Omega}]$ is singular at the Dirac points. The interaction lifts the band degeneracy, and $[\nabla_{\mathbf{k}} \times \mathbf{\Omega}]$ becomes a smooth function which can be calculated using the formula[12] [see also expressions (9) and (10) in Ref. 17 and formula (6.6) in Ref. 18]

$$[\nabla_{\mathbf{k}} \times \mathbf{\Omega}]_z = i\hbar^2 \sum_{l \neq 0} \frac{v_{0l}^x v_{l0}^y - v_{0l}^y v_{l0}^x}{(E_l(\mathbf{k}) - E_0(\mathbf{k}))^2}, \tag{9}$$

which is completely independent of a gauge of the electron Bloch wave functions. Here v_{0l}^i are interband matrix elements of the velocity operator for the bands 0 and l at a point $\mathbf{k}$. Taking into account that Eq. (5) may be rewritten in the form

$$\Phi_B = \int_S dk_x dk_y [\nabla_{\mathbf{k}} \times \mathbf{\Omega}]_z, \tag{10}$$

where the integration is over the surface S spanning the orbit Γ, one can unambiguously calculate the Berry phase for each of the Dirac points in the bilayer.

The effect of the spin-orbit interaction on the spectrum of graphene was considered in Refs. 19 and 20, and the following Hamiltonian for the electron and hole bands in the vicinity of the point K was obtained as

$$\hat{H} = v(k_x\sigma_x + k_y\sigma_y) + \Delta_{so}\sigma_z s_z, \tag{11}$$

where σ_i are the Pauli matrices describing the two bands, v is a matrix element proportional to γ_0, $2\Delta_{so} \sim 0.2$ meV is the gap due to the spin-orbit interaction, and s_z is the Pauli matrix representing electron's spin. Since the interaction be-

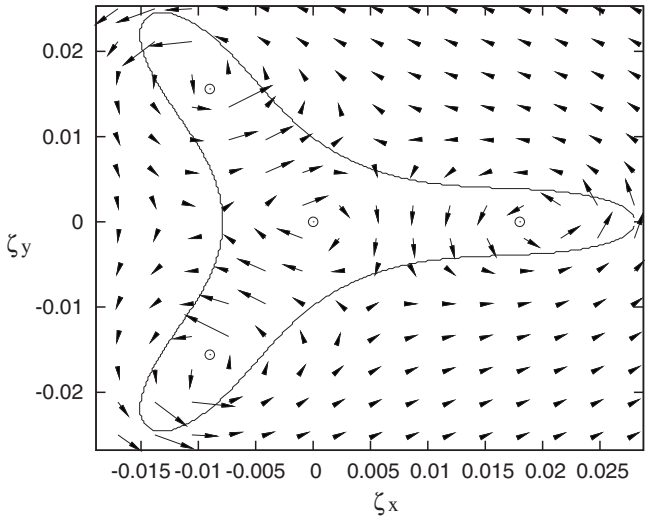

FIG. 2. The field $\mathbf{\Omega}(k_x,k_y)$ (arrows) for the electron band e in the bilayer. The length of the arrows is proportional to $|\mathbf{\Omega}|$. Small circles mark the positions of the Dirac points in the k_x-k_y plane, and the solid line shows an electron orbit with $E>E_c$. Note that near the central and the side Dirac points the vector $\mathbf{\Omega}$ circulates in opposite directions. The components k_i are given in the dimensionless units $\zeta_i=(2\pi/\sqrt{3})(k_i/|\Gamma K|)$ where $|\Gamma K|$ is the distance between the point K and the center of the Brillouin zone, Γ.

tween carbon atoms in a graphite layer is larger than the interaction between the atoms in different graphite layers (i.e., $\gamma_0 \gg \gamma_i$), we use Hamiltonian (11) of a single layer to include the spin-orbit interaction in Hamiltonian (2) and (3) of the bilayer. Then, in the leading order in the small parameter Δ_{so}/γ_1 the matrix elements E_3 in the third and fourth lines of formula (2) should be replaced by $E_3-\Delta_{so}$ and $E_3+\Delta_{so}$, respectively.

Although formulas (9) and (10) clearly demonstrate the invariance of the Berry phase relative to the gauge transformations of the Bloch wave functions, it is more convenient to find the field $\mathbf{\Omega}(k_x,k_y)$ in the bilayer, and to calculate the Berry phase directly from formula (5). This field for a band 0 can be obtained with the formula[15,21]

$$\mathbf{\Omega} = i\left(S^{+}\frac{\partial S}{\partial \mathbf{k}}\right)_{00}, \tag{12}$$

where $S(\mathbf{k})$ is the matrix reducing Hamiltonian (2) and (3) to the diagonal form, S^{+} is the Hermitian conjugate matrix, and the subscript means that one has to consider the diagonal matrix element corresponding to the band 0. Assuming the spin-orbit interaction is infinitesimal, a direct calculation of S leads to the field $\mathbf{\Omega}(k_x,k_y)$ shown in Fig. 2. Note that near the central and the side Dirac points the vector $\mathbf{\Omega}$ "circulates" in opposite directions, which means the opposite signs of the Berry phases generated by these points. The calculation of the integral (5) gives the Berry phase π for electron orbits surrounding each of the three side Dirac points and $-\pi$ for an orbit around the central point. Since the Berry phase of an electron does not depend on a size or a shape of its orbit in the Brillouin zone but is determined only by the Dirac points enclosed by the orbit,[11] one finds the Berry phase $3\cdot\pi-\pi=2\pi$ for electrons with energies $E>E_c$ (i.e., at the electron concentration $N>N_c\approx 5\times 10^{10}$ cm^{-2}) when their orbits surround all these four points. Thus, at $E>E_c$ we arrive at the same Berry phase 2π as in the case of the parabolic spectrum (4) in spite of the change in the energy-band degeneracy. The difference in the Berry phases for the parabolic and real spectra will manifest itself only in the interval $-E_c<E<E_c$ at low magnetic fields when many Landau levels lie in this interval, and hence the trigonal warping is not a small perturbation as compared to the magnetic energy of the electron.

The above considerations also clarify existence of the resistivity maximum discovered in the bilayer.[2] In graphene the universal resistivity maximum $h/4e^2$ was observed at zero magnetic field and low charge-carrier concentration N, and this maximum was explained by the absence of localization for electrons with the Dirac-type spectrum.[22] A similar resistivity maximum was also observed in the bilayer,[2] and Novoselov *et al.*[2] emphasized that this observation is unexpected due to the parabolic spectrum in the bilayer. Although the parabolic spectrum of Ref. 1 and the spectrum with the four Dirac points lead to the same Berry phase at $N>N_c$, existence of the Dirac points seems to shed a light on the appearance of the resistivity maximum in the bilayer. The effect of the trigonal warping on the resistivity maximum in the bilayer was quantitatively analyzed in Refs. 6 and 23.

Finally, let us point out that our result for the Berry phase is reminiscent of the result of Ref. 8. The authors of that paper studied the stability of Fermi points in multilayer graphene relative to perturbations of the crystal potential, and they found that in the bilayer some topological charge Q is equal to 2 for the case of the parabolic spectrum (4), while if one takes into account the trigonal warping, each of the three side Dirac points located near the point K has the charge 1 and the charge of the central Dirac point at K is -1. Nevertheless, it is necessary to emphasize that in general case formula (11) defining Q in Ref. 8 does not coincide with Φ_B/π [compare this formula with our Eqs. (5) and (12)].

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