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ANALYSIS OF THE ZEEMAN EFFECT ON THE ENERGY SPECTRUM IN GRAPHENES

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An analysis of the Zeeman effect with a strong external magnetic field on the energy spectrum in graphene is presented. In general, the Hamiltonian of graphene in applied electric and magnetic fields is not of SO(1,2) invariance even in the nearest-neighbor approximation because of the Zeeman coupling. But an approximate SO(1,2) invariance can be obtained when the applied magnetic field is very strong. This approximate invariance can be used to relate the energy structure of graphene in the presence of both electric and magnetic fields to that when there is only magnetic field. Therefore, it can help explain the recently found quantum Hall conductance $(4q^2/h)L$ for $L = 0, 1$.

Graphene has been one of the major foci in physics because of its simple lattice structure and linear dispersion relation near the Fermi level [1–3] when only nearest-neighbor hopping is taken into account. It has become a new testbed not only for condensed matter physics but also for quantum field theory and mathematical physics [4, 5]. The physical properties of graphene in external field, such as the quantum Hall effect (both integer and fractional [6–11]), spin quantum Hall effect [12], transport theory [13, 14], superconducting [15] and magnetic confinement [16] are under intensive study. Effects of next-nearest-neighbor hopping have also been studied [17]. It is widely recognized that the integer quantum Hall conductance is

$$\sigma_{xy} = \frac{4e^2}{h}\left(L + \frac{1}{2}\right),$$

where $L = 0, 1, \ldots$ [1]. Although disorder and the 4-fold symmetry breaking may be used to explain the recently found quantum Hall structures $n = 0, \pm 1, \pm 4$ [18–22], a unified explanation is still called for and the simple structure of previous formula for σ_{sy} still deserves a simple and fundamental explanation. Not surprisingly, the quantum Hall plateaus at $n = \pm 2$, ± 6, ± 10 in graphenes can be explained by using the Landau levels of a spinless particle in an external magnetic field and the $(1+2)$ Lorentz invariance of the massless Dirac Hamiltonian [23]. Because simple use of the Landau levels disregards the Zeeman energy, which is not negligible compared with low-lying Landau levels, the Zeeman energy might explain some of the recently found plateaus. In this work, we find that although the Zeeman energy breaks the SO(1,2) invariance in general, the system can still have an approximate invariance when the magnetic field is strong enough, and the approximate invariance can be used to relate the physics of one experimental configuration to that of another. Following this line, we found that the newly observed quantum Hall plateaus $(4q^2/h)L$ for $L = 0, 1$ can be attributed to the Zeeman energy.

The direct lattice of graphene is a superposition of two interpenetrated triangular lattices Λ_A, Λ_B. The generators of the lattice Λ_A are [24]

$$\mathbf{a}_1 = \sqrt{3}a\left(\frac{1}{2}, \frac{-\sqrt{3}}{2}\right),$$

$$\mathbf{a}_2 = \sqrt{3}a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$$

[24], where $a \approx 1.42$ Å is the carbon–carbon distance. The vectors

$$\mathbf{s}_1 = a(0, -1), \quad \mathbf{s}_2 = a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \quad \mathbf{s}_3 = a\left(\frac{-\sqrt{3}}{2}, \frac{1}{2}\right)$$

connect each site in the lattice Λ_A to its nearest neighbor sites in the lattice Λ_B. Unlike regular electron

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spin, the pseudospin in graphene represents the two sublattices and there is no magnetic moment associated. Hence the pseudospin does not couple directly to the magnetic field [6]. We here consider only the nearest-neighbor tight-binding Hamiltonian

$$H_0 = -t\sum_{\sigma}\sum_{\mathbf{r}\in\Lambda_A}\sum_{i=1}^{3}\left[A_\sigma^\dagger(\mathbf{r})B_\sigma(\mathbf{r}+\mathbf{s}_i) + B_\sigma^\dagger(\mathbf{r}+\mathbf{s}_i)A_\sigma(\mathbf{r})\right], \quad (1)$$

where σ is pseudospin index and t is the uniform hopping constant. In the presence of an applied magnetic field $\mathbf{B}$ and an electric field $\mathbf{E} = -\nabla\varphi$, the Zeeman energy and Coulomb energy should be included:

$$H_Z = \mu_B\left[\sum_{\mathbf{r}\in\Lambda_A}\mathbf{B}\cdot A^\dagger(\mathbf{r})\boldsymbol{\tau}A(\mathbf{r}) + \sum_{\mathbf{r}\in\Lambda_B}\mathbf{B}\cdot B^\dagger(\mathbf{r})\boldsymbol{\tau}B(\mathbf{r})\right], \quad (2)$$

$$H_C = q\left[\sum_{\mathbf{r}\in\Lambda_A}\varphi(\mathbf{r})A^\dagger(\mathbf{r})A(\mathbf{r}) + \sum_{\mathbf{r}\in\Lambda_B}\varphi(\mathbf{r})B^\dagger(\mathbf{r})B(\mathbf{r})\right], \quad (3)$$

where

$$\mu_B = \frac{|e|\hbar}{2m_e}$$

is the Bohr magneton. In momentum space, we have

$$a_\mathbf{k} = \frac{1}{\sqrt{N_\Lambda}}\sum_{\mathbf{r}\in\Lambda_A}e^{-i\mathbf{k}\cdot\mathbf{r}}A(\mathbf{r})$$

and

$$b_\mathbf{k} = \frac{1}{\sqrt{N_\Lambda}}\sum_{\mathbf{r}\in\Lambda_B}e^{-i\mathbf{k}\cdot\mathbf{r}}B(\mathbf{r}),$$

where N_Λ is the number of lattice points of the sublattice Λ_A (or Λ_B). Introducing two-component spinors

$$\psi_\mathbf{k} = (a_\mathbf{k}, b_\mathbf{k})^T, \quad \psi_\mathbf{k}^\dagger = (a_\mathbf{k}^\dagger, b_\mathbf{k}^\dagger), \quad \psi_{\mathbf{k}\sigma 1} = a_{\mathbf{k}\sigma},$$
$$\psi_{\mathbf{k}\sigma 2} = b_{\mathbf{k}\sigma}, \quad \sigma = \pm 1$$

allows linearizing H_0 near the two Dirac points $\mathbf{K}_\pm$. Considering $\mathbf{K}_+$, we have

$$H = \sum_\mathbf{p}\xi_\mathbf{p}^\dagger(v_F\boldsymbol{\alpha}\cdot\mathbf{p} + \mu_B B)\xi_\mathbf{p} + \sum_\mathbf{p}\eta_\mathbf{p}^\dagger(v_F\boldsymbol{\alpha}\cdot\mathbf{p} - \mu_B B)\eta_\mathbf{p} + H_C. \quad (4)$$

Using the γ-matrices $\gamma^\mu = (\sigma_3, i\sigma_2, i\sigma_1)$ and incorporating the $U(1)$ gauge invariance, we write the Hamiltonian as

$$H = \int d^2\mathbf{x}\bar{\xi}(x)[\hbar v_F\boldsymbol{\gamma}\cdot\left(-i\nabla - \frac{q}{\hbar}\mathbf{A}\right) + \mu_B B\gamma^0 + q\gamma^0\varphi]\xi(x) + \int d^2\mathbf{x}\,\bar{\eta}(x) \times [\hbar v_F\boldsymbol{\gamma}\cdot\left(-i\nabla - \frac{q}{\hbar}\mathbf{A}\right) - \mu_B B\gamma^0 + q\gamma^0\varphi]\eta(x). \quad (5)$$

Let

$$x^\mu = (x^0, \mathbf{x}) = (v_F t, x, y), \quad A^\mu = (A^0, \mathbf{A}).$$

Setting

$$D_\mu = \partial_\mu + i\frac{q}{\hbar}A_\mu, \quad A^0 = \frac{\varphi}{v_F},$$

we have

$$\mathcal{L} = \xi^\dagger i\hbar\partial_t\xi - \mathcal{H} = \bar{\xi}(x)(i\hbar\not{D} + gB\gamma^0)\xi(x) + \bar{\eta}(x)(i\hbar\not{D} - gB\gamma^0)\eta(x), \quad (6)$$

where $g = \mu_B/v_F$. The $U(1)$ gauge invariance is preserved, but the Lorentz SO(1,2) invariance is broken by the Zeeman term. Because

$$-\varepsilon^{\mu\nu\tau}\partial_\mu A_\nu\gamma_\tau = B\gamma^0 + \frac{1}{v_F}E_x\gamma^2 - \frac{1}{v_F}E_y\gamma^1 \quad (7)$$

we can write

$$B\gamma^0 \approx -\varepsilon^{\mu\nu\tau}\partial_\mu A_\nu\gamma_\tau \quad (8)$$

for $|\mathbf{E}| \ll v_F|\mathbf{B}|$, and in this case,

$$L = \int d^3x\Big[\bar{\xi}(x)(i\hbar\not{D} - g\varepsilon^{\mu\nu\tau}\partial_\mu A_\nu\gamma_\tau)\xi(x) + \bar{\eta}(x)(i\hbar\not{D} + g\varepsilon^{\mu\nu\tau}\partial_\mu A_\nu\gamma_\tau)\eta(x)\Big], \quad (9)$$

which shows the (1+2) Lorentz invariance. The current is

$$j^\mu = -\frac{\delta L}{\delta A_\mu} = q\bar{\xi}\gamma^\mu\xi + q\bar{\eta}\gamma^\mu\eta + g\varepsilon^{\mu\nu\tau}\partial_\nu(\bar{\xi}\gamma_\tau\xi) - g\varepsilon^{\mu\nu\tau}\partial_\nu(\bar{\eta}\gamma_\tau\eta). \quad (10)$$

We first consider a constant applied magnetic field. In this case, $\varphi = 0$ and we want to calculate the grand canonical partition function

$$Z = \mathrm{Tr}\,e^{-\beta K},$$

where

$$K = H - \mu N.$$

The Dirac equation is

$$\left[\hbar v_F \boldsymbol{\alpha}\cdot\left(-i\nabla - \frac{q}{\hbar}\mathbf{A}\right) + \mu_B B - \mu\right]\xi = K\xi, \tag{11}$$

which is written as the second order equation

$$\left(-D_i D_i + \frac{q}{\hbar}B\sigma_3\right)\xi = \frac{(K-\mu_B B+\mu)^2}{\hbar^2 v_F^2}\xi. \tag{12}$$

Using standard Landau levels (assuming $qB = |qB|$), we have

$$(K-\mu_B B+\mu)^2 = \hbar v_F^2 2qB(\ell + 1/2 - s_z), \tag{13}$$

whence

$$K_{\ell,s_z} = \pm\hbar v_F\sqrt{2\frac{q}{\hbar}B(\ell+1/2-s_z)} + \mu_B B - \mu. \tag{14}$$

The partition function is

$$Z = \prod_{\ell,s_z}[1+e^{-\beta K_{\ell,s_z}}]^{\Delta_L}, \tag{15}$$

where

$$\Delta_L = \frac{|qB|}{2\pi\hbar}$$

is the Landau degeneracy per unit area. For $B = 1$T, we have $\Delta_L \approx 2.4\cdot 10^{14}/m^2$. The grand canonical thermo-potential is

$$-\Gamma = \Delta_L\sum_\ell\sum_{s_z}\ln[1+e^{-\beta K_{\ell,s_z}}]. \tag{16}$$

For $\mu = 0$, we have the energy levels

$$K_{\ell,s_z} = \pm\hbar v_F\sqrt{2\frac{q}{\hbar}B(\ell+1/2-s_z)} + \mu_B B. \tag{17}$$

Corresponding to the field η, we have

$$K_{\ell,s_z} = \pm\hbar v_F\sqrt{2\frac{q}{\hbar}B(\ell+1/2-s_z)} - \mu_B B, \tag{18}$$

and therefore the energy levels are symmetric under $+\leftrightarrow -$. Therefore, if graphene is undoped, the Fermi level is still at $\mu = 0$. We suppose that $\mu_B B > 0$. Careful analysis shows that negative levels come from both the ξ and η fields ($[A]$ denotes the integer part of A),

$$\xi : K_{\ell,1/2} : \mu_B B - \hbar|v_F|\sqrt{2\frac{q}{\hbar}B\ell}, \quad \ell = \left[\frac{\mu_B^2 B}{2q\hbar v_F^2}\right] + 1,\ldots,\infty, \tag{19}$$

$$\xi : K_{\ell,-1/2} : \mu_B B - \hbar|v_F|\sqrt{2\frac{q}{\hbar}B(\ell+1)}, \quad \ell = \left[\frac{\mu_B^2 B}{2q\hbar v_F^2}\right],\ldots,\infty, \tag{20}$$

$$\eta : K_{\ell,1/2} : \begin{cases} -\mu_B B + \hbar|v_F|\sqrt{2\frac{q}{\hbar}B\ell}, & \ell = 0,1,\ldots,\left[\frac{\mu_B^2 B}{2q\hbar v_F^2}\right], \\ -\mu_B B - \hbar|v_F|\sqrt{2\frac{q}{\hbar}B\ell}, & \ell = 1,2,\ldots,\infty, \end{cases} \tag{21}$$

$$\eta : K_{\ell,-1/2} : \begin{cases} -\mu_B B + \hbar|v_F|\sqrt{2\frac{q}{\hbar}B(\ell+1)}, & \ell = 0,1,\ldots,\left[\frac{\mu_B^2 B}{2q\hbar v_F^2}\right] - 1, \\ -\mu_B B - \hbar|v_F|\sqrt{2\frac{q}{\hbar}B(\ell+1)}, & \ell = 0,1,2,\ldots\infty. \end{cases} \tag{22}$$

For $t = 3.033$ eV, $v_F = 3ta/2\hbar \approx 10^6$ m/s. Defining

$$B_0 := \frac{2qv_F^2\hbar}{\mu_B^2},$$

we have $B_0 \approx 1.1\cdot 10^6$ T. For laboratory field $B \sim 10$ T, it therefore follows that $[B/B_0] = 0$. Hence, for the ξ field, the negative $K_{\ell,1/2}$ levels are

$$s_z = 1/2 : \left\{ \mu_B B - \hbar|v_F|\sqrt{2\frac{q}{\hbar}B\ell}, \quad \ell = 1,\ldots,\infty, \right. \tag{23}$$

and the negative $K_{\ell,-1/2}$ levels are

$$s_z = -1/2 : \left\{ \mu_B B - \hbar|v_F|\sqrt{2\frac{q}{\hbar}B(\ell+1)}, \quad \ell = 0,\ldots,\infty. \right. \tag{24}$$

For the η field, the negative $K_{\ell,1/2}$ levels are

$$s_z = 1/2 : \begin{cases} -\mu_B B, \quad \ell = 0, \\ -\mu_B B - \hbar|v_F|\sqrt{2\frac{q}{\hbar}B\ell}, \quad \ell = 1,2,\ldots,\infty, \end{cases} \tag{25}$$

and the negative $K_{\ell,-1/2}$ levels are

$$s_z = -1/2 : \left\{ -\mu_B B - \hbar|v_F|\sqrt{2\frac{q}{\hbar}B(\ell+1)}, \quad \ell = 0,1,2,\ldots\infty. \right. \tag{26}$$

It follows that the levels

$$\mu_B B - \hbar|v_F|\sqrt{2\frac{q}{\hbar}B\ell}, \quad \ell = 1,\ldots,\infty,$$

and the levels

$$-\mu_B B - \hbar|v_F|\sqrt{2\frac{q}{\hbar}B\ell}, \quad \ell = 1,2,\ldots,\infty$$

are doubly degenerate (apart from the Landau degeneracy). We cannot have an infinite number of filled negative levels, and hence a cut-off is necessary. We suppose that among the levels

$$\mu_B B - \hbar|v_F|\sqrt{2\frac{q}{\hbar}B\ell}, \quad \ell = L_1^u \ldots, L_1^l$$

are filled, and among the levels

$$-\mu_B B - \hbar|v_F|\sqrt{2\frac{q}{\hbar}B\ell}, \quad \ell = L_2^u, \ldots L_2^l$$

are filled. If $-\mu_B B$ is also filled, then at $T = 0$ K,

$$N = \Delta_L \left(2(L_1^l - L_1^u + 1) + 2(L_2^l - L_2^u + 1) + 1\right) = = 2\Delta_L \left(L_1 + L_2 + \frac{1}{2}\right), \tag{27}$$

where

$$L_1 = L_1^l - L_1^u + 1, \quad L_2 = L_2^l - L_2^u + 1.$$

If $-\mu_B B$ is not filled, i.e., $\mu < -\mu_B B$, then

$$N = \Delta_L \left(2(L_1^l - L_1^u + 1) + 2(L_2^l - L_2^u + 1)\right) = = 2\Delta_L(L_1 + L_2). \tag{28}$$

The physics near $\mathbf{K}_-$ makes an equal contribution. The magnetization is

$$M = \mu_B(N_\xi - N_\eta), \tag{29}$$

where

$$N_\xi = \sum_{\mathbf{p}} \langle \xi_{\mathbf{p}}^\dagger \xi_{\mathbf{p}} \rangle, \quad N_\eta = \sum_{\mathbf{p}} \langle \eta_{\mathbf{p}}^\dagger \eta_{\mathbf{p}} \rangle. \tag{30}$$

The thermo-potential for the ξ fields should be regularized. The sum in the second term in the following formula actually extends not to infinity but only L_1:

$$-\frac{\Gamma_\xi}{\Delta_L} = \ln\left[1 + \exp\{\beta(\mu - \mu_B B)\}\right] + 2\sum_{\ell=1}^{\infty} \ln\left[1 + \exp\left\{\beta\left(\mu - \hbar v_F\sqrt{2\frac{q}{\hbar}B\ell} - \mu_B B\right)\right\}\right] + \\ + 2\sum_{\ell=1}^{L_1} \ln\left[1 + \exp\left\{\beta\left(\mu + \hbar v_F\sqrt{2\frac{q}{\hbar}B\ell} - \mu_B B\right)\right\}\right]. \tag{31}$$

With

$$\langle N \rangle = \beta^{-1}\frac{\partial \ln Z}{\partial \mu} = -\beta^{-1}\frac{\partial \Gamma}{\partial \mu},$$

we have

$$\langle N\rangle_\xi = \Delta_L \left[\frac{1}{1+\exp\{\beta(\mu_B B-\mu)\}} + 2\sum_{\ell=1}^{\infty}\frac{1}{1+\exp\left\{\beta(\hbar v_F\sqrt{2\frac{q}{\hbar}B\ell}+\mu_B B-\mu)\right\}} + \right.$$
$$\left. + 2\sum_{\ell=1}^{L_1}\frac{1}{1+\exp\left\{\beta\left(-\hbar v_F\sqrt{2\frac{q}{\hbar}B\ell}+\mu_B B-\mu\right)\right\}}\right]. \quad (32)$$

Similarly,

$$\langle N\rangle_\eta = \Delta_L \left[\frac{1}{1+\exp\{\beta(-\mu_B B-\mu)\}} + 2\sum_{\ell=1}^{\infty}\frac{1}{1+\exp\left\{\beta(\hbar v_F\sqrt{2\frac{q}{\hbar}B\ell}-\mu_B B-\mu)\right\}} + \right.$$
$$\left. + 2\sum_{\ell=1}^{L_2}\frac{1}{1+\exp\left\{\beta(-\hbar v_F\sqrt{2\frac{q}{\hbar}B\ell}-\mu_B B-\mu)\right\}}\right]. \quad (33)$$

At zero temperature, $\mu = 0$, and we have

$$\langle N\rangle = \langle N\rangle_\xi + \langle N\rangle_\eta = \Delta_L[1+2(L_1+L_2)], \quad (34)$$

and the manetization

$$M = \Delta_L\mu_B(2L_1 - 2L_2 - 1). \quad (35)$$

Since

$$L_1 = L_2, L_2+1,$$

we have

$$M = \pm\Delta_L\mu_B.$$

An intensive discussion of pseudospin paramagnetism in graphene was given in [25] very recently.

We next consider perpendicular magnetic and electric fields with $|\mathbf{E}| \ll v_F|\mathbf{B}|$. In this case, we can use the approximate SO(1,2) invariance and the above results. We suppose that the system Σ' is moving with a velocity $\mathbf{v}$ relative to the system Σ. For $\mathbf{v} = (v,0)$, the SO(1,2) transformation is

$$A'_\mu = \Lambda_\mu{}^\nu A_\nu, \quad (36)$$

$$\Lambda_\mu{}^\nu = \begin{pmatrix} \gamma & -\beta\gamma & 0 \\ -\beta\gamma & \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (37)$$

where

$$\beta = \frac{v}{v_F}, \quad \gamma = \frac{1}{\sqrt{1-\beta^2}}.$$

We have

$$E'_y = -\gamma v B, \quad B'_z = \gamma B,$$

whence

$$v = -\frac{E'_y}{B'_z}.$$

Therefore,

$$j^{0\prime} = \gamma j^0, \quad j^{x\prime} = -\gamma\beta j^0 = \gamma\frac{E'_y}{v_F B'_z}j^0$$

in Σ. We note that

$$j^\mu = q(v_F\rho, \mathbf{j}). \quad (38)$$

The Hall conductance is

$$\sigma'_{xy} = \frac{\gamma}{v_F B'_z}j^0 = \frac{q^2}{h}(2L+1), \quad (39)$$

if $-\mu_B B$ is filled or

$$\sigma'_{xy} = \frac{\gamma}{v_F B'_z}j^0 = \frac{q^2}{h}2L, \quad (40)$$

if $-\mu_B B$ is not filled, where $L = L_1 + L_2$. The physics near $\mathbf{K}_-$ makes equal contribution, we hence

$$\sigma'_{xy} = \frac{\gamma}{v_F B'_z}j^0 = $$
$$= \begin{cases} \dfrac{4q^2}{h}\left(L+\dfrac{1}{2}\right), & -\mu_B B \text{ is filled,} \\ \dfrac{4q^2}{h}L, & -\mu_B B \text{ is not filled.} \end{cases} \quad (41)$$

The above SO(1,2) transformation breaks down when $v \geq v_F$, i.e. when $|E'_y| \geq v_F|B'_z|$. The magnetic moment current

$$j_s^\mu = \mu_B(v_F(\rho_\xi - \rho_\eta), \mathbf{j}_\xi - \mathbf{j}_\eta) \quad (42)$$

is then given by

$$j_s^{x\prime} = (-\gamma\beta)v_F M = \mu_B \frac{qE'_y}{h}. \quad (43)$$

So far, the sequence of Hall conductance

$$\sigma_{xy} = \frac{4q^2}{h}\left(L + \frac{1}{2}\right)$$

has been observed; we here predict the existence of the sequence

$$\sigma_{xy} = \frac{4q^2}{h}L,$$

the recently observed $L = 0, 1$ being just part of this sequence [22]. According to above analysis, the filling of Zeeman levels makes the difference.

To summarize, we discussed the Hamiltonian and energy levels of graphene in general constant external electric and magnetic fields. The systems is not SO(1,2) Lorentz invariant when the Zeeman energy is taken into account. But when the magnetic field is strong enough, the SO(1,2) Lorentz invariance is well preseved. Using the symmetry, we predicted a sequence

$$\sigma_{xy} = \frac{4e^2}{h}L$$

and explained the recently observed Hall conductance

$$\sigma_{xy} = \frac{4e^2}{h}L, \quad L = 0, 1,$$

which is an indication that the Zeeman levels are not filled at zero temperature.

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