Zero-temperature Phase Diagram of Two Dimensional Hubbard Model

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Abstract. We investigate the two-dimensional Hubbard model on the triangular lattice with anisotropic hopping integrals at half filling. By means of a self-energy functional approach, we discuss how stable the non-magnetic state is against magnetically ordered states in the system. We present the zero-temperature phase diagram, where the normal metallic state competes with magnetically ordered states with \((\pi, \pi)\) and \((2\pi/3, 2\pi/3)\) structures. It is shown that a non-magnetic Mott insulating state is not realized as the ground state, in the present framework, but as a meta-stable state near the magnetically ordered phase with \((2\pi/3, 2\pi/3)\) structure.

Geometrical frustration in strongly correlated electron systems has attracted current interest. One of the typical examples is an organic material \(\kappa\)-(BEDT-TTF)\(_2\)Cu\(_2\)(CN)\(_3\) with the triangular lattice structure, where a non-magnetic insulating state is realized down to low temperatures \(T \sim 32\text{mK}\)\([1]\). This suggests that a novel spin-liquid insulating state is stable against magnetically ordered states, which stimulates further theoretical investigations on frustrated electron systems \([2–9]\). Although a non-magnetic insulating state was shown to be a probable candidate for the ground state of the Hubbard model on the triangular lattice \([2–4, 6]\), it has not been discussed how this state competes with an antiferromagnetic insulating state with \(120^\circ\) spin structure (\(120^\circ\)-AFI) expected naively. Recently, it was claimed that the \(120^\circ\)-AFI state is, instead of the nonmagnetic insulating state, stabilized in the strong coupling regime by means of variational Monte Carlo (VMC) simulations \([7]\). However, this method may not deal with non-local correlations properly, which should be important in the two-dimensional frustrated systems. Therefore, it is highly desirable to deal with intersite correlations as well as onsite correlations on an equal footing in order to clarify the ground-state properties of the frustrated systems.

Motivated by this, we study the two-dimensional half-filled Hubbard model with geometrical frustration. The model Hamiltonian is given by \(\mathcal{H} = \mathcal{H}_0(\mathbf{t}) + \mathcal{H}'(\mathbf{U})\) with

\[
\mathcal{H}_0(\mathbf{t}) = \sum_{rr'} \sum_{\sigma} t_{rr'} c^\dagger_{r\sigma} c_{r'\sigma},
\]

\[
\mathcal{H}'(\mathbf{U}) = \sum_{r} U n_{r\uparrow} n_{r\downarrow},
\]

and \(\mathbf{t} (\mathbf{U})\) is the parameter-matrix of the one-particle (two-particles) term, where \(c^\dagger_{r\sigma} (c_{r\sigma})\) creates (annihilates) an electron with spin \(\sigma(=\uparrow, \downarrow)\) at site \(r\), and \(n_{r\sigma}\) is the number operator. Here,
\(t_{rr'} = t(t')\) is the nearest-neighbor (second nearest-neighbor) hopping, which is schematically shown in Fig. 1 (a), and \(U\) the on-site Coulomb interaction. We also give a sketch of the square lattice with specific diagonal hopping in Fig. 1 (b), which is topologically equivalent to the triangular lattice with anisotropic hopping. When \(t = t'\), the system is equivalent to the Hubbard model on the triangular lattice. In the following, we set \(t = 1\) as the energy unit.

To study the ground-state properties of the system, we make use of a self-energy functional approach (SFA), which is based on the Luttinger-Ward variational principle \([10]\). It provides us with a non-perturbative treatment of strong correlations, and an efficient and tractable way to investigate the metal-insulator transition (MIT) with and without symmetry breaking \([3, 11–13]\). An advantage in this method is to take into account intersite correlations as well as local electron correlations on an equal footing, which enables us to discuss the competition between the nonmagnetic insulating state and the magnetically ordered states.

In this method, the ground potential \(\Omega\) is given as a function of a reference self-energy \(\Sigma(t')\),

\[
\Omega[\Sigma(t')] = \Omega(t') + \text{Tr} \ln \left\{ -\left[ \omega + \mu - t - \Sigma(t') \right]^{-1} \right\} - \text{Tr} \ln \left\{ -\left[ \omega + \mu - t' - \Sigma(t') \right]^{-1} \right\}
\]

where \(\Omega(t')\) is the ground potential for a reference system with the Hamiltonian \(\mathcal{H}_{ref} = \mathcal{H}_0(t') + \mathcal{H}'(U)\). We note that the Hamiltonian of the reference system is defined by the substitution of the parameter-matrix \(t'\) for \(t\) in the original Hubbard Hamiltonian, where we should keep \(U\) unchanged. The variational condition \(\partial \Omega[\Sigma(t')] / \partial t' = 0\) provides us with an approximate self-energy which properly describes physical properties of the original model. When one applies the SFA to the present system, a cluster Anderson impurity model is one of the most appropriate reference systems. It is described by the following Hamiltonian,

\[
\mathcal{H}_0(t') = \sum_{\mathbf{R}} \left\{ \sum_{\mathbf{r}\mathbf{r}'} \sum_{\sigma} t_{\mathbf{r}\mathbf{r}'} c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} + \sum_{\ell=1}^{N_b} \sum_{\mathbf{r}} \sum_{\sigma} \varepsilon_{\ell\mathbf{r}a\mathbf{r}\sigma} a^\dagger_{\ell\mathbf{r}\sigma} a_{\ell\mathbf{r}\sigma} + \sum_{\ell=1}^{N_b} \sum_{\mathbf{r}} \sum_{\sigma} V_{\ell}(c^\dagger_{\ell\mathbf{r}+\mathbf{R}\sigma} a_{\ell\mathbf{r}\sigma} + H.c.) + \sum_{\mathbf{r}} \exp(i \mathbf{r} \cdot \mathbf{Q}) \mathbf{H}_Q \cdot \mathbf{S}_{\mathbf{r}+\mathbf{R}} \right\},
\]

where \(\sum_{\mathbf{r}} (\sum_{\mathbf{R}})\) sums up sites (clusters) in the cluster (the whole lattice) and \(\{t_{\mathbf{r}\mathbf{r}'}\}, \varepsilon_{\ell\mathbf{r}a\mathbf{r}\sigma}, V_{\ell}, \mathbf{H}_Q\) are variational parameters. \(a^\dagger_{\ell\mathbf{r}\sigma}(a_{\ell\mathbf{r}\sigma})\) creates (annihilates) an electron with spin \(\sigma\) at the \(\ell(= 1, \cdots, N_b)\)th site in the effective bath, which is connected to the original lattice at site \(\mathbf{r}\). In order to deal with magnetically ordered states, we introduce the effective magnetic field \(\mathbf{H}_Q\) in the reference system. Here, \(\mathbf{S}_{\mathbf{r}} = \frac{1}{2} \sigma_{\gamma\gamma} c_{\mathbf{r}\gamma} c^\dagger_{\mathbf{r}\gamma'}\), where \(\sigma\) is the Pauli matrix. In this study, we mainly discuss the triangular lattice, \(t = t'\). In the following, to investigate the MIT of the half-filled Hubbard model, we examine a free energy \(F = \Omega - \mu N\) with an additional variational condition \(\partial F / \partial \mu = 0\), where \(\mu\) is the chemical potential and \(N\) is the total number of electrons.

Before addressing a magnetic instability, we first consider the zero-temperature properties in the paramagnetic state. This might be important at very low temperatures since magnetically ordered states become unstable in two dimensions. Here, we use a two-site cluster with \(\mathbf{H}_Q = 0\). 

![Figure 1](Link to image) 

\textbf{Figure 1.} (a) [(b)] Sketch of the structure of the model Hamiltonian (a topologically equivalent structure of the model). 

\(H_{substitution}\) of the parameter-matrix \(U\) should keep the triangular lattice with anisotropic hopping. When \(t = t'\), the system is equivalent to the Hubbard model on the triangular lattice. In the following, we set \(t = 1\) as the energy unit.

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Figure 2. (a) [(c)] Lattice structure for two-(three-)site clusters, which are represented by rectangles (triangles). (b) [(d)] Cluster impurity model to describe a magnetically ordered state in the original model, where arrows indicate the direction of the effective magnetic field. Dark (white) circles correspond to the impurity-(bath-)site.

Figure 3. (a) Free energy $F$ as a function of the variational parameter $V$ for $t' = 1$. Triangles (crosses) correspond to the stationary points for the paramagnetic insulating (paramagnetic metallic) states. (b) Free energies $F$ for several states as a function of $U$ when $t' = 1$. The inset shows an enlarged picture around $U \sim 9.5$.

as a reference system, which is illustrated in Fig. 2 (b). The obtained free energy is shown in Fig. 3 (a). In the small $U$ region ($U \lesssim 7.8$), we find one stationary point with a large $V$, which should represent the paramagnetic metallic (PM) state. The increase in $U$ gradually changes the stationary point and decreases its variational parameter $V$, which implies that the heavy quasi-particle state is realized in the case $U \lesssim 7.8$. On the other hand, the paramagnetic insulating (PI) state appears in the strong coupling region ($U \gtrsim 10.3$), which is shown as another stationary point in the figure. Thus, these two phases compete with each other and a first-order MIT between the PI and the PM states occurs around $U \sim 9.6$ as far as the paramagnetic states are concerned.

However, this result does not necessarily imply that the PI state is stable against magnetically ordered states at zero temperature. To make this clear, we discuss the magnetic instability in the system. Potential candidates for the ordered states are the $(\pi, \pi)$-antiferromagnetic insulating (AFI) state and the 120$^\circ$-AFI state. By using two kinds of the reference systems illustrated in Figs. 2 (b) and (d), we obtain the free energies for paramagnetic and magnetically ordered states, as shown in Fig. 3 (b). We can see that the PM state is stable in the small $U$ region. On the other hand, it is found that in the strong coupling limit, the 120$^\circ$-AFI state is stabilized, which is consistent with the results for the Heisenberg model. At $U_c \sim 8.4$, the free energies for these states cross each other, suggesting the first-order MIT accompanied by symmetry breaking. We also find that the non-magnetic insulating state is no longer realized as the ground state within the present approach. Nevertheless in the PM region ($7.7 \lesssim U \lesssim 8.4$), the non-magnetic insulating state exists as a meta-stable state. Therefore, if the interacting system
is adiabatically cooled down, the meta-stable non-magnetic insulating state could emerge down to zero temperature.

By performing SFA calculations with several values of $t'$, we obtain the ground-state phase diagram of the half-filled Hubbard model, which is shown in Fig. 4. The PM state is stable in the weakly correlated region with $t' \neq 0$. In the strongly correlated region, the $(\pi, \pi)$-AFI state competes with the $120^\circ$-AFI state and the phase transition occurs at $t'_c \sim 0.8$. These results are consistent with those obtained by the VMC calculations [7]. In Fig. 4, we show the region where the non-magnetic insulating state is not realized as the ground state, but appears as a meta-stable state.

In summary, we have investigated the half-filled Hubbard model on the triangular lattice with anisotropic hopping integrals by means of a self-energy functional approach. We have clarified how the normal metallic state competes with the magnetically ordered states with $(\pi, \pi)$ and $(2\pi/3, 2\pi/3)$ structures. When $t \neq t'$, another type of magnetically ordered state with an incommensurate wave vector $\mathbf{Q}$ might be also possible [14], which has not been addressed in this paper. Therefore, it remains an important problem to explore the stability of such ordered states, which is now under consideration. Furthermore, it has been suggested that in the square-lattice model with next-nearest hopping, which is another important frustrated system slightly different from the present one, the collinear ordered phase with $(\pi, 0)$ or $(0, \pi)$ is stabilized for large frustration[5, 9]. Comprehensive investigations including such frustrated systems are important, which are left for the future study.

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