Modulation effects on Landau levels in a monolayer graphene

J H Ho, Y H Lai, Y H Chiu and M F Lin

Department of Physics, National Cheng Kung University, Tainan 701, Taiwan

E-mail: mflin@mail.ncku.edu.tw

Received 2 August 2007, in final form 20 September 2007
Published 14 December 2007
Online at stacks.iop.org/Nano/19/035712

Abstract

Magnetoelectronic properties of a single-layer graphene are studied by the Peierls tight-binding model. A new numerical technique is developed to obtain a band-like Hamiltonian matrix. A spatially modulated magnetic field \( B' \) could drastically alter the Landau levels due to a uniform magnetic field \( B \). The modulation effects include enhancement in dimensionality, change of energy dispersions, destruction of state degeneracy and creation of band-edge states. The dispersionless Landau levels, those at the Fermi levels excepted, become the 1D parabolic bands. The density of states thus exhibits many pairs of asymmetric prominent peaks. The height, frequency and number of pronounced peaks strongly depend on the modulation strength. These characteristics are hardly affected by the period and direction when \( B' \) is much weaker than \( B \). The predicted results could be verified by experimental measurements on magneto-optical absorption spectra.

Recently, the discovery of few-layer graphenes [1, 2] has inspired considerable theoretical and experimental studies in condensed-matter physics and material science. The nanoscaled graphenes not only have academic value, but also promise to be potentially important candidates for the next generation of electronic devices [1]. Any advances in understanding their essential physical properties, such as band structures [3–10], transport properties [11–19], optical spectra [20–24] and electronic excitations [4, 25, 26] would be very valuable in finding these possible applications. The production of few-layer graphenes means that they can be controlled to a single-atom thickness. It motivates the idea of engineering band structures [1, 3], since electronic properties of few-layer graphenes strongly depend on the hexagonal symmetry, number of layers, stacking sequence, topological defects and external fields. One can further tune the electronic properties by applying a gate voltage. A static external field has been shown to induce a carrier transition between electrons and holes in a monolayer graphene [1] and lead to opening energy gaps in multi-layer graphenes [3, 7, 27, 28].

A 2D monolayer graphene has many parabolic bands and two linear bands intersecting at the Fermi level (\( E_F = 0 \)). It is an exotic zero-gap semiconductor, mainly due to a vanishing density of states at \( E_F = 0 \). The low-energy physical properties can be described by the massless Dirac equation [11]. In a uniform magnetic field, electronic states flock together and all 2D energy bands become the unusual 0D Landau levels [29]. The Landau-level energies, unlike those of a 2D electron gas [30], are proportional to the square root of the quantum number and the field strength, rather than being equally spaced or proportional to the field strength. Recently, these features have been verified by optical measurements from infrared absorption spectroscopy [20]. The Landau-level quantization reflects the Dirac nature of massless quasiparticles, and is deduced to be responsible for the unconventional integer quantum Hall effect [11, 13]. The periodic electric and magnetic fields are predicted to cause drastic changes in the band structures, such as state degeneracy, energy dispersion, band-edge state and band width [31, 32]. In this work, we mainly study the effects of a spatially modulated magnetic field on the Landau levels. The dependence of magnetoelectronic properties on the field strength, period and direction will be investigated in detail. The Peierls tight-binding model is used to calculate band structures. In general, a Hamiltonian matrix is too large to be solved for a realistic magnetic field, e.g. a \( 32000 \times 32000 \) matrix for a uniform magnetic field \( B = 10 \) T. A new numerical technique is developed to diagonalize the Hamiltonian matrix more efficiently. It would be very useful in understanding other physical properties, such as magneto-absorption spectra and Coulomb excitations.

A single-layer graphene is a honeycomb lattice of carbon atoms. The \( \pi \)-band structure formed by 2p\(_x\) orbitals can be...
calculated through the tight-binding model within the nearest-neighbor hopping interactions. There are two carbon atoms in a primitive unit cell, so the Hamiltonian is represented by a $2 \times 2$ Hermitian matrix in the space expanded by Bloch functions of two crystalline sublattices. When Bloch electrons exist in a magnetic field, an extra Peierls phase characterized by the vector potential $A$ needs to be included in the tight-binding functions. Within the tight-binding scheme [33], the magneto-electronic wavefunction is expressed as

$$
|\Phi_n^\parallel_r\rangle = \frac{1}{N} \sum_{R_m} \exp \left( i k \cdot R_m + i e / h G_{R_m} \right) |\varphi_{p}(r - R_m)\rangle.
$$

$R_m$ is the lattice vector with sublattice index ($n = 1$ and 2) and $\varphi_p$, the atomic orbital. $e G_{R_m} / h \equiv (e / h) \int_{R_m} A(\xi) \cdot d\xi$ is the extra phase associated with a magnetic field and would lead to the breakdown of the Bloch condition. If the magnetic field changes slowly as a function of the lattice constant, the Hamiltonian matrix element is given by

$$
H^\parallel_{kk'}^{m} = \langle \Phi_{m}^{\parallel} | H_{BZ} | \Phi_{n}^{\parallel}\rangle
= \frac{1}{N} \sum_{R_m, R_{m'}} \exp \{-i(k \cdot R_m - k' \cdot R_{m'}) - i\Omega(R_m, R_{m'})\} H_{R_m R_{m'}}.
$$

$H_{R_m R_{m'}} = \langle \varphi_{p}(r - R_m) | p^2 / 2m + V | \varphi_{p}(r - R_{m'})\rangle$ is the hopping integral for a single particle in a periodic crystal potential $V$ and is assumed to be nonvanishing only for two nearest-neighbor position vectors $R_m$ and $R_{m'}$. The phase difference $\Omega(R_m, R_{m'}) = e(G_{R_m} - G_{R_{m'}}) / h$ due to a magnetic field would result in the coupling among states with different $k$'s. The calculations of band structures would become more complicated. Generally, the Hamiltonian matrix in $k$ space would be irreducible. In other words, a magnetic field completely destroys the crystal symmetry and $k$ is no longer a good quantum number. But, when $\Omega(R_m, R_{m'})$ is a periodic function of $R_m$, the crystal periodicity will be preserved. The dimension of a primitive unit cell is in turn determined by the period of $\Omega$.

A monolayer graphene is present in a uniform magnetic field $B = B_0$ and a spatially modulated magnetic field $B' = B' \sin K x$ along the armchair direction with a period $l_B = 2\pi / K$ (figure 1). $B$ is much stronger than $B'$; that is, $B'$ serves as a perturbed magnetic field. The magnetic flux, the product of field strength and hexagon area, is $\Phi = (3\sqrt{3}b^2 B_0^2) / (hc/e)$ in units of flux quantum $(\Phi_0 = hc/e = 4.1356 \times 10^{-15} \text{T m}^2)$, $b = 1.42$ Å is the C-C bond length. The vector potential, which is chosen as $A = (B x - B' \cos K x / K) \hat{y}$, leads to a new periodicity along the armchair direction. The unit cell is thus enlarged and its dimension is determined by $R_B = 1 / \Phi$ and $R_B' = l_B / 3b$. The dimensionality of the Hamiltonian matrix corresponds to the least common multiple ($2R_m$) of $2R_B$ and $2R_B'$. The enlarged unit cell contains $4R_m$ carbon atoms and the Hamiltonian matrix is a $4R_m \times 4R_m$ Hermitian matrix. The base functions in the unit cell are chosen from outside to inside rather than from left to right, as shown in figure 1. Their special arrangement would make the Hamiltonian matrix display the band form:

$$
\begin{pmatrix}
0 & q^* & 0 & \cdots & 0 & 0 \\
q & 0 & 0 & \cdots & 0 & 0 \\
p_1 & 0 & 0 & \cdots & 0 & 0 \\
p_2 & \cdots & q & 0 & \cdots & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & \cdots & \cdots & \cdots & \cdots & q \\
0 & 0 & 0 & \cdots & \cdots & 0 \\
p_{R_m+1} & 0 & 0 & \cdots & q^* & 0
\end{pmatrix}
$$

$p_{\parallel} \equiv t_{1k}(n) + t_{2k}(n)$ and $q \equiv t_{1k} \cdot t_{2k}(n) = \gamma_0 \exp((ik, b/2 + i\sqrt{3b^2 / 2}) + G_{R_m})$, $t_{1k}(n) = \gamma_0 \exp((ik, b/2 - i\sqrt{3b^2 / 2}) - G_{R_m})$ and $t_{2k} = \gamma_0 \exp(-ik, b)$ are three nearest-neighbor hopping integrals. $\gamma_0 = 2.5 eV$ [34] is the nearest-neighbor hopping integral at zero field. $G_{R_m} = |[\tau \Phi(n - 1) + 1/6] + [-i[6(R_B)^2 \Phi / \pi \cos[\pi(n - 5/6)]/R_B] \sin[\pi/6R_B^2] |$ is the Peierls phase caused by the magnetic fields. The magnetic flux $\Phi = (3\sqrt{3}b^2 B_0^2 / (hc/e)$, due to a modulated magnetic field, is used to characterize its strength. The $\gamma$-electronic structure might rely on the modulation direction because of the geometric anisotropy. If the magnetic field is modulated along the zigzag direction, the corresponding Hamiltonian matrix can be derived in a similar way (not shown). Energy bands are obtained by diagonalizing the Hamiltonian matrix. For the armchair direction, the range of $k_y$ is $|k_y| < \pi / 3b R_B$ ($|k_y| < \pi / 3b R_{B'}$) at $R = R_B / R_{B'} < 1(R > 1)$ and that of $k_x = |k_x| < \pi / b \equiv \pi / \sqrt{3}b$. The unoccupied conduction bands ($E^c$)'s are symmetric to the occupied valence bands ($E^v$)'s about the Fermi level. Only the former are discussed in this work. Because the range of $k_x$ is much smaller than that of $k_y$ for a large $R_m$, it is sufficient only to consider the dispersion along $k_y$ in the following discussion. A uniform magnetic field could make electronic states flock together and preform the Landau levels $E^c(n)'s$ ($n$ a nonnegative integer), as shown in figure 2(a) by open circles at $B = 40 \text{T}$. Such levels are dispersionless and fourfold degenerate. These well-separated energy levels suggest that graphene under $B$ could be regarded as a zero-dimensional system. In addition, the Landau-level energies obey a simple relation $E^c(n) \propto \sqrt{nB}$. The perturbed modulated magnetic field ($B' \neq 0$) leads to drastic changes in energy dispersions, state degeneracies and band-edge states.
Figure 2. The energy bands of \((B = 40 \text{T}, B' = 4 \text{T}, R = 1)\) at low-energy (a) and high-energy (b) regimes. Those of stronger strength \(B' = 8 \text{T}\), shorter period \(R = 1/2\), longer period \(R = 2\), along different directions (zigzag), respectively, are shown in (c)–(f). The low-energy bands of \((B = 40 \text{T}, B' = 0)\) are also shown in (a) by the dotted curves. Notice that \(b' \equiv \sqrt{3}b\) for the armchair (zigzag) direction.

as shown in figure 2(a) by the solid circles at \(B' = 4 \text{T}\) and \(R = 1\). All the dispersionless Landau levels with \(n \geq 1\) become 1D parabolic bands, the Landau level \(E^c(n = 0)\) at \(E_F = 0\) excepted. The stronger energy dispersions indicate that most of the localized electronic states are transformed into extended states. The latter are purely caused by a modulated magnetic field; that is, one dimensionality is recovered by \(B'\). The fourfold degeneracy is thoroughly destroyed; furthermore, each nondegenerate parabolic band has one band-edge state at \(k_y \neq 0\). The magnetoelectronic structures at high- and low-energy regimes are similar to each other (figures 2(b) and (a)). At \(B' = 0\), the high-energy Landau levels with \(E^c(n) > \gamma_0\) are doubly degenerate, and they are much closer to one another [35] than the low-energy Landau levels are. Under a modulated magnetic field, these Landau levels are totally transformed into pairs of 1D parabolic bands. Each pair of parabolic bands is nondegenerate and owns two band-edge states at the zone boundary \((k_y = \pm \pi/\sqrt{3}b\) for the armchair direction).

The strength, period and direction of the modulated magnetic field strongly affect the low-energy bands, as shown in figures 2(c)–(f). The strength would significantly alter the band curvature \((\propto \text{the inverse of the effective mass})\) and shift the band-edge state energies \((E_{\text{be}}'s)\). The stronger \(B'\) is, the
larger the band curvature is. The energies of local maxima (minima) grow (decline) with the increase of $B'$. On the other hand, the number ($n_{be}$) of band-edge states is independent of the modulation strength (figure 2(c)). The period presents diverse effects on the band-structure characteristics, as shown in figure 2(d) with shorter period ($R < 1$) and figure 2(e) with longer period ($R > 1$). As the period varies, the band curvature increases for $R < 1$, whereas it almost remains the same for $R > 1$. The number of bands, however, exhibits the opposite behavior. When $R > 1$, the band number is proportional to $R$, while it remains unvaried when $R < 1$. Despite the unchanged number of bands, more band-edge states are created with $n_{be}$ inversely proportional to $R$ at $R < 1$. In contrast, $n_{be}$ is invariable even though there are more bands at $R > 1$. State degeneracy is affected by the period in a particular manner. Energy bands are nondegenerate for most $R$’s, but they are doubly degenerate as $1/R$ is an even integer. Notice that the band-edge state energies hardly depend on the period.

The density of states (DOS), which directly reflects the main features of electronic structures, is defined as

$$D(\omega) = \sum_{\sigma, h, c, v} \int_{1\text{st} BZ} \frac{dk_x dk_y}{(2\pi)^2} \frac{\Gamma}{\pi |E^b(k_x, k_y) - \omega|^2 + \Gamma^2} \frac{1}{\Gamma}.$$  

$\Gamma = 10^{-4} \gamma_0$ is the phenomenological broadening parameter. The integration on $k_x$, basically, could be neglected because of a very small range. The density of states in the presence of a uniform magnetic field exhibits many delta-function-like peaks, as shown by the dashed curve in figure 3(a). Such symmetric prominent peaks come from the 0D Landau levels at $B = 40$ T. The distribution of peaks is nonuniform, mainly owing to the unequally spaced Landau levels. When a spatially modulated magnetic field ($B' = 4$ T, $R = 1$) is applied along the zigzag direction, each symmetric pronounced peak at

**Figure 3.** The low-frequency density of states along the armchair direction at (a) ($B = 40$ T, $B' = 4$ T, $R = 1$), (b) ($B = 40$ T, $B' = 8$ T, $R = 1$), (c) ($B = 40$ T, $B' = 12$ T, $R = 1/2$) and (d) along the zigzag direction at ($B = 40$ T, $B' = 4$ T, $R = 1$). That at $B = 40$ T is also shown in (a) for comparison.
\( \omega \neq 0 \) is changed into a pair of asymmetric prominent peaks except for the \( n = 0 \) Landau level at \( E_F = 0 \), as shown by the solid curve in figure 3(a). Such divergent structures are caused by band-edge states (maxima and minima) of 1D parabolic bands. Each pair of asymmetric prominent peaks is located around the original Landau-level energy. The number of peaks is independent of the modulated magnetic field. The peak height is mainly determined by the band curvature and the number of band-edge states, both of which might rely on the strength and period, as mentioned earlier. The field strength could enhance the band curvature, so that the peak height gets weaker when \( B' \) grows. On the other hand, the period and direction hardly affect the peak height for \( B' \ll B \). At \( R \ll 1 \), the period could increase the band curvature and the number of band-edge states. The former and the latter make the peak weaker and stronger, respectively. The increasing compensates for the decreasing, therefore; there is no net effect on the peak height. As for \( R \gg 1 \), the band curvature and range of \( k_x \) are reduced simultaneously. The competitive relation between them also leads to the unchanged peak height. The low-energy bands at zero fields \([36]\) and a uniform magnetic field \([29]\) are isotropic. This property almost remains unchanged for \( B' \ll B \) (figures 3(a) and (d)). The anisotropy of the low-frequency DOS will be strong only when \( B' \) is comparable to \( B \). It is deduced that the low-energy spectrum of DOS is only affected by the strength of the modulated magnetic field even though the period has complicated effects on the Landau levels.

The frequencies of pronounced peaks in DOS deserve a closer investigation. Figure 4(a) shows the relation between \( E_{be} \)'s of the first six peaks and the modulation strength for \( B = 40 \) T and \( R = 1 \). The frequency of the first peak is fixed because of its robustness against the modulated magnetic field as stated earlier. For other peaks, as the strength increases, the frequencies grow or decline depending on whether the corresponding band-edge states are local maxima or minima. The frequency difference between a pair of neighboring peaks is enhanced by the increasing strength. Furthermore, it is appreciable even for a very small \( B'/B \) (\( \sim 1/40 \) in figure 4(a)). Similarly, the influence of the period is illustrated by its relation with \( E_{be} \)'s of the first six peaks in figure 4(b). The frequencies of those peaks remain almost the same when the period varies.

The above-mentioned results show that a weakly modulated magnetic field could dramatically alter the Landau levels caused by a uniform magnetic field. The drastic changes
include modification of one dimensionality, alternation of band curvature, splitting of state degeneracy and production of band-edge states. They will be directly reflected in optical absorption spectra due to the Landau levels exhibit a lot of prominent symmetric peaks [20]. The main features of absorption peaks (form, intensity, number and frequency) are expected to be thoroughly changed by a modulated magnetic field [37]. The modulation effects have also been investigated for a 2D electron gas [38–41]. In experimental measurements, the ratio between the modulated and uniform magnetic fields is \( B'/B \sim 1/10 \), and the maximal modulation strength is \( B' \sim 0.5 \) T [39]. Two parameters used in this work are \( 1 \) T \( \leq B' \leq 6 \) T and \( B = 40 \) T. The theoretical ratio \( B'/B \) is comparable to the experimental value; therefore, the predicted electronic properties are deduced to remain similar even for \( B' \ll 0.5 \) T. Experimental measurements from the magneto-optical absorption spectroscopy could be utilized to directly test the theoretical prediction.

In summary, the modulation effects on the Landau levels of a monolayer graphene are investigated through employing the Peierls tight-binding model. Magneto-electronic properties are mainly determined by the strength, period and direction of a spatially modulated magnetic field. Such a perturbed field thoroughly changes the magneto-electronic structures in a uniform magnetic field. It could recover one dimensionality, alter energy dispersions, lift state degeneracy and produce band-edge states. The 0D Landau levels are transformed into 1D parabolic bands except for those at the Fermi energy. The density of states thus exhibits many pairs of asymmetric prominent peaks. Among various factors influencing the density of states, only the field strength is important when \( B' \ll B \). The strength, but not the period and direction, strongly affects the band-edge state energies, in which local maxima (minima) grow (decline) with the increase of \( B' \). The predicted electronic properties could be directly examined by experimental measurements on magneto-optical absorption spectra [37]. The band-like Hamiltonian matrix developed in this work would be very useful in understanding the other essential physical properties, such as optical absorption spectra, electronic excitations and transport properties. It could be further generalized to multi-layer graphenes, e.g. bilayer and trilayer graphenes. Such problems are under current investigation.

Acknowledgment

This work was supported by the National Science Council of Taiwan, under grant no. NSC 95-2112-M-006-002.

References

[1] Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2004 Science 306 666

[2] Berger C et al 2004 J. Phys. Chem. B 108 19912

[3] Ohta T, Bostwick A, Seyller T, Horn K and Rotenberg E 2006 Science 313 951

[4] Bostwick A, Ohta T, Seyller T, Horn K and Rotenberg E 2007 Nat. Phys. 3 36

[5] Guinea F, Neto A H C and Peres N M R 2006 Phys. Rev. B 73 245426

[6] Latil S and Henrard L 2006 Phys. Rev. Lett. 97 036803

[7] McCann E 2006 Phys. Rev. B 74 161403

[8] Nilsson J, Neto A H C, Guinea F and Peres N M R 2006 Phys. Rev. Lett. 97 266801

[9] Partoens B and Peeters F M 2006 Phys. Rev. B 74 075404

[10] Peres N M R, Guinea F and Neto A H C 2006 Ann. Phys. 321 1559

[11] Novoselov K S, Geim A K, Morozov S V, Jiang D, Katsnelson M I, Grigorieva I V, Dubonos S V and Firsov A A 2005 Nature 438 197

[12] Novoselov K S, McCann E, Morozov S V, Fal’ko V I, Katsnelson M I, Zeitler U, Jiang D, Schedin F and Geim A K 2006 Nat. Phys. 2 177

[13] Zhang Y, Tan Y-W, Stormer H L and Kim P 2005 Nature 438 201

[14] Bunch J S, Yaish Y, Brink M, Bolotin K and McEuen P L 2005 Nano Lett. 5 287

[15] Gusynin V P and Sharapov S G 2005 Phys. Rev. B 71 125124

[16] Gusynin V P and Sharapov S G 2005 Phys. Rev. Lett. 95 146801

[17] Gusynin V P and Sharapov S G 2006 Phys. Rev. B 73 245411

[18] McCann E and Fal’ko V I 2006 Phys. Rev. Lett. 96 086805

[19] Hwang E H, Adam S and Sarma S D 2007 Phys. Rev. Lett. 98 186806

[20] Sadowski M L, Martinez G, Potenski M, Berger C and de Heer W A 2006 Phys. Rev. Lett. 97 266405

[21] Ferrari A C et al 2006 Phys. Rev. Lett. 97 187401

[22] Gusynin V P, Sharapov S G and Carbotte J P 2007 J. Phys.: Condens. Matter 19 026222

[23] Neto A H C and Guinea F 2007 Phys. Rev. B 75 045404

[24] Abergel D S L and Fal’ko V I 2007 Phys. Rev. B 75 155430

[25] Sarma S D, Hwang E H and Tse W-K 2007 Phys. Rev. B 75 121406

[26] Wang X-F and Chakraborty T 2007 Phys. Rev. B 75 041404

[27] Lu C L, Chang C P, Huang Y C, Ho J H, Hwang C C and Lin M F 2007 J. Phys. Soc. Japan 76 024701

[28] Lu C L, Chang C P, Huang Y C, Lu J M, Hwang C C and Lin M F 2006 J. Phys.: Condens. Matter 18 5849

[29] McClure J W 1956 Phys. Rev. 104 666

[30] Kittel C 1996 Introduction to Solid State Physics 7th edn (New York: Wiley)

[31] Ho J H, Lai Y H, Lu C L, Hwang J S, Chang C P and Lin M F 2006 Phys. Lett. A 359 70

[32] Ho J H, Lai Y H, Tsai S J, Hwang J S, Chang C P and Lin A F 2006 J. Phys. Soc. Japan 75 114703

[33] Luttinger J M 1951 Phys. Rev. 84 814

[34] Charlier J C, Michenaud J P and Gonze X 1992 Phys. Rev. B 46 4531

[35] Ho J H, Lai Y H, Chiu Y H and Lin M F 2007 Preprint 0706.0078

[36] Wallace P R 1947 Phys. Rev. 71 622

[37] Cin S, Whittaker D M, Arnone D D, Burke T, Hughes H P, Leadbeater M, Pepper M and Ritchie D A 1999 Phys. Rev. Lett. 83 4425

[38] Carmona H A, Geim A K, Novaretto A, Main P C, Foster T J, Benini M, Beaumont S P and Blamire M G 1995 Phys. Rev. Lett. 74 3009

[39] Novareto A, Carlton S, Gallagher B L, Main P C, Benini M, Wirtz R, Newbury R, Howson M A and Beaumont S P 1997 Phys. Rev. B 55 R16037

[40] Peeters F M and Vasilopoulos P 1993 Phys. Rev. B 47 1466

[41] Peeters F M, Vasilopoulos P and Shi J 2002 J. Phys.: Condens. Matter 14 8803–16