Mott Transition in the Two-Dimensional Flux Phase

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I. INTRODUCTION

There has been a proposal that an order takes place on a link in several interacting lattice-fermion systems. Especially when the link order has a phase factor, it brings an effective magnetic field. Sometime the order can be topological in the sense that the phase factor itself is not a well defined order parameter but the flux characterizes the phase. One of such systems is the flux phase which was proposed to describe the ground state properties of several interacting lattice-fermion systems e.g. the Hubbard model, the t-J model, and their variants. Recently there has been a resurgence of interest in the flux phase and evidences are accumulating for its reality. For example, it was revealed a bond order takes place in the one-dimensional extended Hubbard model at half filling which can be understood by the one-dimensional analog of the flux phase. Further, it has been discussed that a hidden topological order exists in cuprates, which shares some aspects with the flux phase. In general, however, the flux phase competes with other instabilities e.g. superconductivity, antiferromagnetism, charge order and localization due to disorder (see refs. for the effects of disorder on the flux phase). In particular, the flux phase often competes with superconductivity, which is a direct consequence from the SU(2) symmetry at half filling. We also note that the flux phase can emerge dynamically as well as in a static form.

In this paper, we report effects of the interaction in the two-dimensional flux phase. We choose the two-dimensional Hubbard model with a magnetic flux \( \phi = \pi \) per square plaquette and compare the results with the standard Hubbard model (\( \phi = 0 \)). In the standard Hubbard model at half filling, it is believed that an infinitesimally small interaction drives the ground state to the Mott insulator, where a finite charge gap opens and an antiferromagnetic long-range order exists. This is consistent with the nesting argument in the weak coupling region. On the the hand, in the flux phase without the interaction, the density of state disappear linearly at the Fermi energy, which suggests that the structure of the low energy excitations is singular as compared with a simple Fermi liquid and the nesting instability is absent. Therefore one can expect an interaction-driven quantum phase transition from a singular quantum liquid (density of state is linearly vanishing without interaction) to a gapped insulator (Mott insulator).

II. FLUX PHASE

The flux phase is given by the ground state of the following simple Hamiltonian,

\[
H_F = \sum_{\langle j,k \rangle, \sigma} \left( c_{j \sigma}^\dagger t_{jk} c_{k \sigma} + c_{k \sigma}^\dagger t_{kj} c_{j \sigma} \right),
\]

where \( \langle j,k \rangle \) denotes a nearest-neighbor link. The amplitude of \( t_{jk} \) is constant but its phase factor \( t_{jk}/|t_{jk}| = e^{i\theta_{jk}} \) satisfies a condition \( \theta = \sum_{\text{plaquette}} \theta_{jk} \). It leads to a uniform magnetic flux per plaquette. The phase factor \( \theta_{jk} \) itself is not fixed but the flux \( \phi \) is fixed, which is the gauge independent quantity. This Hamiltonian was proposed as an effective model (in the mean field level) of several correlated electron systems and discussed in many different contexts. One of the focuses was the stability of the flux state. Following the discussion, the optimum, energy-minimizing, magnetic flux at half filling (this is the simplest case) is considered as \( \pi \) per square plaquette. Furthermore, we note that Lieb gave some rigorous results for the stability in a general form.

At half filling, the low-lying excitations of the flux phase is described by massless Dirac fermions. There is a gauge freedom for the phase factor \( \theta_{jk} \) but let us fix them by choosing as \( t_{j + \hat{x},j} = (-1)^{\hat{x}i} t, t_{j + \hat{y},j} = t \) and otherwise zero where \( j = (j_x, j_y) \in \mathbb{Z}^2, \hat{x} = (1,0), \hat{y} = (0,1) \). The energy bands in this gauge are given by

\[
E(k) = \pm 2t \sqrt{\cos^2 k_x + \cos^2 k_y} \quad (2)
\]

\[
\approx \pm 2t \sqrt{(k_x^2 - k_i^2)^2 + (k_y^2 - k_i^2)^2} \quad (i = 1, 2) \quad (3)
\]

where \( (k_x, k_y) \in [-\pi, \pi] \times [0, \pi] \), \( k^1 = (k_x^1, k_y^1) = (\pi/2, \pi/2) \) and \( k^2 = (k_x^2, k_y^2) = (-\pi/2, \pi/2) \). Therefore the low-lying excitations are described by massless Dirac...
fermions at these two gap-closing points and the density of states \( D(\epsilon) \) near the Fermi energy vanishes linearly, \( D(\epsilon) \propto |\epsilon| \). The density of states \( D(\epsilon) \) is singular and it leads to the suppression of the instability against the Mott insulator as discussed below. Note that the dispersion is gauge dependent but the density of state is gauge independent. We focus on only the gauge independent quantity in this paper.

### III. MODEL AND METHOD

We investigate effects of the interaction in the flux phase by the following Hamiltonian,

\[
\mathcal{H} = \sum_{\langle j,k \rangle, \sigma} (c_{j\sigma}^\dagger t_{jk} c_{k\sigma} + c_{k\sigma}^\dagger t_{kj} c_{j\sigma}) + U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2),
\]

where \( \langle j,k \rangle \) denotes a nearest-neighbor link and \( U \) a on-site Coulomb repulsion. The geometry is set to be a two-dimensional square lattice and a periodic boundary condition is imposed. The grand-canonical ensemble is employed and we put the system half-filled by the particle-hole symmetry. The \( |t_{jk}| \) is set to be constant (= 1) and, based on the Lieb’s theorem \[14\], the phase factor \( e^{i\theta_{jk}} \) is chosen so that the magnetic flux \( \phi \) is \( \pi \) per plaquette i.e. \( \pi \)-flux phase \( (\phi = \sum_{\text{plaquette}} \theta_{jk} = \pi) \). We always try to compare the results of the flux phase \( (\phi = \pi) \) with those of the standard Hubbard model \( (\phi = 0) \). It is to be noted that neither the translational nor time-reversal symmetry is broken in the \( \pi \)-flux phase.

In order to study the system based on a non-perturbative approximation free method, the quantum Monte Carlo (QMC) technique is applied \[17,18\]. We use the grand-canonical scheme at finite temperatures. Due to the particle-hole symmetry in the Hamiltonian \[10\], the negative-sign problem does not occur. The simulations were performed on a square lattice with a size up to \( N = 12 \times 12 \) at a temperature down to \( T = 0.05t \). The Trotter decomposition is performed in the imaginary-time direction and the time slice is \( \Delta \tau \approx 0.10/t \). We have checked that the systematic errors due to the Trotter decomposition are almost independent of temperatures and does not change the essential features after the extrapolation. We have typically performed 500 Monte Carlo sweeps in order to reach a thermal equilibrium followed by 5000 measurement sweeps. The measurements are divided into 10 blocks and the statistical error is defined by the variance among the blocks.

The Mott insulator is characterized by the following two features. One is a strong suppression of the charge fluctuation and the other is a presence of the strong antiferromagnetic spin correlation. In order to detect signals of the Mott transition, we have calculated the charge compressibility and the magnetic structure factor. The charge compressibility is defined by

\[
\kappa = \frac{1}{N} \frac{\partial N_e}{\partial \mu} = \frac{\beta}{N} (\langle N_e^2 \rangle - \langle N_e \rangle^2),
\]

where \( N_e \) is the number of electrons and \( \beta \) an inverse temperature. The charge compressibility \( \kappa \) measures the charge fluctuation directly. If the system has a finite charge gap, \( \kappa \) shows a thermally-activated behavior and vanishes at zero temperature. The magnetic structure factor is given by

\[
S(q) = \frac{1}{N} \sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \langle (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow}) \rangle.
\]

If the system has an antiferromagnetic long-range order, \( S(\pi, \pi) \) shows a diverging behavior as the temperature decreases.

### IV. RESULTS

First let us discuss effects of the interaction on the charge compressibility. We compare the result with those of the standard Hubbard model to clarify the effects of the flux, that is, the structure of the low energy excitations. Fig.\[4\] shows results of the charge compressibility \( \kappa \). Since the \( \pi \)-flux state at \( U/t = 0 \) has gapless points in the Brillouin zone and the density of states \( D(\epsilon) \) near the Fermi energy vanishes linearly, \( D(\epsilon) \propto |\epsilon| \), the compressibility \( \kappa \) does not show thermally-activated behavior. Even at \( U/t = 4 \), our data show that effects of the flux is still relevant and the charge gap is not well defined in the flux phase. This implies that the singular spectrum of the excitations seems to survive even with the interaction. Then this possible phase is clearly not a simple Fermi liquid but a singular quantum liquid. As the strength of the interaction increases, effects of the flux becomes irrelevant. If the interaction is sufficiently strong \( (U \gg t) \), the system becomes the Mott insulator with a finite charge gap which is the order of the interaction. Therefore the results suggest the existence of a finite value of the interaction strength, \( U_c \), which separates from a gapless singular phase from the gapped one.

Fig.\[2\] shows the antiferromagnetic structure factor \( S(\pi, \pi) \) versus temperatures. For the standard half-filled Hubbard model, since the ground state has an antiferromagnetic long-range order, \( S(\pi, \pi) \) shows a diverging behavior as the temperature decreases (it saturates when the antiferromagnetic correlation length is longer than the lattice size). On the other hand, for the flux phase, the formation of the long-range antiferromagnetic order is not observed for \( U/t \leq 4 \). According to the spin-wave theory, \( S(\pi, \pi) \) at the zero temperature increases with a lattice size as

\[
\frac{S(\pi, \pi)}{N} = \frac{m^2}{3} + O(N^{-1/2}),
\]

with \( m \) the staggered magnetization which is an order parameter of an antiferromagnetic long-range order. Using
this relation, we try to obtain $m^2$ by plotting $S(\pi, \pi)/N$ versus $N^{-1/2} = L^{-1}$. Fig. shows the plots for $U/t = 4$. The temperature is set to be $T = 0.05t$ where the system reaches the zero temperature limit for the system size. For the standard Hubbard model, the data follow the relation (3) and the extrapolation value is finite indicating the existence of the antiferromagnetic long-range order. On the other hand, for the flux phase, the relation (3) with $m > 0$ does not hold i.e. there is no antiferromagnetic long-range order, which is in contrast to the standard Hubbard model. When one discuss perturbatively, in the flux phase, the stoner instability is strongly suppressed due to the absence of the low energy excitations. The numerical results are consistent with this discussion at least in the weak coupling.

Fig. shows the antiferromagnetic structure factor $S(\pi, \pi)$ for a variety of $U/t$. The antiferromagnetic correlation enhances as $U/t$ increases. As noted above, when $U/t$ is sufficiently large, effects of the flux become irrelevant and one can expect that the antiferromagnetic long-range order appears. Due to the numerical difficulties, we can not perform simulations for stronger interaction ($U/t > 10$) regime. However, if the interaction is sufficiently strong ($U/t > t$), the model (3) is essentially described by the antiferromagnetic Heisenberg model. Therefore the antiferromagnetic long-range order also may appear at some finite value of the interaction strength.

V. DISCUSSION AND SUMMARY

We have studied effects of the interaction in the flux phase. The Mott transition is focused using the quantum Monte Carlo method. Our results on the charge compressibility shows that effects of the flux is relevant for small $U/t$, while it becomes irrelevant when $U/t$ is sufficiently large. The antiferromagnetism, which is characteristic of the Mott insulator, is also strongly suppressed in the weak coupling region. This is due to the structure of the low energy excitations in the flux phase. It implies that the flux state with interaction leads to a new singular phase for $U < U_c$. This is in contrast to the standard two-dimensional Hubbard model. Effects of the doping is also an interesting future issue in connection with the competition with the superconductivity.

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FIG. 1. Temperature dependence of the compressibility for a $N = 10 \times 10$ lattice with interaction strengths $U/t = 0$ (squares), 4 (circles), 6 (diamonds), and 8 (triangles). Solid symbols are for $\phi = \pi$ and open symbols for $\phi = 0$. When the interaction is small ($U/t \leq 4$), the difference between $\phi = 0$ and $\phi = \pi$ is large over wide range of temperatures.

FIG. 2. The antiferromagnetic structure factor $S(\pi, \pi)$ as a function of temperature for $U/t = 4$ on a $N = 10 \times 10$ lattice. In the case of $\phi = 0$, $S(\pi, \pi)$ diverges at low temperatures due to the formation of the antiferromagnetic order. On the other hand, for $\phi = \pi$, $S(\pi, \pi)$ does not show a diverging behavior.

FIG. 3. Extrapolation of antiferromagnetic long-range order. The dashed line is a least-squares fit to the data for $\phi = 0$. For $\phi = 0$, the points extrapolate to a finite value, indicating that the ground state has an antiferromagnetic long-range order. On the other hand, for $\phi = \pi$, $S(\pi, \pi)$ versus $1/L$ suggests the absence of an antiferromagnetic long-range order.

FIG. 4. The antiferromagnetic structure factor $S(\pi, \pi)$ versus the inverse of temperature $\beta$ for $\phi = \pi$ on a $N = 10 \times 10$ lattice with interaction strengths $U/t = 4$ (circles), 6 (diamonds), and 8 (triangles). The antiferromagnetic correlation enhances as $U/t$ increases.