Effect of impurity potentials on antiferromagnetism in two-dimensional Hubbard model

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Abstract. Recent numerical studies have shown that antiferromagnetism (AF) prevails widely near half filling in the two-dimensional Hubbard ($t$-$t'$-$U$) model, contrary to the experiments on cuprate superconductors. In cuprates, disorders owing to the dopants, which are usually disregarded in theory, are possibly intrinsic and considerable. Thus, as a first step, we consider the effects of point-type impurity potentials, which are randomly distributed on the lattice sites, on the stability of AF. It is found that a moderate impurity potential does not modify the stability of AF, but a sufficiently strong attractive potential ($U < -U$) appreciably weakens an antiferromagnetic state owing to an insufficient screening of $V$.

1. Introduction

Recent theoretical studies using various refined methods \cite{1, 2} have argued that antiferromagnetism (AF) and phase separation widely prevail in areas near half filling of two-dimensional Hubbard ($t$-$t'$-$U$) models, by which the cuprate superconductors (SCs) have been considered to be well described. And $d_{x^2-y^2}$-wave superconductivity ($d$-SC) appears only in the edge of these areas mainly in the overdoped regime. A similar result was reported for the $d$-$p$ model \cite{3}. Such a situation apparently contradicts the experiments on cuprates. This discrepancy indicates that some common mistakes exist or some essential factors are missed in common in the above theories.

A factor often disregarded in the theories of cuprates is the effect of disorder owing to the carrier dopants, which are inherent in the cuprate SCs and are usually situated in the so-called block layers, namely, off the conducting CuO$_2$ layers. They will work as weak scatterers, in contrast to the in-plane substitutions for Cu sites (strong scatterers). Although the effects of disorder in Hubbard models have been studied by many theorists in various contexts—for instance, Anderson-Mott transitions and vortex core problems—, to our knowledge there are a small number of studies from the viewpoint of how the weak scatterers affect an already existing AF order in the CuO$_2$ plane \cite{4}.

In this publication, we discuss preliminary results of a study in this line obtained using a standard variational Monte Carlo (VMC) method \cite{5, 2}, which is useful to solve a model with strong correlation in a reliable manner. As a primary step, we introduce a point-type impurity potential $V$, which acts on the single site close to an impurity, into the standard Hubbard ($t$-$t'$-$U$) model, and check whether or not the impurity potential destabilizes an antiferromagnetic (AF) state by varying $V$ and other model parameters. Here, however, we focus on a few cases of specific parameter settings.

2. Model and method

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As a simplified model of cuprate SCs, we study the following Hubbard model \((U \geq 0)\) with spin-independent point impurity potentials on extended square lattices:

\[
H = H_{\text{kin}} + H_{U} + H_{\text{imp}} = - \sum_{(i,j),\sigma} t_{ij} \left( c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.} \right) + U \sum_{j} n_{j\uparrow} n_{j\downarrow} + V \sum_{\ell=1}^{N_{\text{imp}}} \sum_{\sigma} n_{\ell\sigma},
\]

where \(n_{j\sigma} = c_{j\sigma}^{\dagger} c_{j\sigma}\), and \((i,j)\) indicates the sum of pairs on sites \(i\) and \(j\). In this work, the hopping integral \(t_{ij}\) is \(t\) for nearest neighbors \((\geq 0)\), \(t'\) for diagonal neighbors, and 0 otherwise \((H_{\text{kin}} = H_{t} + H_{t'})\). We use \(t\) and the lattice spacing as the units of energy and length, respectively. Because the value of \(t'/t\) is estimated as \(-0.1\)\(-0.4\) for hole-doped cuprate SCs, we use a typical value \(t'/t = -0.3\) in the following. Because the value of \(U/t\) in hole-doped cuprates is considered larger than the Mott-transition points \(U_{c}/t = 6\)\(-8\), we discuss the \(V\) dependence for \(U/t = 12\).

In this work, we assume that the impurity potential \(V\) comes from the carrier dopants situated in adjacent block layers (weak scatterers), and acts on respective single sites for simplicity. Therefore, the index \(\ell\) in \(H_{\text{imp}}\) runs over the "impurity sites" \(r_{\ell} (\ell = 1, \cdots, N_{\text{imp}})\), and the number of impurities is equal to that of doped holes: \(N_{\text{imp}} = N_{s} - N\) with \(N\) and \(N_{s}\) being the numbers of electrons and sites, respectively. We also assume that the impurity sites are randomly distributed. Practically, \(V\) may be positive and weak, but we widely varies it to grasp overall features. In this publication, we mainly consider cases for \(V < 0\), because the calculations have not yet been stable for large positive \(V/t\). Thus, we also discuss \(U/t\) dependence for \(V/t = -4\). Although the present setting of impurity potential may be simplistic, we believe that fundamental aspects of impurity potentials can be captured. We will treat more realistic settings in coming publications. We impose the periodic-antiperiodic boundary conditions for the consistency with previous studies.

To the Hamiltonian Eq. (1), we apply a variational Monte Carlo (VMC) method [5], which enables us to exactly estimate expectation values with respect to many-body wave functions. As a trial wave function, we use a Jastrow type: \(\Psi = P \Phi\), where \(P\) indicates a product of many-body projection (Jastrow) factors and \(\Phi\) is a mean-field-type one-body wave function. For the many-body factor, we use \(P = P_{Q}P_{G}\). In the onsite (Gutzwiller) projection \(P_{G}\), we distinguish ordinary and impurity sites as

\[
P_{G} = \prod_{j \neq \ell} \left[ 1 - (1 - g) n_{j\uparrow} n_{j\downarrow} \right] \prod_{\tau=1}^{N_{\text{imp}}} \left[ 1 - (1 - g_{\text{imp}}) n_{\tau\uparrow} n_{\tau\downarrow} \right],
\]

where \(g\) and \(g_{\text{imp}}\) are variational parameters. If the optimized value of \(g\) (or \(g_{\text{imp}}\)) is smaller [larger] than 1, the effective onsite interaction is repulsive (attractive). \(P_{Q}\) is an asymmetric projection between a nearest-neighbor doubly occupied site (doublon) and an empty site (holon) [6, 7, 8],

\[
P_{Q} = \prod_{j} \left[ 1 - \zeta_{d} d_{j} \prod_{\tau} \left[ (1 - h_{j+\tau}) - \zeta_{h} h_{j} \prod_{\tau} (1 - d_{j+\tau}) \right] \right],
\]

where \(d_{j} = n_{j\uparrow} n_{j\downarrow}\), \(h_{j} = (1 - n_{j\uparrow})(1 - n_{j\downarrow})\), and \(\tau\) runs over the nearest-neighbor sites of site \(j\). Here, \(\zeta_{d}\) and \(\zeta_{h}\) are variational parameters. As shown before [9], the doublon-holon binding factor is crucial for appropriately treating Mott physics for \(U \geq U_{c}\) \((U_{c}:\text{Mott transition point})\). For simplicity, we do not distinguish impurity sites from ordinary sites in \(P_{Q}\) in this paper.
For obtaining the one-body part $\Phi$, we diagonalize the following mean-field Hamiltonian,

$$ H_{MF} = H_{kin}^{BR} + U \sum_{j,\sigma} \langle n_{j\sigma} \rangle n_{j-\sigma} + V_{eff} \sum_{\ell=1}^{N_{imp}} \sum_{\sigma} n_{\ell\sigma} . $$

Following Ref. [2], a band-renormalization effect (BRE) is introduced in the kinetic part as

$$ H_{kin}^{BR} = -t \sum_{(i,j),\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H. c.}) - \sum_{(i,j),\sigma} t_{\eta}(c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H. c.}) $$

where the first term indicates the nearest-neighbor hopping and the second term virtual hoppings up to fifth neighbors as shown in Fig. 1. Here, $t_{\eta}$'s ($\eta = 1 \sim 4$) are variational parameters; $t_1$ is optimized independently of $t'$ in Eq. (1). For $U/t \to 0$, the optimized band parameters are reduced to $t_1 \to t'$ and $t_{\eta} \to 0$ for $\eta = 2 \sim 4$. As shown before [2], BRE up to $t_4$ should be included for a state with an AF order. In the second term of Eq. (4), we take account of AF order of the nesting vector $Q = (\pi, \pi)$ as

$$ \langle n_{j\sigma} \rangle = \frac{n}{2} + \delta_{AF} \text{sign}(\sigma) e^{iQ \cdot r_j}, $$

where $n = N/N_s$, \text{sign}(\sigma) = 1 or $-1$ according to $\sigma = \uparrow$ or $\downarrow$, and $\delta_{AF}$ is a variational parameter that controls the magnitude of AF order. In the last term of Eq. (4), a screening of impurity potential owing to electron correlation is considered; $V_{eff}/V$ is an important parameter.

Diagonalizing $H_{MF}$ of an $N_s \times N_s$ matrix, we obtain eigenenergies $\varepsilon_n$ and eigenvectors $\phi_n$ with corresponding quasiparticle operators $\alpha_{n,\sigma}^{\dagger}$, which are linear combinations of $c_{j\sigma}^{\dagger}$. Using $\alpha_{n,\sigma}^{\dagger}$, one-body part is written as

$$ \Phi = \prod_{n} \prod_{\sigma} \langle \alpha_{n,\sigma}^{\dagger} | 0 \rangle, $$

where $\varepsilon_F$ indicates the energy of the highest occupied level (HOMO). The trial wave function $\Psi (= P\Phi)$ is reduced to the exact noninteracting ground state of Eq. (1) for $U = 0$, and becomes identical to the correlated AF state with BRE used in a preceding study for the pure state [2] for $V = 0$, a large $U/t$ and a small $\delta$. We represent a correlated AF [paramagnetic (PM)] state as $\Psi_{AF}$ [$\Psi_{PM} = \Psi_{AF}(\delta_{AF} = 0)$].

We compute expectation values of $\Psi$ using a VMC method similarly to Ref. [2]. In this paper, we exhibit preliminary data for a system with $N_s = 10 \times 10$ sites and 92 electrons, namely, impurity density and doping rate (hole density) are $N_{imp}/N_s = \delta = 0.08$. In most cases, we will simultaneously display the data for 4–8 configurations of impurity sites $\{r_i\}$, which are randomly created. We found that $\{r_i\}$ dependence is small except for special cases, where, for instance, plural impurity clusters are accidentally created.

3. Results

3.1 $U/t$ dependence in attractive potential
We start with $U/t$ dependence in a moderate attractive potential ($V/t = -4$). In the previous study for the pure model ($V/t = 0$) [2], we found that an AF order is absent for $U < U_{AF} \approx 3.75t$ for $t'/t = -0.3$ and $\delta = 0.08$. In the main panel of Fig. 2, the total energy per site for $V/t = -4$ are compared between the AF and PM states. Corresponding to the case of $V = 0$, the AF state has a lower energy than that of the PM state for $U > U_{AF} \approx 4t$ and the staggered magnetization (an order parameter for AF)

$$m = \frac{2}{N_s} \sum_j e^{i Q j} \langle S_j^z \rangle,$$

becomes finite as shown in the inset of Fig. 2. For intermediate values of $U/t$, $m$ in the present case ($V/t = -4$) is somewhat smaller than that in the pure case, but for $U/t \gtrsim 10$, $m$ is almost identical in the two cases. This is because the screening for $V$ becomes effective for strongly correlated cases, as we will discuss shortly.

In Fig. 3, the optimized onsite correlation parameters are plotted. The parameter for the ordinary sites $g$ is almost identical between $V/t = 0$ and $-4$ for any $U/t$ and irrespective of whether the state is AF or PM; $g$ monotonically decreases as the repulsive interaction $U/t$ increases. On the other hand, the onsite factor for the impurity sites $g_{imp}$ becomes $g_{imp} > 1$ for $U \lesssim |V|$; the effective correlation in the impurity sites is attractive in this regime. For $U > |V|$, however, $g_{imp}$ also monotonically decreases and approaches the value of the pure case. This is again screening effect owing to the electron correlation on the impurity potential. In the main panel of Fig. 4, we show $U/t$ dependence of $V_{eff}/V$ for the two states. As $U/t$ increases, $V_{eff}/V$ rapidly decreases and almost vanishes for $U \gtrsim W$ ($W = 8t$: band width). Thus, the attractive impurity potential $V$ is almost completely screened in the strongly correlated regime. Such a tendency of the screening effect on impurity potentials owing to strong correlations has been known in various contexts [10].

### 3.2 $V/t$ dependence in strongly correlated regime

Let us consider how the effect of $V$ evolves as $V$ varies in a strongly correlated regime ($U/t = 12$). First, we look at the energy difference between $\Psi_{AF}$ and $\Psi_{PM}: \Delta E = E(\text{PM}) - E(\text{AF})$, which is plotted in Fig. 5. The energy gain by the AF order $\Delta E$ changes only very slightly for $-W \leq V \leq t$. Corresponding to this behaviour of $\Delta E$, the gap parameter $\delta_{AF}$ and the order parameter $m$ also vary.
only very slightly in this range of $V/t$. Thus, a point impurity potential does not affect the robustness of the AF state realized for the pure state ($V/t = 0$) at least for moderate (especially attractive) values of $V/t$. This is because the screening of impurity potential is very effective and $V_{\text{eff}}/V$ almost vanishes in this regime both for $\Psi_{\text{PM}}$ and $\Psi_{\text{AF}}$, as shown in the inset of Fig. 4.

**Figure 4.** The effective impurity potential ($V_{\text{eff}}/V$) is shown as a function of $U/t$ for $V/t = -4$ in the main panel, and as a function of $V/t$ for $U/t = 12$ in the inset. In both, the values of the AF and PM states are compared.

On the other hand, in the regime of strong impurity potential of $V \leq -U$, $m$ and especially $\Delta E/t$ decrease as $|V|/t$ increases. This is because the screening effect becomes somewhat weak, as seen in the inset of Fig. 4. Consequently, effective onsite correlation in the impurity sites again becomes attractive as shown in Fig. 6, where $g$ and $g_{\text{imp}}$ are plotted as functions of $V/t$. The change in $g$ is very small, whereas $g_{\text{imp}}$ monotonically increases as $V/t$ decreases for $V/t < 0$ and becomes larger than 1 for $V \leq -U$. The relation $g_{\text{imp}}(\text{AF}) > g_{\text{imp}}(\text{PM})$ holds for $V < 0$. This feature is better understood by the behaviour of double occupancy $d$ and electron density at impurity sites $n_{\text{imp}}$ defined as

$$d = \frac{1}{N} \sum_j \langle n_{j\uparrow} n_{j\downarrow} \rangle, \quad n_{\text{imp}} = \frac{1}{N_{\text{imp}}} \sum_{\xi=1}^{N_{\text{imp}}} \sum_{\sigma} \langle n_{\xi\sigma} \rangle. \quad (9)$$

$V/t$ dependence of these quantities are shown in Fig. 7. Note that, as $V/t$ decreases, $n_{\text{imp}}$ approaches 2, for which all impurity sites are doubly occupied. This is reflected in the marked increases of average double occupancy $d$ for $V \leq -U = -12t$. To conclude, in the cases of strong attractive impurity potential ($V \leq -U$), stability of the AF state appreciably deteriorates owing to the decrease in number of singly occupied (spin-alive) sites as a result of the increase in double occupancy in the impurity sites.

### 4. Summary

In this paper, we discussed the effect of a point-type impurity potential on a PM and an AF states in the two-dimensional Hubbard model on the basis of preliminary VMC calculations. The impurity potential is almost completely screened by the electron correlation for $U/t \gtrsim 8$ and moderate potential strength ($-U \leq V \leq 2t$). In this case, the features of the AF and PM states is not modified by the impurity potential, namely the AF state remains very stable as in the pure model ($V = 0$). However, if
the attractive impurity potential is sufficiently strong \((V \lesssim -U)\), the AF state is appreciably destabilized. In this case, the screening becomes insufficient and effective onsite interaction in the impurity sites becomes attractive, resulting in a marked increase in double occupancy. This leads to the decrease in number of spin-alive (singly occupied) sites necessary for the AF order. Here, we mainly treated cases of \(V/t < 0\). In future publications, we will discuss more realistic cases \((V/t > 0)\) for cuprates in detail.

![Graph 1](image1.png)  

**Figure 6.** The optimized onsite correlation factors \((g, g_{\text{imp}})\) for \(U/t = 12\) are shown as functions of \(V/t\). The data of \(\Psi_{\text{AF}}\) and \(\Psi_{\text{PM}}\) are compared.

![Graph 2](image2.png)  

**Figure 7.** Double occupancy and electron density at the impurity sites are plotted as functions of \(V/t\) for AF and PM states. \(n_{\text{imp}} = 0.92\) for \(V = 0\).

**References**

[1] Otsuki J, Hafermann H and Lichtenstein A I 2014 *Phys. Rev. B* **90** 235132; Misawa T and Imada M 2014 *Phys. Rev. B* **90** 115137; Zheng B-X and Chan G K-L 2016 *Phys. Rev. B* **93** 035126

[2] Sato R and Yokoyama H 2016 *J. Phys. Soc. Jpn.* **85** 074701

[3] Tamura S 2016 Dr. Thesis, Faculty of Science, Tohoku University, Sendai [in Japanese], and in preparation

[4] For instance, Tamaki H and Miyake K 2012 *J. Phys. Soc. Jpn.* **81** 124712

[5] Yokoyama H and Shiba H 1987 *J. Phys. Soc. Jpn.* **56** 1490; Umrigar C J, Wilson K G and Wilkins J W 1988 *Phys. Rev. Lett.* **60** 1719

[6] Kaplan T A, Horsch P and Fulde P 1982 *Phys. Rev. Lett.* **49** 889

[7] Yokoyama H and Shiba H 1990 *J. Phys. Soc. Jpn.* **59** 3669

[8] Yokoyama H, Ogata M, Tanaka Y, Kobayashi K and Tsuchiura H 2013 *J. Phys. Soc. Jpn.* **82** 014707

[9] Yokoyama H, Tanaka Y, Ogata M and Tsuchiura H 2004 *J. Phys. Soc. Jpn.* **73** 1119; Yokoyama H, Ogata M and Tanaka Y 2006 *J. Phys. Soc. Jpn.* **75** 114706

[10] For instance, Fukushima N, Chou C-P and Lee T K 2009 *Phys. Rev. B* **79** 184510; Farhoodfar A, Chen X, Gooding R J and Atkinson W A 2009 *Phys. Rev. B* **80** 045108