Theory of Electronic Diamagnetism in Two-Dimensional Lattices

Y. Hasegawa,[(1),(a)] P. Lederer,[(1),(b)] T. M. Rice,[(1)] and P. B. Wiegmann[(2)]
[(1)]*Theoretische Physik, Eidgenössische Technische Hochschule Hönggerberg, CH 8093 Zürich, Switzerland*
[(2)]*The Landau Institute for Theoretical Physics, Academy of Sciences of U.S.S.R., 117940, GSP-1, Moscow, U.S.S.R.*
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The problem of tight-binding electrons in a two-dimensional lattice with a magnetic flux p/q in each plaquette is investigated for $p=0,1,3$, $q=2,3,4,6,8$. For fixed electron filling, ν, the total kinetic energy of the electrons has an absolute minimum for one flux quantum per particle, i.e., when $p/q=\nu\alpha$, where α is $1,\frac{1}{2},2$ for square, triangular, and honeycomb lattices, respectively.

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It is known from the early days of quantum mechanics that the energy spectrum of a charged particle in a magnetic field in two dimensions is quantized.[1] The zero-field dispersion $\epsilon(\mathbf{k})=\hbar^2k^2/2m$ becomes

$$\epsilon_n=\hbar\omega_c(n+\tfrac{1}{2}),$$

with $\omega_c=eH/mc$ and each Landau level is Φ-fold degenerate, where Φ is the flux per unit area in units of the flux quantum. The ground-state energy of spinless electrons in a magnetic field is not less than the energy in zero magnetic field. However, if a number of Landau levels is completely filled, there is a remarkable degeneracy: The total energy

$$E(B,\nu)-E(0,\nu)\propto\nu(\nu-\nu_n),$$

where the electron density ν satisfies the condition $\nu_n<\nu<\nu_{n+1}$, with $\nu_n=n\phi$ and ϕ is the flux per plaquette so that

$$E(B,\nu_n)=E(0,\nu_n).$$

This degeneracy can be lifted by a perturbation. In particular, a periodic potential splits the Landau levels into subbands in an asymmetric way and destroys this fine tuning.

The purpose of this Letter is to point out that in the presence of a periodic potential the ground-state energy of electrons in a magnetic field in the vicinity of the filled lowest Landau level is *lower* than in zero field. More precisely, the ground-state energy $E(B,\nu)$ of spinless noninteracting electrons in a two-dimensional periodic potential with fixed density ν, considered as a function of an external magnetic field, has an absolute minimum at a uniform magnetic field which corresponds to the Hall conductance (we set $e=c=\hbar=m=1$)

$$\sigma_{xy}(B,\nu)=1.$$

It corresponds to one flux quantum per particle and to a commensurate value of the flux per plaquette $\phi=\alpha\nu$, with $\alpha=1,\frac{1}{2},2$ for square, triangular, and honeycomb lattices, respectively.

We consider electrons in the presence of magnetic flux with a Hamiltonian,

$$H=-\sum_{i,j\in\text{n.n.}}t_{ij}c_i^\dagger c_j, \tag{1}$$

where

$$t_{ij}=t\exp\left(-i2\pi\int_i^j\mathbf{A}\,d\mathbf{l}\right). \tag{2}$$

If we use the Landau gauge, $\mathbf{A}=B(0,x,0)$, the energy dispersion $\epsilon(\mathbf{k})$ in a square lattice of spacing a and $Ba^2=\phi=p/q$ is given by the equation ($t=1$)

$$\det\begin{pmatrix} M_1 & -e^{ik_xa} & & & -e^{-ik_xa} \\ -e^{-ik_xa} & M_2 & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & M_{q-1} & -e^{ik_xa} \\ -e^{ik_xa} & & & -e^{-ik_xa} & M_q \end{pmatrix}=0, \tag{3}$$

where

$$M_n=-2\cos(k_ya+2\pi\phi n)-\epsilon(\mathbf{k}). \tag{4}$$

Equation (3) is known as Harper's equation and has been studied extensively.[2–5] Explicit equations for several p and q are given in Table I. In general, if integers p and q are chosen to represent the flux (with no common factor in p and q), then the dependence on the wave vector $\mathbf{k}$ always appears through the combination $\gamma_q\equiv\cos(qk_xa)+\cos(qk_ya)$.

The density of states $D(\epsilon)$ for $p=1,3$ and $q=2,3,4,8$ as well as for the no flux state are shown in Fig. 1. Since the density of states is symmetric in the square lattice, we plot only $D(\epsilon)$ for $\epsilon\le0$. The total energy for filling factor ν is

$$E=\int_{-4}^{\mu}d\epsilon D(\epsilon)\epsilon, \tag{5}$$

where μ is determined by

$$\nu=\int_{-4}^{\mu}d\epsilon D(\epsilon). \tag{6}$$

TABLE I. Energy dispersion in the square, triangular, and honeycomb lattices with magnetic flux p/q per plaquette. $\gamma_n = \cos(nk_x a) + \cos(nk_y a)$, $\delta_n = \cos(nk_x a) + \cos(nk_y a) + \cos(nk_x a + nk_y a)$, $\tilde{\delta}_n = -\cos(nk_x a) - \cos(nk_y a) + \cos(nk_x a + nk_y a)$.

p	q	$\epsilon(k)$
		Square lattice
1	2	$\epsilon^2 - 2\gamma_2 - 4 = 0$
1	3	$\epsilon^3 - 6\epsilon + 2\gamma_3 = 0$
1	4	$\epsilon^4 - 8\epsilon^2 - 2\gamma_4 + 4 = 0$
1	5	$\epsilon^5 - 10\epsilon^3 + [15 - 10\cos(2\pi/5)]\epsilon + 2\gamma_5 = 0$
1	6	$\epsilon^6 - 12\epsilon^4 + 24\epsilon^2 - 2\gamma_6 - 4 = 0$
1	8	$\epsilon^8 - 16\epsilon^6 + (72 - 8\sqrt{2})\epsilon^4 - (96 - 32\sqrt{2})\epsilon^2 - 2\gamma_8 + 4 = 0$
3	8	$\epsilon^8 - 16\epsilon^6 + (72 + 8\sqrt{2})\epsilon^4 - (96 + 32\sqrt{2})\epsilon^2 - 2\gamma_8 + 4 = 0$
		Triangular lattice
1	1	$\epsilon_3 + 2\delta_1 = 0$
1	2	$\epsilon_3 - 2\tilde{\delta}_1 = 0$
1	3	$\epsilon_3^3 - 9\epsilon_3 + 2\delta_3 - 6 = 0$
1	4	$\epsilon_3^2 - 2\delta_2 - 6 = 0$
1	6	$\epsilon_3^3 - 9\epsilon_3 - 2\tilde{\delta}_3 + 6 = 0$
		Honeycomb lattice
1	1	$\epsilon^2 - 2\delta_1 - 3 = 0$
1	2	$\epsilon^4 - 6\epsilon^2 + 2\tilde{\delta}_2 + 3 = 0$
1	3	$\epsilon^6 - 9\epsilon_4 + 18\epsilon^2 - 2\delta_3 - 3 = 0$
1	4	$\epsilon^8 - 12\epsilon^6 + 42\epsilon^4 - 44\epsilon^2 + 2\tilde{\delta}_4 + 3 = 0$
1	6	$\epsilon^{12} - 18\epsilon^{10} + 117\epsilon^8 - 342\epsilon^6 + 450\epsilon^4 - 216\epsilon^2 + 2\tilde{\epsilon}_6 + 3 = 0$

We calculated the total energies for fixed ν and different fluxes ϕ. The results are quoted in Table II. The energy is minimized by choosing the flux so that $\phi = \nu$. This result can be understood by looking at Hofstadter's subbands. Wannier[4] has shown that, in general, if one draws a line entirely within a gap in the Hofstadter

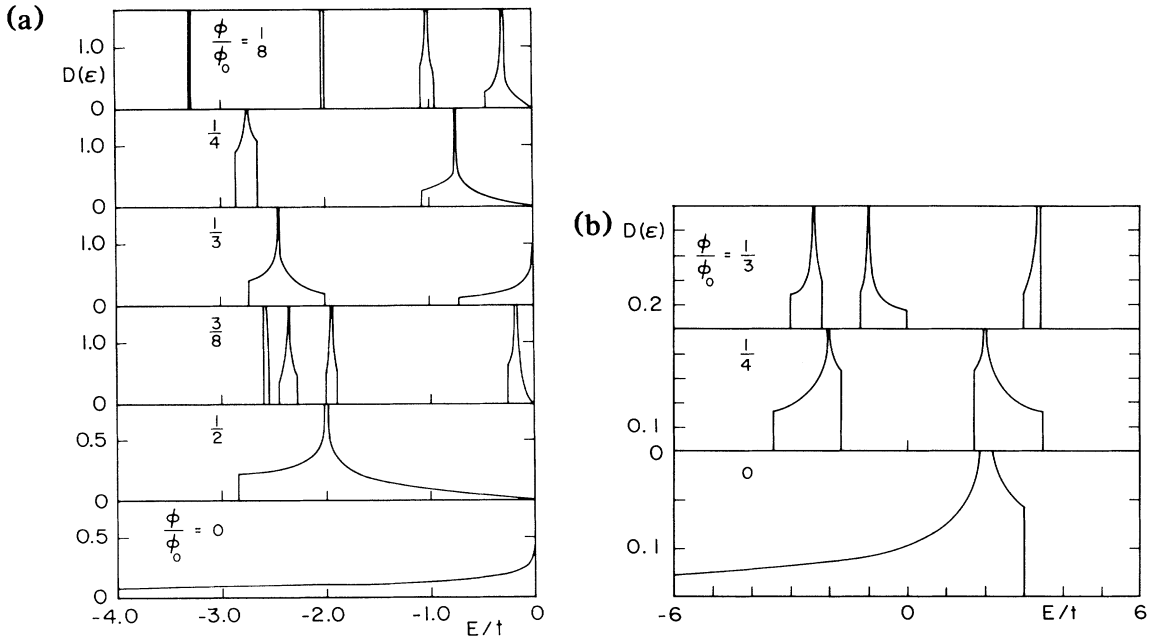

FIG. 1. Density of states in the (a) square and (b) triangular lattices with magnetic flux p/q. The density of states for flux $\frac{1}{2}$ ($\frac{1}{6}$) in the triangular lattice is the same as that for flux 0 ($\frac{1}{3}$) with changing $E \rightarrow -E$.

TABLE II. Total energy per site for filling ν in the square, triangular, and honeycomb lattices with various values of the magnetic flux. Notice that $E(\phi,\nu)=E(\phi,1-\nu)$ for square and honeycomb lattices and $E(\phi,\nu)=E(\frac{1}{2}-\phi,1-\nu)$ for triangular lattice. Energies for $\phi=a\nu$ shown in boldface are the absolute minima for each ν.

ν \ ϕ	0	$\frac{1}{8}$	$\frac{1}{6}$	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{3}{8}$	$\frac{1}{2}$
				Square lattice			
$\frac{1}{8}$	−0.408	**−0.411**	−0.386	−0.348	−0.326	−0.323	−0.321
$\frac{1}{6}$	−0.507	−0.495	**−0.514**	−0.460	−0.428	−0.423	−0.416
$\frac{1}{4}$	−0.656	−0.663	−0.643	**−0.682**	−0.628	−0.617	−0.590
$\frac{1}{3}$	−0.750	−0.749	−0.766	−0.760	**−0.810**	−0.780	−0.748
$\frac{3}{8}$	−0.779	−0.790	−0.790	−0.792	−0.834	**−0.859**	−0.819
$\frac{1}{2}$	−0.811	−0.826	−0.835	−0.859	−0.857	−0.880	**−0.958**
				Triangular lattice			
$\frac{1}{8}$	−0.592	−0.479	−0.423	−0.388	−0.349	−0.335	−0.336
$\frac{1}{6}$	−0.727	−0.637	−0.562	−0.499	−0.455	−0.440	−0.432
$\frac{1}{4}$	−0.915	**−0.954**	−0.835	−0.701	−0.658	−0.644	−0.608
$\frac{1}{3}$	−1.011	−0.994	**−1.095**	−0.881	−0.850	−0.797	−0.765
$\frac{3}{8}$	−1.030	−1.013	−1.089	−0.969	−0.897	−0.896	−0.835
$\frac{1}{2}$	−0.988	−1.046	−1.017	**−1.201**	−1.017	−1.046	−0.988

ν \ ϕ	0	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$
		Honeycomb lattice		
$\frac{1}{8}$	−0.321	**−0.324**	−0.311	−0.302
$\frac{1}{6}$	−0.406	−0.403	**−0.413**	−0.399
$\frac{1}{4}$	−0.547	−0.556	−0.555	**−0.578**
$\frac{1}{3}$	−0.654	−0.670	**−0.684**	−0.674
$\frac{3}{8}$	−0.698	**−0.722**	−0.713	−0.704
$\frac{1}{2}$	**−0.787**	−0.753	−0.751	−0.754

energy-flux diagram, the electron count ν, or integrated density of states below the gap, is of the form

$$\nu=M+N\phi,$$

where M and N are integers. The largest gap in the structure corresponds to $M=0$, $N=1$. Thus at the filling corresponding to $\nu=\phi$, the kinetic energy is lowered by the largest commensurability gap above the lowest group of states of the Hofstadter spectrum. For $\phi=p/q$ this lower group of states has p subbands containing each $1/q$ electrons per site. Therefore we believe the numerical results have general validity.

Note the lowest-energy state corresponds to the integer quantum Hall effect with quantum number 1.

The triangular lattice (considered as a square lattice with all diagonals in the NE direction) is also interesting. The energy dispersion without flux is given by

$$\epsilon_3(\mathbf{k})=-2[\cos(k_x a)+\cos(k_y a)+\cos(k_x+k_y)a]. \quad (7)$$

The density of states has a logarithmic singularity at $\epsilon_3=2$, the Fermi energy for the half-filled case is at $\epsilon=0.84$. Note that a flux of $\phi=\frac{1}{2}$ per plaquette is equivalent to setting $t\rightarrow -t$. For the half-filled case in the triangular lattice, the $\frac{1}{2}$ flux state has the same energy ($E=-0.99$) as the no flux state.

For flux $\phi=p/q$ the spectrum is given by

$$\det\begin{pmatrix} N_1 & A_1 & & & A_m^* \\ A_1^* & N_2 & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & N_{m-1} & A_{m-1} \\ A_m & & A_{m-1}^* & & N_m \end{pmatrix}=0, \quad (8)$$

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

$$N_n=-2\cos(k_y a+4\pi\phi n)-\epsilon_3, \quad (9)$$

and

$$A_n=-(e^{ik_x a}+e^{i2\pi\phi(2n+1)}e^{i(k_x a+k_y a)}). \quad (10)$$

With $\frac{1}{4}$ flux, the dispersion is

$$\epsilon_3(\mathbf{k}) = \pm 2[\cos^2(k_x a) + \cos^2(k_y a) + \cos^2(k_x a + k_y a)]^{1/2}. \quad (11)$$

The energy of the $\frac{1}{4}$ flux state in the half-filled case is $E = -1.20$, therefore substantially lower than for no flux or $\frac{1}{2}$ flux state. More results are reported for the triangular and honeycomb lattices in Table II. Further calculations will be reported in a future publication.

In conclusion, we examined the electron energy in the presence of a uniform flux of p/q. The energy has an absolute minimum when $p/q = \nu\alpha$. This can be considered as a generalization of the Peierls instability to orbital magnetic instabilities in two-dimensional lattices. (It should be noticed that since the energy associated with the external magnetic field is not included, the present result does not mean the spontaneous orbital ferromagnetism in real system.) An implication is the failure in this case of the usual theory of Landau diamagnetism based on an increase in electron kinetic energy in an external field.

The possibility that high-T_c superconductivity derives from electrons moving in a flux state on a square lattice has been proposed by several authors.[6-10] It has been emphasized that there will be commensurability effects whenever the density is such that the Fermi energy lies in a gap between subbands. In this Letter we have shown that not only is there a local minimum in the energy, but that if the flux can be chosen arbitrarily, the absolute minimum occurs when the Fermi energy lies in a gap corresponding to a flux per plaquette equal to the electron density per site.

The results of this paper should play a role in clearing up the dynamics of parity violation in the strongly correlated electron problem, and *CP* violation in gauge theories with fermions. If we take a particular mean-field decoupling in the interaction term in the t-J model, it reduces to Eq. (1); our treatment then corresponds to taking the flux as a variable parameter. This is known to yield a low-energy state at half-filling.[11] The p/q flux state with electron filling p/q will be an interesting basis in the strong correlation problem.

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[a]On leave of absence from Institute for Solid State Physics, The University of Tokyo, 7-22-1 Roppo4gi Minato-ku, Tokyo 106, Japan.

[b]On leave of absence from Physique des Solides, Universite Paris Sud, Orsay, France.

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