Antiferromagnetic Correlation under the External Magnetic Field in the Hubbard Model

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By deriving a generalized Harper’s equation, we investigate the effects of temperature $T$ and hole doping $\delta$ on antiferromagnetically correlated electrons under the influence of an applied magnetic field. We obtain a phase diagram in a $T-\delta$ plane for staggered magnetization under the external field. We find that away from half filling the maximum values of staggered magnetization occur with rapid convergence to a finite temperature constant near half filling. We discover the reentrant behavior of the staggered magnetization in the presence of the magnetic field.

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Hubbard model is one of the most widely used model for studying the systems of correlated electrons. The original Harper’s equation does not contain the effects of electron correlations and thus it takes into account only non-interacting electrons under external fields. To the best of our knowledge, there is no study of Harper’s equation which takes into account such correlation effects. By considering an infinite square lattice, we derive a generalized Harper’s equation which allows to investigate antiferromagnetic electron correlations under the applied magnetic field. Earlier, our study was limited only to zero temperature and half filling. Here we study how the applied magnetic field affects the system of antiferromagnetically correlated electrons at finite temperatures and away from half filling.

The Hubbard model describing the two-dimensional system (square lattice) of electron correlations under an external magnetic field given by

$$H = -t \sum_{\langle ij \rangle \sigma} \exp \left(-i \frac{2\pi}{\phi_0} \int A \cdot d\ell\right) c_{i \sigma}^\dagger c_{j \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow} - \mu \sum_{\sigma} n_{i \sigma},$$

where $t$ is the hopping integral; $A$, the electromagnetic vector potential; $\phi_0 = \frac{h}{e}$ the elementary flux quantum; $U$, the on-site Coulomb repulsion energy, and $\mu$, the chemical potential. $\langle ij \rangle$ stands for summation over nearest neighbor sites $i$ and $j$. $c_{i \sigma}^\dagger$ ($c_{i \sigma}$) is the creation (annihilation) operator of an electron of spin $\sigma$ at site $i$, and $n_{i \uparrow}$ ($n_{i \downarrow}$), the number operator of an electron of spin up (down) at site $i$.

We are interested in a uniform staggered magnetization (antiferromagnetic (AF) order),

$$m = e^{iQ \cdot r_i} (c_{i \uparrow}^\dagger c_{i \downarrow} - c_{i \downarrow}^\dagger c_{i \uparrow}),$$

where $Q = (\pi, \pi)$, and $r_i = (i_x, i_y)$ with $i_x$ and $i_y$ being integers including 0. The lattice spacing is set to be a unity. Introducing the mean field (Hartree-Fock) approximation,

$$n_{i \uparrow} n_{i \downarrow} \simeq (c_{i \uparrow}^\dagger c_{i \uparrow}) (c_{i \downarrow}^\dagger c_{i \downarrow}) + (c_{i \downarrow}^\dagger c_{i \downarrow}) (c_{i \uparrow}^\dagger c_{i \uparrow}) - (c_{i \uparrow}^\dagger c_{i \downarrow}) (c_{i \downarrow}^\dagger c_{i \uparrow}) (c_{i \uparrow}^\dagger c_{i \downarrow}) - (c_{i \downarrow}^\dagger c_{i \uparrow}) (c_{i \uparrow}^\dagger c_{i \downarrow}) (c_{i \downarrow}^\dagger c_{i \uparrow}),$$

and using the Landau gauge $A = B(0, x, 0)$, we obtain, in the momentum space,

$$H = \sum_{\mathbf{k} \sigma} \left[ 2 \cos k_x c_{\mathbf{k} \sigma}^\dagger c_{\mathbf{k} \sigma} + e^{-i k_y} c_{\mathbf{k} - \mathbf{g} \sigma}^\dagger c_{\mathbf{k} \sigma} + e^{i k_y} c_{\mathbf{k} + \mathbf{g} \sigma}^\dagger c_{\mathbf{k} \sigma} \right]$$

$$-\frac{mU}{2} \sum_{\mathbf{k} \sigma} \sigma c_{\mathbf{k} + \mathbf{g} \sigma}^\dagger c_{\mathbf{k} \sigma} + \left[ \frac{U}{2} (1 - \delta) - \mu \right] \sum_{\mathbf{k} \sigma} c_{\mathbf{k} \sigma}^\dagger c_{\mathbf{k} \sigma},$$

where $\mathbf{g} = 2 \pi \left( \frac{\phi_0}{e}, 0 \right) = 2 \pi \frac{\phi_0}{e}$ with $\phi_0$, the number of flux quanta per plaquette. For simplicity we considered a uniform doping $\delta = 1 - \frac{n}{n_0}$ in the expression above. The first bracketed term in (4) represents hopping processes; the first term in the bracket is contributed from the nearest neighbor hopping in the $x$-direction and the last two terms in the bracket, from the nearest neighbor hopping in the $y$-direction. The external vector potential $A$ shifts the wave vector of electron by $\mathbf{g}$ during its hopping in the $y$-direction. The second term results from the antiferromagnetic electron correlations, and the third term shifts the total energy of the system as a result of hole doping. We do not consider the magnon excitation. Thus the exchange terms in (4) above vanish due to the global SU(2) symmetry.

The diagonalization of (4) yields the following generalized Harper’s equation which now incorporates electron correlations,

$$\det (\mathcal{M} - \epsilon \mathbf{I}) = 0,$$

with

$$\mathcal{M} = \begin{bmatrix} T & \mathbf{U} \\ \mathbf{U} & -T \end{bmatrix},$$

where by setting $M_n = -2 \cos (k_x + ng)$ and $t = 1$,

$$T = \begin{bmatrix} M_1 & -e^{i k_y} & 0 & 0 & -e^{i k_y} \\ -e^{-i k_y} & M_2 & \ddots & \vdots & \vdots \\ 0 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ -e^{-i k_y} & 0 & \cdots & M_{q-1} & -e^{-i k_y} \\ -e^{i k_y} & 0 & \cdots & 0 & -e^{i k_y} \end{bmatrix}.$$
and

$$U = \begin{bmatrix}
-\frac{mU_2}{2} & 0 & 0 & 0 & 0 \\
0 & -\frac{mU_2}{2} & 0 & 0 & 0 \\
0 & 0 & \ddots & 0 & 0 \\
0 & 0 & 0 & -\frac{mU_2}{2} & 0 \\
0 & 0 & 0 & 0 & -\frac{mU_2}{2}
\end{bmatrix} \quad (8)
$$

Here the matrix $T$ is associated with electron hopping, involving phase modulation due to the external field, and $U$, with the antiferromagnetic electron correlations.

$$E_k^{(\pm)} = \pm \sqrt{4t^2 (\cos^2 k_x + \cos^2 k_y) + \left(\frac{mU_2}{2}\right)^2} + \frac{U}{2} (1 - \delta) - \mu \quad (9)$$

Here the staggered magnetization (AF order) $m$ is affected by the applied field. The self-consistent mean field equations for $m$ and $\mu$ are given by

$$1 = \int \frac{d^2k}{(2\pi)^2} \frac{U}{\epsilon_k} \left[ \tanh \left( \frac{E_k^{(+)}}{2T} \right) - \tanh \left( \frac{E_k^{(-)}}{2T} \right) \right], \quad (10)$$

$$\delta = 2 \int \frac{d^2k}{(2\pi)^2} \left[ \tanh \left( \frac{E_k^{(+)}}{2T} \right) + \tanh \left( \frac{E_k^{(-)}}{2T} \right) \right], \quad (11)$$

where the prime denotes integration over the reduced Brillouin zone of $(k_x, k_y)$ with $-\frac{\pi}{2} \leq k_x, k_y \leq \frac{\pi}{2}$, as shown in Fig. 1(a).

Now in order to realistically investigate the effect of an applied magnetic field on the two-dimensional system of antiferromagnetically correlated electrons we consider a case of half a flux quantum per plaquette, that is, $\frac{p}{q} = \frac{1}{2}$. The energy dispersion relation is then obtained as

$$E_k^{(\pm)} = \pm \sqrt{4t^2 (\cos^2 k_x + \cos^2 k_y) + \left(\frac{mU_2}{2}\right)^2} + \frac{U}{2} (1 - \delta) - \mu \quad (9)$$

Here the elementary flux quantum $\phi_0$ is set to be a unity.}

FIG. 1. Reduced Brillouin zone (shaded region) for the computation of energy dispersion relation with (a) half a flux quantum per plaquette, $\frac{p}{q} = \frac{1}{2}$, and (b) no magnetic field, $\frac{p}{q} = 0$. Here the elementary flux quantum $\phi_0$ is set to be a unity.

FIG. 2. Phase diagram of the staggered magnetization (AF order) in the $(T, \delta)$ plane with (a) $U = 4t$ (b) $U = 8t$. The dashed and solid lines indicate the boundary of antiferromagnetic states for the magnetic flux quanta per plaquette, $\frac{p}{q} = 0$ and $\frac{p}{q} = \frac{1}{2}$ respectively. Here the elementary flux quantum $\phi_0$ is set to be a unity.
In order to examine the dependence of the external magnetic field (the solid lines in Fig. 2) on the staggered magnetization (AF order) \( m \) in the \( T-\delta \) plane we solved numerically Eqs. (10) and (11). We find that the reentrant behavior of the staggered magnetization (AF order) persists at a certain region of doping rate \( \delta \) despite the application of the external magnetic field. The reentrant behavior appears at smaller doping rates for weaker correlations (see the case of \( U = 4t \)), as shown in Fig. 2. The domain of antiferromagnetic phase is smaller compared to the case of zero external field (the dotted lines in Fig. 2). The band gap \( mU \) owing to the antiferromagnetic correlations gets smaller in the presence of the external magnetic field as a consequence of reduced magnetization \( m \). Such effect of reduction was predicted to be much larger with \( U = 4t \) than with \( U = 8t \), as shown in the figure.

We now investigate the reentrant behavior of staggered magnetization more in detail. In Fig. 3(a) we display the staggered magnetization \( m \) as a function of both temperature \( T \) and doping rate \( \delta \). At exactly half filling, i.e., \( \delta = 0 \), \( m \) reaches the maximum at zero temperature. We find that the temperature at which it reaches a maximum value quickly increases and converges to a finite temperature near half filling, as shown in Fig. 3(b). The reentrant behavior with \( U = 8t \) occurs more clearly at a region of higher doping rates (say \( 0.42 < \delta < 0.48 \)), as shown in Fig. 3(b). We see more readily from Fig. 3(c) the variation of reentrant behavior with the increasing doping rate. We find explicitly the rapid decrease of the AF order (staggered magnetization) with doping rate at a given temperature, e.g., \( kT = 1t \), as shown in Fig. 3(c).

Let us now consider the limiting case of vanishing external magnetic field (\( B = 0 \)). We obtain from (4) the following expression,

\[
H = -2t \sum_{k,\sigma} (\cos k_x + \cos k_y) c_{k\sigma}^{\dagger} c_{k\sigma} \\
- \frac{mU}{2} \sum_{k,\sigma} \sigma c_{k+Q,\sigma}^{\dagger} c_{k\sigma} + \frac{U}{2}(1 - \delta) - \mu \sum_{k,\sigma} c_{k\sigma}^{\dagger} c_{k\sigma}
\]

(12)
as a result of \( g = 0 \). The dispersion relation is then, by diagonalizing the Hamiltonian above \( \mathcal{H} \),

\[
E_k^{(\pm)} = \pm \sqrt{4t^2(\cos k_x + \cos k_y)^2 + \left( \frac{mU}{2} \right)^2}
+ \frac{U}{2}(1 - \delta) - \mu
\]

(13)
The self-consistent equations for \( m \) and \( \mu \) are, in form, the same as (14) and (15) above. However the integral is now over the reduced Brillouin zone of \( (k_x, k_y) \) with \( |k_x| + |k_y| \leq \pi \) as shown in Fig. 3(b).
ally lower. Now for the limiting case of the zero external field (the dotted lines in Fig. 2), we find that there exists a reentrant behavior with a larger domain of staggered magnetization (AF order) in the $T-\delta$ plane compared to the case of the applied external field (the solid lines in Fig. 2). In qualitative agreement with our present results, Halvorsen et al. [6] also showed the reentrant behavior using a different approach. They used the Hubbard model within the self-consistent second-order weak $U$-perturbation treatment, thus allowing to study only a limited region of small $U$. Lately, Inaba et al. [7] found qualitatively a similar reentrant behavior using the $t$-$J$ Hamiltonian in the slave-boson representation, permitting to investigate only the large $U$ limit case. On the other hand, our present approach allows to examine the full range of $U$, although we are not able to display all details due to a limited space. Further, unlike our present case, their studies were limited only to the case of zero external magnetic field.

In the present study we derived the generalized Harper’s equation which incorporates correlation effects between electrons. Unlike other studies [6,7] we were able to examine as a function of both temperature and doping rate the variation of the staggered magnetization $m$ for the system of antiferromagnetically correlated electrons under the external magnetic field. By deducing the phase diagram in the $T-\delta$ plane, we explored staggered magnetization $m$ as a function of both temperature and doping rate and found the reentrant behavior even in the presence of the applied magnetic field. Finally, it is of note that the staggered magnetization or the AF order for other values of magnetic flux $\frac{q}{q_0}$ can be investigated in a similar manner. Further studies regarding this problem will be resumed on.

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