Massless Dirac fermions in graphene under an external periodic magnetic field

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Abstract

By solving the two-component spinor equation for massless Dirac fermions, we show that graphene under a periodic external magnetic field exhibits a unique energy spectrum. At low energies, Dirac fermions are localized inside the magnetic region with discrete Landau energy levels, while at higher energies, Dirac fermions are mainly found in non-magnetic regions with continuous energy bands originating from wavefunctions analogous to particle-in-box states of electrons. These findings offer a new methodology for the control and tuning of massless Dirac fermions in graphene.

(Some figures may appear in colour only in the online journal)

Due to the honeycomb lattice structure, the low-energy quasi-particles in graphene behave as massless Dirac fermions, which leads to peculiar electronic properties and lots of exciting new phenomena [1,2]. Recently, controlling and tuning properties of massless Dirac fermions in graphene by an external field has become a hot subject, which may lead to novel applications of graphene in nanoscale devices. It has been found by theoretical calculations that with an external periodic electric field, interesting phenomena such as anisotropic group velocities of Dirac fermions [3], emerging zero-energy states [4], a new type of massless charge carriers [5], unusual Landau levels and quantum Hall effects [6] and bandgap opening or quenching [7] may appear. With an external local magnetic field, previous studies suggested that the confinement of massless Dirac fermions in graphene is possible [8–10]. Interesting transport properties [11–14] and energy spectrum [14–17] of graphene under a one-dimensional (1D) periodic magnetic field have also been reported. In the current study, we theoretically investigated the behaviors of low-energy quasi-particles in graphene under an external periodic magnetic field. The method we used can be applied to both 1D and two-dimensional (2D) cases. Our studies showed that a unique energy spectrum of massless Dirac fermions occurs in periodic magnetic fields consisting of alternating magnetic and non-magnetic regions, which offers new opportunities for future applications of graphene.

When under an external magnetic field, the properties of massless Dirac fermions in graphene can be described by a spinor equation [2,18]

\[ \psi(x, y) = E\psi(x, y). \]  

(1)

where \( v_F \) is the Fermi velocity in graphene, \( \sigma = (\sigma_x, \sigma_y) \) are two-component Pauli matrices and \( A \) is the vector potential corresponding to the magnetic field that is normal to the graphene (xy plane). In the case of uniform magnetic field, the vector potential can be written as \( A(x) = Bx\hat{y} \), and then equation (1) has analytical solutions [18] which read

\[ \psi_{n,k_x} \propto e^{ik_xx} \begin{cases} \text{sgn}(n)\psi_{n-1}(\xi), & n \neq 0 \\ i\psi_n(\xi), & n = 0 \end{cases}, \]  

(2)

where \( k_x = \frac{\sqrt{n^2 + 2\hbar Bv_F}}{l_c}, \xi = \frac{1}{2}(x + \xi k_x) \), \( n \) are integers and \( \psi_n(\xi) \) are harmonic oscillator eigenfunctions. The solutions in equation (2) perfectly explain the experimentally observed unusual \( \sqrt{|n|} \) dependence of discrete Landau levels in graphene [19].

In this paper, we focus on the effects of external periodic magnetic fields, with both magnetic and non-magnetic regions, on the properties of massless Dirac fermions. The external periodic magnetic field can be either 1D or 2D.
In figure 1(a), we show an example of 1D magnetic field consisting of alternating magnetic and non-magnetic regions. The corresponding periodic vector potential under the Landau gauge is also plotted in the figure. An example of 2D magnetic fields is shown in figure 1(b). For the 2D case, the symmetric gauge is used in calculations. In both examples, the average magnetic field in one unit cell is zero. The resultant periodic system is referred to as an anti-ferromagnetic (AF) superlattice in this paper. We would like to mention here that the theoretical techniques we will discuss later can also be applied to ferromagnetic superlattices with non-zero average magnetic field, and the major physics presented in the paper remains the same in ferromagnetic cases.

Here we describe the theoretical method of solving the spinor equation (equation (1)) with an external periodic magnetic field. In this case, the solution takes the format of the Bloch function, $\psi(x, y) = e^{i(k_x x + k_y y)} \phi_m(x, y)$, where $\phi_{1,2}(x, y)$ are periodic. The discrete Fourier expansion can then be applied,

$$\phi_1(x, y) = \sum_{m,n=-N}^{N} a_{mn} e^{i(m\omega_x x + n\omega_y y)},$$

$$\phi_2(x, y) = \sum_{m,n=-N}^{N} b_{mn} e^{i(m\omega_x x + n\omega_y y)},$$

where $\omega_x = \frac{2\pi}{T_x}$, $\omega_y = \frac{2\pi}{T_y}$ with $T_x$ and $T_y$ the period of the superlattice. If we insert the above Fourier expansion into equation (1) and use the orthogonality condition, we obtain an eigenvalue equation in matrix form that can be numerically solved:

$$\begin{pmatrix} 0 & \hbar^2 \gamma \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = E \begin{pmatrix} a \\ b \end{pmatrix}$$

(3)

where

$$a = (a_{0,0} \cdots a_{2N+1,2N+1})^T,$$

$$b = (b_{0,0} \cdots b_{2N+1,2N+1})^T,$$

and

$$h_{m'm''n'} = (m'\omega_x - in'\omega_y + k_x - ik_y)\delta_{m'm'}\delta_{n'n'} + A_{x(m'n''n)} - iA_{y(m'n''n)}.$$

Equation (3) is the key equation of this paper and it provides the theoretical basis for understanding the properties of massless Dirac fermions under periodic magnetic field with different gauges. In our calculations, we used the Landau gauge in the 1D case and the symmetric gauge in the 2D case. We now solve equation (3) for different magnetic superlattices.

In figure 2, we show the calculated energy spectrum at different energies of Dirac fermions for the 1D AF superlattice depicted in figure 1(a). As a test of our calculations, we first calculated the energy spectrum for a limiting case with a very large size of magnetic regions (1250 nm) and also lattice constant (5000 nm). This limiting case can be compared with the graphene under a uniform magnetic field. The calculated energy as a function of level index is shown in figure 2(c) (red circle). For comparison, analytic Landau energy levels (equation (2)) with the same magnetic field ($B = 0.1$ T) are also plotted in the same panel (solid lines). Clearly, our numerical calculations exactly reproduced the well-known Landau levels of graphene under uniform field. Note that, in our case, each of these Landau levels is double degenerate. The double degeneracy comes from the fact that in the AF superlattice we studied, there are two magnetic traps with opposite magnetic fields in one unit cell. We then set the lattice constant to 1850 nm and the size of magnetic region to 462.5 nm. Under the same magnetic field, the calculated energy dispersion in the Brillouin zone is plotted in figure 2(a) and the energies at the $\Gamma$ point are shown in figure 2(c). At low energy dispersion, the spectrum is similar to the graphene under a uniform magnetic field.
Figure 2. The energy spectrum of massless Dirac fermions in the 1D magnetic superlattice as depicted in figure 1(a). (a) The energy spectrum: discrete Landau levels at lower energies and continuous energy bands at higher energies. (b) An enlarged picture for the continuous spectrum: the energy dispersion of free Dirac fermions (dotted line) is also plotted for comparison. (c) Energies calculated at the $\Gamma$ point (the center of the Brillouin zone). The calculated Landau energy levels under a limiting case with large lattice constant and magnetic regions (red circle) are also plotted for comparison. In this case, the calculated energies are almost exactly the same as the analytic solutions shown in equation (2) (horizontal solid lines).

energies (less than the energy of the $n = 4$ Landau level in the uniform field), the energy spectrum of the AF superlattice is the same as the well known discrete Landau levels in graphene. Starting from $n = 5$, the Landau level develops into a continuous band which can be seen from figure 2(a). The transition of the energy spectrum (from a discrete Landau level to continuous bands) can also be seen in the plot of the energies at the $\Gamma$ point in figure 2(c). In figure 2(b), we show an enlarged version of the calculated continuous energy bands. The linear energy dispersion of free massless Dirac fermions is also imposed for comparison.

To understand the above-mentioned transition of the energy spectrum, we calculated the wavefunctions of different energy levels at the $\Gamma$ point. The wavefunction for the Landau level $n = 4$ is plotted in figure 3(a), where we can see that in this case, the Dirac fermions are mainly localized inside the magnetic region. The wavefunction is just the usual harmonic oscillator function (Hermite function). For these Landau levels, we can define the ‘cyclotron’ size of the Dirac fermion as the distance between the two outermost peaks of the Hermite wavefunction. Obviously, the cyclotron size is a function of magnetic field $B$ and the level index $n$. The size decreases with $B$ and increases with $n$. The transition of the energy spectrum can then be understood as a consequence of the competition between the cyclotron size of Dirac fermions and the width of the magnetic region. In the case shown in figure 3(a), for the Landau level $n = 4$, the cyclotron size has almost been the same as the width of the magnetic region. When $n$ is bigger than 4, Dirac fermions escape from the magnetic trap, resulting in the transition of the energy spectrum. Wavefunctions for $n = 5$ and 6 are
Figure 4. The first component of the pseudospinor, $|\phi_1|^2$, for the 2D superlattice as depicted in figure 1(b). The amplitude increases from purple to burgundy. The corresponding energies for the four eigenstates are $E_a = 10.1 \text{ meV}$, $E_b = 16.1 \text{ meV}$, $E_c = 21.4 \text{ meV}$, $E_d = 41.4 \text{ meV}$.

plotted in figures 3(b) and (c), respectively. In these cases, the Dirac fermion is mainly found in non-magnetic regions. For $n = 5$, the wavefunction outside the magnetic trap is similar to the ground state of an electron confined in a box. For $n = 6$, the wavefunction has two peaks and is analogous to the first excited state of electrons confined in box. The analogy between these Landau-level derived states of massless Dirac fermions and particle-in-box states of electrons is also correct for other cases with higher $n$.

One convenient thing about the predicted transition of the energy spectrum is that the transition energy where the particle-in-box states occur can be controlled by the magnetic field together with the size of the magnetic region. With the magnetic field of 0.04 T, our calculations show that for the case of lattice constant 1500 nm and in the magnetic region 375 nm, the transition occurs at the $n = 1$ Landau level, which means that in the energy spectrum there is only one flat band corresponding to the lowest Landau level ($n = 0$). If the size of the magnetic region decreases to 250 nm, the lowest Landau level also becomes a particle-in-box state with a continuous energy band. With a weaker magnetic field, the lattice constant and the size of the magnetic region can be bigger for the transitions to occur. These findings offer a new and also practical methodology for controlling/tuning massless Dirac fermions in graphene that may have major implications for the future design of graphene-based devices.

In summary, by numerically solving the spinor equation, we show that graphene under periodic magnetic field exhibits a unique energy spectrum with the discrete Landau levels at low energies and continuous energy bands at higher energies. The continuous energy bands originate from the wavefunctions analogous to the particle-in-box states of electrons. The transition energy where the particle-in-box states occur can be controlled by the magnetic field together with the geometry of the superlattice structures, which offers new avenues for the design of graphene-based systems with unique properties. The magnetic superlattice structures discussed in this paper may be readily fabricated by putting graphene onto a magnetic substrate with pre-designed 1D or 2D periodic surface patterns. The strength of the magnetic field (around 0.1 T) as well as the detailed superlattice structures (for example, 1850 nm of lattice constant) are all within the capabilities of current experimental techniques. We expect our findings to stimulate new experiments along this direction.

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