Berry phase, semiclassical quantization and Landau levels

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We propose the semiclassical quantization for complicated electron systems governed by a many-band Hamiltonian. An explicit analytical expression of the corresponding Berry phase is derived. This impact allows us to evaluate the Landau magnetic levels when the rigorous quantization fails, for instance, for bilayer graphene and graphite with the trigonal warping. We find that the magnetic breakdown can be observed for the certain type of classical electron orbits.

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The most accurate investigation of the band structure of metals and semiconductors is studying the Landau levels in magneto-transport and magneto-optical experiments. However, the theoretical solution of the band problem in magnetic fields cannot often be exactly found. A typical example is presented by graphene layers. For bilayer graphene and graphite, the effective Hamiltonian is a $4 \times 4$ matrix giving four energy bands. Fig. 1 shows nearest two bands of the level structure together with semiclassical orbits. The trigonal warping described by the effective Hamiltonian with a relatively small parameter $\gamma_3$ provides an evident effect (see right panel). Another important parameter is the gate-tunable bandgap $U$ in bilayer graphene. In this situation, the quantization problem cannot be solved within a rigorous method. To overcome this difficulty one can use a perturbation theory, however this theory becomes quite complicated for the many-band Hamiltonian.

Alternatively, the semiclassical quantization can be applied. Thus, we can use the Bohr-Zommerfeld condition as

$$S(\varepsilon) = \frac{e}{\hbar} S(\varepsilon) = 2\pi \left[ n + \frac{T}{4} + \delta(\varepsilon) \right].$$

where $S(\varepsilon)$ is the cross-section area of the electron orbit in the $k$ space for the energy $\varepsilon$ in absence of the magnetic field $B$ and for the constant momentum projection $k_z$ on the magnetic field, $n$ is an integer number, $T$ is the number of the smooth turning points on the electron orbit. There are two smooth turning points for the Landau levels and only one for skipping electrons reflected by the hard edge.

The goal of this letter is an explicit analytical expression for the $\delta(\varepsilon)$—phase within the band scheme of the matrix Hamiltonian. The semiclassical approach is used for the magnetic field normal to the layered system when the quantization of in-layer momentum components is only essential and the size of the Fermi surface is small compared with the Brillouin zone size. We illustrate our results for bilayer graphene. Notice, that the $\delta(\varepsilon)$—phase depends on the energy and can be taken in the interval $0 \leq |\delta| \leq 1/2$. If the spin is neglected, $\delta = 0$ and $T = 2$ for the Landau levels, and $\delta = 1/2$ and $T = 2$ for monolayer graphene. In these two cases, the semiclassical result coincides with the rigorous quantization and it is closely connected with the topological Berry phase $\Pi$. This $\delta$—phase was evaluated for bismuth in Ref. [4], preceding Berry’s work by almost two decades, and it was considered again for bismuth in Ref. [3]. For graphene, the semiclassical quantization was applied in Ref. [7]. However, in the general case, the evaluation of the $\delta$—phase is still attracted a widespread interest [11].

The problem under consideration is described by the Hamiltonian in the band representation

$$(\mathbf{V} \cdot \mathbf{k} + \mathbf{\Gamma} + \varepsilon) \Psi = 0,$$

where the column $\Psi$ consists of functions corresponding with a number of bands included and is labelled by the band subscript which we omit together with the matrix as

![FIG. 1: (Color online) (a) The energy dispersion $\varepsilon(k, \alpha)$ of two nearest bands (the electron band shown in solid line and the hole band in dashed line) in bilayer graphene for two polar angles $\alpha$ with the local extrema at $k \neq 0$ ("mexican hat") represented. The band parameters are given in the figure, others are $\gamma_0 = 3.05$ eV, $\gamma_1 = 360$ meV, $\gamma_4 = -150$ meV. (b) Cross-sections $k(\alpha, \varepsilon)$ of the electron band for energies of 80 meV (dashed-dotted line) and 40 meV (solid line).]
subscripts on Γ and V; a summation over them is implied in Eq. (2). Matrices Γ and V are the first two terms in a series expansion of the Hamiltonian in the power of quasi-momentum \( k \).

In the magnetic field, the momentum operator \( \tilde{k} \) depends on the vector-potential \( \mathbf{A} \) by means the Peierls substitution,

\[
\tilde{k} = -i\hbar \nabla - e\mathbf{A}/c,
\]

providing the gauge invariance of the theory. The magnetic field can also enter explicitly describing the magnetic interaction with the spin of a particle. However, for the graphene family, the magnetic interaction is weak and omitted here.

A simple example of Eq. (2) is given by the graphene monolayer. There are two sublattices in it, and Eq. (2) is represented by a \( 2 \times 2 \) matrix if the spin of carriers is neglected. Another example considered below is bilayer graphene with the \( 4 \times 4 \) matrix Hamiltonian. For the monolayer and bilayer graphene, both \( V \) and \( \tilde{k} \) are two-dimensional vectors, e.g., with \( x \) and \( y \) components.

We seek for \( \Psi \) in the form

\[
\Psi = \Phi \exp \left( is/\hbar \right),
\]

where the function \( s \) is assumed to be common for all components of the column \( \Psi \). The equation for \( \Phi \) is reduced to

\[
\begin{align*}
|V \cdot (\mathbf{k} - i\hbar \nabla) + \Gamma - \varepsilon| \Phi &= 0, \\
&\text{with } \mathbf{k} = \nabla s - e\mathbf{A}/c.
\end{align*}
\]

The function \( \Phi \) is expanded in series of \( \hbar/ i \):

\[
\Phi = \sum_{m=0}^{\infty} \left( \frac{\hbar}{i} \right)^m \varphi_m.
\]

Comparing the terms involving the same powers of \( \hbar \) in Eq. (4) we have

\[
(V \cdot \mathbf{k} + \Gamma - \varepsilon)\varphi_m = -V \nabla \varphi_{m-1}.
\]

For \( m = 0 \), we get a homogeneous system of algebraic equations

\[
(V \cdot \mathbf{k} + \Gamma - \varepsilon)\varphi_0 = 0
\]

which has a solution under the condition

\[
\text{Det}(V \cdot \mathbf{k} + \Gamma - \varepsilon) = 0.
\]

This equation determines the classical electron orbit, \( \varepsilon(k_x, k_y) = \varepsilon \), in presence of the magnetic field while the electron energy \( \varepsilon \) is constant. At the same time, the equation yields the electron dispersion equation with \( \mathbf{k} \) as the momentum without any magnetic field. In 3d case, the electron dispersion depends as well on the momentum projection \( k_z \) on the magnetic field and our scheme can be implied in this case without the expansion in \( k_z \).

It is convenient to choose the vector-potential in the Landau gauge \( A_x = -By, A_y = A_z = 0 \) in such a way that the Hamiltonian does not depend on the \( x \)-coordinate. Then, the \( x \)-momentum component \( K_x \) becomes a conserved quantum number and the function \( s \) in Eq. (5) can be written as

\[
s = xK_x + \sigma(y) .
\]

The equations (5) are reduced to

\[
k_x = K_x + \frac{e}{c} By, \quad k_y = \frac{d\sigma}{dy}.
\]

These equations enable us to use the variable \( k_x \) instead of \( y \) and to obtain

\[
\sigma(k_x) = \frac{c}{eB} \int k_y(k_x')dk_x',
\]

where \( k_y \) as a function of \( k_x \) is determined by the dispersion equation (8).

The eigenfunction column obeying Eq. (7) can be multiplied by the scalar function \( C \) common for all elements of the column

\[
\varphi_0 \to C \varphi_0
\]

where \( \varphi_0 \) is any eigen-column of Eq. (7). The function \( C \) is determined by Eq. (6) with \( m = 1 \). Left-to-right multiplying both sides of this equation by \( \varphi_0^* \) and using the Hamiltonian hermiticity, i.e. the complex conjugations of Eq. (7), we get the consistency condition

\[
\varphi_0^* V \nabla (C \varphi_0) = 0 ,
\]

where the derivative with respect to \( y \) (i.e. to \( k_x \)) is only to be taken. The left hand-side of this equation can be written as

\[
\frac{1}{C} \frac{dC}{dk_x} + \frac{1}{2\varphi_0^* V_y \varphi_0} \frac{d\varphi_0^* V_y \varphi_0}{dk_x} + \frac{i}{\varphi_0^* V_y \varphi_0} \text{Im} \varphi_0^* V_y \frac{d\varphi_0}{dk_x}
\]

Using the identity \( \varphi_0^* V \varphi_0 = \varphi_0^* \varphi_0 v \) with the electron velocity \( v = \partial \varepsilon/\partial k \), one can write the solution of Eq. (11) as

\[
C = c_0 (\varphi_0^* \varphi_0 v_y)^{-1/2} \exp(-i\theta) ,
\]

where

\[
\theta = \text{Im} \int \frac{dk_x}{\varphi_0^* \varphi_0 v_y} \varphi_0^* V_y \frac{d\varphi_0}{dk_x}.
\]

and \( c_0 \) is the normalization factor.

The quantization condition can be written as usual from the requirement that the wave function has to be single-valued. Continuing Eqs. (10), (12), and (13) along
the orbit and making the bypass in the complex plane around the turning points where \( v_y = 0 \) to obtain the decreasing solutions in the classically inaccessibile region, one obtains \( \mathcal{T} = 2 \) and \( \delta \)-phase as a contour integral along the classical orbit

\[
\delta(\epsilon) = \frac{1}{2\pi} \text{Im} \oint \frac{dk_x}{\varphi_0^* \varphi_0 v} \varphi_0 V_y \frac{d\varphi_0}{dk_x} .
\]  

(14)

Using the Hamiltonian hermiticity, after the simple algebra (see Ref. [2]), Eq. (14) can be rewrite as

\[
\delta(\epsilon) = \frac{1}{4\pi} \oint \frac{dk}{\varphi_0^* \varphi_0 v} \varphi_0 \left[ V \times \frac{d}{dk} \right] \varphi_0
\]

called usually the Berry phase.

Now let us calculate the \( \delta \)-phase for bilayer graphene. In simplest case, the effective Hamiltonian can be written (see, for instance Refs. [12 [13]) as

\[
H(k) = \begin{pmatrix}
U & q_+ & \gamma_1 & 0 \\
q_- & U & 0 & 0 \\
\gamma_1 & 0 & -U & q_- \\
0 & 0 & q_+ & -U
\end{pmatrix},
\]

(15)

where the parameter \( U \) describes the tunable gap, \( \gamma_1 \) is the nearest-neighbor hopping integral energy, the matrix elements are expanded in the momentum \( k_\pm = \mp ik_x - k_y \) near the \( K \) points of the Brillouin zone, and the constant velocity parameter \( v \) is incorporated in the notation \( q_\pm = vk_\pm \).

Here, the orbit is the circle defined by Eq. (13), written in the following form

\[
(U + \epsilon)^2 - q^2[(U - \epsilon)^2 - q^2] - \gamma_1^2(\epsilon^2 - U^2) = 0. \]  

(16)

The eigenfunction \( \varphi_0 \) of the Hamiltonian (15) can be taken as

\[
\varphi_0 = \begin{pmatrix}
(U - \epsilon)[(U + \epsilon)^2 - q^2] \\
q_-[q^2 - (U + \epsilon)^2] \\
\gamma_1(U^2 - \epsilon^2) \\
\gamma_1 q_+(U - \epsilon)
\end{pmatrix},
\]

(17)

with the norm squared

\[
\varphi_0^* \varphi_0 = \frac{\gamma_1^2(\epsilon - U)^2[(U + \epsilon)^2 + q^2]}{\gamma_1 q_+(U - \epsilon)} .
\]

(18)

The derivatives for Eq. (14) are calculated along the trajectory where the energy \( \epsilon \) and consequently the trajectory radius \( q \) are constant. The equation (14) has only one solution for \( q^2 \) if \( |U| < |\epsilon| < \sqrt{U^2 + \gamma_1^2} \). First, let us consider this case.

(i) there is only one orbit at given energy \( \epsilon \) with the radius squared

\[
q^2 = U^2 + \epsilon^2 + \sqrt{4U^2\epsilon^2 + (\epsilon^2 - U^2)\gamma_1^2} .
\]

The matrix \( V_y = \partial H/\partial k_y \) in Eq. (14) has only four nonzero elements \( V_{y12} = V_{y21} = V_{y34} = V_{y43} = -1 \). Using Eqs. (16) and (17), we find

\[
\text{Im} \varphi_0^* V_y \frac{d\varphi_0}{dk_x} = 4U\epsilon(U - \epsilon)[(\epsilon + U)^2 - q^2].
\]

(19)

This expression is constant on the trajectory as well as \( \varphi_0^* \varphi_0 \), Eq. (18). Therefore, in order to find \( \delta \), Eq. (14), we have to integrate along the trajectory

\[
\oint \frac{dk_x}{\varphi_0 v}.
\]

This integral equals \(-dS(\epsilon)/d\epsilon\), where \( S(\epsilon) = \pi q^2 \) is the cross-section area, Eq. (11), with

\[
\frac{dS(\epsilon)}{d\epsilon} = \pi \epsilon \frac{2(\epsilon^2 + U^2 - \epsilon^2) + \gamma_1^2}{(\epsilon^2 - U^2 - \epsilon^2)^2} .
\]

(20)

Now we have to substitute Eqs. (18), (19), and (20) into Eq. (14). Thus, we find the Berry phase

\[
\delta(\epsilon) = -\frac{-\epsilon U}{q^2 - \epsilon^2 - U^2} = \frac{-\epsilon U}{\sqrt{4U^2\epsilon^2 + (\epsilon^2 - U^2)^2}} .
\]

(21)

shown in Fig. 2 where \( \delta \)-phase of bilayer graphene with trigonal warping is also shown, the detailed calculations will be elsewhere published. For the ungapped bilayer, \( U = 0 \), the Berry phase \( \delta(\epsilon) = 0 \). The Berry phase depends on the energy and \( \delta = \mp \pi/2 \) at \( \epsilon = \pm U \). At the larger energy, \( \epsilon \gg U \), the Berry phase \( \delta \rightarrow \mp U/\gamma_1 \).

Substituting Eq. (21) in the semiclassical quantization condition, Eq. (11), and solving the equation obtained for \( \epsilon \), we get energy levels as a function of the magnetic field. We have to notice that the Landau numbers \( n_L \)

![FIG. 2: (Color online) Semiclassical phase vs energy in the conduction band of bilayer graphene without trigonal warping (solid line) and with warping (dashed line).](image-url)
listed in Fig. 3 do not coincide with the numbers $n$ in the semiclassical condition (11). The rigorous quantization shows that there are only one Landau level with $n_L = 0$ and three Landau levels with $n_L = 1$ (14). These levels are not correctly described within the semiclassical approach. However, for $n_L \geq 2$, there are levels in all four bands $s$ (two nearest bands with $s = 2, 3$ are shown in Fig. 3). They correspond with the quantum number $n = n_L - 1$, and the semiclassical levels become in excellent agreement with the rigorous solution for the larger $n$.

(ii) for $|U|/\sqrt{1 + (2U/\gamma_1)^2} < |\varepsilon| < |U|$, at the given energy, there are two orbits with the radius squared

$$q_{1,2}^2 = U^2 + \varepsilon^2 \pm r,$$

where $r = \sqrt{4U^2\varepsilon^2 + (\varepsilon^2 - U^2)\gamma_1^2}$.

This is an effect of "the mexican hat". Then we seek for the general solution as a sum of two solutions $\phi^j_0(1)$ and $\phi^j_0(2)$ corresponding to these two contours,

$$\phi^j_0 = C_1 \phi^j_0(1) + C_2 \phi^j_0(2)$$

with two scalars $C_1$ and $C_2$. Instead of Eq. (11) we have a system of two equations written in the $2 \times 2$ matrix form as follows

$$\begin{align*}
a \frac{dC}{dq_x} + bC & = 0 \\
C & = \begin{pmatrix}
a_{11} & a_{12} \\
a_{21} & a_{22}
\end{pmatrix}
\end{align*}$$

where the notations of the matrix elements are introduced

$$a_{ik} = \phi^*_i(i)V_y \phi_0(k), \quad b_{ik} = \phi^*_i(i)V_y \frac{d\phi_0(k)}{dq_x}.$$  

The off-diagonal matrix elements $a_{ik}$ vanish, $a_{12} = a_{21} = 0$. Thus, the first equation of the system (22) becomes

$$2q_1q_y \frac{dC_1}{dq_x} + (2i\varepsilon U - rq_x/q_{1y})C_1 + i(2\varepsilon U + r)C_2 = 0,$$

and the second equation can be obtained with the index replacement $1 \leftrightarrow 2$ and $r \rightarrow -r$.

These equations can be simplified with the substitution

$$C_i = \tilde{C}_i (q_1^2 - q_x^2)^{-1/4}.$$  

For the new functions $\tilde{C}_i$, we get the equation system

$$\begin{align*}
q_{1y} \frac{d\tilde{C}_1}{dq_x} + iE\tilde{C}_1 & + i \sqrt{\frac{q_{1y}}{q_{2y}}}(E + \frac{1}{2})\tilde{C}_2 = 0, \\
q_{2y} \frac{d\tilde{C}_2}{dq_x} - iE\tilde{C}_2 & - i \sqrt{\frac{q_{2y}}{q_{1y}}}(E - \frac{1}{2})\tilde{C}_1 = 0,
\end{align*}$$

where the parameter $q_{1y} = \sqrt{q_1^2 - q_x^2}$, $i = 1, 2$ and $E = \varepsilon U/r$.

For the minimum of conduction band (maximum of valence band), where $r \rightarrow 0$, there is a simple limit,

$$q_{1y} \frac{d\tilde{C}_1}{dq_x} - \frac{i}{2} \tilde{C}_1 = 0 \quad \text{with} \quad \tilde{C}_2 = -\tilde{C}_1.$$

Solving this equation, one gets

$$\tilde{C}_1 = c_0 \exp \left( \frac{i}{2} \arcsin \frac{q_x}{q_1} \right).$$  

Going with $q_x$ along the trajectories and making the bypass in the complex plane around the turning points $q_x = \pm q_1$ and $q_x = \pm q_2$, we see that both $\tilde{C}_1$ and $\tilde{C}_2$ acquire from two turning points in Eq. (24) the additional phase $-\pi$ with $T = 2$. At the same time, we have $1/2$ from Eq. (24) for $\delta$-phase. Thus, at the boundaries of the narrow interval considered, the $\delta$-phase obtains the same value, $\delta = -1/2$.

Taking into account the phases of the functions $\phi^j_0(i)$, we see, that the area $S(\varepsilon)$ in Eq. (11) can play the different role. In weak magnetic fields, slower oscillations with the smaller $S(\varepsilon)$ corresponding to $q_2$ should be observed in oscillating phenomena. However, when the magnetic field becomes larger and the semiclassical condition is fulfilled only for the larger cross-section $S(\varepsilon)$, calculated with $q_1$, the larger frequency oscillations should be observed. This is nothing but the magnetic breakdown (13) which should be utilized if the chemical potential belongs to the interval where the effect of "the mexican hat" appears.

In conclusion, our study shows that the semiclassical approach gives a powerful tool for probing the electron magnetic properties in metals. The Berry phase depending on the energy can be calculated and observed even for complicated band scheme. The method presented here should be useful for many electron systems.
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