Stabilization of flux states on two-dimensional lattices

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The total energy of two-dimensional electrons in a uniform magnetic field is systematically calculated for the square lattice, the triangular lattice, and the honeycomb lattice for various ratios of transfer integrals. It has many cusps as a function of the magnetic field at which the Fermi energy jumps across a gap. For a fixed electron density, the lowest energy with respect to the magnetic field (including the zero-field case) is realized when the magnetic field gives one flux unit per electron in agreement with the proposal of Hasegawa, Lederer, Rice, and Wiegmann [Phys. Rev. Lett. **63**, 907 (1989)]. The density of states is calculated analytically for the square lattice. The anyon lattice gas, which obeys fractional statistics, is discussed. In the mean-field treatment of the flux, the boson gas has the lowest energy.

I. INTRODUCTION

The spectrum of tight-binding electrons on the square lattice in a magnetic field¹ has an extremely rich structure as shown by Hofstadter² and Wannier.³ When the magnetic flux ϕ (in units of ch/e) through a plaquette is a rational number p/q (p and q being mutually prime integers), the spectrum has q subbands. The *r*th gap from the bottom can be labeled by two integers s_r and t_r which are related to p, q, and r by a Diophantine equation³

$$r = qs_r + pt_r , \qquad (1.1)$$

with $|t_r| \leq q/2$. The Hall conductance where the Fermi energy is in the gap is given by $\sigma_{xy} = (e^2/h)t_r$, thus it is quantized.^{4,5} The integer has a topological origin.^{6,7} It is the Chern number of a fiber bundle which is defined by the wave functions on a two-torus, the reciprocal space of this problem.

Recently, there has been a renewal of interest on this subject because this spectrum has been shown to be related to the ground-state energy of a mean-field theory of the *t-J* model.⁸⁻¹⁰ This connection is also studied numerically.^{11,12} Hasegawa, Lederer, Rice, and Wiegmann¹³ studied the stability of the state with respect to the magnetic field. From the results on a few rational values of $\phi = p/q$ (q = 2, 3, 4, 6, and 8), they argue that, if the number of electrons per site v is fixed, the total kinetic energy of the electrons has an absolute minimum when $\phi = v$, i.e., one flux per electron. This is an important and interesting result especially in relation to the flux state model for high-temperature superconductivity.¹⁴⁻¹⁸

A preliminary work¹⁹ has shown that this minimum is cusplike and that other cusplike local minima exist whenever the Fermi energy is in a gap, that is, $v=r/q=s_r+\phi t_r$. In the low-density limit, the local minimum at $v=t_r\phi$ ($s_r=0$, $t_r>0$) correspond to filled Landau levels of a continuum system. The other gaps are due to the commensurability between the lattice periodicity and the magnetic field.

The isotropic case (isotropy of the transfer integrals) is known to be a special case.²⁰⁻²³ For irrational flux, the total bandwidth of the spectrum is zero which implies a singular continuous spectrum.

In this paper we study the spectrum both in the isotropic case and in the anisotropic case which has not been analyzed in detail.^{24,25} This study may be relevant to various physical interesting problems: quasi-onedimensional conductors in a magnetic field or anisotropic high- T_c superconductors to which an anisotropic *t-J* model would apply. We calculate analytically the density of states (DOS).

We also calculate the total energies on the triangular and honeycomb lattices. The lattices which are topologically equivalent to these lattices are obtained from the square lattice by adding bonds (triangular lattice) or removing bonds (honeycomb lattice).

II. SPECTRUM OF THE SQUARE LATTICE

The two-dimensional tight-binding Hamiltonian on the square lattice in a magnetic field

$$H = -\sum_{i,j} t_{ij} c_j^{\dagger} c_i e^{i2\pi\phi_{ij}} , \qquad (2.1)$$

where *i* and *j* are nearest-neighbor sites and c_i (c_j^{\dagger}) is a fermion annihilation (creation) operator at site *i* (*j*). The phase factor is given by the line integral of the vector potential as

$$\phi_{ij} = \frac{e}{ch} \int_1^j \mathbf{A} \cdot \mathbf{d}l \; \; .$$







FIG. 1. Energy spectra for two-dimensional tight-binding electrons in uniform magnetic flux $\phi = p/307$. The dashed lines are Fermi energies for densities $v = \frac{51}{307}$, $\frac{102}{307}$, $\frac{154}{307}$, $\frac{205}{307}$, and $\frac{256}{307}$ which are approximations for $\frac{1}{6}$, $\frac{1}{3}$, $\frac{1}{2}$, $\frac{2}{3}$, and $\frac{5}{6}$, respectively. The large gaps are labeled by sets of integers (s_r, t_r) [see (1.1)]. (a) $t_a = t_b = 1$. (b) $t_a = 2$ and $t_b = 1$. (c) $t_a = 10$ and $t_b = 1$.

If the Landau gauge $\mathbf{A} = (0, Bx, 0)$, is used, the wave function is written

$$\psi_{nm}(k_x,k_y) = \psi_n(k_x,k_y)e^{ik_xn + ik_ym}$$

where n and m are integers representing x and y coordinates of the square lattice, respectively. The Schrödinger equation

$$H|\psi\rangle = E|\psi\rangle \quad \left\{ |\psi\rangle = \sum_{n,m} \psi_{nm}(k_x,k_y)c_{nm}^{\dagger}|0\rangle \right\}$$

$$E(k_{x},k_{y})\psi_{n} = -2t_{b}\cos(k_{y}+2\pi n\phi)\psi_{n}$$
$$-t_{a}(e^{ik_{x}}\psi_{n-1}+e^{-ik_{x}}\psi_{n+1}). \qquad (2.2)$$

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For a rational flux $\phi = p/q$, we have $\psi_{n+q} = \psi_n$, and

$$\{\mathbf{k} | 0 \leq k_x < 2\pi/q, 0 \leq k_v < 2\pi\}$$

0

 M_{q-} $-t_{a}e$

.

 $-t_a e^{ik_x}$

is the magnetic Brillouin zone which is reduced due to the effect of the magnetic field (see, for example, Ref. 26). This equation can be regarded as a one-dimensional tight-binding model with on-diagonal modulation.²⁷ The secular equation for this linear system is

 $-t_a e^{ik_x}$

$$F_{p/q}(E,k_x,k_y) = \det \begin{pmatrix} M_1 & -t_a e^{-ik_x} & 0 & \cdots \\ -t_a e^{ik_x} & M_2 & -t_a e^{-ik_x} & \cdots \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots \\ -t_a e^{-ik_x} & 0 & 0 & \cdots \end{pmatrix}$$

$$\begin{bmatrix} 0 \\ \vdots \\ 1 & -t_a e^{-ik_x} \\ ik_x & M_q \end{bmatrix} = 0 , \qquad (2.3)$$

where

$$M_n = -2t_b \cos(k_v + 2\pi n \phi) - E \quad . \tag{2.4}$$

Since (2.3) is of *q*th order, the spectrum of the original two-dimensional (2D) problem has *q* bands. Each band is *q*-fold degenerate since

$$E(k_x, k_v + 2\pi j/q) = E(k_x, k_v)$$

 $(j=1,2,\ldots,q-1)$ as seen from (2.2). Here it is straightforward to see the structure

$$F_{p/q}(E,k_x,k_y) = F_{p/q}(E,0,k_y) - 2t_a^q [\cos(qk_x) - 1] .$$

By duality $k_x \leftrightarrow k_v$, $t_a \leftrightarrow t_b$ we obtain,

$$F_{p/q}(E,k_x,k_y) = F_{p/q}(E,0,0) + 2(t_a^q + t_b^q) - \alpha_q ,$$

where

$$\alpha_q = 2t_a^q \cos qk_x + 2t_b^q \cos qk_y \ . \tag{2.5}$$

The eigenvalue equation now takes a simple form

$$G(E) \equiv F_{p/q}(E,0,0) + 2(t_a^q + t_b^q) = \alpha_q . \qquad (2.6)$$

The spectra for several values of anisotropy ratio $(t_b/t_a=1, 0.5, \text{ and } 0.1)$ are shown in Fig. 1. The spectrum is unchanged when ϕ is shifted by an integer since $2\pi\phi$ appears as a phase factor in (2.1). This symmetry is more easily seen from (2.2). The spectrum is also invariant under a reversal of the magnetic field, i.e., $\phi \rightarrow -\phi$. Therefore, it is enough to show the spectra for $0 \le \phi \le \frac{1}{2}$. The spectrum for $\frac{1}{2} \le \phi \le 1$ is obtained by the symmetry

 $\phi \rightarrow 1 - \phi$. Also, it is shown from (2.3) that the spectrum is symmetric with respect E = 0.

III. DENSITY OF STATES OF THE SQUARE LATTICE

From (2.6), one can write the DOS $\rho(E)$ as

$$\rho(E) = \rho_G \left| \frac{dG}{dE} \right| , \qquad (3.1)$$

where the associated density of states ρ_G is defined by

$$\rho_G dG = \frac{d^2 k}{\left(2\pi\right)^2} \ . \tag{3.2}$$

For the isotropic case, it is given analytically as

$$\rho_G = \frac{1}{2\pi^2 q t^8} K' \left[\frac{G}{4} \right] , \qquad (3.3)$$

where $K'(k) = K[(1-k^2)^{1/2}]$ and K is the complete elliptic integral of the first kind.³ The DOS for $\phi = p/q$ thus has q bands with a pagoda shape which is characteristic of the 2D electron gas on the square lattice. There is a Van Hove singularity (logarithmic divergence) at each half-filled subband. See Fig. 2. The linear variation $\rho(E) \propto E$ near E = 0 when q is even corresponds to the zero mode described by Kohmoto²⁶ and Wen and Zee.²⁸

When anisotropy is introduced, each Van Hove singularity is split into two singularities [for $\phi=0$ the separation is $4(t_a-t_b)$ in energy]. The associated density of

ratio t_b/t_a .



FIG. 2. The DOS for isotropic cases. (a) $\phi = \frac{1}{3}$. (b) $\phi = \frac{1}{8}$.



FIG. 3. The DOS for anisotropic cases when $\phi = \frac{1}{4}$. (a) $t_b / t_a = 0.7$. (b) $t_b / t_a = 0.1$.

states ρ_G is still known analytically²⁹ so that one can deduce the DOS as

$$\rho(E) = \frac{1}{2\pi^2 q (t_a \gamma^{1/2})^q} \left| \frac{dG}{dE} \right| \beta(G) , \qquad (3.4)$$

with

β

$$(G) = K \left[\left(\frac{(\gamma+1)^2 - x^2}{4\gamma} \right)^{1/2} \right] \text{ for } |G| < 2(1-\gamma)t_a ,$$

$$= K \left\{ \left[\frac{\gamma+1}{2\sqrt{\gamma}} \left(1 - \frac{x^2}{(\gamma+1)^2 t^2} \right)^{1/2} \right] \right\}$$

$$\text{ for } 2(1-\gamma)t_a < |G| < 2(1+\gamma)t_a , \quad (3.5)$$

where $x = G/(2t_a)$. The DOS is plotted in Fig. 3 for $\phi = \frac{1}{4}$ and $t_b/t_a = 0.7$ and 0.1. When t_b/t_a is small, the DOS evolves toward the 1D DOS, although the logarithmic Van Hove singularities always remain unless $t_b = 0$.

IV. TOTAL ENERGY

In this section, we study the total energy of electrons for a fixed density as a function of the magnetic flux ϕ for the square, the triangular, and the honeycomb lattices. The total energy per particle will be denoted by $E_T(\phi)$. When varied continuously, ϕ is irrational almost everywhere and the spectrum consists of infinitely many subbands with zero widths (Cantor set). In numerical calculation, however, we can handle only rational points $\phi = p/q$, so we take large values of q to deduce the behavior $E_T(\phi)$. For a large value of q each subband is narrow and we can approximate the DOS by δ functions with a weight 1/q'

$$\rho(E) = \frac{1}{q'} \sum_{n=1}^{q'} \delta(E - E_n) , \qquad (4.1)$$

where q' is the number of subbands (which is equal to q for the square lattice) and E_n is the center of *n*th band. Since the total width of the subbands is of the order 1/q for the isotropic square lattice,²¹ we get the total energy very accurately when q > 10. For an anisotropic transfer integral case of the square lattice, however, the sum of the bandwidths is nonzero as q goes to infinity although each bandwidth approaches zero. Therefore, the δ -function approximation for the DOS is less accurate. We must take a much larger q to get an accurate result.

A. Square lattice

We set q to a large prime number 307 and vary p from 1 to (q-1)/2=153. The spectra are shown in Fig. 1 together with the Fermi energies for fixed electron densities. The corresponding total energy per particle E_T is shown in Fig. 4. From these data for the rational points, one can expect that E_T is a continuous function of ϕ . We also calculated the total energy for several values of rational ϕ whose q is not 307 (note that if ϕ is continuously changed, p and q vary wildly). The total energy is always



FIG. 4. Total energies per particle for fixed densities $v = \frac{51}{307}, \frac{102}{307}, \frac{154}{307}, \frac{205}{307}$, and $\frac{256}{307}$ (from bottom to top) which are approximations for $\frac{1}{6}, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}$, and $\frac{5}{6}$, respectively. The corresponding Fermi energies are shown in Fig. 1. Typical cusps observed in the figures are labeled by (s_r, t_r) . (a) $t_a = t_b = 1$. (b) $t_a = 2$ and $t_b = 1$. (c) $t_a = 10$ and $t_b = 1$.



FIG. 5. Total energy per electron at densities ν $(\frac{1}{307}, \frac{3}{307}, \frac{5}{307}, \dots, \frac{305}{307})$ for the isotropic square lattice.

in between the two energies of the two nearby points of ϕ with q = 307. This supports that $E_T(\phi)$ is continuous. Figure 4 clearly shows that the total energy has a cusp (local minimum) at the position where the Fermi energy jumps across a gap. Thus, a cusp is labeled by s_r and $t_r = h/e^2 \sigma_{xy}$ which are given in Fig. 4. For an irrational ϕ , the spectrum is a Cantor set, namely the gaps are dense.² Since ϕ is almost always irrational, we expect that $E_T(\phi)$ has cusps everywhere and is nondifferentiable. The cusps get less pronounced as the anisotropy is increased.

In the cases shown above, the lowest energy state is realized for $\phi = v$ ($s_t = 0$, $t_r = h/e^2\sigma_{xy} = 1$) and $\phi = 1 - v$ ($s_r = 1$, $t_r = h/e^2\sigma_{xy} = -1$), which has the same spectrum as for $\phi = v$. In Fig. 5, $E_T(\phi)$ for other values of v ($\frac{1}{307}$, $\frac{3}{307}$, $\frac{5}{307}$, ..., $\frac{305}{307}$) for the isotropic case are shown. It can be seen that the lowest energy is always realized when $\phi = v$. We believe that this result holds for all the values of v including irrational fillings.

B. Triangular lattice

Let us add bonds with transfer integrals t_c between next-nearest-neighbor sites of the square lattice in only one direction as shown in Fig. 6(a). Since this lattice is topologically equivalent (namely, it can be continuously deformed) to the triangular lattice, the electronic properties are the same as those for the triangular lattice. We consider this lattice and use the same Landau gauge as for the square lattice. So the new bonds between (n,m)and (n+1,m+1) gets a phase $\exp\{i(2n+1)\pi\phi\}$. Here,



FIG. 6. (a) A lattice which is topologically equivalent to the triangular lattice. (b) When the bonds which have a transfer integral t_b is removed from this square lattice, it becomes topologically equivalent to the honeycomb lattice.

 ϕ is the flux per square, and the flux per triangular plaquette is $\phi/2$. The energy spectrum for a rational flux $\phi = p/q$ is obtained by the secular equation of a $q \times q$ matrix:

$$\det \begin{vmatrix} N_1 & A_1 & 0 & \cdots & 0 & A_q^* \\ A_1^* & N_2 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & A_{q-2}^* & N_{q-1} & A_{q-1} \\ A_q & 0 & 0 & \cdots & A_{q-1}^* & N_q \end{vmatrix} = 0, \quad (4.2)$$

where

$$N_n = -2t_b \cos(k_v + 2\pi n\phi) - E \tag{4.3}$$

and

$$A_n = -t_a e^{ik_x} - t_c e^{i(k_x + k_y)} e^{i\pi(2n+1)\phi} .$$
 (4.4)

The total energy per particle for $v = \frac{25}{151}$ ($\approx \frac{1}{6}$) is plotted in Fig. 7 for $t_a = t_b = 1$ and $t_c / t_a = 0$, 0.5, and 1. The flux per a unit cell (triangle) is now $\phi/2$, so the spectrum is invariant when ϕ is shifted by an even integer. Therefore, the degeneracy between $\phi = v$ and 1 - v for the square lattice is lifted by taking a finite t_c and the absolute minimum of the total energy is obtained at $\phi = v$. The triangular lattice with uniform transfer integrals is realized when $t_c / t_a = 1$.



FIG. 7. Total energies per particle for fixed densities $v = \frac{1}{6}$. Line *a*: honeycomb lattice, namely, $t_a = t_b = t'_a = 1t'_b = 0$ in Fig. 6(b). Line *b*: $t_a = t_b = t'_a = 1t'_b/t_a = 0.5$. Line *c*: square lattice with $t_a = t_b = 1$. Line *d*: the triangular lattice in Fig. 6(a) with $t_a = t_b = 1$ and $t_c/t_a = 0.5$. Line *e*: the triangular lattice in Fig. 6(a) with $t_a = t_b = t_c = 1$.

C. Honeycomb lattice

Let us consider transfer integrals t_a , t_a' , t_b , and t_b' at the bonds on the square lattice as shown in Fig. 6(b). Note that a lattice which is topologically equivalent to the honeycomb lattice is obtained from the square lattice by removing the bonds which have a transfer integral t_b' . When a gauge $\mathbf{A} = [0, \phi(x + y), 0]$ is chosen, the wave function may be written as

$$\psi_{nm}(k_1,k_2) = e^{i(k_1n+k_2m)} \widetilde{\psi}_{n+m}(k_1,k_2) .$$

Then the secular equation for the energy spectrum is

$$\det \begin{vmatrix} -E_1 & B_1 & 0 & \cdots & 0 & B''_m \\ B_1^* & -E & B'_1 & \cdots & 0 & 0 \\ 0 & B'_1^* & -E & & & \\ \vdots & \vdots & \vdots & & & \vdots \\ 0 & 0 & 0 & \cdots & B'_{m-1} & -E & B_m \\ B'_m & 0 & 0 & \cdots & 0 & B_m^* & -E \end{vmatrix} = 0 ,$$

$$(4.5)$$

where
$$m = q/2$$
 for q even, $m = q$ for q odd,

$$B_{n} = -t_{a}e^{ik_{x}} - t_{b}e^{ik_{y}}e^{i4\pi n\phi}$$
(4.6)

$$B'_{n} = -t'_{a}e^{ik_{x}} - t'_{b}e^{ik_{y}}e^{i2\pi(2n+1)\phi} . \qquad (4.7)$$

The energy per particle for $t_a = t_b = t'_a = 1$, $t'_b / t_a = 0$, 0.5, 1, and $v \approx \frac{1}{6}$ is plotted in Fig. 7. When $t'_b = 0$, we have the spectrum for the honeycomb lattice with uniform transfer integrals. Note that the unit cell is doubled and the flux per unit cell is 2ϕ . Thus, the spectrum is unchanged when ϕ is shifted by an integer or a half integer. The absolute minimum is obtained at $\phi = \frac{1}{2} - v$, v, 1 - v, $\frac{1}{2} + v$. Note that all these minima are related to $\phi = v$ by the symmetries.

V. ANYON ON THE LATTICE

It is worthwhile to comment on the problem of anyons. In two dimensions, statistics for quantum-mechanical particles can be exotic and characterized by the braid group.^{30,31} If two particles are interchanged, the wave function gains a phase factor $e^{i\theta}$. Bosons have $\theta=0$ and fermions have $\theta=\pi$. For other values of θ , the statistics is called θ fractional statistics. The system obeying this θ fractional statistics has been recently studied by the several authors¹⁴⁻¹⁸ in relation to high-temperature superconductivity. In this paper, we follow the conventional notation³⁰ and consider an anyon obeying θ statistics to be a fermion with a confined flux attached to it.

The Hamiltonian of a free-anyon gas in continuous space is written

$$H = \frac{1}{2m} \sum_{i} (\mathbf{p}_i - \mathbf{a}_i)^2 , \qquad (5.1)$$

where \mathbf{a}_i is a statistical vector potential of the *i*th particle defined by

$$\mathbf{a}_{i} = \left[1 - \frac{\theta}{\pi}\right] \sum_{j \neq i} \frac{\mathbf{\hat{z}} \times (\mathbf{r}_{i} - \mathbf{r}_{j})}{|\mathbf{r}_{i} - \mathbf{r}_{j}|^{2}} .$$
(5.2)

The ground state of this anyon gas is speculated to be superconductive. $^{8-17}$

Let us define anyons on the square lattice.^{32,33} If a flux of $\overline{\theta}/2\pi$ goes through an adjacent plaquette of a fermion, the particle with the flux obeys θ statistics with $\theta = \pi - \overline{\theta}$. Let us consider a string which starts from the plaquette and extends to $x = \infty$ (see Fig. 8). For a bond which



FIG. 8. Definition of anyons on the lattice.

and

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crosses the string, we assign a phase. The Hamiltonian for free anyons on the square lattice is thus written

$$H = -t \sum_{\langle ij \rangle} c_j^{\dagger} e^{-i\theta_{ij}} c_i , \qquad (5.3)$$

where the summation is over the nearest-neighbor sites and θ_{ij} is $\overline{\theta}$ multiplied by the number of strings which cross the bond (ij).

In the following we average these strings in the spirit of the mean-field approximation. $^{14-16}$ We want to replace the system of anyons by the fermion system with a uniform magnetic flux ϕ . If an anyon moves around another anyon anticlockwise, the wave function changes the phase by $2\overline{\theta}$. This is easily seen from the string configuration in Fig. 8. Thus, if an anyon moves around an area S, the wave function gets a phase $2\overline{\theta}vS$ on the average, where v is the density of the anyons. In order to get the same phase change by a fermion system with a uniform flux, the flux is $\phi = \overline{\theta} v / \pi$. If we write $\theta = \pi(1-1/n)$, we have $\overline{\theta} = \pi/n$ and $\phi = \nu/n$. When n is an integer, the Fermi energy is in a gap with $s_r = 0$ and $t_r = h/e^2 \sigma_{xy} = n$. So the total energy has a local minimum as a function of n (or equivalently θ) at an integer value of n. As shown in Sec. II, the absolute minimum energy state is realized when $v = \phi$, namely, n = 1. This corresponds to a boson system. The local minimum value increases as an integer n is increased. In the low-density limit, the lattice system corresponds to a continuum system, where n Landau levels are filled. The fermion system is given by $n = \infty$.

Until now we have considered spinless particles, i.e., only one species for anyon and electron. Here, we take into account the internal degree of freedom for both electrons and anyons. If we consider two species of anyons and electrons, then the absolute minimum of the electrons is obtained at $v=2\phi$, because in this case $v=v_1+v_2$ and the absolute minimum is realized at $v_1=v_2=\phi$, where v_1 and v_2 are the densities of each species of particles. This absolute minimum corresponds to anyon system with n = 2, i.e., semion, which was argued to be relevant to the high- T_c superconductivity by Laughlin.¹¹

VI. SUMMARY

We studied numerically noninteracting electrons on two-dimensional lattices (square, triangular, and honeycomb lattices) in a uniform magnetic field. The triangular lattice is obtained from the square lattice by introducing next-nearest bonds as shown in Fig. 6(a). The honeycomb lattice is obtained by removing bonds from the square lattice as shown in Fig. 6(b). Thus, these lattices are transformed continuously by each other. We fixed particle density v and calculated the total energy per particle E_T as a function of flux per square cell ϕ . The function $E_T(\phi)$ is continuous but has cusps everywhere. These cusps correspond to a point where the Fermi energy jumps across a gap. For all cases we examined (square, triangular, and honeycomb lattices with a various ratio of the transfer integrals), the minimum of E_T occurs when $\phi = v$, namely one flux per electron.

Anyons on the lattice are considered. In the mean-field approximation in which statistical flux attached to particles is replaced by a uniform magnetic field, the boson system has the lowest energy. Nori and Doucot³⁴ also calculated the total energy on the square lattice. Yoshioka and co-workers³⁵ studied the triangular charge-density wave in two dimensions under a magnetic field and got a cusplike minimum of the energy. Their results are consistent with ours.

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