Effects of Electron Correlations on Hofstadter Spectrum

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Abstract

By allowing interactions between electrons, a new Harper's equation is derived to examine the effects of electron correlations on the Hofstadter energy spectra. It is shown that the structure of the Hofstadter butterfly for the system of correlated electrons is modified only in the band gaps and the band widths, but not in the characteristics of self-similarity and the Cantor set.

1 Introduction

Numerous studies have been made to study two dimensional quantum systems of electrons in a magnetic field, including the Hofstadter energy spectrum [1] and the quantum Hall effects [2]. Hofstadter studied the energy spectrum for non-interacting electrons on a two dimensional square lattice in a perpendicular uniform magnetic field, namely the energy spectrum vs. magnetic flux per plaquette known as the Hofstadter butterfly. The energy spectrum was found to critically depend on the ratio p/q (p and q are positive integers) of the magnetic flux per plaquette to the flux quantum. If p/q is a rational number, each energy band is split into q sub-bands by the magnetic field. The Hofstadter butterfly displays a recursive structure over rational (number) fields and a Cantor set at any irrational number of p/q [1].

The gap structure predicted by the Hofstadter butterfly is known to play an important role on the magnetoresistance of the laterally modulated two-dimensional electron systems in GaAs-AlGaAs heterostructure [3]. Such gap structure can be sensitive to the strength of interactions between electrons. Lately, based on the Hartree approximation Gudmundsson and Gerhardts [4] studied the effects of interacting electrons on the Hofstadter butterfly. In the present study we derive a new Harper's equation which will allow us to study the Hofstadter energy spectrum as a function of Coulomb repulsion by properly taking into account electron interactions. As an illustration we pay a special attention to the interesting system of antiferromagnetically correlated electrons on a square lattice.

2 Hofstadter Spectrum of Interacting Electrons

Earlier Hasegawa et al.[5] studied the Harper's equation [6] and the energy spectrum only for spinless non-interacting electrons. In the present study we derive a new Harper's equation in order to study the Hofstadter butterfly, that is, the energy spectrum vs. magnetic flux as a function of interaction strength (Coulomb repulsion U) between electrons.

In order to treat interacting electrons in a two dimensional square lattice in a perpendicular uniform magnetic field, we consider the one-band Hubbard model Hamiltonian,

$$H = - \sum_{\langle ij \rangle \sigma} t_{ij} C^{\dagger}_{i\sigma} C_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} C^{\dagger}_{i\sigma} C_{i\sigma}, \tag{1}$$

with

$$t_{ij} = -t \exp \left(-i \frac{2\pi}{\phi_0} \int_j^i \mathbf{A} \cdot d\mathbf{l} \right). \tag{2}$$

Here $C^{\dagger}_{i\sigma} (C_{i\sigma})$ is the creation (annihilation) operator of an electron with spin σ at site $i = (i_x, i_y)$. $\langle ij \rangle$ denotes only the nearest neighbor hopping with lattice spacing a. ϕ_0 is the unit flux. The choice of the Landau gauge, $\mathbf{A} = B(0, j_x a, 0)$ for a uniform magnetic field B leads to the hoping integrals, $t_{ij} = t_{(j_x \pm 1, j_y)(j_x, j_y)} = t$ for the x-direction of hopping and $t_{ij} = t_{(j_x, j_y \pm 1)(j_x, j_y)} = t \exp \left(\mp i 2\pi j_x \frac{\phi}{\phi_0} \right) = t \exp \left(\mp 2\pi j_x \frac{p}{q} \right)$ for the y-direction of hopping, where $\phi \equiv Ba^2$. $\frac{\phi}{\phi_0} = \frac{p}{q}$ with p and q integers is the number of flux quanta per plaquette which is equivalent to the gain of phase by a particle as a result of hopping round the closed path of a plaquette.

We now introduce the staggered magnetization at site i,

$$m(i) = e^{i\mathbf{Q} \cdot \mathbf{r}} \sum_{\sigma} \sigma \langle C^{\dagger}_{i\sigma} C_{i\sigma} \rangle$$

with $\mathbf{Q} \equiv (\frac{\pi}{a}, \frac{\pi}{a})$, $\mathbf{r} = a(j_x, j_y)$ and the hole doping rate δ,

$$1 - \delta(i) = \sum_\sigma \langle C_{i\sigma}^\dagger C_{i\sigma} \rangle.$$

Considering a uniform doping and a uniform staggered magnetization, i.e., $\delta(i) = \delta$ and $m(i) = m$ respectively, we obtain from (1) the following mean field Hamiltonian for interacting electrons in the square lattice,

$$H = - \sum_{\langle ij \rangle \sigma} t_{ij} C_{i\sigma}^\dagger C_{j\sigma} + \sum_{i\sigma} \left[\frac{U}{2}(1 - \delta) - \frac{\sigma m U}{2} e^{i\mathbf{Q}\cdot\mathbf{r}} - \mu \right] C_{i\sigma}^\dagger C_{i\sigma} + \sum_i U \left[(\frac{m}{2})^2 - \frac{1}{4}(1 - \delta)^2 \right].$$
$$(3)$$

Here the exchange correlation is properly introduced [7]. The third term represents a constant energy shift. Ignoring the third term, we rewrite (2) explicitly

$$
\begin{aligned}
H &= -t \sum_{(j_x, j_y)\sigma} \left[C_{(j_x+1,j_y)\sigma}^\dagger C_{(j_x,j_y)\sigma} + C_{(j_x-1,j_y)\sigma}^\dagger C_{(j_x,j_y)\sigma} + e^{-2\pi\frac{p}{q}j_x i} C_{(j_x,j_y+1)\sigma}^\dagger C_{(j_x,j_y)\sigma} \right. \\
&\quad \left. + e^{2\pi\frac{p}{q}j_x i} C_{(j_x,j_y-1)\sigma}^\dagger C_{(j_x,j_y)\sigma} \right] \\
&\quad - \sum_{(j_x,j_y)\sigma} \frac{\sigma m U}{2} e^{i\mathbf{Q}\cdot\mathbf{r}} C_{(j_x,j_y)\sigma}^\dagger C_{(j_x,j_y)\sigma} + \sum_{(j_x,j_y)\sigma} \left[\frac{U}{2}(1-\delta) - \mu \right] C_{(j_x,j_y)\sigma}^\dagger C_{(j_x,j_y)\sigma} \quad (4)
\end{aligned}
$$

Omitting the third term which represents the shift of constant energy, the Hamiltonian (4) is reduced to

$$
\begin{aligned}
H &= -t \sum_{(j_x, j_y)\sigma} \left[C_{(j_x+1,j_y)\sigma}^\dagger C_{(j_x,j_y)\sigma} + C_{(j_x-1,j_y)\sigma}^\dagger C_{(j_x,j_y)\sigma} \right. \quad (5) \\
&\quad \left. + e^{-2\pi\frac{p}{q}j_x i} C_{(j_x,j_y+1)\sigma}^\dagger C_{(j_x,j_y)\sigma} + e^{2\pi\frac{p}{q}j_x i} C_{(j_x,j_y-1)\sigma}^\dagger C_{(j_x,j_y)\sigma} \right] \\
&\quad - \sum_{(j_x,j_y)\sigma} \frac{\sigma m U}{2} e^{i\mathbf{Q}\cdot\mathbf{r}} C_{(j_x,j_y)\sigma}^\dagger C_{(j_x,j_y)\sigma}
\end{aligned}
$$

Now we denote $|(j_x, j_y)\rangle$ as a single (one) particle state in number representation,

$$|(j_x, j_y)\rangle = |1_{(j_x,j_y)}\rangle = C_{(j_x,j_y)}^\dagger |0\rangle \qquad (6)$$

4

and define

$$|(j_x\pm1, j_y)\rangle = |1_{(j_x\pm1,j_y)}\rangle = C^\dagger_{(j_x\pm1,j_y)}C_{(j_x,j_y)}|1_{(j_x,j_y)}\rangle.$$

$$|(j_x, j_y\pm1)\rangle = |1_{(j_x,j_y\pm1)}\rangle = C^\dagger_{(j_x,j_y\pm1)}C_{(j_x,j_y)}|1_{(j_x,j_y)}\rangle. \tag{7}$$

We now use the Schrödinger equation, $H|\psi\rangle = E|\psi\rangle$ where H is the Hamiltonian (5) and $|\psi\rangle$, the eigenstate in number representation. We then obtain from the use of (6) and (7),

$$-t\left[\langle(j_x-1,\ j_y)|\psi\rangle + \langle(j_x+1,\ j_y)|\psi\rangle + e^{-2\pi\frac{p}{q}j_x i}\langle(j_x,\ j_y-1)|\psi\rangle + e^{2\pi\frac{p}{q}j_x i}\langle(j_x,\ j_y+1)|\psi\rangle\right] \tag{8}$$

$$-(-1)^{j_x+j_y}\frac{mU}{2}\langle(j_x,\ j_y)|\psi\rangle = E\langle(j_x,\ j_y)|\psi\rangle$$

Here $j_x = 1, \cdots, q$ acts as a coordinate in the magnetic cell. The one-dimensional quasi-periodic boundary condition is satisfied; $\langle(j_x, j_y)|\psi\rangle = e^{iqk_x a}\langle(j_x+q, j_y)|\psi\rangle$. There exists q plaquettes per magnetic unit cell. Accordingly the energy spectrum has q sub-bands as a result of the applied magnetic field. Here for the range of k vector one magnetic Brillouin zone is equivalent to one original Brillouin zone divided by q.

The above Hamiltonian (5) is invariant under the translation $j_y \rightarrow j_y + 2$ for the system of antiferromagnetically correlated electrons. Thus using the Bloch theorem,

$$\langle(j_x,\ j_y)|\psi\rangle = e^{ik_y a j_y}\langle(j_x,\ 0)|\psi\rangle \qquad \text{for even } j_y,$$

$$\text{and}$$

$$\langle(j_x,\ j_y)|\psi\rangle = e^{ik_y a j_y}\langle(j_x,\ 1)|\psi\rangle \qquad \text{for odd } j_y,$$

we write

$$\langle(j_x,\ j_y)|\psi\rangle = e^{ik_y a j_y}\left(\frac{1+(-1)^{j_y}}{2}\langle(j_x,\ 0)|\psi\rangle + \frac{1-(-1)^{j_y}}{2}\langle(j_x,\ 1)|\psi\rangle\right) \tag{9}$$

$$= e^{ik_y a j_y}\left(\frac{\langle(j_x,\ 0)|\psi\rangle + \langle(j_x,\ 1)|\psi\rangle}{2} + (-1)^{j_y}\frac{\langle(j_x,\ 0)|\psi\rangle - \langle(j_x,\ 1)|\psi\rangle}{2}\right)$$

By defining

$$u(j_x) = \frac{\langle(j_x,\, 0)|\psi\rangle + \langle(j_x,\, 1)|\psi\rangle}{2}, \qquad (10.a)$$

and

$$v(j_x) = (-1)^{-j_x}\frac{\langle(j_x,\, 0)|\psi\rangle - \langle(j_x,\, 1)|\psi\rangle}{2}, \qquad (10.b)$$

we rewrite (9) above,

$$\langle(j_x,\, j_y)|\psi\rangle = e^{ik_y a j_y}\left(u(j_x) + (-1)^{j_x+j_y}v(j_x)\right). \qquad (11)$$

Using (11), we readily find from (8),

$$-t\left[u(j_x-1) + u(j_x+1) + \{e^{-(2\pi\frac{p}{q}j_x+k_ya)i} + e^{(2\pi\frac{p}{q}j_x+k_ya)i}\}u(j_x)\right] - \frac{mU}{2}v(j_x) \qquad (12)$$

$$+(-1)^{j_x+j_y}\, t\left[v(j_x-1) + v(j_x+1) + \{e^{-(2\pi\frac{p}{q}j_x+k_ya)i} + e^{(2\pi\frac{p}{q}j_x+k_ya)i}\}v(j_x)\right]$$

$$-(-1)^{j_x+j_y}\frac{mU}{2}u(j_x) = E\left(\left(u(j_x) + (-1)^{j_x+j_y}v(j_x)\right)\right)$$

The expression (12) above leads to the following new Harper's equations which are simply

the coupled one-dimensional quasiperiodic difference equations.

$$-t\left[u(j_x-1) + u(j_x+1) + 2\cos(2\pi\frac{p}{q}j_x+k_ya)u(j_x)\right] - \frac{mU}{2}v(j_x) = Eu(j_x) \qquad (13)$$

$$t\left[v(j_x-1) + v(j_x+1) + 2\cos(2\pi\frac{p}{q}j_x+k_ya)v(j_x)\right] - \frac{mU}{2}u(j_x) = Ev(j_x)$$

The coupled difference equations here arise due to the antiferromagnetically correlated elec-

trons.

Defining the reduced energy $\epsilon = E/t$, and the reduced energy gap $\Delta = mU/t$, we rewrite

(13) above to explicitly show the following recursion relations,

$$u(j+1) \;=\; (-\epsilon - 2\cos(2\pi\frac{p}{q}j + k_ya))u(j) - u(j-1) - \frac{\Delta}{2}v(j)$$

$$v(j+1) \;=\; (\epsilon - 2\cos(2\pi\frac{p}{q}j + k_ya))v(j) - v(j-1) + \frac{\Delta}{2}u(j)$$

or in matrix form,

$$
\begin{pmatrix} u(j+1) \\ u(j) \\ v(j+1) \\ v(j) \end{pmatrix} = \begin{pmatrix} -\epsilon - 2\cos(2\pi\frac{p}{q}j+k_ya) & -1 & \frac{\Delta}{2} & 0 \\ 1 & 0 & 0 & 0 \\ -\frac{\Delta}{2} & 0 & \epsilon - 2\cos(2\pi\frac{p}{q}j+k_ya) & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} u(j) \\ u(j-1) \\ v(j) \\ v(j-1) \end{pmatrix}
$$ (14)

Since there is no possible confusion below, we omit the subscript x of j_x in the expression (14).

To block-diagonalize the square matrix in (14) above, we introduce the following transformation,

$$
\begin{pmatrix} u'(j) \\ v'(j) \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ -\beta & \alpha \end{pmatrix} \begin{pmatrix} u(j) \\ v(j) \end{pmatrix}
$$

where

$$
\alpha = \sqrt{\frac{1 + \sqrt{1 - (\frac{\Delta}{2\epsilon})^2}}{2}}
$$

$$
\beta = \sqrt{\frac{1 - \sqrt{1 - (\frac{\Delta}{2\epsilon})^2}}{2}}
$$

Thus the square matrix above is block-diagonalized as

$$
\begin{pmatrix} -\epsilon_0 - 2\cos(2\pi\frac{p}{q}j+\nu) & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & \epsilon_0 - 2\cos(2\pi\frac{p}{q}j+\nu) & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}
$$ (15)

where $\epsilon_0 \equiv \sqrt{\epsilon^2 - (\frac{\Delta}{2})^2}$.

Using (14) and (15) above, we readily find

$$
\begin{pmatrix} u'(j+1) \\ u'(j) \end{pmatrix} = \begin{pmatrix} -\epsilon_0 - 2\cos(2\pi\frac{p}{q}j+k_ya) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u'(j) \\ u'(j-1) \end{pmatrix}
$$ (16.a)

7

$$\begin{pmatrix} v'(j+1) \\ v'(j) \end{pmatrix} = \begin{pmatrix} \epsilon_0 - 2\cos(2\pi\frac{p}{q}j+k_ya) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} v'(j) \\ v'(j-1) \end{pmatrix} \tag{16.b}$$

ϵ_0 here represents the energy spectrum of non-interacting electrons. The energy dispersion relation [8] for the system of interacting electrons is readily obtained from (16) above,

$$\epsilon(\mathbf{k}) = \frac{U}{2t}(1-\delta) - \frac{\mu}{t} \pm \sqrt{\epsilon_0(\mathbf{k})^2 + \left(\frac{\Delta}{2}\right)^2}, \tag{17}$$

with the energy gap, $\frac{mU}{2}$. Here we reintroduced the first term which was omitted in (5). As seen in (17) above, the energy spectrum ϵ shows the variation of energy gap with both the staggered magnetization m and the Coulomb interaction U. However the dispersion relation (17) indicates that the self-similarity and homeomorphism to the Cantor set are not affected by such electron correlations.

Now using in (16) the translation matrix

$$Q(\epsilon; k_y) \equiv \prod_{j=1}^{q} A_j(\epsilon; k_y), \tag{18}$$

made of q successive products of

$$A_j(\epsilon; k_y) \equiv \begin{pmatrix} -\epsilon_0 - 2\cos(2\pi\frac{p}{q}j+k_ya) & -1 \\ 1 & 0 \end{pmatrix},$$

we obtain

$$\begin{pmatrix} g(q+1) \\ g(q) \end{pmatrix} = Q(\epsilon; k_ya) \begin{pmatrix} g(1) \\ g(0) \end{pmatrix} \tag{19}$$

where $g(j) = u'(j)$ or $v'(j)$. Note that in the expression (18), ϵ_0 is replaced by ϵ due to relation (17). Further we note from the Bloch theorem,

$$\begin{pmatrix} g(q+1) \\ g(q) \end{pmatrix} = e^{iqk_xa} \begin{pmatrix} g(1) \\ g(0) \end{pmatrix}. \tag{20}$$

8

Thus we readily find from (19) and (20),

$$\det(Q(\epsilon; k_y) - e^{iqk_x a} I) = 0.$$

One of the eigenvalues of Q is complex conjugate to the other in order to have a real value of tr Q. Thus we have

$$\text{tr } Q(\epsilon; k_y) = 2\cos(qk_x a). \tag{21}$$

The k_y dependency of the trace is additively separable as shown by Buther and Brown [9], and thus we write

$$\text{tr } Q(\epsilon) \equiv \text{tr } Q(\epsilon; \frac{\pi}{2q}) = 2\cos(qk_x a) + 2\cos(qk_y a). \tag{22}$$

Since tr $Q(\epsilon)$ is simply the q-th polynomial of ϵ, there exist q sub-bands for a given k. Here k is readily obtained for given ϵ. ϵ should satisfy the following condition,

$$|\text{tr } Q(\epsilon)| \leq 4. \tag{23}$$

One can determine from the condition (23) whether a state of a given energy ϵ is possible or not. Using the relations (22) and (23) above, we compute the Hofstadter energy spectrum as a function of $\frac{p}{q}$ for the square lattice of antiferromagnetically correlated electrons at half-filling, that is, $\delta = 0$. In principle, the self consistent equations for m and μ can be derived for a lattice of infinite size [8]. For the case of finite size lattices we obtain m and μ numerically for arbitrary values of p and q. It is important to thoroughly check numerical precision of the computed staggered magnetization m in order to accurately evaluate dispersion relation (17). This is because m in the dispersion relation is very sensitive to the variation of p/q. In order to check numerical accuracy, in Fig. 1 we show the computed results of staggered

9

magnetization m as a function of Coulomb repulsion U for the two cases of finite (10×10, 20×20 and 30×30 square lattices) and infinite size lattices. For both zero magnetic field and the non-zero magnetic field (corresponding to half a flux quantum per plaquette), the computed results of m with the finite size lattices (denoted as solid or open circles in Fig. 1) are nearly the same as the exact values obtained from the use of the infinite size lattice (denoted as a solid line in Fig. 1). Encouraged by such numerical accuracy, we computed the Hofstadter energy spectra of interacting electrons for various values of U by using the finite size lattice of 10×10. They are shown in Fig. 2 through 4. We find that the structure of the Hofstadter energy spectrum for interacting electrons is greatly modified only in the band gaps and the band widths (the bars in the figures stand for the band width) which depend on the strength of the Coulomb interaction U, as well displayed in Figs. 2 through 4. Indeed this is clearly understood from the expression of the energy dispersion relation (17). Although not shown here, at higher values of U we find no other changes but larger band gaps and narrower band widths in the Hofstadter energy spectrum. The self-similarity of the Hofstadter butterfly is preserved at all values of Coulomb interaction U.

The band gap in the structure of the Hofstadter spectrum is predicted to be undulatory particularly at the low value of $U = 2t$ as shown in Fig. 3. For the sake fo clarity, undulatory feature of the band gap as a function of magnetic flux is explicitly shown in Fig. 5. It is noted that this undulatory behavior seen at a low value of $U \simeq 2t$ originates from the oscillatory variation of the staggered magnetization m as a function of p/q. At larger values of U such oscillatory behavior disappears as seen in Fig. 4. This is because the staggered magnetization (or antiferromagnetic order) becomes increasingly stable and thus insensitive

to the variation of magnetic field. The Hofstadter spectrum yields an additional sub-band only for odd q. This is caused by the Coulomb interaction which splits the band containing the fermi level into two bands. In short, one can readily see from the dispersion relation (17) that only the band gaps and the band widths in the Hofstadter spectrum but not the essential characters of the self-similarity and the Cantor set can be affected by interactions between electrons.

3 Conclusion

In the present study we derived a new generalized Harper's equation to deal with both the undoped (half-filling, $\delta = 0$) and doped ($\delta \neq 0$) systems by allowing interactions between electrons, and examined the Hofstadter energy spectrum as a function of Coulomb repulsion U for the square lattice of correlated electrons at half-filling. We found that such Coulomb interactions between electrons affect only the band gaps and band widths in the structure of the Hofstadter butterfly. Judging from the dispersion relation (17), the inclusion of electron correlation effects beyond the mean field level will modify only the band gaps and band widths in the Hofstadter spectrum, but not the self-similarity of the Hofstadter spectrum and the homeomorphism to the Cantor set.

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Figure Captions

Fig. 1 Staggered Magnetization with and without magnetic field; solid line for the infinite

   size lattice and dots, for the finite size lattices.

Fig. 2 Hofstadter spectrum of non-interacting electrons at half-filling.

Fig. 3 Hofstadter spectrum of interacting electrons at half-filling with $U = 2t$.

Fig. 4 Hofstadter spectrum of interacting electrons at half-filling with $U = 4t$.

Fig. 5 Band gap Δ as a function of $\frac{p}{q}$.