Energy quantization at the “three-quarter Dirac point” in a magnetic field

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The quantization of the energy in a magnetic field (Landau quantization) at a three-quarter Dirac point is studied theoretically. The three-quarter Dirac point is realized in the system of massless Dirac fermions with the critically tilted Dirac cone in one direction, where a linear term disappears and a quadratic term \( \alpha_2 q_x^2 \) with a constant \( \alpha_2 \) plays an important role. The energy is obtained as \( E_n \propto \alpha_2^2 (nB)^{\frac{2}{5}} \), where \( n = 1, 2, 3, \ldots \) by means of numerically and analytically solving the differential equation, as well as by the semiclassical quantization rule. The existence of the \( n = 0 \) state is studied by introducing the energy gap due to the inversion-symmetry-breaking term, and it is obtained that the \( n = 0 \) state exists in one of a pair of three-quarter Dirac points, depending on the direction of the magnetic field when the energy gap is finite.

I. INTRODUCTION

Massless Dirac fermions are observed in condensed matter physics, in graphene [1, 2], organic conductors [3–5], and the surface of the 3D topological insulators [6, 7].

When a two-dimensional system has an inversion symmetry and a time reversal symmetry, massless Dirac points (\( \pm k_D \)) appear as a pair. The minimal model for the massless Dirac fermions is written as [8–10]

\[
\mathcal{H}_D = \begin{pmatrix} w_{0x} q_x + w_{0y} q_y & w_x q_x \mp iw_y q_y \\ w_x q_x \pm iw_y q_y & w_{0x} q_x + w_{0y} q_y \end{pmatrix},
\]  

where

\[
q = k \mp k_D.
\]

Two bands touch at the Dirac points. When \( w_{0x} = 0 \) and \( w_{0y} = 0 \), the linear energy dispersion near the Dirac point (Dirac cone) is not tilted. By the finite \( w_{0x} \) or \( w_{0y} \), the Dirac cone is tilted, and if the condition

\[
\left( \frac{w_{0x}}{w_x} \right)^2 + \left( \frac{w_{0y}}{w_y} \right)^2 = 1,
\]

is fulfilled, the Dirac cone is critically tilted, i.e., the conical edge of the Dirac cone is horizontal in one direction. In that case we have to take into account the quadratic terms in the tilted direction, except for the special case that the quadratic terms vanish by symmetry or by accident. Generally the quadratic terms exist as we have found previously [11] in the tight-binding model with pressure-dependent hoppings for the organic conductor, \( \alpha \)-\( \text{(BEDT-TTF)}_2I_3 \). The energy near the critically tilted Dirac point is shown in Fig. 1. Since the energy of the upper band depends linearly in three directions (for example, \( -q_x \) and \( \pm q_y \)) and quadratically in one direction (for example, \( q_x \)) in that case, we call the critically tilted Dirac point as the three-quarter Dirac point [11].

It has been known that when two-Dirac points merge at the time-reversal-invariant momentum, the energy depends linearly in two directions and quadratically in two directions, and it is called the semi-Dirac point [12–16].

Previously we have shown that the energy in the magnetic field (the Landau level) at the three-quarter Dirac point depends on the quantum number \( n \) and the magnetic field \( B \) as

\[
\epsilon_n \propto (nB)^{\frac{2}{5}},
\]

by calculating the energy of the tight-binding model for \( \alpha \)-\( \text{(BEDT-TTF)}_2I_3 \) in a magnetic field numerically [11]. In that paper we have explained these \( n \) and \( B \) dependences of Landau levels by using the semi-classical quanti-
tization rule. In this paper we study the Landau quantization at the three-quarter Dirac point in numerical and analytical treatment. The Dirac cone is taken to be critically tilted in the $k_x$ direction, i.e., $w_{0x} = -w_x$, and $w_{0y} = 0$. For simplicity we take $w_x > 0$, $w_y > 0$, and we introduce the quadratic terms in the $q_x$ direction ($\alpha'_2 q_x^2$ in diagonal elements and $\alpha''_2 q_x^2$ in off-diagonal elements). Then the three-quarter Dirac Hamiltonian we study in this paper is

$$
H_{\text{tqD}} = \begin{pmatrix}
-w_x q_x + \alpha'_2 q_x^2 & w_x q_x + \alpha''_2 q_x^2 - i w_y q_y \\
w_x q_x + \alpha'_2 q_x^2 + i w_y q_y & -w_x q_x + \alpha''_2 q_x^2
\end{pmatrix}.
$$

(5)

II. THREE-QUARTER DIRAC POINT

A. energy at $B = 0$

In the absence of the magnetic field the energy is obtained by

$$
H_{\text{tqD}} \Psi = E(q) \Psi,
$$

(6)

where $\Psi$ is a wave function which has two components, $\psi_1$ and $\Psi_2$. The eigenvalues of $H_{\text{tqD}}$ is obtained as $E(q) = \varepsilon_{q_{\text{tqD}}}(q)$;

$$
\varepsilon_{q_{\text{tqD}}}(q) = -w_x q_x + \alpha'_2 q_x^2 \\
\pm \sqrt{(w_x q_x + \alpha''_2 q_x^2)^2 + (w_y q_y)^2},
$$

(7)

which are plotted in Fig. [1]. There exist the upper band ($\varepsilon_{q_{\text{tqD}}+}(q)$) and the lower band ($\varepsilon_{q_{\text{tqD}}-}(q)$). These two bands touch at $q = (0, 0)$. Along the $q_x$ axis, the linear term disappears in $\varepsilon_{q_{\text{tqD}}+}(q)$ and $\varepsilon_{q_{\text{tqD}}-}(q)$ for $q_x > 0$ and $q_x < 0$, respectively, whereas in other three directions the linear term exists;

$$
\varepsilon_{q_{\text{tqD}}+}(q_x, q_y = 0) = \begin{cases} 
\alpha'_2 q_x^2 & \text{if } q_x > 0 \\
2 w_x |q_x| + \tilde{\alpha}_2 q_x^2 & \text{if } q_x < 0
\end{cases}
$$

(8)

$$
\varepsilon_{q_{\text{tqD}}-}(q_x = 0, q_y) = w_y |q_y|,
$$

(9)

$$
\varepsilon_{q_{\text{tqD}}-}(q_x, q_y = 0) = \begin{cases} 
-2 w_x q_x + \tilde{\alpha}_2 q_x^2 & \text{if } q_x > 0 \\
\alpha''_2 q_x^2 & \text{if } q_x < 0
\end{cases}
$$

(10)

$$
\varepsilon_{q_{\text{tqD}}-}(q_x = 0, q_y) = -w_y |q_y|,
$$

(11)

where

$$
\alpha_2 = \alpha'_2 + |\alpha''_2|,
$$

(12)

and

$$
\tilde{\alpha}_2 = \alpha'_2 - |\alpha''_2|.
$$

(13)

If $\alpha_2 > 0$, $q = 0$ is a local minimum of $\varepsilon_{q_{\text{tqD}}+}$ with the linear dispersion in three directions ($q_x < 0$, $q_y > 0$ and $q_x < 0$) and quadratic dispersion in one direction ($q_x > 0$). Note that the “three-quarter Dirac point” is neither the local maximum nor the local minimum of $\varepsilon_{q_{\text{tqD}}}$ if $\alpha_2 > 0$. If $\alpha_2 < 0$, the “three-quarter Dirac point” is the local maximum of $\varepsilon_{q_{\text{tqD}}}$, but it is neither the local maximum nor the local minimum of $\varepsilon_{q_{\text{tqD}}}$.

B. numerical results of the energy at $B > 0$, using boundary condition at $y > 0$

Hereafter we study the case $\alpha_2 > 0$, i.e., the three-quarter Dirac point is the minimum of $\varepsilon_{q_{\text{tqD}}+}$, as shown in Fig. [1]. In this case it is expected that when the magnetic field is applied, there are the almost-localized bound states (Landau levels) at $E > 0$, which is obtained by the Landau quantization of $\varepsilon_{q_{\text{tqD}}+}$. Since $\varepsilon_{q_{\text{tqD}}+}$ becomes positive as $q_y < 0$, the Landau levels couple to the continuous energy band by quantum tunneling. In this subsection we show that the Landau levels couple to the continuous energy band by tunneling.

In the presence of the magnetic field $B$ ($B = \nabla \times A$, where $A$ is the vector potential), we replace $q_x$ and $q_y$ as

$$
q_x \rightarrow i \hbar \frac{\partial}{\partial x} + e A_x, \\
q_y \rightarrow i \hbar \frac{\partial}{\partial y} + e A_y.
$$

(14)

(15)

Hereafter, we set the absolute value of the electron charge and the Planck constant divided by $2\pi$ to be 1 ($e = \hbar = 1$) for simplicity. We study the case that the uniform magnetic field $B > 0$ is applied along the $z$ direction. We take the vector potential as

$$
A = (-B y, 0, 0).
$$

(16)

Since there are no explicit $x$ in Eq. (6), we can write

$$
\Psi(x, y) = e^{i \tilde{q}_x x} \begin{pmatrix} \Psi_1(y) \\ \Psi_2(y) \end{pmatrix}.
$$

(17)

In this case we take

$$
q_x \rightarrow \tilde{q}_x - B y \equiv -B \tilde{y}.
$$

(18)

We write $\tilde{y}$ as $y$ hereafter for simplicity. Then the equation we study is

$$
\begin{pmatrix} \hat{H}_{\text{tqD}} & 11 \\ \hat{H}_{\text{tqD}} & 12 \end{pmatrix} \begin{pmatrix} \Psi_1(y) \\ \Psi_2(y) \end{pmatrix} = E \begin{pmatrix} \Psi_1(y) \\ \Psi_2(y) \end{pmatrix},
$$

(19)

where

$$
(\hat{H}_{\text{tqD}})_{11} = w_x B y + \alpha'_2 (B y)^2, \\
(\hat{H}_{\text{tqD}})_{12} = -w_x B y + \alpha''_2 (B y)^2 - w_y \frac{d}{d y}, \\
(\hat{H}_{\text{tqD}})_{21} = -w_x B y + \alpha''_2 (B y)^2 + w_y \frac{d}{d y}, \\
(\hat{H}_{\text{tqD}})_{22} = \hat{H}_{\text{tqD}}_{11}.
$$

(20)

(21)

(22)

(23)

We seek the solution of Eq. (19) with $E \geq 0$ and the boundary conditions

$$
\Psi_1(y) \rightarrow 0, \\
\Psi_2(y) \rightarrow 0,
$$

(24)

(25)
For given \( s \), there are no strict quantization for boundary condition. The lower band becomes positive when \( q \to 0 \) as seen in Eq. (18). When \( q \to +\infty \), \( \Psi_1(y) \) and \( \Psi_2(y) \) do not have to vanish because the lower band becomes positive when \( q_x \to -\infty \) at \( B = 0 \) as seen in Fig. 1. We solve the differential equations, Eq. (19), numerically by the Runge-Kutta method in this study.

We adopt the boundary condition at \( y = 20 \) to be Eq. (20).

\[
\Psi_2(y = 20) / \Psi_1(y = 20) = \tan \theta. \tag{26}
\]

Note that \( \theta \) and \( \theta + n\pi \) with integer \( n \) are the same boundary condition. The lower band becomes positive at \( q_x \to -\infty \) at \( B = 0 \) as shown in Fig. 1. As a result, there are no strict quantization for \( E \) at \( B \neq 0 \). For given \( E \) we determine \( \theta \). The numerically obtained solution diverges as \( y \) becomes a negative large value, if the chosen \( \theta \) is not suitable. Only when \( \theta \) is the correct value for \( E \), the numerically obtained solution becomes zero as \( y \to -\infty \). We show some examples of the solutions for \( 0.3 \leq E \leq 0.33 \) in Fig. 2 and Fig. 3 and for \( 0.52906 \leq E \leq 0.52907 \) in Fig. 4 where we have normalized the wave functions numerically as

\[
\int_{-10}^{20} (|\Psi_1(y)|^2 + |\Psi_2(y)|^2) \, dy = 1. \tag{27}
\]

Nearly bound states in \( y \lesssim 0 \) exist at \( E \approx 0.3108 \) and 0.529065. The wave functions \( (\Psi_1(y), \Psi_2(y)) \) at \( E = 0.3105 \) and 0.3108 with the suitable boundary conditions have one node of \( \Psi_1(y) \) and \( \Psi_2(y) \) in \( y \lesssim 0 \), as seen in Fig. 3 (a) and (b), and the wave functions at \( E = 0.52906, 0.529065, \) and 0.52807 have two nodes in \( y \lesssim 0 \), as seen in Fig. 4 (a) - (c). Therefore, \( E \approx 0.3108 \) and \( E \approx 0.529065 \) are the bound state energies with \( n = 1 \) and \( n = 2 \), respectively. Due to the tunneling these bound states are not completely localized in the region \( y \lesssim 0 \), which corresponds to the region \( q_x \gtrsim 0 \) in the case of \( B = 0 \) (see Eq. (18) and Fig. 1). This interpretation of the bound states in three-quarter Dirac point is justified by plotting \( \theta \) as a function of energy (Fig. 5). As seen in Fig. 5 \( \theta \) changes continuously as \( E \) increases. When the energy is close to one of the energies of the bound states, \( \theta \) changes by \( \pi \) in a narrow region of \( E \). At \( n = 2 \) \( E \approx 0.529065 \) \( \theta \) changes in a narrower region than at \( n = 1 \) \( E \approx 0.3108 \). The narrowing of the region in \( \theta \) is reasonable because the tunneling of the almost-localized state at \( y \lesssim 0 \) into the region of \( y > 0 \) is weaker at \( n = 2 \) than at \( n = 1 \). As the bound-state energy becomes larger, the tunneling of the bound state at \( y \lesssim 0 \) into \( y > 0 \) becomes smaller. Therefore, the numerical solutions of the bound states \( n \geq 3 \) are difficult to obtain by using the boundary condition Eq. (20), since \( \theta \) changes in a
very narrow region. In the next subsection we use the boundary condition at \( y < 0 \) to obtain the energy of the bound states.

### C. numerical results of energy at \( B > 0 \), using boundary condition at \( y < 0 \)

As shown in the previous subsection, it is difficult to obtain the energy of the almost-localized states at \( y < 0 \) for large quantum number \( n \) in Eq. (19) by using the boundary condition at \( y > 0 \), since the boundary condition changes in a very narrow region and the energy of the almost-localized states at \( y < 0 \) may be overlooked. Therefore, we try to obtain the energy by using the boundary conditions at \( y < 0 \). We study the solutions of Eq. (19) at \( y \to -\infty \), assuming

\[
\Psi_j(y) = c_j(y)e^{-g(y)}, \quad (j = 1, 2)
\]

(38) and

\[
\frac{d\Psi_j}{dy} = \left( \frac{dg(y)}{dy} c_j(y) + \frac{dc_j(y)}{dy} \right) e^{-g(y)} \\
\sim -\frac{dg(y)}{dy} c_j e^{-g(y)},
\]

as \( y \to -\infty \). Then we obtain the equation

\[
\begin{pmatrix}
(\hat{H}_{\text{tqD}})_{11} & (\hat{F}_{\text{tqD}})_{12} \\
(\hat{F}_{\text{tqD}})_{21} & (\hat{H}_{\text{tqD}})_{22}
\end{pmatrix}
\begin{pmatrix}
\Psi_1(y) \\
\Psi_2(y)
\end{pmatrix}
\approx E \begin{pmatrix}
\Psi_1(y) \\
\Psi_2(y)
\end{pmatrix},
\]

(39)

where \((\hat{H}_{\text{tqD}})_{11}\) and \((\hat{H}_{\text{tqD}})_{22}\) are given in Eqs. (20) and (23) and

\[
(\hat{F}_{\text{tqD}})_{12} = -w_x By + \alpha_2'(By)^2 + w_y \frac{dg}{dy},
\]

(40)

and

\[
(\hat{F}_{\text{tqD}})_{21} = -w_x By + \alpha_2'(By)^2 - w_y \frac{dg}{dy}.
\]

The nontrivial solution exists when the condition

\[
\det \begin{pmatrix}
(\hat{H}_{\text{tqD}})_{11} - E & (\hat{F}_{\text{tqD}})_{12} \\
(\hat{F}_{\text{tqD}})_{21} & (\hat{H}_{\text{tqD}})_{22} - E
\end{pmatrix} = 0,
\]

(41)

is fulfilled, i.e.,

\[
\left( \frac{w_y}{w_x} \frac{dg}{dy} \right)^2 = (-2w_x B y + \tilde{\alpha}_2(By)^2 - E),
\]

(42)

where \( w_x = w_y = 1, w_{0x} = -1, w_{0y} = 0, \alpha_2' = \alpha_2 = 0.01, B = 1 \). (b) and (c) are the close-up of (a) near the energy of the almost-localized states at \( y \lesssim 0 \).
between the nearly-localized state at \( y \lesssim 0 \) and the continuous state as \( y \gtrsim 0 \) is small for \( n \geq 2 \). In section II B we first fixed the energy and obtain the correct bound state as \( y > 0 \) (\( y = 20 \)). In this section we first take the approximate boundary condition at \( y = -10 \), and obtain the energy which gives the smallest amplitude of oscillations of the wave function at \( y > 0 \). Even though the boundary condition is not exact, suitable linear combination of the nearly-localized state at \( y \lesssim 0 \) and continuous state as \( y \gtrsim 0 \) may give the non-divergent solution if the energy is a discrete energy of the nearly-localized state at \( y \lesssim 0 \).

In Fig. 6 we show the wave functions for nearly-localized states with quantum numbers \( n = 0 - 6 \). For \( n = 0 \), i.e. \( E = 0 \), two components of the wave function have broad peak at \( y = 0 \), although they are not small at \( y > 0 \) as shown in Fig. 7(a). The oscillation of the wave function at \( y > 0 \) can be understood as the continuous energy states at \( y > 0 \). Since the upper band touches the lower band at the three-quarter Dirac point without the boundary barrier, the bound state at \( y < 0 \) goes through to the region \( y > 0 \). We will discuss the \( n = 0 \) state in the next section.

The eigenstate for \( n \geq 1 \) is obtained by taking the suitable value of \( E \), which minimize the amplitude of oscillation of the wave function in the region \( y > 0 \). We find the tunneling through the barrier is smaller as \( n \) becomes larger, which is expected since the forbidden energy region at \( B = 0 \) becomes wider as the energy becomes higher (see Fig. 1).

We also calculate the energy as a function of quantum number \( n \) with different choice of parameters \( \alpha'_2 = 0.02 \) and \( \alpha''_2 = 0 \) from these used in Fig. 7(a) (\( \alpha'_2 = \alpha''_2 = 0.01 \)).

We plot the energy as a function of \( n \) in Fig. 8. We obtain

\[
E_n \propto n^\frac{3}{2}.
\]  

(39)

In Figs. 3 and 10 we plot the energy as a function of \( \alpha_2 \) and \( B \), respectively. We obtain

\[
E_n \propto \alpha'^2_2 \left(nB\right)^\frac{3}{2}.
\]  

(40)

We have previously obtained \( n \) and \( B \) dependence at the three-quarter Dirac point (Eq. (10)) in the tight-binding model of \( \alpha-(BEDT-TTF)_2I_3 \) at the critical pressure [11]. We plot the wave functions as a function of \( By \) in Fig. 10 in which we also plot \( \varepsilon_{\pm qD+}(q_x, q_y = 0) \) at \( B = 0 \) (Eqs. 8).
Parameters are $w$, $n$. FIG. 8. (Color online) Energy as a function of the quantum number $n$ for the three-quarter Dirac point. Parameters are $w_x = w_y = 1$, $w_{ox} = -1$, $w_{oy} = 0$, and $B = 1$. We take two choices of parameters giving the same $\alpha$, $B$ and (10) with replacing $q_x \rightarrow -By$ (Eq. (18)). Classically, electrons can exist in the green-striped regions in Fig. 11 and they can exist only by the quantum tunneling effect in the white regions.

and (10) with replacing $q_x \rightarrow -By$ (Eq. (18)). Classically, electrons can exist in the green-striped regions in Fig. 11 and they can exist only by the quantum tunneling effect in the white regions.

D. analytical study of the magnetic-field- and $\alpha_2$-dependence of the Landau levels at the three-quarter Dirac point

The $B$ and $\alpha_2$ dependences of the energy are obtained as follows. We take

$$y = \alpha_2 \delta B^\eta Y,$$  \hspace{1cm} (41)

in Eq. (19) and we obtain

$$\begin{align*}
\left(\alpha_2 \delta B^{1+\eta} Y + \alpha_2 \alpha_2 \delta B^{2+2\eta} Y^2 - E\right) \Psi_1 \\
+ \left(-\alpha_2 \delta B^{1+\eta} Y + \alpha_2 \delta B^{2+2\eta} Y^2 - \alpha_2 \delta B^{-\eta} \frac{d}{dY}\right) \Psi_2 = 0, \\
\left(-\alpha_2 \delta B^{1+\eta} Y + \alpha_2 \delta B^{2+2\eta} Y^2 + \alpha_2 \delta B^{-\eta} \frac{d}{dY}\right) \Psi_1 \\
+ \alpha_2 \delta B^{1+\eta} Y + \alpha_2 \delta B^{2+2\eta} Y^2 + \alpha_2 \delta B^{-\eta} \frac{d}{dY}\right) \Psi_2 = 0.
\end{align*}$$  \hspace{1cm} (42)

We assume

$$-1 < \eta < 0,$$  \hspace{1cm} (44)

in order to make all terms go to zero as $B \rightarrow 0$. From Eqs. (42) and (43) we obtain

$$\begin{align*}
\left(\alpha_2 \delta B^{2+2\eta} Y^2 - E\right) (\Psi_1 + \Psi_2) \\
+ \alpha_2 \delta B^{-\eta} \frac{d}{dY}(\Psi_1 - \Psi_2) = 0
\end{align*}$$  \hspace{1cm} (45)
and

\[(2\alpha_0^2 \beta^{1+\gamma} Y + \tilde{a}_2 \alpha_0^{2\gamma} B^{2+2\gamma} Y^2 - E) (\Psi_1 - \Psi_2) - \alpha_0^{-\gamma} B^{-\gamma} \frac{d}{dY}(\Psi_1 + \Psi_2) = 0.\] (46)

From Eq. (45) there should be the solution,

\[E = O(\alpha_0^2 B^{1+2\gamma})\] (47)

\[\Psi_1 + \Psi_2 = O(\alpha_0^2 B^0)\] (48)

in the limit \(B \to 0\). Then we can neglect \((\tilde{a}_2 \alpha_0^{2\gamma} B^{2+2\gamma} Y^2 - E)\) with respect to \(2B^{1+\gamma} Y\) in Eq. (49), to obtain

\[\Psi_1 - \Psi_2 \sim \alpha_0^{-2\gamma} B^{-1-2\gamma} \frac{1}{2Y} \frac{d}{dY}(\Psi_1 + \Psi_2),\] (49)

and inserting it in Eq. (45) we obtain

\[
\left(\alpha_0^{1+2\gamma} B^{2+2\gamma} Y^2 - E\right) (\Psi_1 + \Psi_2) + \frac{1}{2} \alpha_0^{-2\gamma} B^{-1-2\gamma} \frac{d}{dY} \left(\frac{1}{Y} \frac{d}{dY}(\Psi_1 + \Psi_2)\right) \sim 0.
\] (50)

In order to let each terms to be the same order in \(B, \eta\) should be

\[\eta = -\frac{3}{5}.\] (51)

Similarly, we obtain

\[\delta = -\frac{1}{5}\] (52)

in order to make all terms to be the same order in \(\alpha\), and we obtain

\[E \propto \alpha_0^{2\gamma} B^{2\gamma}.\] (53)

In Appendix we give a simpler derivation of Eq. (53).

This result is the same as the result obtained by the semiclassical quantization rule\(^{[11]}\), in which the energy is quantized as

\[A(E_n) \propto (n + \gamma) B,\] (54)

where \(\gamma\) is a phase factor \((\gamma = 1/2\) for 2D free electrons and semi-Dirac fermions and \(\gamma = 0\) for Dirac fermions and three-quarter Dirac fermions) and \(A(e)\) is the area of the Fermi surface in the 2D momentum space at \(B = 0\) with the Fermi energy \(e\), i.e.

\[\frac{dA(e)}{de} = D(e),\] (55)

where \(D(e)\) is a density of states. We plot \(A(e)\) and \(D(e)\) in Fig. 12. In the three-quarter Dirac case, we obtain

\[A(e) \propto \alpha_0^{-\frac{1}{2}} e^\frac{\gamma}{2},\] (56)

in the limit \(e \to 0\), and

\[\epsilon_n \propto \alpha_0^{2\gamma} (nB)^{\frac{\gamma}{2}}.\] (57)

### III. Finite Energy Gap and \(n = 0\) State

In this section we study the \(n = 0\) state by introducing the energy gap in the three-quarter Dirac point, which may be caused by a difference of the site energy in two sublattices.

\[\mathcal{H}_{tqD} = \mathcal{H}_{tqD} + \begin{pmatrix} \Delta & 0 \\ 0 & -\Delta \end{pmatrix}\] (58)

where \(2|\Delta|\) is the energy gap at the three-quarter Dirac point. Note that the minimum of the upper band is not at the three-quarter Dirac point \((q = 0)\) and the minimum energy of the upper band is not \(|\Delta|\). Then the equation we study at \(B \neq 0\) is

\[
\begin{pmatrix}
(\mathcal{H}_{tqD})_{11} + \Delta & (\mathcal{H}_{tqD})_{12} \\
(\mathcal{H}_{tqD})_{21} & (\mathcal{H}_{tqD})_{22} - \Delta
\end{pmatrix}
\begin{pmatrix}
\Psi_1(y) \\
\Psi_2(y)
\end{pmatrix}
= E
\begin{pmatrix}
\Psi_1(y) \\
\Psi_2(y)
\end{pmatrix}.
\] (59)

Although the energy dispersion at \(B = 0\) does not depend on the sign of \(\Delta\), the quantized energies at \(B \neq 0\) are not the same for \(\pm \Delta \neq 0\). We take \(\alpha_0 = \alpha_0'' = 0.01\) and \(B = 1\) and we calculate the wave functions numerically with the boundary condition at \(y = 20\), as in Section 11B. We plot the boundary condition \(\theta\) as a function of energy in Fig. 11. For \(\Delta \lesssim -0.1, \theta\) changes in a narrow region of \(E\), which indicate that an almost-localized state exists at \(y \lesssim 0\) as shown in Fig. 13(a) and (b), while the variation of \(\theta\) as a function of \(E\) becomes broad for \(\Delta \gtrsim -0.1\), which indicate that an almost-localized state does not exist at \(y \lesssim 0\) as shown in Fig. 13(c) and (d). We think that the eigenstate with \(n = 0\) does not exist when \(\Delta > 0\), but the almost-localized state exists at \(y \lesssim 0\) when \(\Delta \leq 0\). The effect of the tunneling would become important as \(\Delta\) approaches to zero and the almost-localized \(n = 0\) state at \(y \lesssim 0\) couples strongly to the continuous energy levels in \(y > 0\). This situation that the \(n = 0\) mode exists only when \(\Delta \leq 0\) is similar to the model studied by Haldane\(^{[17]}\), where the zero mode exists either upper band or lower band depending on the sign of the mass, which is \(\Delta\) in the present model, and the direction of the magnetic field. In our model the
FIG. 13. (Color online) Energy at $B = 0$ as a function of $q_x$ and $q_y$ with parameters $w_x = w_y = 1$, $\alpha_2 = \alpha_2' = 0.01$, and $\Delta = \pm 0.3$.

FIG. 14. (Color online) Boundary condition $\theta$ at $y = 20$ (Eq. (26)), which makes $|\Psi_{1,2}(y)| \to 0$ at $y \to -\infty$, as a function of the energy. We take parameters $w_x = w_y = 1$, $\alpha_2 = \alpha_2' = 0.01$, $\Delta = 0.3, 0.2, \cdots, -0.3, -0.4$, and $B = 1$.

nearly bound state with $n = 0$ exists when $\Delta \leq 0$. The $n = 0$ ($E = 0$) state at $\Delta = 0$ in Fig. 7(a) is understood as the zero-mode of the almost-localized state at three-quarter Dirac point, which couples strongly to the continuous states at $y \gtrless 0$. Note that the simultaneous changes of $B \leftrightarrow -B$, $y \leftrightarrow -y$, $\Psi_1 \leftrightarrow \Psi_2$, and $\Delta \leftrightarrow -\Delta$ do not change Eq. (59).

IV. SUMMARY

We study the quantized energy at the three-quarter Dirac point in the presence of external magnetic field $B$. We obtain that the quantized energy is proportional to $\alpha_2' (nB)^{\frac{1}{2}}$ (Eq. (10)) by calculating the solution of the differential equation (Eq. (19)) numerically. We also obtain the same result analytically in the limit of $B \to 0$ in Eq. (59), except the $n$-dependence. We have obtained the same result by using the semiclassical quantization rule [11]. We show that the zero mode exists by studying the finite gap system. The quantization of the energy in the three-quarter Dirac point in a magnetic field can be observed experimentally in quasi-two-dimensional organic superconductor $\alpha$-(BEDT-TTF)$_2$I$_3$ [11] and ultra cold Fermi gas on a tunable optical lattice [13].

Appendix: another derivation of $E \propto \alpha_2' B^{\frac{1}{2}}$

From Eq. (10), we formally obtain the equation

$$\det \begin{pmatrix} By + \alpha_2' (By)^2 - E & -By + \alpha_2'' (By)^2 - \frac{d}{dy} \\ -By + \alpha_2'' (By)^2 + \frac{d}{dy} & By + \alpha_2' (By)^2 - E \end{pmatrix} = 0$$

(A.1)

to get

$$E = By + \alpha_2' (By)^2 \pm \sqrt{(-By + \alpha_2'' (By)^2)^2 - \frac{d^2}{dy^2}}$$

(A.2)
The bound states in the upper band is obtained by taking the expansion

\[ |\alpha''|, \quad |\alpha| \ll 1, \quad (A.3) \]

\[ \left| \frac{d}{dy} \right| \ll |By|, \quad (A.4) \]

Then we obtain for \( y < 0 \),

\[ E \sim \alpha(By)^2 - \frac{1}{2By \ dy^2}. \quad (A.5) \]

Take a new variable \( Y \) as

\[ y = \alpha^2 B^n Y, \quad (A.6) \]

we obtain

\[ E \sim \alpha^2 \gamma(B^{2+2\eta}Y^2 - \frac{1}{2} \alpha^{-3\eta} B^{-1-3\eta} \frac{d^2}{dY^2}). \quad (A.7) \]

We take \( \eta \) and \( \delta \) in order to let two terms to be zero in the same order as \( B \) and \( \alpha \) become zero, i.e.,

\[ \delta = -\frac{1}{5}, \quad (A.8) \]

and

\[ \eta = -\frac{3}{5}. \quad (A.9) \]

We obtain

\[ E \sim \alpha^2 \gamma \left( Y^2 - \frac{1}{2Y} \frac{d^2}{dY^2} \right). \quad (A.10) \]

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