Impurity effects on \(d_{x^2-y^2}\)-wave superconducting state in strongly correlated Hubbard model

Ryo Sato and Hisatoshi Yokoyama

Department of Physics, Tohoku University, Sendai 980-8578, Japan
E-mail: satoryo@cmpt.phys.tohoku.ac.jp

Abstract. With cuprate superconductors in mind, we study the effects of point-type impurity potential \(V\) on a \(d_{x^2-y^2}\)-wave superconducting (\(d\)-SC) state in a strongly correlated square-lattice Hubbard model \((U/t = 12)\) with a diagonal transfer \((t')\), using a variational Monte Carlo method. At half filling, insulator-to-conductor (filling-control-type Mott) transitions occur at \(V \approx V_U^{(+)} \sim \pm U\). The phase realized for \(V < V_U^{(-)}\) is robust \(d\)-SC and the charge carriers are holes, whereas for \(V > V_U^{(+)}\) a metallic (or weak \(d\)-SC) state appears with charge carriers of electrons. For a partially-filled case where the impurity density is equal to the doping rate, a \(d\)-SC-to-insulator transition arises at \(V \approx V_M \sim 4t\). In the weak-\(|V|\) phases, the impurity effects in the electron distribution are smeared out by the screening effect, whereas in the strong-\(|V|\) phases, the electron distribution directly depend on the impurity configurations.

1. Introduction

Cuprate superconductors (SCs) [1] are inherently inhomogeneous systems in that the charge carriers are necessarily introduced with charged dopants, which randomly enter into the block layers and affect the carriers, in addition to other disorders specific to individual compounds. In most of relevant theoretical studies, such disorder potential has been treated with Anderson-Hubbard-type models [2], in which the local one-body potential \(V\) in each site is randomly distributed in the range \(-D \geq V \geq D\) \((D: a\ constant)\), instead of the (more simple) impurity Hubbard model [3], in which the impurity sites with a one-body potential of fixed \(V\) are randomly chosen. Since the understanding of disorder in the strongly correlated systems is still insufficient, it seems better to start with primitive cases in the impurity Hubbard model. Actually, the effects of positive and negative potential are found distinct.

In previous reports [4, 5, 6], we considered the impurity effects on the antiferromagnetic (AF) and paramagnetic (PM) or normal states in a strongly correlated Hubbard model, using a variational Monte Carlo (VMC) method. We found that in weak or intermediate attractive potential the impurity effects are almost completely screened out in a strongly correlated regime. And that a metal-to-insulator (Mott) transition occurs for weak repulsive potential. However, the trial states used in Ref. [4, 5] are insufficient for treating strong repulsive potential.

In this study, we modify the trial state to be applicable to any model parameter set [8, 6]; in addition, we formulate the VMC scheme applicable to the \(d_{x^2-y^2}\)-wave superconducting (SC) state. In this report, we represent some preliminary results at half filling and for a special partially-filled case, where the impurity density is equal to the doping rate.
2. Model and Method

In this series of research [4, 5, 6], we consider a Hubbard model \((U \geq 0)\) with a point-type spin-independent impurity potential \((V)\) on extended square lattices:

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

where \(n_{j\sigma} = c_{j\sigma}^+ c_{j\sigma}\), \((i,j)\) indicates the pairs on sites \(i\) and \(j\), and \(N_{\text{imp}}\) is the number of impurity sites, which we will explain shortly. Here, we set the hopping integral \(t\) and the lattice spacing as the units of energy and length, respectively. We define the electron density \(n\) and the doping rate \(\delta\) as \(n = N/N_s\) and \(\delta = |1 - n|\) \((N:\) number of electrons, \(N_s:\) number of sites). For simplicity, we assume that the impurity potential \(V\) comes from a single species and act on a nearby single site (“impurity site”). If we grant this simplification, the index \(\ell\) in \(H_{\text{imp}}\) runs over the impurity sites \(r_{\ell}\) \((\ell = 1, \ldots, N_{\text{imp}})\). Furthermore, we assume that \(r_{\ell}\) are randomly distributed. In this report, we concentrate on the cases of impurity densities, \(\delta_{\text{imp}} = N_{\text{imp}}/N_s \sim 0.08\) in strong correlation \((U/t = 12)\). We widely varies \(V\) (even for \(V < 0\)) to grasp overall features of impurity effects. Although the above setting of impurity potential is possibly simplistic, we believe that the essence of impurity effects with strong correlation can be captured.

To the above model, we apply a variational Monte Carlo (VMC) method [7], which enables us to exactly treat many-body wave functions. As a trial wave function, we use a Jastrow type: \(\Psi = \mathcal{P}\Phi\). In the previous studies [4, 5], we distinguished the impurity and host sites in the (many-body) projection factor \(\mathcal{P}\). We found, however, that this leads to the uncontrollable fluctuation in the VMC optimization for \(V \gtrsim 2t\). Therefore, in the new trial state here, we do not distinguish the impurity and host sites in the many-body projection factors, \(\mathcal{P} = \mathcal{P}_{H}\mathcal{P}_{\sigma}\mathcal{P}_{Q}\mathcal{P}_{G}\), where \(\mathcal{P}_{H}, \mathcal{P}_{\sigma}, \mathcal{P}_{Q}, \) and \(\mathcal{P}_{G}\) are a nearest-neighbor charge [5] and spin \((\mathcal{P}_{\sigma} = \beta^\sigma\) with \(\beta\) being a parameter and \(\sigma = 4 \sum_{(i,j)} S_i^z S_j^z\) \()\) correlators, a nearest-neighbor doublon-holon binding factor, and onsite (Gutzwiller) factor, respectively. For \(\mathcal{P}_{Q}\) and \(\mathcal{P}_{G}\), we adopt the same forms as those used for the uniform systems [7]. Instead of indirectly controlling the effect of \(V\) using many-body correlators, we introduce a one-body projector [8]

\[
\mathcal{P}_\theta = \theta^\kappa, \quad \text{with} \quad \kappa = \sum_{\ell,\sigma} n_{\ell\sigma},
\]

and \(\theta\) being a parameter. The new trial state becomes \(\Psi(\theta) = \mathcal{P}\mathcal{P}_\theta\Phi\), which is found to be well convergent for any \(V\).

To obtain the Slater-determinantal part \(\Phi\), we diagonalize the following mean-field Hamiltonian,

\[
H_{\text{MF}} = H_{\text{kin}}^{\text{BR}} + H_{d-\text{SC}} + H_{\text{imp}}.
\]

In the kinetic part \(H_{\text{kin}}^{\text{BR}}\), a band-renormalization effect is introduced in the same manner as in Refs. [4, 5, 6, 7]. In the impurity term, we use the raw form in the Hamiltonian \([\text{a constant } V_{\text{imp}} (=V)\] instead of a parameter \(V_{\text{eff}}\)] to avoid the redundancy of the screening effect, which is also introduced by \(\mathcal{P}_\theta\). The second term is the mean-field pair potential term for \(d\)-SC,

\[
H_{d-\text{SC}} = - \sum_{\mathbf{k}} \left( \Delta_{\mathbf{k}} c_{\mathbf{k}\uparrow}^+ c_{\mathbf{k}\downarrow}^+ + \text{h.c.} \right),
\]

\[
\Delta_{\mathbf{k}} = \Delta_d (\cos k_x - \cos k_y).
\]
To treat the site-dependent SC state, we follow a general mean-field scheme of the Bogoliubov-de Gennes (BdG) equation [9]. We rewrite $H_{MF}$ for the BdG equation as

$$H_{\text{BdG}} = \sum_{i,j} \left( \begin{array}{cc} c^\dagger_i & c_i \end{array} \right) \left( \begin{array}{cc} H_{ij} & F_{ij}^* \\ F_{ji} & -H_{ij} \end{array} \right) \left( \begin{array}{c} c^\dagger_i \\ c_i \end{array} \right).$$

(6)

In diagonalizing $H_{\text{BdG}}$, we solve the equation,

$$\sum_j \left( \begin{array}{cc} H_{ij} & F_{ij}^* \\ F_{ji} & -H_{ij} \end{array} \right) \left( \begin{array}{c} U_{ij} \\ V_{ij} \end{array} \right) = E \left( \begin{array}{c} U_{ij} \\ V_{ij} \end{array} \right)$$

(7)

with $U_{ij}$ and $V_{ij}$ being the coefficients of two sets of eigenfunctions corresponding to $E^\alpha$ and

$$H_{ij} = -t \sum_{\tau} \delta_{j,i+\tau} - \sum_{m=1}^{4} \sum_{\tau_m} t_m \delta_{j,i+\tau_m} - \mu \delta_{i,j} + V_{\text{imp}} \sum_{\ell=1}^{N_{\text{imp}}} \delta_{i,j} \delta_{\ell,\ell},$$

(8)

$$F_{ij} = -\frac{2}{N_s} \Delta_d \sum_{k(y>0)} (\cos k_x - \cos k_y) \cos [k \cdot (r_i - r_j)],$$

(9)

where $\tau$ and $\tau_m$ (m = 1–4) run over the first to fifth nearest-neighbor sites, respectively, and $\ell$ the impurity sites. After diagonalization, the operators corresponding to the eigenvalue $E^\alpha$ are written as

$$\gamma_{\alpha\uparrow} = \sum_i U_{\alpha i} c_{i\uparrow} + \sum_i V_{\alpha i} c_{i\downarrow},$$

(10)

$$\gamma_{\alpha\downarrow} = -\sum_i V_{\alpha i} c_{i\uparrow} + \sum_i U_{\alpha i} c_{i\downarrow}.$$  

(11)

Using $\gamma_{\alpha\sigma}$, the ground-state wave function within the BdG equation is given as

$$|\Phi_{\text{BdG}}\rangle = \prod_{\alpha (\alpha>N_s)} \gamma_{\alpha\uparrow} \gamma_{\alpha\downarrow} |0\rangle = \text{(const.)} \times \exp \left[ \sum_{i,j} (U^{-1} V)_{ij} c^\dagger_i c_{j\uparrow} c^\dagger_j c_{i\downarrow} \right] |0\rangle,$$

(12)

which is written for a fixed-electron-number form, which we use, as [10, 11]

$$|\Phi_{d-\text{SC}}\rangle = \left[ \sum_{i,j} (U^{-1} V)_{ij} c^\dagger_i c_{j\uparrow} c^\dagger_j c_{i\downarrow} \right]^{N_e} |0\rangle.$$  

(13)

Equation (13) is reduced to the usual BCS form for $V_{\text{imp}} \to 0$. The $d$-SC state $\Psi_{d-\text{SC}} = \mathcal{P} \mathcal{P}_0 \Phi_{d-\text{SC}}$ is reduced to the normal state $\Psi_N = \mathcal{P} \mathcal{P}_0 \Phi_{\text{FS}}$ ($\Phi_{\text{FS}}$: Fermi sea) for $\Delta_d \to 0$ and the bare chemical potential.

We compute expectation values with respect to $\Psi_{d-\text{SC}}$ using a VMC method similar to that in Ref. [7]. The optimization is performed using the stochastic reconfiguration method [12]. In calculating physical quantities, we average $2.5 \times 10^5$ samples. We use systems of $N_s = L \times L$ sites with $L = 10 - 20$ and the periodic-antiperiodic boundary conditions. A configuration of impurities $\{r_\ell\}$ is randomly chosen and fixed throughout a single sweep of VMC calculation (optimization and measurement). In most cases, we will display data of a typical $\{r_\ell\}$. 


3. Results

Before discussing physics, we touch on a celebrated electron-hole (unitary) transformation

$$U^{-1}c_{j\sigma}^\dagger U \rightarrow e^{i(Q\cdot r_j)}\tilde{c}_{j\sigma}, \text{ or } U^{-1}c_{k\sigma}^\dagger U \rightarrow \tilde{c}_{Q-k\sigma},$$

(14)

to confirm the correctness of VMC calculations, as well as to make good use of the symmetrical relations quantities have, especially, at half filling. Since some details are described in another report [6], here we summarize resultant relations relevant to the present subject. If we define a shifted energy as $\mathcal{E}(V, t') = E - V\delta_{\text{imp}}$ ($E$: total energy per site) and average electron densities on the impurity and host sites as,

$$n_{\text{imp}} = \frac{1}{N_{\text{imp}}} \sum_{l=1}^{N_{\text{imp}}} \sum_{\sigma} \langle n_{l\sigma} \rangle, \quad n_{\text{host}} = \frac{N - N_{\text{imp}}n_{\text{imp}}}{N_s - N_{\text{imp}}},$$

(15)

they have symmetrical relations,

$$\mathcal{E}(V, t') = \mathcal{E}(-V, -t'),$$

(16)

$$n_{\text{imp}}(V, t') = 2 - n_{\text{imp}}(-V, -t'),$$

(17)

$$n_{\text{host}}(V, t') = 2 - n_{\text{host}}(-V, -t'),$$

(18)

at half filling. Similarly, because the present system has inversion symmetry, the $d_{x^2-y^2}$-wave SC correlation function $P_d(\mathbf{r})$ and the optimized $d_{x^2-y^2}$-wave pairing parameter $\Delta_k$ should satisfy the relation, $P_d(\mathbf{r})(V, t') = P_d(\mathbf{r})(-V, -t')$ and $\Delta_d(V, t') = \Delta_d(-V, -t')$, respectively, at half filling. $P_d(\mathbf{r})$ is the real-space $d$-SC correlation function for the nearest-neighbor-site pairing

$$P_d(\mathbf{r}) = \frac{1}{N_s} \sum_i \sum_{\tau, \tau' = x, y} (-1)^{1-\delta(\tau, \tau')} \left\langle \Delta^\dagger(R_i)\Delta_{\tau'}(R_i + \mathbf{r}) \right\rangle,$$

(19)

$\mathbf{x}$ ($\mathbf{y}$) denotes the lattice vector in the $x$ ($y$) direction, $\delta(\tau, \tau')$ is the Kronecker delta, and $\Delta^\dagger(R_i)$ is the creation operator of a nearest-neighbor singlet pair at site $R_i$,

$$\Delta^\dagger(R_i) = (c_{i\uparrow}^\dagger c_{i+\tau\downarrow}^\dagger + c_{i+\tau\uparrow}^\dagger c_{i\downarrow}^\dagger)/\sqrt{2}. $$

(20)

Here, $\Delta_d(V, t')$ indicates the optimized $\Delta_d$ [Eq. (5)] for $V$ and $t'$ with the other model parameters fixed. $P_d(\mathbf{r})(V, t')$ indicates the average with respect to the optimized trial state for the model.
parameters $V$ and $t'$ with the other model parameters fixed. In Fig. 1, $E(V,t')$ is shown for $t' = \pm 0.3$. The symmetric relation Eq. (16) is basically satisfied, indicating the VMC calculations are correct.

We start with the half-filled case. In Fig. 1, we find that the behavior of $E(V,t')$ exhibits abrupt changes at $V \equiv V^{(\pm)}_U \sim \pm 12t$, indicating some transitions or crossovers occur. To study this anomaly, we consider the momentum distribution function

$$n(k) = \frac{1}{2} \sum_{\sigma} \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle.$$  \hspace{1cm} (21)

For recalling the behavior of $n(k)$, we show in Fig. 2, $U/t$ dependence of $n(k)$ at half filling in the uniform cases ($V = 0$). For $V = 0$ and $\delta = 0$, it is known that the d-SC state (unless an AF order is assumed) evolves as $U/t$ increases from metallic (normal) or weak d-SC ($U \lesssim 5t$) to d-SC ($5t \lesssim U < U_c \sim 6.5t$) and finally to Mott insulating ($U > U_c$) [13]. In Fig. 2, $n(k)$ exhibits discontinuities (Fermi surfaces, FSs) both near the antinode ($\pi, 0$) and near ($\pi/2, \pi/2$) in the nodal direction for the metallic state. In d-SC states, the FS near ($\pi, 0$) disappears but the FS near ($\pi/2, \pi/2$) remains, corresponding to opening a $d$-wave gap. In Mott insulating states, all FSs disappear, corresponding to opening of a full gap.

In Fig. 3(a), the evolution of $n(k)$ as $V/t$ changes is shown for $U/t = 12$ and $t'/t = -0.3$. For $V^{(-)}_U < V < V^{(+)}_U$ (indicated with greenish colors), $n(k)$ exhibits no discontinuity, indicating that the Mott-insulating state for $V = 0$ continues within this range of $V$. For $V < V^{(-)}_U$ (warm colors), a FS appears near ($\pi/2, \pi/2$) but $n(k)$ is continuous near ($\pi, 0$), indicating that d-SC is realized. Thus, an insulator-to-SC (Mott) transition is considered to occur at $V = V^{(-)}_U$. On the other hand for $V > V^{(+)}_U$ (cold colors), it seems that FSs appear both near ($\pi, 0$) and ($\pi/2, \pi/2$), indicating that the state becomes metallic (or weak d-SC). In this case, an insulator-to-metal (Mott) transition is considered to arise at $V = V^{(+)}_U$.

It is important to check the order parameter of d-SC ($P_d$), and the $d$-wave pairing-gap parameter ($\Delta_d$), which are shown in Fig. 4. As expected from $n(k)$, d-SC coherence vanishes ($P_d = 0$) in the range of $V^{(-)}_U < V < V^{(+)}_U$, but becomes finite for $V < V^{(-)}_U$. For $V > V^{(+)}_U$, $P_d$ is small or almost vanishes, indicating that the state is weak d-SC or metallic. Thus, the interpretation of the behavior of $n(k)$ is confirmed. Note in Fig. 4 that $\Delta_d$ is robust in the insulating regime $|V| \lesssim |V^{(\pm)}_U|$, whereas the pairing gap becomes small in the conducting regime $|V| \gtrsim |V^{(\pm)}_U|$. This behavior of $\Delta_d$ will be understood in the same manner as in the uniform
cases [14, 7]: The origin of d-wave pairing is the AF spin correlation, which becomes largest in carrier-less cases and decreases as the carrier density increases. The d-SC coherence $P_d$ is suppressed as the carrier density decreases because charge fluctuation is suppressed by Mott physics.

Therefore, we next consider the electron densities at the impurity and host sites. In Fig. 5(a), $n_{\text{imp}}$ and $n_{\text{hst}}$ are plotted as functions of $V/t$. In the insulating regime $|V| \lesssim |V_U^{(+)}|$, electron density both in the impurity and host sites are almost unity, namely, a “half-filled” state is preserved in this range of $V$. On the other hand in the conductive regime $|V| \gtrsim |V_U^{(+)}|$, the impurity sites are occupied by holons (empty sites) for $V > 0$ or doublons (doubly occupied sites) for $V < 0$. Correspondingly, the charge carriers (doublons for $V > 0$ or holons for $V < 0$) appears in the host sites and enable currents to flow. Thus, the Mott transitions arising at $V = V_U^{(\pm)}$ are filling-control-type. Because the basic mechanism of the Mott transition is the same as in the case of AF and normal states, for detailed explanation, refer to Ref. [6].

We can further discuss the reason of asymmetry in $P_d$ with respect to $V = 0$ in Fig. 4 on the basis of the sign of charge carriers. Because the charge carriers for $V \gtrsim V_U^{(-)}$ are holons, the mechanism of SC is parallel to the hole-doped case of $t'/t = -0.3$, in which d-SC is robust up to
high doping rate [14, 7, 15]. On the other hand, the charge carriers for $V > V_U^{(+)}$ are doublons (electrons), the mechanism corresponds to the electron-doped case of $t'/t = +0.3$, in which $d$-SC is weak and nearly vanishes. Thus, the robustness of $d$-SC becomes markedly different whether the impurity potential is attractive or repulsive even at half filling, in contrast to the AF order.

Next, we take up a doped case in which the impurity density is equivalent to the doping rate ($\delta_{\text{imp}} = \delta$). This case is experimentally special, but theoretically simple to consider the metal-to-insulator (Mott) transition arising at small $V/t$. It is known for homogeneous systems ($V = 0$) that the $d$-SC state is conductive ($d$-SC or metallic) for any $U/t$ and $\delta > 0$ [14]. Below, we mainly consider the effect of repulsive $V$. The behavior of total energy abruptly changes at $V = V_M$ (not shown). We again expect that some transition occurs at $V = V_M$. In Fig. 3(b), $n(k)$ is shown for various values of $V/t$ for $\delta = 0.08$. For $V < V_M$, $n(k)$ has a jump at a point near $(\pi/2, \pi/2)$ but is smooth around $(\pi, 0)$, showing a feature characteristic of $d$-SC. On the other hand for $V > V_M$, $n(k)$ is always smooth on the path. It means that a $d$-SC-to-insulator (Mott) transition occurs at $V = V_M$. We corroborate this point by referring to $P_d$ in Fig. 4, where $P_d$ is finite for $V < V_M$ but abruptly vanishes and remains null for $V > V_M$. In Fig. 5(b), we find $n_{\text{imp}}$ and $n_{\text{hst}}$ becomes 0 and 1, respectively for $V > V_M$. The half-filled state is realized in the host sites. Thus, this transition is again a filling-control-type Mott transition. The mechanism is parallel to the corresponding transition in the AF state; see Fig. 3 in Ref [5] for details. Incidentally, in Fig. 4, $\Delta_d$ is found damped together with $P_d$ for $V > V_M$, suggesting that the AF correlation becomes weak in this insulating state.

Finally, let us look at the charge-density structure factor defined as

$$\tilde{N}(\mathbf{q}) = \frac{1}{N_s} \sum_{i,j} e^{i\mathbf{q}(\mathbf{r}_i - \mathbf{r}_j)} \langle n_i n_j \rangle - n^2.$$  \hspace{1cm} (22)

Fig. 6 shows the evolution of $N(\mathbf{q})$ as $V/t$ changes for the doped case. It shows that the charge distribution hardly alters from the uniform case for $V < V_M$, probably owing to the screening effect. On the other hand, $N(\mathbf{q})$ exhibits scattered pattern depending upon the impurity configuration. This scattered property in the large-$V/t$ phase does not depend on whether the large-$V/t$ phase is conducting or insulating. In this case, the phase is insulating,
but the scattered property in $N(q)$ appears in the conductive states at half filling (not shown). See Fig. 2(b) in Ref. [6] for the AF state.

4. Summary and discussions

We studied the effect of point-type impurity potential on a superconducting state on a two-dimensional Hubbard model, using a variational Monte Carlo method. We found that filling-control-type insulator-to-conductor (Mott) transitions occur at $V = V_U^{(+)} \sim \pm U$ at half filling ($U/t = 12$). The state for $V < V_U^{(-)}$ is $d$-wave superconducting and the charge carriers are holes, whereas the state for $V > V_U^{(+)}$ is metallic (or weak $d$-SC) and the carriers are electrons. This large asymmetry in the $d$-SC state is in contrast to the AF state. At a partially filling, we find a $d$-SC-to-insulator (Mott) transition at $V = V_M \sim 4t$, which is somewhat larger than that for the AF state ($V_M \sim 0 - 2t$). In this report, we took up a specific case of $\delta_{\text{imp}} = \delta$ as a doped example. We found that the behavior considerably differs in other conditions. We will publish this point and other development elsewhere in near future. We acknowledge the support by Grants-in-Aid from the Ministry of Education, Culture, Sports, Science and Technology, Japan.

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Figure 6. The charge-density structure factor $N(q)$ along the path of $q$: $(0,0)-(\pi,0)-((\pi,\pi)-(0,0)$ is shown for several positive values of $V/t$. We use a certain impurity configuration for all values of $V/t$. As a result, the scattered forms for $V > V_M$ becomes similar. If we use distinct impurity configurations, the patterns become random. It follows that the impurity configurations regulate the charge distribution for $V > V_M$. 

![Figure 6](image-url)