Berry phase and pseudospin winding number in bilayer graphene

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Ever since the novel quantum Hall effect in bilayer graphene was discovered, and explained by a Berry phase of $2\pi$ [K. S. Novoselov et al., Nat. Phys. 2, 177 (2006)], it has been widely accepted that the low-energy electronic wave function in this system is described by a nontrivial Berry phase of $2\pi$, different from the zero phase of a conventional two-dimensional electron gas. Here, we show that (i) the relevant Berry phase for bilayer graphene is not different from that for a conventional two-dimensional electron gas (as expected, given that Berry phase is only meaningful modulo $2\pi$), and (ii) what is actually observed in the quantum Hall measurements is not the absolute value of the Berry phase but the pseudospin winding number.

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I. INTRODUCTION

A conventional two-dimensional electron gas (2DEG) under a high magnetic field and low temperature shows a quantized Hall conductance $\sigma_{xy} = n e^2 / h$ per spin degree of freedom where $n$ is an integer, $e$ the charge of an electron, and $h$ Planck’s constant. For graphene, it has been predicted that the Hall conductance per spin and valley degrees of freedom is $\sigma_{xy} = (n + 1/2) e^2 / h$. This prediction has then been proven by experiments performed on mechanically exfoliated samples. Such half-integer quantum Hall effect is the most decisive evidence that the sample is actually a single atomic layer of carbon atoms effectively decoupled from the substrate, and is a direct manifestation of a nontrivial Berry phase of $\pi$ in the electron wave function. This half-integer quantum Hall effect is different from the fractional quantum Hall effect in a conventional two-dimensional electron gas. Here, we focus on the Berry phase in bilayer graphene. Half-integer quantum Hall effect has been observed in graphene epitaxially grown on the carbon-rich surface and the silicon-rich surface of silicon carbide or graphene grown by chemical vapor deposition.

When a second layer is added, thus forming bilayer graphene [Fig. 1(a)], the electronic structure changes dramatically. The dispersion for low-energy quasiparticles in graphene is linear [Fig. 2(a)], whereas in bilayer graphene it becomes quadratic [Fig. 2(b)]. The quantum Hall conductance for low-energy quasiparticles in bilayer graphene effectively decoupled from the substrate, and is a direct manifestation of a nontrivial Berry phase of $2\pi$ in the electron wave function. The sign of the Berry phase is not a nontrivial Berry phase of $2\pi$ and is not different from that for a conventional two-dimensional electron gas (as expected, given that Berry phase is only meaningful modulo $2\pi$).

II. BERRY PHASE

For electrons in a periodic system, the Berry phase is a phase acquired by the wave function over the course of a cyclic evolution of the Hamiltonian—such a concept has had a fundamental role in developing the modern theory of polarization and of magnetization. The evolving parameter that we consider here is the 2D Bloch wave vector $\mathbf{k} = (k_x, k_y)$. The Berry phase $\Gamma$ described in the wave-vector evolution of Fig. 3 is given by

$$\Gamma = -i \lim_{N \to \infty} \sum_{j=0}^{N-1} \log(j | j + 1),$$

(1)
K' (a) y x (b) k k B (A') A y x B' (a) Graphene (b) Bilayer graphene (c) 2D electron gas FIG. 2. (a) Upper panel: Energy dispersions for low-energy electrons in graphene. Lower panel: Pseudospin distribution for electronic eigenstates in graphene on an equienergy contour specified by the dashed curve in the upper panel. The arrows represent the direction of pseudospin. Here, we consider the electronic states with wave vectors near the Dirac point \( K \). (b) and (c): Similar quantities as in (a) for bilayer graphene and a conventional 2DEG, respectively. Note that the electrons in a 2DEG have an energy minimum at the center of the Brillouin zone and do not have a pseudospin degree of freedom.

where \( m \) is an arbitrary integer. Now using Eqs. (1), (3), and (4), the Berry phase \( \Gamma' \) for the new set of wave functions [Eq. (3)] is

\[
\Gamma' = -i \lim_{N \to \infty} \sum_{j=0}^{N-1} \log \langle j | j + 1 \rangle' = \Gamma + \lim_{N \to \infty} \sum_{j=0}^{N-1} (\theta_{j+1} - \theta_j)
\]

\[
= \Gamma + 2\pi m,
\]

i.e., the Berry phase can be defined for modulo 2\( \pi \) only. In the following, we paraphrase this general argument using the language of graphene.

For graphene, let us consider the case where \( \mathbf{k} \) is very close to the Dirac point \( K \) [Fig. 1(b)], and define \( \mathbf{q} = \mathbf{k} - K \) \((|\mathbf{q}| \ll |K|)\). Then, if we use a basis set composed of the Bloch sums of \( p_z \) orbitals localized on the two sublattices \( A \) and \( B \) [Fig. 1(a)], the effective Hamiltonian reads

\[
H_{\text{mono}}(\mathbf{q}) = \frac{\hbar v_0}{2} \begin{pmatrix} 0 & \exp(-i\theta_q) \\ \exp(i\theta_q) & 0 \end{pmatrix},
\]

where \( v_0 \) is the band velocity and \( \theta_q \) the angle between \( \mathbf{q} \) and the \(+k_x\) direction. The energy eigenvalue and wave function of Eq. (6) are given by

\[
E_{s\mathbf{q}} \text{mono} = \hbar v_0 s |\mathbf{q}| \quad \text{and} \quad |\psi_{s\mathbf{q}}^{\text{mono}}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ s \exp(i\theta_q) \end{pmatrix},
\]

respectively, where \( s = \pm 1 \) is the band index. As shown before, the Berry phase \( \Gamma_{\text{mono}} \) of the electron wave function in graphene when the Bloch wave vector undergoes a full

where \( |N\rangle = |0\rangle \). (2)

Here, \( \mathbf{k} \) is determined by the state index \( j \).

We first show that the Berry phase [defined in Eq. (1)] is in general meaningful only for modulo 2\( \pi \). After multiplying each of the wave functions by a position-independent overall phase factor \( \exp(i\theta_j) \), we obtain another set of wave functions which satisfies the equation of motion

\[
|j\rangle' = \exp(i\theta_j) |j\rangle.
\]

(3)

In order to have a well-defined set of wave functions for Berry phase evaluation [Eq. (2)], we have to impose

\[
\theta_N - \theta_0 = 2\pi m,
\]

(4)
rotation around the Dirac point (Fig. 3) can be obtained from Eq. (1):

\[
\Gamma_{\text{mono}} = -i \lim_{N \to \infty} \sum_{j=0}^{N-1} \log \left( \frac{1 + \exp[i(\theta j+1 - \theta j)]}{2} \right)
= -i \int_{0}^{2\pi} d\theta \frac{i}{2} = \pi , \tag{8}
\]

where we have substituted \( \mathbf{q} \) by the corresponding state index \( j \) (\( j = 0, 1, 2, \ldots, N-1 \)) as shown in Fig. 3.

Now we show that Eq. (1) is not affected by an arbitrary phase factor of each electronic wave function. Suppose that we use a new form for an electron wave function in graphene

\[
|\psi_{j,0}^{\text{mono}}\rangle' = e^{-i\theta_j/2} |\psi_{j,0}^{\text{mono}}\rangle = \sqrt{\frac{1}{2}} \left( e^{-i\theta_j/2} + e^{i\theta_j/2} \right), \tag{9}
\]

for \( j = 0, 1, \ldots, N-1 \), and of course \(|\psi_{0,0}^{\text{mono}}\rangle' = |\psi_{0,0}^{\text{mono}}\rangle'\) (Fig. 3). Then the Berry phase \( \Gamma_{\text{mono}}' \) is given by

\[
\Gamma_{\text{mono}}' = -i \lim_{N \to \infty} \sum_{j=0}^{N-1} \log \left( \frac{1 + \exp[2i(\theta j+1 - \theta j)]}{2} \right)
= -i \left\{ i \pi + \int_{0}^{2\pi} d\theta \ 0 \right\} = \pi, \tag{10}
\]

i.e., we obtain the same result as in Eq. (8). The physical reason for this invariance of the Berry phase with respect to an arbitrary gauge phase of each electronic state evaluated from Eq. (1) is that each state appears twice (once as a bra state and once as a ket state), thus canceling out any arbitrary phase in each wave function. Since the Berry phase obtained from Eq. (1) is \textit{not} affected by any arbitrary phase of each state \(|j\rangle\), we can choose for convenience a gauge such that the state varies smoothly over the course of parameter evolution.

Similarly, for bilayer graphene, if we use a basis set composed of Bloch sums of localized Wannier-like \( p_z \) orbitals on each of the two sublattices \( A \) and \( B' \) [Fig. 1(a)], and consider only the nearest-neighbor intralayer hopping and vertical interlayer hopping (characterized by the hopping integral \( t_{11} \)) processes, the effective Hamiltonian of low-energy electronic states in bilayer graphene becomes

\[
H_{\text{bi}}(\mathbf{q}) = \frac{\hbar^2 q^2}{2m^*} \begin{pmatrix} 0 & \exp(-2i\theta_q) \\ \exp(2i\theta_q) & 0 \end{pmatrix}, \tag{11}
\]

where \( m^* = 3a^2 t_{11}/8\hbar^2 \) is the effective mass and \( a \) the lattice parameter. The energy eigenvalue and wave function of Eq. (11) are given by \( E_{\text{bi}}^{s} = s\hbar^2 q^2/2m^* \) and

\[
|\psi_{s, q}^{\text{bi}}\rangle = \frac{1}{\sqrt{2}} \left( e^{2i\theta_q} \right), \tag{12}
\]

respectively \( (s = \pm 1) \). The Berry phase \( \Gamma_{\text{bi}} \) of the electron wave function in bilayer graphene can again be obtained from Eq. (1):

\[
\Gamma_{\text{bi}} = -i \lim_{N \to \infty} \sum_{j=0}^{N-1} \log \left( \frac{1 + \exp[2i(\theta j+1 - \theta j)]}{2} \right)
= -i \int_{0}^{2\pi} i d\theta = 2\pi, \tag{13}
\]

which is the result of previous studies.\(^{16,17}\)

Now we consider another form for the wave function

\[
|\psi_{s, q}^{\text{bi}}\rangle' = \frac{1}{\sqrt{2}} \left( e^{-i\theta_q} \right), \tag{14}
\]

whose only difference from the original one is the position-independent overall phase \(|\psi_{s, q}^{\text{bi}}\rangle' = e^{-i\theta_q} |\psi_{s, q}^{\text{bi}}\rangle\). Because the two wave functions are different only in the overall coefficient, they both are perfectly good solutions of the effective Hamiltonian of bilayer graphene [Eq. (11)]. Moreover, both the original [Eq. (12)] and new [Eq. (14)] wave functions satisfy the gauge condition that the wave function varies smoothly in the course of cyclic evolution; hence, in the evaluation of the Berry phase, one does not have to consider any branch cut, as we did in the derivation of Eq. (10). The Berry phase \( \Gamma_{\text{bi}}' \) for \(|\psi_{s, q}^{\text{bi}}\rangle'\) evaluated from Eq. (1) is

\[
\Gamma_{\text{bi}}' = 0; \tag{15}
\]

in other words, the Berry phase of the electronic wave function of bilayer graphene is the same as that of a conventional 2DEG.

In fact, the Berry phase of an electronic wave function in bilayer graphene evaluated from Eq. (1) is \( 2m \pi \), with \( m \) an arbitrary integer. Or, in other words, any Berry phase of \( 2m \pi \) is equivalent to a trivial Berry phase of 0. [Similarly, this Berry phase for graphene obtained from Eq. (1) is \( (2m + 1) \pi \), with \( m \) an arbitrary integer.] This statement is related also to the well-known application of Berry-phase physics to the modern theory of polarization,\(^{23,24}\) according to which the electrical polarization in a periodic system can only be determined for modulo \( e \mathbf{R}/\Omega \), where \( \mathbf{R} \) is a lattice vector and \( \Omega \) the unit cell volume.

Our claim that the Berry phase in bilayer graphene is \textit{not} nontrivial and is equivalent to that of a conventional
2DEG remains valid even if we consider a more complex model Hamiltonian. If, for example, second-nearest-neighbor interlayer hopping processes are considered in the tight-binding model of bilayer graphene, the low-energy electronic states can be described by four Dirac cones. It was suggested that the central Dirac cone contributes $-\pi$ to the Berry phase and each of the three satellite Dirac cones contribute $\pi$ to the Berry phase, and hence the total “nontrivial” Berry phase is $-\pi + 3 \times \pi = 2\pi$. According to our discussion, this view is not correct, again because a Berry phase of $-\pi$ is equivalent to that of $\pi$, etc. In particular, starting from the wave functions used in Ref. 16, one can define a new set of wave functions with additional four phase factors, e.g., $e^{-i\theta_n}$, defined around each of the four Dirac cones in a way similar to Eq. (14). Then, the Berry phase around the $i$th Dirac cone ($i = 1, 2, 3, 4$) obtained by evaluating Eq. (1) would be $(2m_i + 1)\pi$ for an arbitrary integer $m_i$. Thus, the Berry phase for bilayer graphene is of the form $\Gamma_{si} = \sum_{i=1}^4 (2m_i + 1)\pi = 2m\pi$, with $m$ an arbitrary integer, and cannot uniquely be $2\pi$ as suggested in previous studies.16,17

**III. PSEUDOSPIN WINDING NUMBER**

However, these considerations do not mean that there is no qualitative difference between the electronic eigenstates in bilayer graphene and those in a conventional 2DEG. Indeed, a new phenomenon in bilayer graphene was observed and explained: the step size at charge neutrality point in the quantum Hall conductance step at the charge neutrality point of size $n e^2/h$ per spin and valley degrees of freedom. Our interpretation is that what we learn from a measured step size $n e^2/h$ per spin and valley degrees of freedom17 is not the “absolute” value of the Berry phase ($\Gamma = n\pi$) but the pseudospin winding number ($n_w = n$); we also note that the quantum Hall conductance step, which has been correctly obtained in Ref. 17 from Eq. (16), does not need a Berry phase of $\Gamma = n\pi$ for its explanation. In other words, the size of the quantum Hall conductance step at the charge neutrality point is connected directly to the special form of the Hamiltonian in Eq. (16), or, equivalently, to $n$, which can be interpreted, from its wave function [Eq. (17)], as the pseudospin winding number and not to the absolute value of the Berry phase. It should be stressed that our discussion of the pseudospin winding number is confined to systems whose effective Hamiltonian is given by Eq. (16).

On the other hand, the Berry phase still determines the shift of the plateaus, with integer and half-integer quantum Hall effects for $\Gamma = 0$ and $\Gamma = \pi$, respectively.5,8,27 The former and the latter correspond to multilayer graphene with an even and odd number of layers, respectively.20 It has been recently shown within a semiclassical theory that the so-called topological part of the Berry phase, which is determined by the pseudospin winding number, is responsible for this shift.30

**IV. CONCLUSION**

In conclusion, we have shown that the Berry phase of the low-energy quasiparticle wave function of bilayer graphene is the same as that of a conventional two-dimensional electron gas, and that the fundamental difference between the two systems is the pseudospin winding number. Our findings have a broader implication than the cases discussed here. For example, the interpretation of the recent angle-resolved photoemission spectroscopy on bilayer graphene31,32 and that of the recent quantum Hall experiments on trilayer graphene33 should be revisited in view of the present discussion.

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