Peierls stabilization of magnetic-flux states of two-dimensional lattice electrons

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The problem of two-dimensional lattice electrons in a uniform magnetic field is reduced to a one-dimensional Peierls system which is an off-diagonal tight-binding model. Thus, this off-diagonal equation and the usual Harper equation, which has a diagonal modulation, give the same energy spectrum. The stabilization of the state in which the magnetic field gives one flux unit per electron is formally equivalent to the Peierls instability of lattice deformation.

Electrons in a two-dimensional lattice subject to a uniform magnetic field show extremely rich and interesting behavior (see, for example, Wannier,[1] Hofstadter,[2] and references therein). The spectrum is symmetric with respect to $E=0$ and when the flux per unit cell ϕ is a rational number p/q (p and q are integers which are prime to each other) it consists of q bands. As ϕ is changed continuously, p and q change wildly. In fact if ϕ is irrational, the spectrum is a Cantor set which consists of infinitely many "bands" with scaling properties.[3] Thouless, Kohmoto, Nightingale, and den Nijs[4] showed that each band carries an integral Hall conductance.

Recently Anderson[5] proposed the generalized flux phases for the high-T_c superconductors which are related to this so-called Hofstadter problem. Hasegawa, Lederer, Rice, and Wiegmann[6] studied the stability of the states with respect to the magnetic field. From the results of a few rational values of $\phi=p/q$ ($q=2$, 3, 4, 6, and 8), they argue that, if the number of electrons per lattice point ρ is fixed, the lowest energy with respect to the magnetic field (including the zero-field case) is realized when $\phi=\rho$, i.e., one flux unit per electron. Extensive numerical work[7,8] confirmed this proposal. This is a rather unexpected result, since one might naively think that the external magnetic field would increase the total energy. Note that, in the continuum case, however, the total energy when the Landau levels are fully filled is equal to that without magnetic field.

The Harper equation (2) below which is one-dimensional model with diagonal modulation is known to represent the Hofstadter problem. In this paper, we obtain an equation of a different type: one-dimensional tight-binding model with lattice distortion, namely an off-diagonal model. Thus, we have an example in which an on-diagonal model and and off-diagonal model give the same energy spectrum. The case without magnetic field corresponds to an undistorted one-dimensional lattice. The application of a magnetic field is equivalent to an introduction of a lattice distortion. Hence we argue that the stabilization of the flux state is formally equivalent to a Peierls instability in which a lattice distortion lowers the electronic energy by opening a gap in the spectrum at the Fermi energy.

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

$$\mathcal{H}=-t\sum_{\langle i,j\rangle}c_j^{\dagger}c_i e^{i\theta_{ij}}, \tag{1}$$

where c_i is the usual fermion operator on the lattice. The summation is taken over all nearest-neighbor sites. The phase factor $\theta_{ij}=-\theta_{ji}$ is defined on each link and represents the magnetic flux through the lattice, i.e., $\phi=1/2\pi\sum_{\text{plaquette}}\theta_{ij}$ is the magnetic flux through a plaquette in units of the magnetic flux quantum ch/e. Hereafter the transfer integral t will set to unity for simplicity without loss of generality. If we choose a gauge in which $\theta_{ij}=0$ for the link between $i=(n,m)$ and $j=(n+1,m)$ along the x direction and $\theta_{ij}=2\pi\phi n$ for the link between $i=(n,m)$ and $j=(n,m+1)$ along the y direction, we obtain the well-known Harper equation (see, for example, Ref. 9),

$$-\psi_{j+1}-\psi_{j-1}-2\cos(k_x^0+2\pi\phi j)\psi_j=E\psi_j. \tag{2}$$

Here, j is an integer and (2) is defined on a one-dimensional infinite lattice $-\infty<j<\infty$. This equation represents a one-dimensional tight-binding model with a diagonal modulation. When ϕ is a rational number, i.e., $\phi=p/q$ with p and q being integers which are prime to each other, (2) represents a system with period q. The energy dispersion of the original two-dimensional problem is determined by k_x^0 and k_y which is defined by the Bloch condition $\psi_{j+q}=\exp(iqk_y)\psi_j$. The magnetic Brillouin zone is given by $0\le k_x^0\le 2\pi/q$, and $0\le k_y\le 2\pi$. Since there are q solutions to (2) for a given set of k_x^0 and k_y, the spectrum consists of q bands. Also note that the energy is degenerate for k_y and $k_y+2\pi i/q$ where i is an integer.

Now we obtain another one-dimensional equation for the Hofstadter problem which has an off-diagonal modulation. Let us choose a gauge in which $\theta_{ij}=-\pi\phi(n+m)$ for the link between $i=(n,m)$ and $j=(n+1,m)$ along the x direction and $\theta_{ij}=\pi\phi(n+m)$ for the link between $i=(n,m)$ and $j=(n,m+1)$ along the y direction. Then

the Hamiltonian (1) is written

$$\mathcal{H}=\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}dk_x\int_{-\pi}^{\pi}dk_y H(\mathbf{k}), \tag{3}$$

with

$$H(\mathbf{k})=-(e^{ik_x}+e^{-i(k_y+\pi\phi)})c^{\dagger}(k_x+\pi\phi,k_y+\pi\phi)c(k_x,k_y) -(e^{-i(k_x-\pi\phi)}+e^{ik_y})c^{\dagger}(k_x-\pi\phi,k_y-\pi\phi)c(k_x,k_y), \tag{4}$$

where the fermion operator in the reciprocal space is defined by

$$c_{nm}=\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}dk_x\int_{-\pi}^{\pi}dk_y\exp[i(k_x n+k_y m)]c(k_x,k_y). \tag{5}$$

Transform the coordinates by

$$K=\frac{k_x+k_y}{2}+\frac{\pi\phi}{2}, \qquad k=\frac{k_x-k_y}{2}-\frac{\pi\phi}{2}, \tag{6}$$

and write

$$c(k_x,k_y)=\tilde{c}\left(\frac{k_x+k_y}{2}+\frac{\pi\phi}{2},\frac{k_x-k_y}{2}-\frac{\pi\phi}{2}\right)=\tilde{c}(K,k). \tag{7}$$

The first Brillouin zone can be chosen to be $0\le K\le 2\pi, 0<k\le\pi$. Now the $\mathbf{k}$-dependent Hamiltonian may be written

$$H(K,k)=-2e^{ik}\cos K\,\tilde{c}^{\dagger}(K+\pi\phi,k)\tilde{c}(K,k) -2e^{-ik}\cos(K-\pi\phi)\tilde{c}^{\dagger}(K-\pi\phi,k)\tilde{c}(K,k). \tag{8}$$

Note that there is no coupling between different k's and only K's which differ by $\pi\phi$ couple. Hence, we have a one-dimensional discrete system. If we write

$$K=K^0+\pi\phi j \tag{9}$$

and

$$c_j=\tilde{c}(K^0+\pi\phi j,k), \tag{10}$$

then K^0 and k are good quantum numbers. For a given set of K^0 and k, an eigenstate is written

$$|u\rangle=\sum_{j=0}^{2q-1}u_j c_j^{\dagger}|0\rangle. \tag{11}$$

The Schrödinger equation $\mathcal{H}|u\rangle=E|u\rangle$ gives

$$-e^{-ik}t_j u_{j+1}-e^{ik}t_{j-1}u_{j-1}=Eu_j, \tag{12}$$

with

$$t_j=2\cos(K^0+\pi\phi j), \tag{13}$$

where $u_{-1}=u_{2q-1}$ and $u_{2q}=u_0$. Although (12) represents a closed chain with $2q$ sites, it is equivalent to an infinite periodic chain with period q. In order to show this, we need to consider the following cases separately: (i) p even and q odd: We have $t_{j+q}=t_j$. (ii) p odd and q odd: Since the energy spectrum is invariant under $\phi\to 1-\phi$ [note that it is invariant under $\phi\to-\phi$ (reversal of the direction of the magnetic field) and $\phi\to\phi+1$], this case is mapped to case (i). (iii) p odd and q even: We now have $t_{j+q}=-t_j$, but (12) is invariant under a transformation

$$t_j\to -t_j \text{ for } j=q,q+1,\ldots,2q-1$$

$$u_j\to -u_j \text{ for } j=q+1,q+3,\ldots,2q-1.$$

Thus after the transformation, we have $t_{j+q}=t_j$ again.

Now, it is enough to consider the case with $t_{j+q}=t_j$, so we have $u_{j+q}=u_j$ or $u_{j+q}=-u_j$. Let us define

$$\psi_j=e^{-ikj}u_j. \tag{14}$$

Here, ψ_j is defined for $-\infty<j<\infty$ (u_j is extended to have period $2q$). The two types of the solutions $u_{j+q}=\pm u_j$ can be taken into account by expanding the domain of k which was originally $0\le k\le\pi$ to $0\le k\le 2\pi$. By substituting (14) into (12), we get

$$-t_{j-1}\psi_{j-1}-t_j\psi_{j+1}=E\psi_j, \tag{15}$$

where t_j ($j=0,\ q-1$) repeat themselves to make an infinite chain with period q. The magnetic Brillouin zone of the original two-dimensional problem is now represented by $0\le K^0\le\pi/q$ and $0\le k\le 2\pi$. The energy is degenerate for k and $k+2\pi i/q$, where i is an integer.

The numerical result[7,8] shows that, if the number of electrons per lattice point ρ is fixed, the lowest total energy with respect to the magnetic field (including the zero-field case) is realized when $\phi=\rho$, i.e., one flux unit per electron. A large gap exists at the Fermi energy in this case except for $\phi=\frac{1}{2}$ in which the spectrum does not have a gap (two bands touch each other at the center of the spectrum).

Let us first consider the case $\phi=\frac{1}{2}$. Then (15) represents a dimerized system with $t_0=2\cos K^0$ and $t_1=2\cos(K^0+\pi/2)$, where the range of K^0 is chosen to be $-\pi/2\le K^0\le 0$ to make t_0 and t_1 positive. The energy dispersion is given by $E=\pm 2(1+\sin 2K^0\cos 2k)^{1/2}$ and has a gap at the center for all K^0 except $K^0=-\pi/4$. On the other hand, when $\phi=0$ (which has the same energy dispersion as for $\phi=1$), we have $E=-4\cos K^0\cos k$. It is expected then that, if the spectrum is half-filled, $\phi=\frac{1}{2}$ gives a lower energy than $\phi=0$ due to the gap at the Fermi energy. This is confirmed numerically.[6-8] Note that the spectrum for the two-dimensional system does not really have a gap, since it is obtained by superposition of E with respect to K^0.

In order to have some feeling about the above two cases, we average the transfer integral t_j in (15) with respect to K^0. We have $t=\langle t\rangle_{\phi=1}=\langle(t_0+t_1)/2\rangle_{\phi=1/2}=4/\pi$, and $\Delta t=\langle|t_1-t_0|/2\rangle_{\phi=1/2}=4(\sqrt{2}-1)/\pi$. So, roughly speaking, the external magnetic field corresponds to the introduction of a lattice dimerization which causes the transfer integral to deviate from t by Δt.

For $\phi=1/q$ all t_j's can be taken to be positive and the analogy to the one-dimensional system with lattice distortion still holds. If the filling of electrons is $1/q$, a gap is

created at the Fermi energy by the lattice distortion or equivalently by an application of the magnetic field, thus lowering the energy. There is no gap in the part of the spectrum filled by the electrons.

When the filling is p/q ($p \neq 1$), we also find a gap at the Fermi energy, if the magnetic field gives $\phi = p/q$. In this case, we have gaps in the filled portion of the spectrum. Since not all t_j's are positive, the analogy to the Peierls system of lattice distortion is not perfect. However, the mechanism of lowering the energy by opening a gap at the Fermi edge is the same. This has been confirmed numerically.[7,8]

In summary, we have reformulated the problem of two-dimensional lattice electrons in a magnetic field (the Hofstadter problem). The usual gauge leads to the Harper equation (2), which is a one-dimensional tight-binding equation with diagonal modulation. Our reformulation leads to (15), which is also one-dimensional but contains off-diagonal modulation. The Hofstadter spectrum arises in the usual formulation as a superposition over k_x^0 and, equivalently, from (15) as a superposition over K^0. This connection between two apparently quite different one-dimensional equations is not at all evident in the one-dimensional context but emerges in the two-dimensional context as a consequence of the gauge symmetry. In order to obtain the off-diagonal model, we used a gauge which is rotated by 45° from that for deriving the Harper equation. If we rotate the gauge 90°, the same Harper equation is obtained due to the symmetry of the square lattice.[9] This transformation is equivalent to the self-dual transformation by Aubry and Andre.[10]

Using the off-diagonal model, we pointed out that the stabilization of the state with filling ρ when a flux of $\phi = \rho$ is introduced can be explained by a mechanism similar to the Peierls mechanism in which a lattice distortion lowers the energy by opening a gap at the Fermi energy.

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