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Kinetic energy of electrons on a two-dimensional lattice with commensurate flux

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The kinetic energy of tight-binding electrons on a two-dimensional lattice with a perpendicular magnetic field has been studied using a recursion approach. For a fixed filling factor the energy is shown to exhibit several local minima as a function of flux. The minima correspond to the situation where the Fermi level lies in a gap. The absolute minimum corresponds to one flux quantum per particle.

The problem of electrons on a two-dimensional lattice with a perpendicular magnetic field has been well studied during the last few years because of its relation to the integer quantum Hall effect, in particular. Recently, Affleck and Martson[1] and others[2] have suggested that the above problem is also related to high-T_c superconductivity in the t-J model. Hasegawa *et al.*[3] have recently proposed that the energy of noninteracting spinless electrons has an absolute minimum when the flux per plaquette Φ (in units of $\Phi_0 = hc/e$) equals the electron density ν per site. Using this property and a renormalized mean-field theory, Lederer *et al.*[4] have recently shown that commensurate flux phases have special stability for $J/t \gtrsim 1$ and are superconducting.

In this paper we present a study of the kinetic energy of noninteracting spinless electrons on a two-dimensional square lattice as a function of the flux Φ per plaquette. We show that the energy has local minima with cusp when the Fermi level lies in a gap. Further, the energy has an absolute minimum with a cusp for $\Phi = \nu\Phi_0$ and we thus confirm the hypothesis of Hasegawa *et al.*[3] We also present results on the variation of the minimum energy as a function of the filling ν.

Consider a system of tight-binding electrons on a square lattice in the presence of a magnetic field described by a Hamiltonian

$$H = -\sum_{ij \in n\cdot n}{}' t_{ij} |i\rangle\langle j| ,$$

where

$$t_{ij} = t \exp\left(-2\pi i \int_i^j \mathbf{A}\cdot d\mathbf{l}\right)$$

is the hopping integral in the presence of a magnetic field with the vector potential $A = B(0,x,0)$ in the Landau gauge. The electronic structure of the system is described by the density of states $n_i(E)$, which is related to the diagonal element of the Green's function $G_i(E+i\epsilon)$. In this work we determine the Green's function $G_i(z)$ using the recursion approach[5] which allows one to express $G(z)$ as a continued fraction

$$G_i(z) = \cfrac{1}{z-a_0-\cfrac{b_0^2}{z-a_1-\cfrac{b_1^2}{z-a_2-\cdots}}} , \tag{1}$$

where coefficients a_n and b_n^2 are related to the moments[6] of the density of states. It is easy to see that the odd moments and hence the coefficients a_n are zero for the square lattice. In calculating $G_i(z)$ using (1), one is faced with the problem of termination of the continued fraction since only a finite number of coefficients can be numerically calculated. The asymptotic behavior of the coefficients is related to the singularities in the density of states and the presence of gaps leads to undamped oscillations.[7] In general, these oscillations are complicated and, thus, the calculation of $G(z)$ is numerically difficult. However, we empirically found a remarkable behavior of the coefficients $b_n^2 (a_n = 0)$ when the flux is such that

$$\Phi = \Phi_0 \frac{p}{q} ,$$

where p and q are incommensurate integers. In this case the coefficients b_n^2 were found to be periodic as a function of n with a period q. This allowed us a fairly exact termination of the continued fraction and, hence, an accurate determination of the density of states and the energy of the system.

In Fig. 1 we show the coefficients b_n^2 as a function of n for $\Phi/\Phi_0 = \frac{1}{3}$. As is clearly seen, b_n^2 are periodic with a period of 3 and with 100 calculated coefficients the limiting values are very well obtained. In Fig. 2(a) we show the density of states for $\Phi/\Phi_0 = \frac{7}{16}$. There are 16 bands which are symmetric around the energy $E = 0$ and we only

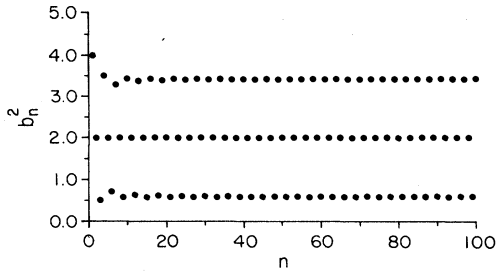

FIG. 1. Coefficients b_n^2 for the square lattice with a flux per plaquette $\Phi=\Phi_0/3$ (Φ_0 is the flux quantum hc/e) as a function of n. The limiting value for $\Phi=0$ is $b_\infty^2=4$.

show the negative-energy region. Figure 2(b) shows the different bands on a magnified scale. We have also studied the progression of the spectrum in the limit of weak magnetic fields. In Fig. 3 we show the density of states and the coefficients b_n^2 for $\Phi/\Phi_0=\frac{1}{32}$. Again the coefficients are periodic (with a period of 32). It is interesting to note that they go periodically to a very small value (which is probably zero for $\Phi/\Phi_0\rightarrow 0$) and that the spectrum has a structure similar to Landau levels. However, the spacing between the subbands decreases while the width increases[8] as one approaches the middle of the band. These results are in agreement with previous studies[8] and indicate that the present approach is well suited for studying density of states as well as the derived quantities in the presence of a magnetic field. We now present our results on the band-filling energy.

In this work we have studied the band energy as a function of flux for various values of filling factor. For each flux, we calculated 300 coefficients b_n^2 which permitted us

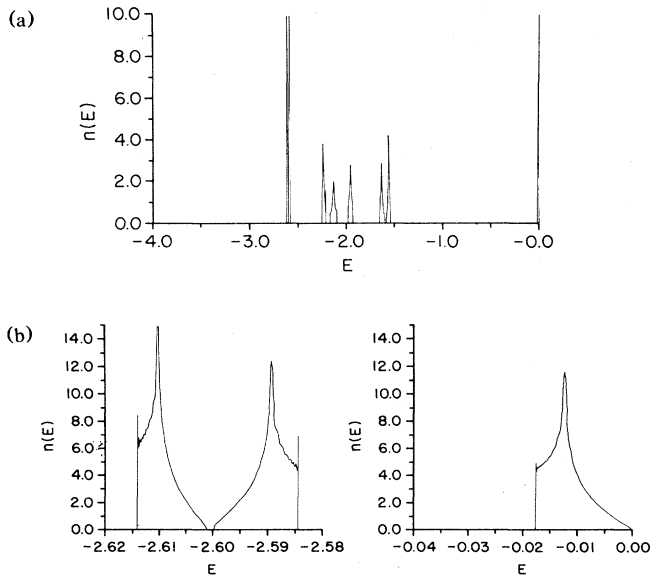

FIG. 2. (a) The density of states for $\Phi/\Phi_0=\frac{7}{16}$ (only negative values of energy are shown since the spectrum is symmetric around $E=0$). (b) Magnified view of the subbands around $E=-2.60$ and $E=-0.01$

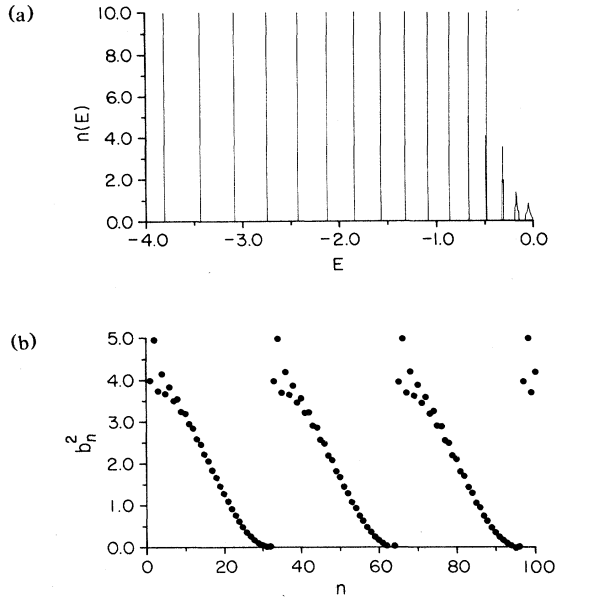

FIG. 3. (a) The density of states for $\Phi/\Phi_0=\frac{1}{32}$. Note that except around $E=0$ the subbands are dispersionless like Landau levels. (b) Coefficients b_n^2 as a function of n. Periodicity with a period of 32 is quite apparent.

to obtain periodicity of b_n^2 and hence the Green's function to a great precision. To calculate band energy as a function of the flux Φ and filling factor ν one has to perform an integration of the density of states. This was accomplished by using analytical properties of the Green's function which permit a replacement of the integrations along the real axis by integrations in the complex plane. We estimate errors in our computed band energy to be less than 10^{-3} in the worst cases and much smaller in most cases.

In Fig. 4 we show the band energy as a function of flux per plaquette for five values of the filling factor $\nu=p/10$ ($1\leq p\leq 5$). It is seen that the minimum energy is obtained for $\Phi=\nu\Phi_0$ as stated by Hasegawa *et al.*[3] Furthermore, the energy apparently has a cusp as a function of flux for this value of the flux. This cusp has important consequences in the theory proposed by Lederer, Poilblanc, and Rice.[4] One also notices that each time the Fermi level lies in a gap, the energy appears to show a local minima. This implies that the curve $E(\Phi)$ has a subtle structure. For the case when the Fermi level lies in a gap, Wannier[9] has shown that

$$\nu=M+N\frac{\Phi}{\Phi_0},$$

where M and N are two integers. From Fig. 4 it is seen that there are well-pronounced local minima (apparently with cusp) when the Fermi level is in the gap corresponding to

$$\nu=N\frac{\Phi}{\Phi_0}.$$

Except for $\nu=0.1$, these minima are clearly visible up to $N=5$ in Fig. 4. We also note that depending on the value

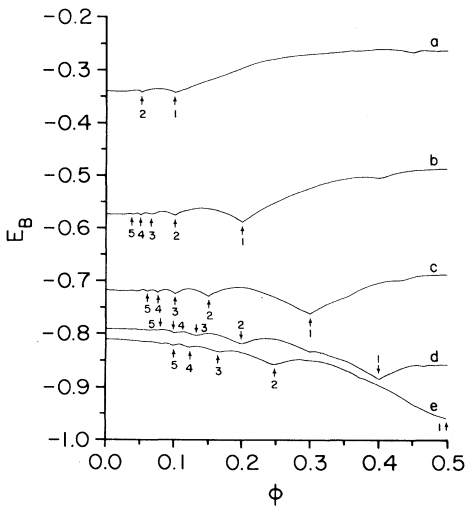

FIG. 4. The energy for filling the band, E_B, as a function of the flux (in units of the quantum flux). Curves *a*, *b*, *c*, *d*, and *e* correspond to filling factors $=0.1$, 0.2, 0.3, 0.4, and 0.5, respectively. The arrows indicate the local minima corresponding to $\Phi = v/n$ (n is an integer).

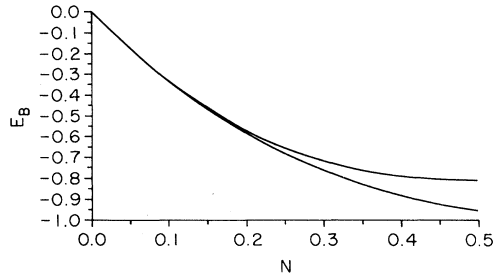

FIG. 5. Energy E_B as a function of the filling N for $\Phi/\Phi_0 = 0$ (upper curve) and $\Phi/\Phi_0 = N$ (lower curve). The difference in energy is maximum for $N = 0.5$.

of the flux, the mean kinetic energy can be higher or lower than in zero field. Indeed, the usual theory of Landau diamagnetism is based on an increase in kinetic energy in an external field.

Finally, in Fig. 5 we show the band energy for $\Phi = 0$ and $\Phi/\Phi_0 = v$ as a function of the filling factor. One notices that the difference in energy increases and is maximum at half filling.

To conclude, we have studied the variation of the kinetic energy of electrons on a two-dimensional lattice as a function of the applied magnetic field. The technique used by us allows studies with small variations in flux ($\Delta\Phi/\Phi_0 = \frac{1}{200}$). We find that the energy presents a lot of local minima with cusps as a function of flux for a given filling factor v. It is likely that the number of these local minima is infinite and that they are obtained when the Fermi level lies in a gap. The absolute minimum of energy is obtained when the flux per plaquette (in units of quantum flux) is equal to the filling factor of the band. This fact is the basis of the theory of high-T_c superconductivity developed recently by Lederer *et al.*[4]

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