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Zero-temperature Phase Diagram of Two
Dimensional Hubbard Model

K. Inaba\textsuperscript{a}, A. Koga\textsuperscript{b}, S. Suga\textsuperscript{a}, and N. Kawakami\textsuperscript{b}

\textsuperscript{a}Department of Applied Physics, Osaka University, Suita, Osaka 565-0871, Japan
\textsuperscript{b}Department of Physics, Kyoto University, Kyoto 606-8502, Japan

E-mail: inaba@tp.ap.eng.osaka-u.ac.jp

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)\textsubscript{2}Cu\textsubscript{2}(CN)\textsubscript{3}
with the triangular lattice structure, where a non-magnetic insulating state is realized down to low temperatures
\(T \sim 32\text{mK}\)\textsuperscript{[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
\textsuperscript{[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 \textsuperscript{[2–4,6]}, it has not been
discussed how this state competes with an antiferromagnetic insulating state with \(120^\circ\) spin
structure \((120^\circ\text{-AFI})\) expected naively. Recently, it was claimed that the \(120^\circ\text{-AFI}\) state is,
instead of the nonmagnetic insulating state, stabilized in the strong coupling regime by means
of variational Monte Carlo (VMC) simulations \textsuperscript{[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 \(\mathcal{H} = \mathcal{H}_0(t) + \mathcal{H}'(U)\) with

\[
\mathcal{H}_0(t) = \sum_{rr'} \sum_{\sigma} t_{rr'} c_{rr' \sigma}^\dagger c_{rr' \sigma}, \tag{1}
\]

\[
\mathcal{H}'(U) = \sum_{r} U n_{r \uparrow} n_{r \downarrow}, \tag{2}
\]

and \(t (U)\) is the parameter-matrix of the one-particle (two-particles) term, where \(c_{rr' \sigma}^\dagger (c_{rr \sigma})\) creates
(annihilates) an electron with spin \(\sigma (\uparrow, \downarrow)\) at site \(r\), and \(n_{r \sigma}\) is the number operator. Here,
Substitution of the parameter-matrix 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.

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

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

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,

$$\mathcal{H}_0(t') = \sum_{\mathbf{R}} \left\{ \sum_{\mathbf{r}'} \sum_{\mathbf{r}} \sum_{\sigma} \epsilon_{\mathbf{r}r} c_{\mathbf{r}r}^\dagger c_{\mathbf{r}r'} + R, \sigma \right\} + \sum_{\ell=1}^{N_b} \sum_{r} \sum_{\sigma} \epsilon_{\mathbf{r}r} a_{\mathbf{r}r\sigma}^\dagger a_{\mathbf{r}r\sigma}$$

$$+ \sum_{\ell=1}^{N_b} \sum_{\mathbf{r}'} \sum_{\mathbf{r}} V_{\ell}(c_{\mathbf{r}r}^\dagger R, \sigma a_{\mathbf{r}'r\sigma} + H.c.) + \sum_{\mathbf{r}} \exp(i\mathbf{r} \cdot \mathbf{Q}) \mathbf{H}_Q \cdot \mathbf{S}_{\mathbf{r}+R},$$

where $\sum_{\mathbf{r}} (\sum_{\mathbf{R}})$ sums up sites (clusters) in the cluster (the whole lattice) and $(t'_{\mathbf{r}r'}, \epsilon_{\mathbf{r}r}, V_{\ell}, \mathbf{H}_Q)$ are variational parameters. $a_{\mathbf{r}r\sigma}^\dagger (a_{\mathbf{r}r\sigma})$ 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 $r$. In order to deal with magnetically ordered states, we introduce the effective magnetic field $\mathbf{H}_Q$ in the reference system. Here, $\mathbf{S}_r = \frac{1}{2} c_{\mathbf{r}r}^\dagger \sigma_{\gamma\gamma} c_{\mathbf{r}r}$, 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 $\mathbf{H}_Q = 0$. 

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**Figure 1.** (a) [(b)] Sketch of the structure of the model Hamiltonian (a topologically equivalent structure of the model).
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 $U \approx 7.8$. 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 $U_c \approx 8.4$, 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 $Q$ 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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