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Energy Spectrum of a Triangular Lattice in a Uniform Magnetic Field: Effect of Next-Nearest-Neighbor Hopping

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The energy spectrum of a triangular lattice in a uniform magnetic field is studied within the tight-binding approximation. The effect of next-nearest-neighbor (NNN) hopping on the energy spectrum is investigated in detail. Numerical calculations show that, when NNN hopping is turned on, most of the subband widths for a rational magnetic flux first decrease to certain critical values of NNN hopping, resulting in a very narrow band structure. Then, the widths increase with increasing NNN hopping strength, and the resultant energy spectrum shows a very complicated, fat band structure. These phenomena are explained by elucidating, in detail, the dependence of the subbands and the gaps on the NNN hopping strength. The symmetry of the energy spectrum in the presence of NNN hopping is also discussed.

I. INTRODUCTION

The problem of the energy spectrum of two-dimensional (2D) electrons in a magnetic field has attracted much interest for several decades in connection with various phenomena such as the quantum Hall effect [1], the flux-state model for high-T_c superconductivity [2], and the mean-field transition temperature of superconducting wire networks or Josephson junction arrays [3]. Recently, by means of the remarkable advent of nanofabrication techniques, studies to find indications of peculiar energy spectra and their effects on the transport and the optical properties have been extensively performed [4].

So far, a number of works have focused on a square lattice, and the energy spectrum of the lattice with isotropic hopping between nearest-neighbor (NN) sites is known to be characterized by Hofstadter's butterfly [5]. The effect of the anisotropy in NN hopping integrals on the energy spectrum has also been studied, and the anisotropy is found to generically lead to the occurrence of band broadening and gap closing [6] and to a dramatic enhancement of the anisotropy in the longitudinal conductivities [7]. Triggered by fascinating results for the square lattice, other works have taken into account various kinds of 2D lattices, including triangular [8-12], honeycomb [13], quasiperiodic [14], fractal [15] and rhombus [16] lattices, in order to investigate the effect of the lattice geometry on the energy spectrum. Among the various lattices, the most extensively studied example has been the triangular lattice, and the energy spectrum of the lattice with isotropic NN hopping is known to exhibit a recursive band structure as in the case of the square lattice [11]. Recently, the effect of NN hopping anisotropy on the energy spectrum was also studied to find behaviors similar to those seen in the case of the square lattice [12].

To date, most of the works studying the energy spectrum of 2D electrons have been performed within the simplest tight-binding (TB) model which only includes the NN hopping integral from the common sense point of view that the hopping integrals decrease exponentially with distance. However, since, to some degree, long-range correlations are inevitably present in every physical system, it may be worth studying the problem of the energy spectrum within a more realistic model that includes hopping terms beyond the NN hopping integral. For a square lattice, the effect of adding extra hopping terms beyond NN hopping has already been studied, and it was demonstrated that turning on next-nearest-neighbor (NNN) hopping not only lowers the symmetry of the energy spectrum but also removes a degeneracy at the band center of the energy spectrum [17]. However, to our knowledge, the effect of NNN hopping on the energy spectrum of a triangular lattice has not been studied yet, the reason for which seems to be in the supposition that results similar to those of the square lattice are expected. However, as we shall show below, the effect of NNN hopping on the energy spectrum of the triangular lattice is much more dramatic than it is in the case of the square lattice, and the resultant energy spectrum exhibits a very complicated and interesting band structure.

In this paper, we examine, in detail, the dependence of the energy spectrum of a triangular lattice on the NNN

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hopping strength. In Section II, a generalized Harper equation, which includes NNN hopping terms, as well as NN hopping terms, is derived. In Section III, numerical results for the effects of NNN hopping on the energy spectrum are presented. The symmetry of the energy spectrum in the presence of NNN hopping is also discussed in this section. Finally, Section IV is devoted to a summary.

II. THE TIGHT-BINDING EQUATION

We consider an electron on a 2D triangular lattice with hexagonal symmetry in the presence of a uniform magnetic field $\vec{B} = B\hat{z}$. Under the Landau gauge, the vector potential is given by $\vec{A} = (0, Bx, 0)$. The TB Hamiltonian is given by

$$H = \sum_{ij} t_{ij} \mathrm{e}^{i\theta_{ij}} |i\rangle\langle j|, \tag{1}$$

where t_{ij} is the hopping integral between sites i and j, $|i\rangle$ is a state of an atomic-like orbital centered at site i, and $\theta_{ij} = (2\pi/\phi_0)\int_i^j \vec{A}\cdot d\vec{l}$ is the magnetic phase factor, $\phi_0 = hc/e$ being the magnetic flux quantum. Let us denote the lattice point as (m, n), i.e., $(x, y) = (mb, nc)$, where $b = a/2$ and $c = \sqrt{3}a/2$, a being the lattice constant. Then, θ_{ij} can be written as

$$\theta_{ij} = \begin{cases} 0 & j = (m \pm 2, n) \\ \pm 2\pi\phi m & j = (m, n \pm 2) \\ \pm\pi\phi(m + 1/2) & j = (m + 1, n \pm 1) \\ \pm\pi\phi(m - 1/2) & j = (m - 1, n \pm 1) \\ \pm\pi\phi(m + 3/2) & j = (m + 3, n \pm 1) \\ \pm\pi\phi(m - 3/2) & j = (m - 3, n \pm 1) \end{cases} \tag{2}$$

where $i = (m, n)$ and $\phi = 2\sqrt{3}Bb^2/\phi_0$ is the magnetic flux through the unit cell. By means of Eqs. (1) and (2), the TB equation $H\psi_{m,n} = E\psi_{m,n}$ reads

$$\begin{aligned} E\psi_{m,n} = \; & t_a(\psi_{m-2,n} + \psi_{m+2,n}) + t'_b(\mathrm{e}^{i2\pi\phi m}\psi_{m,n-2} + \mathrm{e}^{-i2\pi\phi m}\psi_{m,n+2}) \\ & + t_b[\mathrm{e}^{i\pi\phi(m-1/2)}\psi_{m-1,n-1} + \mathrm{e}^{-i\pi\phi(m+1/2)}\psi_{m+1,n+1}] \\ & + t_c[\mathrm{e}^{i\pi\phi(m+1/2)}\psi_{m+1,n-1} + \mathrm{e}^{-i\pi\phi(m-1/2)}\psi_{m-1,n+1}] \\ & + t'_a[\mathrm{e}^{i\pi\phi(m-3/2)}\psi_{m-3,n-1} + \mathrm{e}^{-i\pi\phi(m+3/2)}\psi_{m+3,n+1}] \\ & + t'_c[\mathrm{e}^{i\pi\phi(m+3/2)}\psi_{m+3,n-1} + \mathrm{e}^{-i\pi\phi(m-3/2)}\psi_{m-3,n+1}], \end{aligned} \tag{3}$$

where t_a is the NN hopping integral along the x-direction, $t_{b(c)}$ is the NN hopping integral along the direction which makes an angle of $\pi/3$ ($2\pi/3$) with the x-direction, and $t'_{a(b,c)}$ is the NNN hopping integral along the direction which makes an angle of $\pi/6$ ($\pi/2$, $5\pi/6$) with the x-direction. For the sake of simplicity, we assume that both NN and NNN hoppings are isotropic; i.e., $t_a = t_b = t_c(\equiv t)$ and $t'_a = t'_b = t'_c(\equiv t')$.

Since y is cyclic under the Landau gauge, the wave function $\psi_{m,n}$ can be written as $\psi_{m,n} = \mathrm{e}^{ik_y nc}\varphi_m$. Thus, Eq. (3) can be reduced to a one-dimensional generalization of the Harper equation:

$$E\varphi_m = C_{m-2}\varphi_{m-3} + t\varphi_{m-2} + B_{m-1}\varphi_{m-1} + A_m\varphi_m + B_m\varphi_{m+1} + t\varphi_{m+2} + C_{m+1}\varphi_{m+3}, \tag{4}$$

where

$$A_m = 2t'\cos(2\pi\phi m - 2k_y c), \quad B_m = 2t\cos[\pi\phi(m - 1/2) - k_y c], \quad C_m = 2t'\cos[\pi\phi(m - 1/2) - k_y c]. \tag{5}$$

Denoting $\phi = p/q$ with mutual primes p and q, we have

$$A_{m+q} = A_m, \quad B_{m+M} = B_m, \quad C_{m+M} = C_m, \tag{6}$$

where $M = q$ ($2q$) for an even (odd) p. Thus, m in Eq. (4) satisfies the condition $1 \le m \le q$ ($1 \le m \le 2q$) for an even (odd) p, and the Bloch condition along the x-direction can be written as

$$\varphi_{m+M} = \mathrm{e}^{ik_x Mb}\varphi_m. \tag{7}$$

Using Eqs. (4) and (7), we obtain the eigenvalue equation $\mathbf{A}\psi = E\psi$, where $\psi^\dagger = (\varphi_1, \varphi_2, \cdots, \varphi_M)$ and

$$\mathbf{A} = \begin{pmatrix} A_1 & B_1 & t & C_2 & \cdots & C_{M-1}\mathrm{e}^{-i\delta} & t\mathrm{e}^{-i\delta} & B_M\mathrm{e}^{-i\delta} \\ B_1 & A_2 & B_2 & t & \cdots & 0 & C_M\mathrm{e}^{-i\delta} & t\mathrm{e}^{-i\delta} \\ t & B_2 & A_3 & B_3 & \cdots & 0 & 0 & C_1\mathrm{e}^{-i\delta} \\ C_2 & t & B_3 & A_4 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ C_{M-1}\mathrm{e}^{i\delta} & 0 & 0 & 0 & \cdots & A_{M-2} & B_{M-2} & t \\ t\mathrm{e}^{i\delta} & C_M\mathrm{e}^{i\delta} & 0 & 0 & \cdots & B_{M-2} & A_{M-1} & B_{M-1} \\ B_M\mathrm{e}^{i\delta} & t\mathrm{e}^{i\delta} & C_1\mathrm{e}^{i\delta} & 0 & \cdots & t & B_{M-1} & A_M \end{pmatrix} \quad (8)$$

with $\delta = k_x qa/2$ ($k_x qa$) for an even (odd) p. By diagonalizing Eq. (8), we can obtain M energy eigenvalues for a given $\vec{k}$, as well as the full energy spectrum by sweeping all the $\vec{k}$-points in the magnetic Brillouin zone (MBZ).

III. NUMERICAL RESULTS AND DISCUSSION

Figure 1 shows the energy eigenvalues as a function of ϕ in the absence of NNN hopping, which is consistent with the result of Claro and Wannier [11]. Figures 2(a) – 2(d) show the results in the presence of NNN hopping. In our calculation, we took $\phi = p/199$ ($1 \le p \le 198$). Note that the width of every subband for the rationals ϕ considered in the calculation is so narrow that we only considered $\vec{k} = 0$ instead of scanning all the $\vec{k}$-points in the MBZ. Comparison of Fig. 2 with Fig. 1 shows several interesting features. First, the fractal structure of the energy eigenvalues survives despite introducing NNN hopping, which may be attributed to the isotropy of the hopping integrals. Second, though the bandwidths for $\phi = 0$ and 1 increase monotonically with increasing t', those for other rationals ϕ are so sensitive to t' that the $E-\phi$ diagram exhibits a very complicated structure that depends on t'; the $E-\phi$ diagram for a small (large) value of t' exhibits a narrow (fat) band structure. We explain these interesting phenomena below in more detail. Third, introducing NNN hopping leads to the occurrence of subband crossings in some regions of ϕ; see, for example, the regions of $\phi \le 1/10$ and $\phi \ge 9/10$ in Figs. 2(b) – 2(d) and the region near $\phi = 1/2$ in Fig. 2(d), where the breaking of the 'continuity of a gap boundary' can be seen. This phenomenon is expected to make it difficult to label the gaps divided by the 'crossed' subband lines by using a unique Hall coefficient [9,17]. Since the calculation of the Hall conductance is beyond the scope of this paper, we omit further discussion on the Hall conductance.

Figure 2 shows that the largest gap boundary, which runs from left to right in a downward slope in Fig. 1,

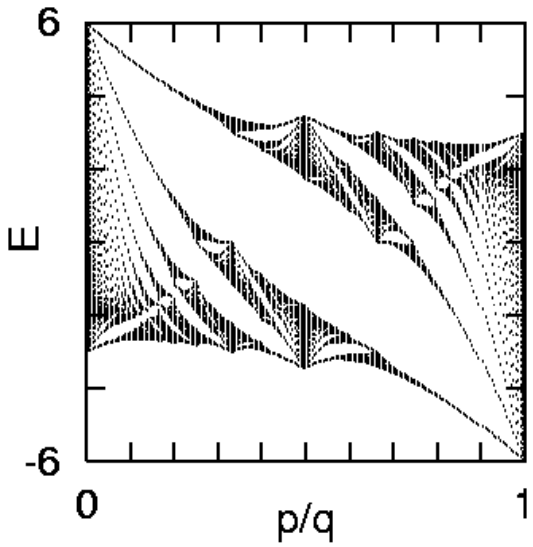

Fig. 1. Energy eigenvalues versus $\phi = p/q$ for a lattice with $t = 1$ and $t' = 0$.

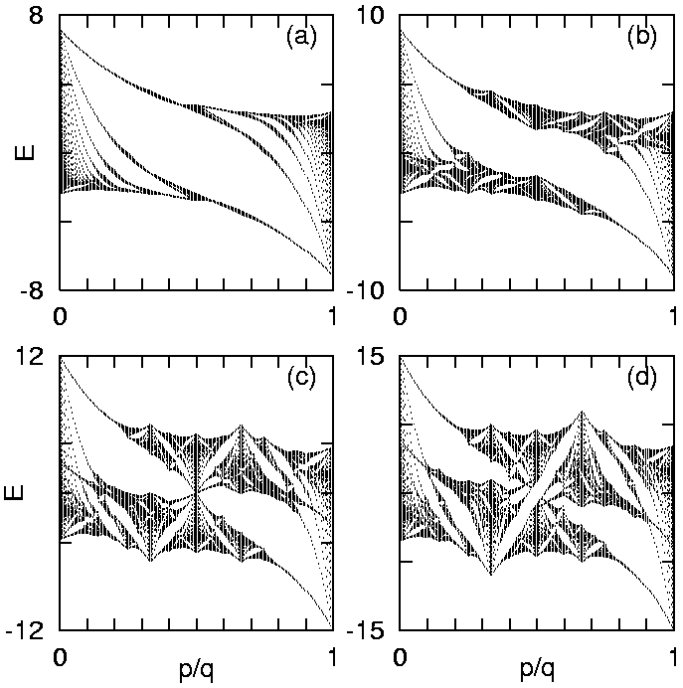

Fig. 2. Energy eigenvalues versus ϕ for a lattice with $t = 1$ and (a) $t' = 0.2$, (b) $t' = 0.5$, (c) $t' = 1.0$, and (d) $t' = 1.2$.

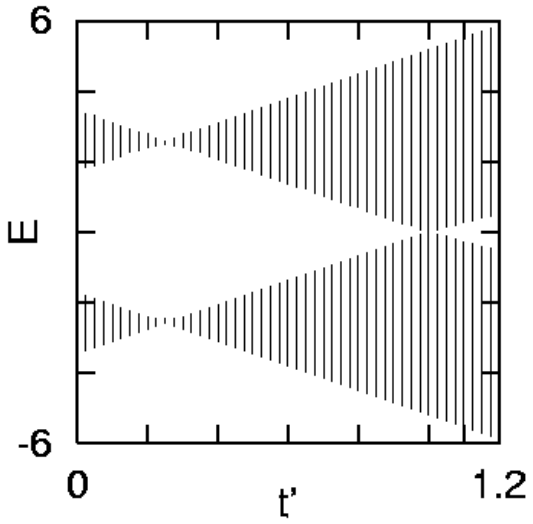

Fig. 3. Energy eigenvalues as a function of t' for $\phi = 1/2$ with $t = 1$.

exhibits a very sensitive t' dependence. To demonstrate this explicitly, we plot in Fig. 3 the energy spectrum for $\phi = 1/2$ as a function of t', where two critical values of t' appear, one at $t'_{c1} = 0.25$ and the other at $t'_{c2} = 1$. The width of the gap increases with increasing t' up to t'_{c1}, and then decreases up to t'_{c2} so that it closes at t'_{c2}. Then, the gap reopens and increases again for $t' > t'_{c2}$. Note that the occurrence of a subband touching (or a gap closing) at $E = 0$ when $t' = t_{c2}$ (i.e., $t' = t$) is a feature that is distinct from the case of the square lattice where NNN hopping removes the subband touching at $E = 0$ for even values of q [17].

The energy spectra for $\phi = 1/3$ and $2/3$ also exhibit an interesting t' dependence. In these cases, there are three subbands and two gaps at $t' = 0$. When t' is turned on, the widths of the subbands decrease up to a certain value of t' [Figs. 2(a) – 2(b)], and then increase so that the widths of the two gaps decrease [Figs. 2(c) – 2(d)] for large values of t'. This kind of t' dependence of the gaps leads us to expect that the energy spectra for $\phi = 1/3$ and $\phi = 2/3$ will exhibit gapless single-band structures in the limit of $t'/t \to \infty$. Besides, the lowest (highest) subband edge for $\phi = 1/3$ $(2/3)$ is expected to go downward (upward) with increasing t' so that $E_l(\phi = 1/3) = E_l(\phi = 1)$ $[E_h(\phi = 2/3) = E_h(\phi = 0)]$ in this limit, where $E_{l(h)}$ means the lowest (highest) subband edge. As a result, the periodicity of the $E - \phi$ diagram in this limit will be reduced by a factor of 3 in ϕ. Figure 4 shows the $E - \phi$ diagram for a lattice with $t = 0$ and $t' = 1$, which confirms our expectation. Note that Fig. 4 is just the $E - \phi$ diagram for a lattice with an isotropic hopping integral ($t' = 1$) and a lattice constant $\sqrt{3}a$. To illustrate the t' dependence of the energy spectra for other rationals ϕ, we plot in Fig. 5 the energy spectra for $\phi = 1/7$ and $\phi = 2/7$ as functions of t', where the phenomena of subband shrinking and broadening, gap closing and reopening, and subband touching are clearly seen. We observed these phenomena for all other rationals ϕ we considered.

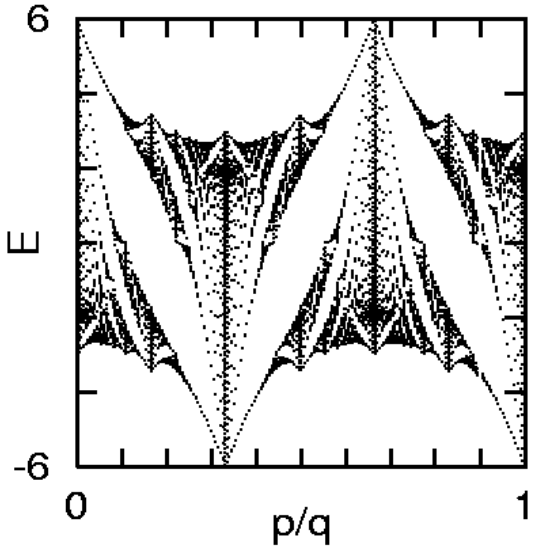

Fig. 4. Energy eigenvalues versus ϕ for $t = 0$ and $t' = 1$.

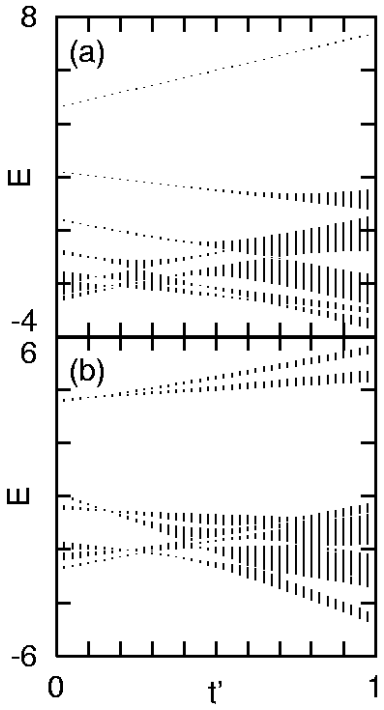

Fig. 5. Energy eigenvalues as a function of t' for (a) $\phi = 1/7$ and (b) $\phi = 2/7$ with $t = 1$.

From now on, let us discuss the reason for the narrow (fat) band structures exhibited in Fig. 2. The complicated, fat structure [Figs. 2(c) – 2(d)] can be easily understood by keeping in mind that the energy spectra for $t \gg t'$ resemble those in Fig. 1 while the spectra for $t \ll t'$ resemble those in Fig. 4, except for the energy

scale. Meanwhile, when t and t' are comparable with each other, the resultant energy spectrum is a mixture of the two energy spectra in Figs. 1 and 4, resulting in spectra as in Figs. 2(c) – 2(d). The t' dependence of the subband widths in Figs. 3 and 5 gives a clue for understanding the narrow structure [Fig. 2(a)]. We can see that, when t' is turned on, most of the subbands first decrease to certain critical values t'_c, and then increase beyond t'_c. We checked that most of the subbands for generic rationals ϕ exhibit a decreasing behavior for small values of t'. As a result, the energy spectrum for a small value of t' exhibits a very narrow band structure as in Fig. 2(a), which is a remarkable feature that was not observed in the case of the square lattice with NNN hopping. This means that introducing NNN hopping leads to a more complicated lattice effect than that for the case of the square lattice [18]. Note that t'_c differs for every subband, even for a given rational ϕ, and there seems to be no universal criterion for t'_c. Note also the fact that, though the widths of the subbands, for example, in Fig. 3 become minimal at $t = t'_{c1}$, they are still nonzero and dispersive. We also checked this behavior for other rationals ϕ, which implies that all Aharonov-Bohm cages [16] remain unbounded even in the presence of NNN hopping, which in turn indicates that the localization properties of the eigenstates are insensitive to NNN hopping.

We are now in position to discuss the symmetry of the energy spectrum in the presence of NNN hopping. Denoting a set of energy eigenvalues for a given $\vec{k}$ as $E(\phi;\vec{k})$ and the full energy spectrum taking into account all the $\vec{k}$-points in the MBZ as $E(\phi)$, we observe the following properties for generic rationals ϕ: (i) $E(\phi;\vec{k}) = E(\phi;-\vec{k})$, which can be easily checked in Eq. (8); $\mathbf{A} \rightarrow \mathbf{A}^{\dagger}$ under the transformation $\vec{k} \rightarrow -\vec{k}$. (ii) $E(\phi) = E(-\phi)$, which implies that there is no way for a 2D Bloch electron to discern the direction of the magnetic field. (iii) $E(\phi) = -E(1-\phi)$ with $0 \leq \phi \leq 1/2$. (iv) $E(\phi) = E(\phi+2)$. Figure 2 shows that properties (iii) and (iv) hold except for the case of $t'/t \rightarrow \infty$; in this case, they should be replaced by $E(\phi) = -E(1/3-\phi)$ with $0 \leq \phi \leq 1/6$ and $E(\phi) = E(\phi+2/3)$, as can be seen in Fig. 4. Properties (i) – (iv) indicate that the symmetry of the energy spectrum is insensitive to introducing NNN hopping, unlike in the case of the square lattice.

IV. SUMMARY

The effect of NNN hopping on the energy spectrum of an electron in a triangular lattice subject to a uniform magnetic field was studied within the TB approximation. The energy spectrum was found to change drastically with the introduction of NNN hopping; the phenomena of subband shrinking and broadening, gap closing and reopening, and subband crossing were observed by turning on NNN hopping. The dependence of the widths of the subbands and the subgaps on the NNN hopping strength was illustrated in detail, and the symmetry of the energy spectrum was also discussed. For better physical insight into the energy spectrum of the triangular lattice, it may be worth studying the effects of, for example, nonuniform magnetic fields [12,19], interband correlations [20], and electron-electron interactions [21].

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