Renormalization of transition matrix elements of particle number operators due to strong electron correlation

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Abstract

Renormalization of non-magnetic and magnetic impurities due to electron double-occupancy prohibition is derived analytically by an improved Gutzwiller approximation. Non-magnetic impurities are effectively weakened by the same renormalization factor as that for the hopping amplitude, whereas magnetic impurities are strengthened by the square root of the spin-exchange renormalization factor, in contrast to results by the conventional Gutzwiller approximation. We demonstrate it by showing that transition matrix elements of number operators between assumed excited states and between an assumed ground state and excited states are renormalized differently than diagonal matrix elements. Deviation from such simple renormalization with a factor is also discussed. In addition, as a related calculation, we correct an error in treatment of the renormalization of charge interaction in the literature. Namely, terms from the second order of the transition matrix elements are strongly suppressed. Since all these results do not depend on the signs of impurity potential or the charge interaction parameter, they are valid both in attractive and repulsive cases.

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1. Introduction

In this paper, we discuss the renormalization of impurities due to a strong electron correlation. Such renormalization may be intuitive in the case of the Hubbard model, where each site has onsite electron repulsion. Namely, sites with higher potential energy have lower electron occupancy, and consequently have less chance of double occupancy. Then, the total energy loss from the impurity potential and the repulsive interaction should be more uniform than in the system without the electron correlation; we call it the renormalization of
impurities. However, when the repulsion is very strong, we need to consider much smaller energy scales. That is, if double occupancy does not occur, the above argument cannot be applied, and thus the renormalization of impurities within the lower Hubbard band is not so trivial.

When electron double occupancy is prohibited at every site, a system with quite densely packed electrons has a good chance to have one electron with up or down spin at each site. If the system has a tendency toward phase separation, small perturbation by an impurity may produce a large effect to separate a system into hole-rich regions and electron-rich regions; it may appear in close vicinity of the half filling in the $t$–$J$-type models, where effective hopping is negligibly small compared to the effective exchange interaction. In contrast, the focus of this paper are systems not that close to the half filling or systems with a relatively weak exchange interaction. Then, electrons are more mobile. Near the half filling, since there is little freedom left to change charge distribution, and sudden spatial change of particle number distribution around impurities is not favorable for the kinetic energy, non-magnetic impurity potentials may have little effect on low-energy eigenstates and only shift their eigenenergies quite uniformly. In other words, impurity potentials can be renormalized by the electron correlation even within the lower Hubbard band.

In previous papers [1, 2], such renormalization of non-magnetic impurity potentials was investigated numerically. That is, (i) to estimate perturbation from an impurity potential, the variational Monte Carlo method was applied to calculation of its matrix elements with respect to assumed excited states in the uniform systems; and (ii) inhomogeneous systems with an impurity or impurities were investigated by a Bogoliubov–de Gennes equation with the double-occupancy prohibition treated by a kind of mean-field approximation called the Gutzwiller approximation (GA) generalized to inhomogeneous systems.

Both (i) and (ii) manifested the strong renormalization of the impurity potential, and its renormalization factor (the ratio between corresponding quantities in systems with and without the double-occupancy prohibition) seems approximately proportional to $g' \equiv 2x/(1 + x)$, which is the renormalization factor of the hopping amplitude obtained by the GA as a function of the hole concentration $x$. Since double-occupancy prohibition inhibits hopping, $g'$ is less than unity and goes to zero as $x \rightarrow 0$. To explain the impurity renormalization factor close to $g'$, we pointed out the similarity between the impurity potential and hopping in the real space, i.e. the Fourier-transformed impurity potential has the form of hopping in the $k$-space.

If electrons are densely packed in the lattice, it must be difficult even in the $k$-space to hop from $k$ to a different $k'$. However, it is a speculation and may not be trivial because double occupancy is prohibited in the real space rather than in the $k$-space. In addition, we do not really know how general the numerical results are because the calculation was done only for limited parameter sets. To complement this argument, an analytic approximation is adopted in this paper, namely (i) is redone using the GA to derive dominant $g'$ dependence and deviation from $g'$ explicitly. In fact, however, the conventional GA [3, 4] fails to derive this renormalization. It compares mean weights of configurations relevant to operators of interest with and without electron repulsion in calculating the renormalization factors. Then, the renormalization factor for the particle number operators is actually unity, i.e. they are not renormalized. The spin rotation invariant slave-boson mean-field theory [5] is known to be equivalent to the conventional GA; the saddle-point approximated boson fields play a role of the weights in the GA. Therefore, we speculate that it may have the same problem as the conventional GA. In addition, we believe that the slave-boson mean-field theory with only one boson, often used for the $t$–$J$ model, can be even less accurate because it does not yield the renormalization of the exchange interaction, which may be an artifact from the lost boson hard-core property.
Let us recall that the GA corresponds to taking the leading order of the Wick expansion with respect to the intersite contractions of creation/annihilation operators \([6, 7]\). In fact, the weights of configurations in the conventional GA are likely to be calculated with the focus only on the lowest order; apparently it breaks down when the lowest order vanishes or when the next lowest order is of interest. An example is a particle number operator as shown in this paper. Although the lowest order is the average particle number, when we discuss transition matrix elements with excited states, this lowest order does not contribute, and the next lowest order is relevant. We will demonstrate that off-diagonal matrix elements between an assumed ground state and excited states, as well as between different excited states, are renormalized differently than diagonal matrix elements.

Furthermore, by slightly modifying the non-magnetic impurity, i.e. by subtraction between up- and down-spin particle number operators, we also consider a simple magnetic impurity. In this case, the direction of the renormalization is reversed, namely the impurity is strengthened by the electron correlation in contrast to the non-magnetic impurity. It must be physically reasonable because electron repulsion increases single occupancy. As a calculation related to the non-magnetic impurity, the renormalization of charge interaction is discussed to correct an error in its treatment in the literature. That is, terms relevant to the mean-field approximation are actually the second order of the transition matrix elements, and they are weakened by a very small renormalization factor \((gt)^2\) although treated usually as not being renormalized.

2. Model

What we have in mind is \(t-J\)-type models with impurities, namely

\[
H \equiv P_G \left[ \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,j} J_{ij} \left( \vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \vec{n}_i \vec{n}_j \right) + H_{\text{imp}} \right] P_G, \tag{1}
\]

where \(c_{i\sigma}^\dagger (c_{i\sigma})\) is the creation (annihilation) operator of the electron with site \(i\) and spin \(\sigma\), and \(\vec{S}_i\) is the spin operator at site \(i\). In addition,

\[
\vec{n}_i \equiv \vec{n}_i^\uparrow + \vec{n}_i^\downarrow, \quad \vec{n}_i^\sigma \equiv \vec{n}_i^\uparrow + \vec{n}_i^\downarrow. \tag{2}
\]

The Gutzwiller projection operator \(P_G \equiv \prod_i (1 - \vec{n}_i^\uparrow \vec{n}_i^\downarrow)\) prohibits electron double occupancy at each site and represents strong Coulomb repulsion. In this paper, we do not use any explicit form of \(t_{ij}\) and \(J_{ij}\) although they are implicitly included in assumed variational ground/excited states. Our main focus here is on the impurity term \(H_{\text{imp}}\).

In sections 3–5, our target is the renormalization of a single non-magnetic \(\delta\)-function impurity potential located at \(i = I\):

\[
H_{\text{imp}} = V_I \vec{n}_I = V_I (\vec{n}_I^\uparrow + \vec{n}_I^\downarrow). \tag{3}
\]

Then, in section 6, we discuss the renormalization of a simple magnetic impurity:

\[
H_{\text{imp}} = -h_I \vec{S}_I^z = - \frac{h_I}{2} (\vec{n}_I^\uparrow - \vec{n}_I^\downarrow). \tag{4}
\]

In addition, the focus in section 7 is not on \(H_{\text{imp}}\) but on the charge interaction \(\vec{n}_I \vec{n}_j\) in Hamiltonian (1).
3. Non-magnetic impurity renormalization

Let us start from a uniform system without impurities. A basic idea of variational theories is that the ground state of the $t$–$J$-type models may be similar to the BCS superconducting state

$$|\Psi_0\rangle = \prod_k (u_k + v_k c_k^\dagger c_{-k}^\dagger)|0\rangle,$$

but somewhat modified by the electron correlation. Simple variational wavefunctions adopted by most of analytic theories have a form of $P_G|\Psi_0\rangle$ with something to control the particle number. One way to control it is to use the projection $P_N$ to the fixed particle number $N$.\(^1\)

Another is to attach fugacity factors to the projector, namely

$$|\Psi\rangle = P|\Psi_0\rangle, \quad P = \prod_i P_i, \quad P_i = \lambda_{i\uparrow}^{\hat{n}_{i\uparrow}} \lambda_{i\downarrow}^{\hat{n}_{i\downarrow}} (1 - \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}).$$

The latter is adopted in this paper. The reason to control the particle number is that $P_G$ changes the average particle number of $|\Psi_0\rangle$ because states with a larger particle number have more chance to be projected out \([8]\). Since the GA relates expectation values before and after the projection,

$$\langle \hat{O} \rangle_0 \equiv \langle \Psi_0 | \hat{O} | \Psi_0 \rangle, \quad \langle \hat{O} \rangle \equiv \frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle},$$

for some operator $\hat{O}$; usually, it is not convenient if $|\Psi\rangle$ and $|\Psi_0\rangle$ are totally different, e.g., if $|\Psi_0\rangle$ has a more-than-half-filled electron band\(^2\). Although our main interest here is perturbation from the uniform state, most of the derivation in this paper is valid also for inhomogeneous systems, and thus we prefer to keep general expressions with site and spin indices throughout the paper, e.g.

$$n_{i\sigma} \equiv \langle \hat{n}_{i\sigma} \rangle_0, \quad n_i \equiv \langle \hat{n}_i \rangle_0 = n_{i\uparrow} + n_{i\downarrow}.$$  \((8)\)

However, we use $0 = \langle c_{i\sigma}^\dagger c_{i\sigma}\rangle_0 = \langle c_{i\sigma}^\dagger c_{j\sigma}\rangle_0 = \langle c_{i\uparrow}^\dagger c_{i\downarrow}\rangle_0$ to avoid making formulas too lengthy. Although the choice of the fugacity factors is not unique, especially in inhomogeneous systems \([7]\), it is convenient to define

$$\lambda_{i\sigma} \equiv \frac{1 - n_{i\sigma}}{1 - n_i},$$

because it satisfies

$$\langle \hat{n}_{i\sigma} \rangle \approx \langle \hat{n}_{i\sigma} \rangle_0,$$  \((10)\)

for any $i$ and $\sigma$ \([6, 7]\), neglecting terms of the ‘fourth order’. Here, and throughout this paper, if not specified, ‘$n$th order’ represents the $n$th order with respect to intersite contractions such as $\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle$ and $\langle c_{i\uparrow}^\dagger c_{j\downarrow}\rangle$ with $i \neq j$. Note that $\langle \hat{O} \rangle$ of any $\hat{O}$ can be in principle calculated by the Wick theorem, which yields many such intersite contractions. High-order terms may be neglected by recalling that onsite contractions are larger than intersite contractions. The GA corresponds to taking the leading order only, e.g.

$$\langle P^2 \rangle_0 \approx \prod_i \langle P_i^2 \rangle_0.$$  \((11)\)

\(^1\) Many different $|\Psi_0\rangle$ correspond to $|\Psi\rangle$ under the projections. For example, $\exp(\lambda N)$ with $N$ the total particle number operator is constant under $P_N$, and thus $\exp(\lambda N)|\Psi_0\rangle$ is equivalent to $|\Psi_0\rangle$.

\(^2\) The variational Monte Carlo method does not have such a restriction. For example, local magnetic moments before and after the projection are different in general, and the chemical potential in a variational mean-field Hamiltonian is a variational parameter under $P_N$ rather than a parameter to control the particle number.
The terms neglected in the approximation in (11) are of fourth order because the second-order terms cancel out when $\lambda_{\pm}$ is defined as (9) [6, 7]. Let us show it explicitly with a notation to treat $c^\dagger$ and $c$ together:

$$c^\dagger_{\pm} \equiv c^\dagger_{\uparrow \sigma}, \quad c_{\pm} \equiv c_{\uparrow \sigma},$$

(13)

by considering contractions between $P^2_i$ and operators at some site(s) $j, j' \neq i$.

$$\langle P^2_i c_{j'\sigma} c_{j'\sigma} \rangle = \langle P^2_i | c_{j'\sigma} c_{j'\sigma} \rangle_0 + (\langle c_{i\uparrow \sigma} c_{j'\sigma} | c_{i\uparrow \sigma} c_{j'\sigma} \rangle_0 - \langle c_{i\downarrow \sigma} c_{j'\sigma} | c_{i\downarrow \sigma} c_{j'\sigma} \rangle_0) \lambda_i,$$

(14)

for arbitrary $\tau, \tau', \sigma$ and $\sigma'$. Then, the quantities in the square brackets vanish.

We assume that $|\Psi\rangle$ is a good variational ground state, and that the excited states are well represented by projected quasiparticles

$$|ks\rangle \equiv \frac{P^{\dagger}_{V_{ks}} |\Psi_0\rangle}{\sqrt{\langle |\Psi_0\rangle P P^{\dagger}_{V_{ks}} |\Psi_0\rangle}} \approx \frac{P^{\dagger}_{V_{ks}} |\Psi_0\rangle}{\sqrt{\langle P^2 \rangle_0}},$$

(15)

where $\gamma_{ks}$ are quasiparticles for $|\Psi_0\rangle$, namely

$$\gamma_{k\uparrow} = u_k^* c_{k\uparrow} - v_k^* c_{-k\downarrow}, \quad \gamma_{-k\downarrow} = v_k c_{k\uparrow} + u_k c_{-k\downarrow}.$$  

(16)

For the denominator of $|ks\rangle$, we have used the approximation $\langle \Psi_0 | P^2 \gamma_{ks} \gamma_{ks} | \Psi_0 \rangle \approx \langle P^2 \rangle_0$ [7, 9], and errors from this approximation are of second order.

By switching on the impurity potential, these excited states should be mixed by matrix elements

$$\frac{V_{k',k}}{N_s} \equiv \langle k'| \hat{n}_{1\sigma} |ks\rangle \approx \frac{\gamma_{k\uparrow} P \hat{n}_{1\sigma} P^{\dagger}_{V_{k\uparrow}} |\Psi_0\rangle}{\langle P^2 \rangle_0},$$

(17)

with $N_s$ the number of sites. The limit of the half filling can be exactly evaluated, $\lambda \to \infty$, $P \hat{n}_{1\sigma} P \to P P$, and thus $V_{k',k}/N_s \to \langle k'| ks \rangle = \delta_{k',k}$. According to the BCS theory, $V_{k',k} = \langle \gamma_{k\uparrow} \gamma_{k'\uparrow} \rangle_0 = u_k^* u_{k'} - v_k^* v_{k'}$. In a previous paper [2], the author noted that $V_{k',k}$ is not renormalized with the conventional GA [4] because it originally comes from a particle number operator. However, more careful analysis here will show that, although the diagonal matrix elements of the particle number operators are not renormalized (e.g. see (10)), their off-diagonal matrix elements with respect to the projected quasiparticle excited states are renormalized.

The Wick expansion of $\langle \gamma_{k\uparrow} P \hat{n}_{1\sigma} P^{\dagger}_{V_{k\uparrow}} |\Psi_0\rangle_0$ yields many terms, and some terms contain onsite contraction of $\hat{n}_{1\sigma}$ at the center as $\hat{n}_{1\sigma} \to n_{1\sigma}$, and the others do not. Let us separate these two groups of terms:

$$\langle \gamma_{k\uparrow} P \hat{n}_{1\sigma} P^{\dagger}_{V_{k\uparrow}} |\Psi_0\rangle_0 = n_{1\sigma} \langle \gamma_{k\uparrow} P^2 |\Psi_0\rangle_0 + \langle \gamma_{k\uparrow} P^2 (\hat{n}_{1\sigma} - n_{1\sigma}) |\Psi_0\rangle_0.$$  

(18)

The first term is proportional to $\langle k' \uparrow | k \uparrow \rangle$, and vanishes when $k \neq k'$. Namely, we can only consider the second term.

Let us first take only $\hat{n}_{1\sigma}$ in the impurity potential term. Since the GA is carried out in the real space, the $k$ representation should be inverse Fourier-transformed into the real space.
representation. Namely, what we should calculate is \(|\langle c^\dagger_{i'\sigma} P \tilde{n}_{I\uparrow} P c_{i\sigma} \rangle_0| \). Let us first take the case of \(i \neq I, i' \neq I\) and \(i \neq i'\), which makes the dominant contribution to \(\mathcal{V}_{ki}\). After using \(P_{\ell} \tilde{n}_{I\uparrow} P_I = \lambda_{I\uparrow} \tilde{n}_{I\uparrow} (1 - \tilde{n}_{I\downarrow})\), we take onsite contractions for all the sites except \(i, i'\) and \(I\) of the numerator neglecting fourth-order terms:

\[
\frac{\langle c^\dagger_{i'\sigma} P \tilde{n}_{I\uparrow} P c_{i\sigma} \rangle_0 \langle \rangle_0}{\langle \rangle_0} \approx \frac{\lambda_{I\uparrow} \langle c^\dagger_{i'\sigma} P^2 \tilde{n}_{I\uparrow} (1 - \tilde{n}_{I\downarrow}) P^2 c_{i\sigma} \rangle_0 \langle \rangle_0}{\langle \rangle_0}.
\]

(19)

Then, let us work on sites \(i\) and \(i'\):

\[
P^2_i c^\dagger_{i\sigma} = \lambda_{i\sigma} (1 - \tilde{n}_{i\sigma}) c^\dagger_{i\sigma}, \quad P^2_i c_{i\sigma} = [(1 - \tilde{n}_{i\sigma}) + \lambda_{i\sigma} \tilde{n}_{i\sigma}] c_{i\sigma}.
\]

(20)

For the moment, we take the onsite contractions for \(i\) to \(i'\) neglecting intersite contractions between \(I \uparrow\) or \(I \downarrow\) and then; the terms neglected here are of third order and will be calculated in the next section. Accordingly, using

\[
\frac{\lambda_{i\sigma} (1 - n_{i\sigma})}{\langle \rangle_0} = \frac{(1 - n_{i\sigma}) + \lambda_{i\sigma} n_{i\sigma}}{\langle \rangle_0} = 1,
\]

(21)

(19) can be approximated as

\[
\frac{\langle c^\dagger_{i'\sigma} P \tilde{n}_{I\uparrow} P c_{i\sigma} \rangle_0 \langle \rangle_0}{\langle \rangle_0} \approx \frac{\lambda_{I\uparrow} \langle c^\dagger_{i'\sigma} \tilde{n}_{I\uparrow} (1 - \tilde{n}_{I\downarrow}) c_{i\sigma} \rangle_0 \langle \rangle_0}{\langle \rangle_0}.
\]

(22)

It is convenient to define mean-value-subtracted operators:

\[
\tilde{n}_{i\sigma} \equiv \tilde{n}_{i\sigma} - n_{i\sigma}.
\]

(23)

Consequently, we obtain

\[
\frac{\langle c^\dagger_{i'\sigma} P \tilde{n}_{I\uparrow} P c_{i\sigma} \rangle_0 \langle \rangle_0}{\langle \rangle_0} \approx \frac{\langle c^\dagger_{i'\sigma} \tilde{n}_{I\uparrow} c_{i\sigma} \rangle_0}{\langle \rangle_0} - \frac{n_{I\uparrow}}{1 - n_{I\downarrow}} \langle c^\dagger_{i'\sigma} \tilde{n}_{I\downarrow} c_{i\sigma} \rangle_0.
\]

(24)

Here, the first term and the second term on the rhs are from the onsite contraction of \(1 - \tilde{n}_{I\downarrow}\) and \(\tilde{n}_{I\downarrow}\), respectively; from the residual operators \(\tilde{n}_{I\uparrow}\) and \(1 - \tilde{n}_{I\downarrow}\), respectively, their mean values are subtracted to cancel their onsite contraction.

For the moment, we neglect deviation from (24) for any \(i\) and \(i'\), which will be discussed in the next section. Then, it is straightforward to Fourier transform back

\[
\frac{\langle \gamma_{k\sigma} P \tilde{n}_{I\uparrow} P \gamma_{k\sigma} \rangle_0 \langle \rangle_0}{\langle \rangle_0} \approx \frac{\langle \gamma_{k\sigma} \tilde{n}_{I\uparrow} \gamma_{k\sigma} \rangle_0}{\langle \rangle_0} - \frac{n_{I\uparrow}}{1 - n_{I\downarrow}} \langle \gamma_{k\sigma} \tilde{n}_{I\downarrow} \gamma_{k\sigma} \rangle_0.
\]

(25)

The formula for \(\tilde{n}_{I\uparrow}\) is obtained by exchanging \(\uparrow\) and \(\downarrow\) at site \(I\), and this formulas represent that \(\tilde{n}_{I\sigma}\) is renormalized into \(\tilde{n}_{I\sigma} = \tilde{n}_{I\sigma} n_{I\sigma}/(1 - n_{I\sigma})\).

In fact, the derivation above is valid also for inhomogeneous systems by replacing \(\gamma_k\) with the Bogoliubov quasiparticles \(\gamma_k\). A difference is that the orthogonality of the Gutzwiller-projected Bogoliubov quasiparticle states is only approximately satisfied [7], i.e. errors from the GA can be larger than those in uniform systems. The renormalization of \(\tilde{n}_{I\uparrow}\) in inhomogeneous systems is obtained by summing up \(\tilde{n}_{I\uparrow}\) and \(\tilde{n}_{I\downarrow}\) for \(\ell \neq \ell'\),

\[
\frac{\langle \gamma_{k\sigma} P \tilde{n}_{I\uparrow} P \gamma_{k\sigma} \rangle_0 \langle \rangle_0}{\langle \rangle_0} \approx \frac{\langle \gamma_{k\sigma} (g'_{I\uparrow} \tilde{n}_{I\uparrow} + g'_{I\downarrow} \tilde{n}_{I\downarrow}) \rangle_0}{\langle \rangle_0},
\]

(26)

where

\[
g'_{I\sigma} \equiv \frac{1 - n_i}{1 - n_{i\sigma}}
\]

(27)

is the Gutzwiller renormalization factor for the hopping amplitude.
Returning to our main target, i.e. the non-magnetic uniform system, we can set \( g'_{I',\sigma} = g'_{I,\sigma} \), and then
\[
V_{k',k} = \langle k'|\hat{n}_I|ks \rangle \approx g'_{I,\sigma}(u_k u_{k'}^* - v_k v_{k'}^*) = g'_{I,\sigma} V_{k',k}^{BCS},
\]
which is exactly the same as the speculation in the previous paper [2] consistent with the numerical results for several \( k \)-points by the variational Monte Carlo method, i.e. the renormalization factor is close to \( g' \) and insensitive to model parameters. The important point here may be \( g' \) appears only after summation of up and down spins, \( \hat{n}_{I\uparrow} + \hat{n}_{I\downarrow} \), which is a difference from the hopping amplitude renormalization in the real space.

According to the conventional GA [4], what is renormalized is an operator rather than its matrix elements, and thus diagonal and off-diagonal matrix elements have the same renormalization factor. In fact, however, what is renormalized should be matrix elements rather than operators, and diagonal and off-diagonal matrix elements with respect to excited states can have different renormalization factors as demonstrated above.

Using exactly the same procedure as above, transition matrix elements between the variational ground state and projected two-quasiparticle excited states can also be calculated. Corresponding to (26),
\[
\left\langle \Psi_0|\gamma_I\gamma_E P \hat{n}_I|\Psi \right\rangle \approx \left\langle \Psi_0|\gamma_I\gamma_E \left( g'_{I\uparrow}\hat{n}_{I\uparrow} + g'_{I\downarrow}\hat{n}_{I\downarrow} \right) |\Psi_0 \right\rangle.
\]

4. Corrections to the simple \( g' \) renormalization

In the cases of \( i = I \neq i', i' = I \neq i \) and \( i = i' = I \), we obtain formulas equivalent to (24). However, for \( i = i' \neq I \), we have
\[
\left\langle c_{i\sigma}^+ P \hat{n}_{I\uparrow} P c_{i\sigma}^\dagger \right\rangle_0 \approx \lambda_{I\uparrow}(1 - \hat{n}_{I\downarrow}) c_{i\sigma}^+ P_{i\sigma}^2 c_{i\sigma}^\dagger_0,
\]
where \( c_{i\sigma}^+ P_{i\sigma}^2 c_{i\sigma}^\dagger \) can be explicitly written as
\[
c_{i\sigma} P_{i\sigma}^2 c_{i\sigma}^\dagger = \lambda_{i\sigma}(1 - \hat{n}_{i\sigma})(1 - \hat{n}_{i\sigma}), \quad c_{i\sigma}^\dagger P_{i\sigma}^2 c_{i\sigma} = [1 - \hat{n}_{i\sigma} + \lambda_{i\sigma}\hat{n}_{i\sigma}] \hat{n}_{i\sigma},
\]
because the other combinations of \( c_{i\sigma}^\dagger \) and \( c_{i\sigma} \) yield zero or very small quantities. Then, although the onsite contraction of \( i\sigma \) with intersite contractions between \( i\sigma \) and \( I \) yields a formula equivalent to (24), the onsite contraction of \( i\sigma \) with intersite contractions between \( i\sigma \) and \( I \) additionally yields the same order of contribution. To write them compactly, let us define
\[
k_{i\sigma}^+ = \frac{1}{1 - n_{i\sigma}}, \quad k_{i\sigma}^- = \frac{n_{i\sigma}}{(1 - n_{i\sigma})(1 - n_{i\downarrow})},
\]
as well as
\[
\eta_{i'\sigma',i\sigma} \equiv \langle \hat{n}_{i'\sigma'}\hat{n}_{i\sigma} \rangle_0 - n_{i'\sigma}n_{i\sigma},
\]
which extracts only intersite contractions in \( \langle \hat{n}_{i'\sigma'}\hat{n}_{i\sigma} \rangle_0 \). Then, \( \langle \hat{n}_{i'\sigma'}(1 - \hat{n}_{i\sigma}) \rangle_0 = n_{i'\sigma'}(1 - n_{i\sigma}) = -\eta_{i'\sigma',i\sigma} \) and \( \langle (1 - \hat{n}_{i'\sigma'})(1 - \hat{n}_{i\sigma}) \rangle_0 = (1 - n_{i'\sigma'})(1 - n_{i\sigma}) = \eta_{i'\sigma',i\sigma} \). More explicitly,
\[
\eta_{i'\sigma',i\sigma} = -\left| c_{i'\sigma'} c_{i\sigma}^\dagger \right|^2, \quad \eta_{i'\sigma',i\sigma}^2 = \left| c_{i'\sigma'} c_{i\sigma}^\dagger \right|^2.
\]
Using these notations,
\[
\left\langle c_{i\sigma}^+ P \hat{n}_{I\uparrow} P c_{i\sigma}^\dagger \right\rangle_0 \approx \frac{1}{n_{I\uparrow}} \left( n_{I\uparrow} - n_{I\downarrow} \eta_{I\downarrow,i\sigma} \right) + k_{i\sigma}^+ \left| c_{i\sigma}^+ c_{i\sigma}^\dagger \right|^2 \left( n_{I\uparrow} - n_{I\downarrow} \eta_{I\downarrow,i\sigma} \right).
\]
By summing up $\hat{n}_{I\uparrow}$ and $\hat{n}_{I\downarrow}$,
\[
\langle c_{i\sigma}^{\dagger} P(\hat{n}_{I\uparrow} + \hat{n}_{I\downarrow}) P c_{i\sigma} \rangle_0 \approx \mathbb{T} \left( g'_{I\uparrow} \eta_{I\uparrow,i\sigma} + g'_{I\downarrow} \eta_{I\downarrow,i\sigma} \right) + \kappa_{i\sigma}^c \langle c_{i\sigma}^{\dagger} \rangle_0 \left( g'_{I\uparrow} \eta_{I\uparrow,i\sigma} + g'_{I\downarrow} \eta_{I\downarrow,i\sigma} \right).
\]

(36)

Since $i \neq i'$ occurs more often than $i = i'$, the third-order terms neglected in the previous section for the case of $i \neq I, i' \neq I$, and $i \neq i'$ may have larger contribution than the newly derived terms above. Such terms are derived by taking into account intersite contraction including $i\bar{\sigma}$ and $i'\bar{\sigma}'$. However, if intersite contractions are taken between $i\bar{\sigma}$ and $i'\bar{\sigma}'$ and the onsite contractions are taken for $I$, then such terms do not contribute as explained around (18). Using the notation above, (20) is rewritten as
\[
\frac{P_2 c_{i\sigma}}{P_2^0} = (1 + \kappa_{i\sigma}^c \eta_{i\sigma}) c_{i\sigma}^c.
\]

(37)

Then, for $t' = -\tau \sigma \sigma'$ ($\uparrow, \downarrow$ and $+1, -1$ are used interchangeably),
\[
\langle c_{i'\sigma'}^{\dagger} P(\hat{n}_{I\uparrow} + \hat{n}_{I\downarrow}) P c_{i'\sigma'} \rangle_0 \approx g'_{I\uparrow}^{i'} \langle c_{i'\sigma'}^{\dagger} \hat{n}_{I\uparrow} c_{i'\sigma'} \rangle_0 + g'_{I\downarrow}^{i'} \langle c_{i'\sigma'}^{\dagger} \hat{n}_{I\downarrow} c_{i'\sigma'} \rangle_0
\]
\[
+ \langle c_{i'\sigma'}^{\dagger} c_{i'\sigma'} \rangle_0 \left( \kappa_{i'\sigma'} \left( g'_{I\uparrow} \eta_{I\uparrow,i'\sigma'} + g'_{I\downarrow} \eta_{I\downarrow,i'\sigma'} \right) + \kappa_{i'\sigma'} \left( g'_{I\uparrow} \eta_{I\uparrow,i'\sigma'} + g'_{I\downarrow} \eta_{I\downarrow,i'\sigma'} \right) \right)
\]
\[
+ \sigma \kappa_{i'\sigma'} \langle c_{i'\sigma'}^{\dagger} c_{i'\sigma'} \rangle_0 \langle c_{i'\sigma'}^{\dagger} c_{i'\sigma'} \rangle_0 \left( g'_{I\uparrow}^{i'} \kappa_{i'\sigma'} c_{i'\sigma'} c_{i'\sigma'} \right) - g'_{I\downarrow}^{i'} \kappa_{i'\sigma'} c_{i'\sigma'} c_{i'\sigma'} \langle c_{i'\sigma'}^{\dagger} c_{i'\sigma'} \rangle_0
\]
\[
+ \sigma \kappa_{i'\sigma'} \langle c_{i'\sigma'}^{\dagger} c_{i'\sigma'} \rangle_0 \left( g'_{I\uparrow}^{i'} \kappa_{i'\sigma'} c_{i'\sigma'} c_{i'\sigma'} \right) - g'_{I\downarrow}^{i'} \kappa_{i'\sigma'} c_{i'\sigma'} c_{i'\sigma'} \langle c_{i'\sigma'}^{\dagger} c_{i'\sigma'} \rangle_0 \right).
\]

(38)

Although all the new terms in (36) and (38) contain the $g_i$ factors, they are not so simple as (24) and inhibit the straightforward analytical transform back to the $k$-representation. In other words, they cause $k$-dependence of the renormalization. Since the ratio between the leading order and the corrections calculated in (38) is only of first order, the influence from the corrections may be larger than those in the GA for the real-space hopping amplitude, where the ratio is of second order.

Other corrections are the terms neglected in (15). We expect that they only slightly change the magnitude of the leading order, and that their contribution is probably not very important.

5. General estimation of higher order terms

Let us estimate the other higher order terms neglected above. The terms appearing in the Wick expansion can be classified into three groups by how to take contractions of $\hat{1}_{I\sigma}(1 - \hat{1}_{I\sigma})$:

(i) Onsite contractions are taken both for $I \uparrow$ and $I \downarrow$. These terms do not contribute to $V_{kk}$ as explained around (18).

(ii) If intersite contractions are taken for $I\sigma$ and the onsite contraction is taken for $I\bar{\sigma}$, then $\lambda_{I\sigma} \hat{n}_{I\sigma}(1 - \hat{n}_{I\sigma})/(P_2^0)$ is reduced to $\hat{n}_{I\sigma}$. Doing the same for $\lambda_{I\bar{\sigma}} \hat{n}_{I\bar{\sigma}}(1 - \hat{n}_{I\bar{\sigma}})/(P_2^0)$ yields $-\hat{n}_{I\sigma} n_{I\sigma}/(1 - n_{I\sigma})$. Then, their summation is $g'_{I\sigma} \hat{n}_{I\sigma}$. Namely, all of these terms are proportional to $g'_{I\sigma}$.

(iii) For the other terms, intersite contractions are taken both for $I \uparrow$ and $I \downarrow$. The naive evaluation of these terms does not yield any explicit factor vanishing at half filling, and we expect that many terms cancel out each other in some way. Instead, to derive explicit
renormalization, let us consider such contractions for \((k's)(1 - \hat{n}_{I}\uparrow)(1 - \hat{n}_{I}\downarrow)|ks\rangle\), which is equivalent to \(V_{k'k}\) for \(k \neq k'\). Then, we can replace as

\[
\frac{(1 - \hat{n}_{I}\uparrow)(1 - \hat{n}_{I}\downarrow)}{\langle P_{I}^{2} \rangle_{0}} \Rightarrow \frac{1 - n_{I}}{(1 - n_{I}\uparrow)(1 - n_{I}\downarrow)} \tilde{n}_{I}\uparrow \tilde{n}_{I}\downarrow, \tag{39}
\]

i.e. all such terms contain \(g_{I\sigma}' / (1 - n_{I\sigma})\) explicitly.

These considerations in (i), (ii) and (iii) above demonstrate that \(V_{k'k}\) contains the overall factor \(g_{I\sigma}'.\)

6. Magnetic impurity renormalization

Let us consider a simple magnetic impurity (4), i.e. the local magnetic field is applied at site \(I\). Its renormalization can be easily calculated by subtraction instead of summation of renormalized \(\hat{n}_{I}\uparrow\) and \(\hat{n}_{I}\downarrow\) using the above formulas. Corresponding to (26) and (28),

\[
\langle y_{r} P_{I}^{2} S_{I}^{z} P_{I} y_{r} \rangle_{0} \approx \frac{1}{2} \left[ \frac{1 - n_{I\uparrow} + n_{I\downarrow}}{1 - n_{I\uparrow}} \langle y_{r} \tilde{n}_{I}\uparrow S_{I}^{z} \rangle_{0} - 1 - n_{I\uparrow} \right] \tag{40}
\]

\[
\rightarrow \frac{1}{1 - n_{I\sigma}} \langle y_{r} S_{I}^{z} y_{r} \rangle_{0} \quad (n_{I} = n_{I}). \tag{41}
\]

The renormalization factor for \(n_{I\uparrow} = n_{I\downarrow}\) is \((1 - n_{I\sigma})^{-1}\), which is the square root of the Gutzwiller renormalization factor for the exchange interaction. Namely, in contrast to the non-magnetic impurity, the magnetic impurity is strengthened by the strong electron correlation. It also makes a good contrast with the unrenormalized diagonal matrix element \(\langle S_{I}^{z} \rangle = \langle S_{I}^{z} \rangle_{0}\).

(To derive this, the limit of \(\lambda_{I\uparrow} - \lambda_{I\downarrow} \to 0\) should be taken at the end starting from \(\lambda_{I\uparrow} \neq \lambda_{I\downarrow}\).)

In fact, also for magnetic systems \((n_{I\uparrow} \neq n_{I\downarrow})\), the factors appearing in (40) are equivalent to those in the renormalization of the exchange interaction derived in [7], i.e.

\[
\langle S_{I}^{+} S_{I}^{-} \rangle \approx \langle S_{I}^{+} \rangle_{0} \langle S_{I}^{-} \rangle_{0} + \frac{1}{4} \sum_{\sigma, \sigma'} \eta_{\sigma, \sigma'} \left( \frac{1}{1 - n_{I\sigma}} \right) \left( \frac{1 - 2\sigma' \langle S_{I}^{+} \rangle_{0}}{1 - n_{I\sigma'}} \right). \tag{42}
\]

Although it is not explicitly noted in [7], in this renormalization of the spin interaction, the first term is from onsite contractions and not renormalized (from diagonal matrix elements of the spin-\(z\) operators), whereas the second term, including intersite contractions, is enhanced by the renormalization factor (from the second order of the transition matrix elements of the spin-\(z\) operators). In fact, as shown in the next section, the charge interaction is also renormalized in a similar manner, although the direction of renormalization is opposite.

7. Charge interaction renormalization

The conventional GA [4] relates \(\langle \hat{O} \rangle_{0}\) for an operator \(\hat{O}\) using a renormalization factor. By following this procedure, the renormalization factor is unity for the charge interaction, namely

\[
\langle \hat{n}_{i} \hat{n}_{j} \rangle \approx \langle \hat{n}_{i} \hat{n}_{j} \rangle_{0} = n_{i} n_{j} + \sum_{\sigma, \sigma'} \eta_{i\sigma, j\sigma'}. \tag{43}
\]

However, this approximation is correct only for the leading term \(n_{i} n_{j}\) and the renormalization factor is likely to be derived by taking only the lowest order into account. Using a procedure
similar to that for the non-magnetic impurity, more careful analysis can be carried out, i.e.

\[
\langle \hat{n}_i \hat{n}_j \rangle \approx \sum_{\sigma, \sigma'} \lambda_i \lambda_j \langle (1 - \hat{n}_i) \hat{n}_j (1 - \hat{n}_j) \rangle_0
\]

\[
\approx n_i n_j + \sum_{\sigma, \sigma'} \left( \frac{n_i}{1 - n_i} \eta_{i \sigma, j \sigma'} - \frac{n_j}{1 - n_j} \eta_{i \sigma, j \sigma'} + \frac{n_i}{1 - n_i} \frac{n_j}{1 - n_j} \eta_{i \sigma, j \sigma'} \right)
\]

\[
= n_i n_j + \sum_{\sigma, \sigma'} g_{i \sigma} g_{j \sigma'} \eta_{i \sigma, j \sigma'}.
\]

At the half filling, any state is an eigenstate of \(\hat{n}_i \hat{n}_j\) with the eigenvalue unity by definition because every site is occupied by one electron and there is no particle number fluctuation, which contradicts (43) but is consistent with (44). In fact, the second term on the rhs of (44) is the second order of (29), namely it comes from a process in which \(\hat{n}_j\) creates two quasiparticles and \(\hat{n}_i\) annihilates them.

To the best of our knowledge, every calculation in the literature on the GA is using (43) instead of (44) including the calculation by the author himself, and this error is probably pointed out for the first time here. However, this charge interaction usually does not give a very important contribution in \(t-J\)-type models, and this correction is likely to make only minor modification to numerical values. Therefore, we expect that main conclusions are not drastically changed by this correction. Following this correction, equations in [7] should be modified, namely \((3g_{ij}^\sigma - 1)\) and \((3g_{ij}^\sigma + 1)\) in (14) and (15) should be replaced by \((3g_{ij}^\sigma - g_{i\sigma}^\sigma g_{j\sigma}^\sigma)\) and \((3g_{ij}^\sigma + g_{i\sigma}^\sigma g_{j\sigma}^\sigma)\), respectively, and the derivative of \(g_{ii}^\sigma\) should also be considered for (16).

8. Conclusion

Since the Gutzwiller approximation (GA) is formulated to (almost) conserve the particle number at the Gutzwiller projection, one may consider that quantities related to particle number operators are not renormalized. However, since the particle number is an expectation value with respect to an assumed ground state, the constraint of its conservation does not restrict transition matrix elements with excited states. Our results here correct the description by the conventional GA in the literature, where such renormalization factors are calculated with a focus on diagonal matrix elements or lowest order terms and regarded as unity. The results in this paper are general and do not depend on parameters. Namely, they are valid both for attractive and repulsive impurity potentials and both for attractive and repulsive charge interactions.

The Fourier-transformed impurity potential has a form of hopping in the \(k\)-space. We have derived similarities and differences between this ‘hopping’ in the \(k\)-space and in the real space under the real-space electron double-occupancy prohibition. As a similarity, they are strongly renormalized to decrease with the hole concentration \(x\), and their renormalization factor is \(g^i = 2x/(1 + x)\) in uniform non-magnetic systems. In addition, the higher order terms also contain \(g^i\). It should represent that not many available seats to hop are left because of the electron repulsion. A difference is that, however, \(\langle c_{j\sigma}^\dagger c_{j\sigma'} \rangle\) of each \(\sigma\) is renormalized in the real space, whereas the renormalization of \(\sum_{\sigma} \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle\) appears only after the summation over spin \(\sigma = \pm\) in the \(k\)-space. If this summation is replaced by subtraction, which corresponds to a magnetic impurity in the real space, then the direction of the renormalization is reversed, i.e. the renormalization factor is larger than unity and equivalent to the square root of that for the exchange interaction. As another difference, the corrections to the leading order term in the \(k\)-space can be larger and have a more complicated expression than those in the real space.
As a related calculation, the renormalization of charge interaction has also been derived. The leading order is rather trivial and unrenormalized, i.e. it is the product of particle densities at the two relevant sites. The next leading order term is the second order of transition matrix elements of the number operators with excited states. Since the transition matrix elements are renormalized by $g'$, these second-order terms are renormalized by $(g')^2$, namely strongly reduced. These terms include hopping and pairing amplitude and are relevant to the mean-field approximation. A similar relation is found also in the $z$-component of the exchange interaction. Namely, the leading order is the product of spin-$z$ densities at the two relevant sites. The next term is the second order of transition matrix elements of the spin-$z$ operator, which is strengthened by the electron repulsion. At the half filling, any state is an eigenstate of $\hat{n}_i\hat{n}_j$, with the eigenvalue unity. In fact, (44) satisfies it even in magnetic systems, which may demonstrate that the choice of fugacity factors by (9) is reasonable. Other choices of fugacity factors also discussed in [7] do not seem to satisfy it in magnetic systems, and their use is likely to be restricted in systems with small magnetic moments.

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