

Zero modes of tight-binding electrons on the honeycomb lattice

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Tight-binding electrons on the honeycomb lattice are studied where nearest-neighbor hoppings in the three directions are t_a , t_b , and t_c , respectively. For the isotropic case—namely, for $t_a=t_b=t_c$ —two zero modes exist where the energy dispersions at the vanishing points are linear in momentum k . Positions of zero modes move in the momentum space as t_a , t_b , and t_c are varied. It is shown that zero modes exist if $|\frac{t_b}{t_a}-1| \leq |\frac{t_c}{t_a}| \leq |\frac{t_b}{t_a}+1|$. The density of states near a zero mode is proportional to $|E|$ but it is proportional to $\sqrt{|E|}$ at the boundary of this condition

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The integer quantum Hall effect has been observed in graphene^{1,2} when the carriers are changed by the gate voltage. The quantization of the Hall effect is observed as $\sigma_{xy}=2n\frac{e^2}{h}$ with $n=\pm 1, \pm 3, \dots$, where the factor of 2 comes from the spin degrees of freedom. These quantum numbers are unusual, since in a usual case $n=0, \pm 1, \pm 2, \dots$. This unusual quantum Hall effect was discussed in terms of relativistic Dirac theory.³ However, it is more natural to be explained by the realization of the quantum Hall effect in periodic systems⁴ in the presence of zero modes.^{5,6} We will use zero modes instead of massless Dirac excitations in this paper because we do not consider relativistic particles. The energy spectrum and the density of states of the honeycomb lattice near half filling and in zero or small magnetic field are similar to these in the square lattice near half filling in a very strong magnetic field, about half flux quantum per each unit cell.⁵

At zero carrier concentration (i.e., half-filled electrons), the resistivity ρ_{xx} is close to the quantum value $h/(4e^2)=6.45k\Omega$ independent of temperature,¹ which has been also attributed to the zero modes.^{1,2,7}

The existence of zero modes has also been proposed for the quasi-two-dimensional organic conductor α -(BEDT-TTF)₂I₃. The conductivity under pressure is almost constant in a wide range of temperature.⁸ Pertinent numerical computations performed by Kobayashi *et al.*⁹ found that, for a certain range of parameters, the Fermi surfaces become points and the density of states is proportional to the energy at 3/4 filling of electrons. The existence of zero modes was also confirmed by a band structure calculation.^{10,11} The unit cell for the model of α -(BEDT-TTF)₂I₃ has four nonequivalent sites. Katayama *et al.*¹² studied a simpler model with two sites in the unit cell, and they obtained a condition for zero modes.

In this paper we study a tight-binding model on the honeycomb lattice and obtain the condition of t_a , t_b , and t_c for the existence of zero modes.

The unit cell of the honeycomb lattice contains two sublattices as shown in Fig. 1(a). The Bravais lattice is a triangular lattice with

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

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

where a is the lattice constant of graphene. We consider only nearest-neighbor hoppings. There are three nearest neighbors for each site, t_a , t_b , and t_c , as shown in Fig. 1. We study the generalized honeycomb lattice model where t_a , t_b , and t_c are not necessarily equal. Under uniaxial pressure, t_a , t_b , and t_c have different values for each other. For example, $t_a > t_b = t_c$ is expected, if the uniaxial pressure along the x direction is applied. The Hamiltonian for the generalized honeycomb lattice is given by

$$\mathcal{H} = \sum_{\mathbf{r}_m} [-t_a(a_{\mathbf{r}_m}^\dagger b_{\mathbf{r}_m} + \text{H.c.}) - t_b(a_{\mathbf{r}_m}^\dagger b_{\mathbf{r}_m+\mathbf{v}_1} + \text{H.c.}) - t_c(a_{\mathbf{r}_m}^\dagger b_{\mathbf{r}_m+\mathbf{v}_2} + \text{H.c.})]. \quad (3)$$

Using the Fourier transform

$$a_{\mathbf{r}_m} = \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_m} a_{\mathbf{k}}, \quad (4)$$

$$b_{\mathbf{r}_m} = \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{r}_m+\mathbf{x})} b_{\mathbf{k}}, \quad (5)$$

where $\mathbf{x}=(\frac{\sqrt{3}}{3}a, 0)$, we obtain

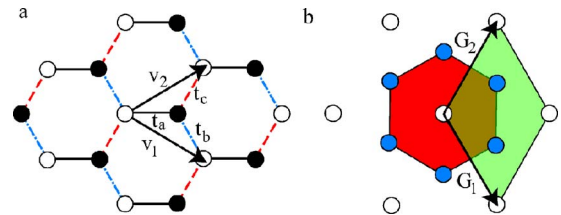


FIG. 1. (Color online) (a) Honeycomb lattice. Unit vectors are $\mathbf{v}_1=(\frac{\sqrt{3}}{2}a, -\frac{1}{2}a)$ and $\mathbf{v}_2=(\frac{\sqrt{3}}{2}a, \frac{1}{2}a)$. Three nearest-neighbor hoppings are t_a , t_b , and t_c . (b) The red hexagon is a Brillouin zone for the honeycomb lattice. The reciprocal lattice vectors are $\mathbf{G}_1=(\frac{2\pi\sqrt{3}}{3a}, -\frac{2\pi}{a})$ and $\mathbf{G}_2=(\frac{2\pi\sqrt{3}}{3a}, \frac{2\pi}{a})$. White circles are Γ points. The Brillouin zone can also be taken by the green diamond.

$$\mathcal{H} = \sum_{\mathbf{k}} \left(\left\{ -t_a \exp\left(-i\frac{\sqrt{3}}{3}ak_x\right) - t_b \exp\left[i\left(\frac{\sqrt{3}}{6}ak_x - \frac{1}{2}ak_y\right)\right] - t_c \exp\left[i\left(\frac{\sqrt{3}}{6}ak_x + \frac{1}{2}ak_y\right)\right] \right\} a_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \text{H.c.} \right). \quad (6)$$

The energy is given by

$$\begin{aligned} \epsilon_{\mathbf{k}}^2 = & t_a^2 + t_b^2 + t_c^2 + 2t_a t_b \cos\left(\frac{\sqrt{3}}{2}ak_x - \frac{1}{2}ak_y\right) \\ & + 2t_a t_c \cos\left(\frac{\sqrt{3}}{2}ak_x + \frac{1}{2}ak_y\right) + 2t_b t_c \cos(ak_y). \end{aligned} \quad (7)$$

If we perform a translation in momentum space,

$$(k_x, k_y) \rightarrow \left(k_x + \frac{2\pi}{\sqrt{3}}, k_y\right), \quad (8)$$

and a replacement $t_a \rightarrow -t_a$ simultaneously, we get the same $\epsilon_{\mathbf{k}}$. Therefore we can take $t_a \geq 0$ without loss of generality. In a similar way one can take $t_b \geq 0$ and $t_c \geq 0$ without loss of generality by taking a translation in momentum space,

$$(k_x, k_y) \rightarrow \left(k_x + \frac{\sqrt{3}}{3}\pi, k_y \pm \pi\right). \quad (9)$$

The reciprocal lattice vectors are

$$\mathbf{G}_1 = \left(\frac{2\pi\sqrt{3}}{3a}, -\frac{2\pi}{a}\right), \quad (10)$$

$$\mathbf{G}_2 = \left(\frac{2\pi\sqrt{3}}{3a}, \frac{2\pi}{a}\right), \quad (11)$$

as shown in Fig. 1(b). Let us write

$$\mathbf{k} = k_1 \mathbf{G}_1 + k_2 \mathbf{G}_2, \quad (12)$$

where

$$k_1 = \frac{\sqrt{3}}{4\pi}ak_x - \frac{1}{4\pi}ak_y, \quad (13)$$

$$k_2 = \frac{\sqrt{3}}{4\pi}ak_x + \frac{1}{4\pi}ak_y. \quad (14)$$

The energy is

$$\begin{aligned} \epsilon_{\mathbf{k}}^2 = & t_a^2 + t_b^2 + t_c^2 + 2t_a t_b \cos(2\pi k_1) + 2t_a t_c \cos(2\pi k_2) \\ & + 2t_b t_c \cos[2\pi(-k_1 + k_2)]. \end{aligned} \quad (15)$$

The minimum of $|\epsilon_{\mathbf{k}}|$ is obtained as follows. Consider the quadrangle $ABCD$ in Fig. 2(a). Then we have

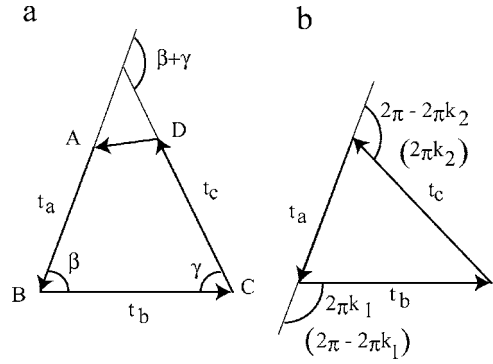


FIG. 2. Graphical explanation for appearance of zero modes. (a) If t_a , t_b , and t_c do not form a triangle, there are no zero modes and gaps at $E=0$ are open. (b) Zero modes exist when t_a , t_b , and t_c form a triangle. Angles k_1 and k_2 are shown.

$$\begin{aligned} |\vec{DA}|^2 = & |\vec{AB} + \vec{BC} + \vec{CD}|^2 = t_a^2 + t_b^2 + t_c^2 - 2t_a t_b \cos \beta \\ & - 2t_b t_c \cos \gamma - 2t_a t_c \cos(\pi - \beta - \gamma) \geq 0. \end{aligned} \quad (16)$$

Put

$$\beta = \pi - 2\pi k_1, \quad (17)$$

$$\gamma = \pi + 2\pi(k_1 - k_2), \quad (18)$$

then

$$\begin{aligned} t_a^2 + t_b^2 + t_c^2 + 2t_a t_b \cos(2\pi k_1) + 2t_a t_c \cos(2\pi k_2) \\ + 2t_b t_c \cos[2\pi(k_1 - k_2)] \geq 0. \end{aligned} \quad (19)$$

The equality is satisfied when t_a , t_b , and t_c form a triangle which can be seen in Fig. 2(b)—i.e.,

$$\cos(2\pi k_1) = \frac{t_c^2 - t_a^2 - t_b^2}{2t_a t_b}, \quad (20)$$

$$\cos(2\pi k_2) = \frac{t_b^2 - t_a^2 - t_c^2}{2t_a t_c}, \quad (21)$$

$$\cos[2\pi(k_1 - k_2)] = \frac{t_a^2 - t_b^2 - t_c^2}{2t_b t_c}. \quad (22)$$

The triangle can be formed when

$$\left| \frac{|t_b|}{|t_a|} - 1 \right| \leq \frac{|t_c|}{|t_a|} \leq \left| \frac{|t_b|}{|t_a|} + 1 \right| \quad (23)$$

is satisfied. See Fig. 3.

In the isotropic case where $t_a = t_b = t_c$, zero modes are at $(k_1, k_2) = \pm(\frac{1}{3}, \frac{2}{3})$, $(k_1, k_2) = \pm(\frac{2}{3}, \frac{1}{3})$, and $(k_1, k_2) = \pm(\frac{1}{3}, \frac{1}{3})$ —i.e., the corners of the first Brillouin zone, $(k_x, k_y) = \pm(\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{3a})$, $(k_x, k_y) = \pm(\frac{2\pi}{\sqrt{3}a}, -\frac{2\pi}{3a})$, and $(k_x, k_y) = \pm(0, \frac{4\pi}{3a})$. See Fig. 4. The density of states is written in

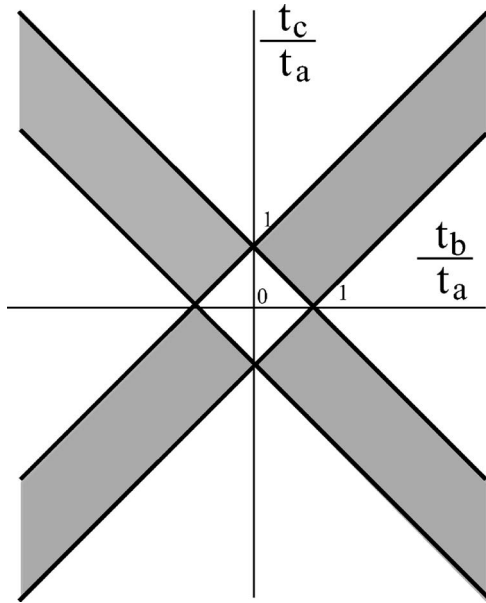


FIG. 3. Zero modes exist in the filled region.

terms of the complete elliptic integral¹³ and it is plotted in Fig. 5(a).¹⁴

If the parameters are in the boundary as seen in Fig. 3, two zero modes merge into a confluent point. For example, $\epsilon_k=0$ at confluent point $(k_x^*, k_y^*) = (\frac{2\pi}{\sqrt{3}a}, 0)$ for $t_a=2$, $t_b=1$, and $t_c=1$ (Fig. 6). Near this point ϵ_k is written as

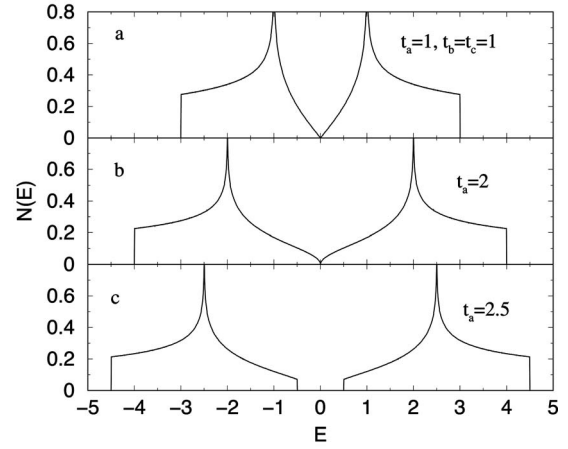


FIG. 5. Density of states of the electrons on a generalized honeycomb lattice.

$$\begin{aligned} \epsilon_k^2 &= 6 - 8 \cos\left(\frac{\sqrt{3}}{2}a(k_x - k_x^*)\right) \cos\left(\frac{1}{2}a(k_y - k_y^*)\right) \\ &+ 2 \cos a(k_y - k_y^*) \approx 3a^2(k_x - k_x^*)^2 \left(1 - \frac{1}{8}a^2(k_y - k_y^*)^2\right) \\ &+ \frac{1}{16}a^4(k_y - k_y^*)^4. \end{aligned} \quad (24)$$

In this case the density of states near $E=0$ becomes

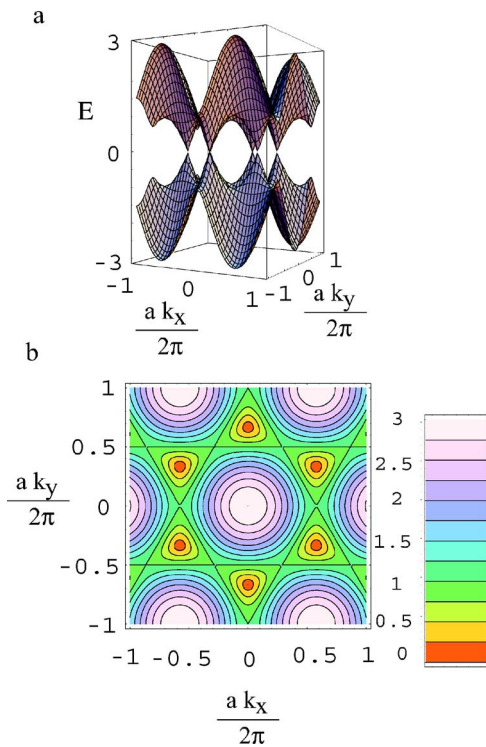


FIG. 4. (Color online) Energy dispersion for the isotropic case ($t_a=t_b=t_c=1$). (a) Three-dimensional plot and (b) contour plot.

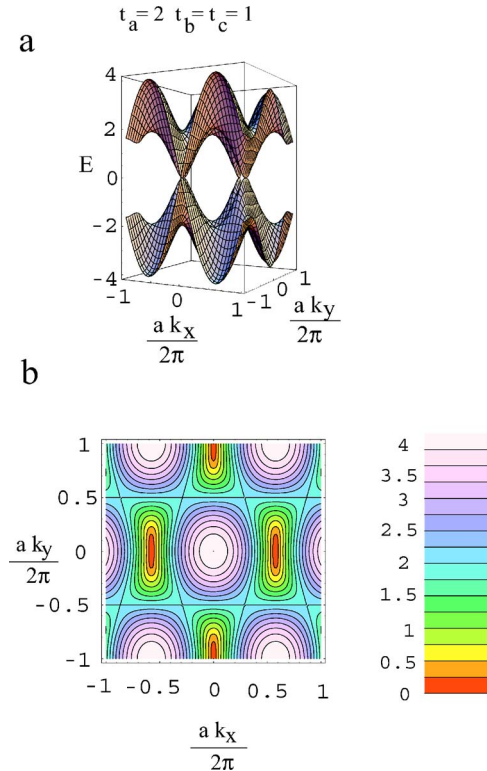


FIG. 6. (Color online) Three-dimensional plot (a) and the contour plot (b) of the energy of the generalized honeycomb lattice with $t_a=2$, $t_b=t_c=1$.

$$N(E) = \frac{\sqrt{\pi}}{4\pi^2} \frac{\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)} \sqrt{|E|}. \quad (25)$$

[see Fig. 5(b)], while $N(E) \propto |E|$ in the case of two zero modes [Fig. 5(a)]. When the inequality (23) is not satisfied, a finite gap opens at $E=0$ as shown in Fig. 5(c).

In conclusion, we have studied the energy of tight-binding

electrons in the generalized honeycomb lattice and found the condition for the existence of zero modes. The zero modes exist at the corners of the hexagonal first Brillouin zone for the usual honeycomb lattice. Two zero modes moved to become a confluent point at the critical values of parameters t_a , t_b , and t_c , where t_a , t_b , and t_c stop to form a triangle.

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¹K. S. Novoselov *et al.*, Nature (London) **438**, 197 (2005).

²Y. Zhang *et al.*, Nature (London) **438**, 201 (2005).

³V. P. Gusynin and S. G. Sharapov, Phys. Rev. Lett. **95**, 146801 (2005).

⁴D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982); M. Kohmoto, Ann. Phys. (N.Y.) **160**, 343 (1985).

⁵Y. Hasegawa and M. Kohmoto, cond-mat/0603345 (unpublished).

⁶N. M. R. Peres, F. Guinea, and A. H. Castro Neto, Phys. Rev. B **73**, 125411 (2006).

⁷K. Ziegler, Phys. Rev. Lett. **80**, 3113 (1998).

⁸N. Tajima, A. Ebina-Tajima, M. Tamura, Y. Nishio, and K. Kajita,

J. Phys. Soc. Jpn. **71**, 1832 (2002).

⁹A. Kobayashi, S. Katayama, K. Noguchi, and Y. Suzumura, J. Phys. Soc. Jpn. **73**, 3135 (2004); A. Kobayashi, S. Katayama, and Y. Suzumura, *ibid.* **74**, 2897 (2005).

¹⁰S. Ishibashi, T. Tamura, M. Kohyama, and K. Terakura, J. Phys. Soc. Jpn. **75**, 015005 (2006).

¹¹H. Kino and T. Miyazaki, J. Phys. Soc. Jpn. **75**, 034704 (2006).

¹²S. Katayama, A. Kobayashi, and Y. Suzumura, J. Phys. Soc. Jpn. **75**, 054705 (2006).

¹³T. Horiguchi, J. Math. Phys. **13**, 1411 (1972).

¹⁴J. P. Hobson and W. A. Nierenberg, Phys. Rev. **89**, 662 (1953).