Grand canonical Gutzwiller approximation for magnetic inhomogeneous systems

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The Gutzwiller approximation (GA) for Gutzwiller-projected grand canonical wave functions with fugacity factors is investigated in detail. Our systems in general contain inhomogeneity and local magnetic moments. In deriving renormalization formulas, we also derive or estimate terms of higher powers of intersite contractions neglected in the conventional GA. We examine several different constraints, i.e., local/global spin-dependent/independent particle-number conservation. Out of the four, the local spin-dependent constraint seems the most promising at present. An improved GA derived from it agrees with the variational Monte Carlo method better than the conventional GA does. The corrections to the conventional GA can be interpreted as two-site correlation including the phase difference of configurations. Furthermore, projected quasiparticle excited states are orthogonal to each other within the GA. Using these states, spectral weights are calculated. We show that asymmetry between electron addition and removal spectra can appear by taking into account the higher powers of the intersite contractions in the case of the *d*-wave superconductors and the Fermi sea; the addition is smaller than the removal. However, the asymmetry is quite weak especially near the Fermi level. In contrast, projected *s*-wave superconductors can have the opposite asymmetry (addition larger than removal) especially near the Fermi level. In addition, formulas from the other three constraints are also derived, which may be useful depending on purposes.

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I. INTRODUCTION

This paper concerns calculation of expectation values using projected wave functions in inhomogeneous systems. In order to study electronic systems with repulsive on-site interactions, Gutzwiller proposed projected wave functions[1] of the form $P_{\mathrm{G}}|\Psi_0\rangle$ with the Gutzwiller projection operator,

$$P_{\mathrm{G}} \equiv \prod_i (1 - \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}), \tag{1}$$

to prohibit electron double occupancy on each site. Here, $\hat{n}_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$ with $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) being the creation (annihilation) operator of site i and spin σ.

Expectation values of operators by this projected wave function can be evaluated by the variational Monte Carlo (VMC) method numerically exactly within statistical errors. However, the VMC requires lots of computational effort for some issues. In addition, it needs one run for each parameter set, whereas an analytical method can generate more general formulas that often provide us some hint to understand the system. Thus, instead of the VMC, an analytical approximation called the Gutzwiller approximation (GA) is used on occasions, i.e.,

$$\frac{\langle\Psi^N|\hat{O}|\Psi^N\rangle}{\langle\Psi^N|\Psi^N\rangle} \approx g^O \frac{\langle\Psi_0^N|\hat{O}|\Psi_0^N\rangle}{\langle\Psi_0^N|\Psi_0^N\rangle}, \tag{2}$$

with $|\Psi^N\rangle \equiv P_{\mathrm{G}}|\Psi_0^N\rangle$, where $|\Psi_0^N\rangle$ have a fixed particle number N. The factor g^O is the Gutzwiller renormalization factor for the operator $\hat{O}$. If one chooses a noninteracting or mean-field approximated wave function as $|\Psi_0^N\rangle$, the expectation value in the right-hand side of Eq. (2) can be easily evaluated. The renormalization factor for the hopping term denoted by g^t is smaller than unity because it is more difficult to hop in the presence of the strong on-site Coulomb repulsion between electrons; that for the exchange interaction denoted by g^s is larger than unity because each site is more often singly occupied to avoid the other electrons. The GA was first introduced for the Hubbard model by Gutzwiller,[2,3] then reformulated by Ogawa *et al.*[4] A clear description of the method has been given by Vollhardt.[5] It was also applied to a mean-field theory for the *t-J* model by Zhang *et al.*[6] Improvements of the GA by taking more intersite correlations have been made by several authors.[7–9] The GA usually produces qualitatively correct results although it is reported that there are also qualitative differences in some cases.[10]

The original formulation of the GA implicitly assumes that a wave function before the projection has a fixed particle number N (in the following, we call it the "canonical scheme"). If the particle number of a wave function has fluctuation (the "grand canonical scheme"), then the Gutzwiller projection reduces the particle number (see Appendix A). Such reduction of the particle number may arouse a question whether the GA as Eq. (2) is valid because this equation seems to say that the wave functions before and after the projection have similar properties except for the double occupancy; are they similar if they have different particle numbers? To avoid such an unclear path, Anderson and Ong,[11] and Edegger *et al.*[12] formulated a grand canonical GA by taking the canonical scheme as a guide. Namely, one can force the projection not to change the *average* particle number, by gluing to P_{G} a fugacity factor that compensates the particle-number reduction. To our knowledge, the fugacity factor was first seen in a preliminary form in the paper by Yokoyama and Shiba[13] to relate the canonical and the grand canonical VMC. Gebhard[14] introduced position- and spin-dependent fugacity factors for calculational convenience of the $1/d$ expansion whose $d\to\infty$ limit corresponds to the GA. They also appear in the construction of the gossamer superconductivity by Laughlin.[15] Then, Wang *et al.*[16] used

position-dependent but spin-independent fugacity factors for inhomogeneous systems.

The fugacity factors allow us freedom to choose a relation between the particle numbers before and after the projection, and the renormalization depends on this choice. Recently, Ko *et al.*[17] pointed out that two contradictory formulas of the Gutzwiller renormalization factors in the literature actually come from two different choices of the fugacity factors. That is, (i) the fugacity factors are determined so that the projection conserves the *local* particle density of each spin direction at each site, or (ii) so that the projection conserves the *total* particle number for each spin direction (this is the usual canonical-scheme constraint). Mainly for the square lattice antiferromagnet, they used the canonical scheme, and introduced additional position- and spin-dependent fugacity factors, then calculated each renormalization factor as a ratio of probabilities for the physical process.

In this paper, we examine in detail several different choices of fugacity factors that impose local/global spin-dependent/independent particle-number conservation. We adopt the grand canonical scheme, and derive general formulas. Some of our formulas are different from those by the canonical derivation. Furthermore, corrections to the conventional GA are also estimated or derived by taking intersite correlations into account. The structure of the paper is as follows: Secs. II and III are devoted for case (i), and Sec. IV for case (ii). First in Sec. II, we derive renormalization of the hopping and the pairing amplitude, the local spin moments and the exchange interaction from the local spin-dependent constraint. We test the formulas of the hopping amplitude by comparing with the VMC. Physical interpretations are given for newly derived terms. Subsequently in Sec. III, we also check orthogonality and excitation energies of projected Bogoliubov quasiparticle states, and discuss asymmetry between positive and negative bias spectra. Next, in Sec. IV, formulas from the global spin-dependent constraint are derived. The formulation there includes cases where the particle numbers before and after the projection are unequal. In addition, grand canonical GAs with local/global spin-*independent* constraints are briefly discussed in Sec. V.

In our impression, the grand canonical scheme simplifies calculation in many cases because it is free from complicated configuration counting. Furthermore, systematic improvement is straightforward by including terms from larger clusters in the linked-cluster expansion.[1] The formulation we use is similar to the $1/d$ expansion by Metzner and Vollhardt,[18] and Gebhard.[14] The lowest-order theory in the uniform nonsuperconducting limit of our formulation for case (i) is equivalent to the $d\rightarrow\infty$ limit of the $1/d$ expansion. However, in inhomogeneous systems and in the presence of the second and the third neighbor hopping, it is not clear if $1/d$ is a good expansion parameter. In addition, considering future improvements of the theory, it may be difficult to define terms of very high order in $1/d$. Therefore, we naively use the linked-cluster expansion as Gutzwiller's original formulation,[1] then expand it in a power series of intersite contractions and neglect high-order terms. Furthermore, we do not adhere to making derived formulas into the form of Eq. (2).

Throughout this paper, we use the following notation: A wave function before a projection is denoted by $|\Psi_0\rangle$ and it does not have a definite particle number and may have some inhomogeneity in general. Then, the wave function after the projection is represented by $|\Psi\rangle=P|\Psi_0\rangle$, where P is a generalized projector that includes fugacity factors defined later. The expectation values of an arbitrary operator $\hat{O}$ by these wave functions are denoted by

$$\langle\hat{O}\rangle \equiv \frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \quad \langle\hat{O}\rangle_0 \equiv \frac{\langle\Psi_0|\hat{O}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}. \tag{3}$$

Furthermore,

$$n_{i\sigma} \equiv \langle\hat{n}_{i\sigma}\rangle_0, \ \ n_{ij\sigma} \equiv \langle c_{i\sigma}^{\dagger}c_{j\sigma}\rangle_0, \ \ \Delta_{ij} \equiv \langle c_{j\downarrow}c_{i\uparrow}\rangle_0, \tag{4}$$

$$n_i \equiv n_{i\uparrow} + n_{i\downarrow}, \quad m_i \equiv \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}). \tag{5}$$

In addition, $\mathbf{S}_i$ denotes the spin operator at site i.

II. LOCAL CONSTRAINT

The Gutzwiller projection changes electron-density distribution in inhomogeneous systems in general. However, by introducing fugacity factors, one can force desired electron-density distribution. We prefer to start from the grand canonical GA with a local constraint for each spin direction, namely,

$$\langle\hat{n}_{i\sigma}\rangle = \langle\hat{n}_{i\sigma}\rangle_0, \tag{6}$$

for any i and σ. Note that this local constraint is different from the canonical-scheme constraint that conserves the *total* particle number. However, this "local canonical" constraint simplifies the resultant formulas as shown in the following. For example, some of low-order corrections to the GA vanish automatically. Furthermore, with this constraint, projected Bogoliubov quasiparticle states are approximately orthogonal to each other, and excitation energies are approximately obtained by diagonalizing a renormalized Hamiltonian (shown in Sec. III).

In general, $\langle S_i^x\rangle_0$ and $\langle S_i^y\rangle_0$ can be finite. Such cases will be discussed only in Sec. II D, and otherwise $\langle S_i^x\rangle_0=\langle S_i^y\rangle_0=0$ and $\langle c_{i\sigma}^{\dagger}c_{j\bar{\sigma}}\rangle_0=0$ are assumed. Furthermore, although we have d-wave superconductors in mind, there may be deviation from d wave in inhomogeneous magnetic systems, and $\langle c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}\rangle_0$ (on-site pairing *before* the projection) can be nonzero. We discuss effect of $\langle c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}\rangle_0\neq 0$ in Sec. III G, and otherwise assume $\langle c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}\rangle_0=0$ for any i. We also do not consider triplet pairing of the form $\langle c_{i\sigma}^{\dagger}c_{j\sigma}^{\dagger}\rangle_0$ and set it to zero for any i, j, and σ. The generalization to $\langle c_{i\sigma}^{\dagger}c_{j\sigma}^{\dagger}\rangle_0\neq 0$ is straightforward.

A. Condition for fugacity factors

The projected wave function is defined as $|\Psi\rangle=P|\Psi_0\rangle$ with $P\equiv\Pi_i P_i$, where

$$P_i \equiv \lambda_{i\uparrow}^{\hat{n}_{i\uparrow}/2}\lambda_{i\downarrow}^{\hat{n}_{i\downarrow}/2}(1-\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}). \tag{7}$$

The local up and down particle numbers are controlled by $\lambda_{i\sigma}^{\hat{n}_{i\sigma}/2}$, and the fugacity factors $\lambda_{i\sigma}$ will be determined later to

satisfy Eq. (6). In order to derive their explicit forms, let us calculate the density of σ-spin electron at site i,

$$\langle \hat{n}_{i\sigma} \rangle = \frac{\left\langle \lambda_{i\sigma} \hat{n}_{i\sigma} (1 - \hat{n}_{i\bar{\sigma}}) \prod_{l \neq i} P_l^2 \right\rangle_0}{\left\langle \prod_l P_l^2 \right\rangle_0}. \tag{8}$$

In principle, by applying the Wick theorem, these expectation values can be exactly evaluated. In practice, however, such calculation is quite difficult to carry out because too many terms appear by the Wick decomposition. To approximate it, remember that intersite contractions, $n_{ij\sigma}$ and Δ_{ij}, are much smaller than on-site contractions, $n_{i\sigma}$. An approximation to take the leading order with respect to the intersite contractions corresponds to the GA. Here, we take only on-site contractions. Then, $l \neq i$ terms cancel out between the numerator and the denominator, namely,

$$\langle \hat{n}_{i\sigma} \rangle \approx \frac{\lambda_{i\sigma}(1 - n_{i\bar{\sigma}})}{\Xi_i} n_{i\sigma}, \tag{9}$$

$$\Xi_i \equiv \langle P_i^2 \rangle_0 = (1 - n_{i\uparrow})(1 - n_{i\downarrow}) + \lambda_{i\uparrow} n_{i\uparrow}(1 - n_{i\downarrow}) + \lambda_{i\downarrow} n_{i\downarrow}(1 - n_{i\uparrow}). \tag{10}$$

Therefore, the condition to determine $\lambda_{i\sigma}$ is given by $\lambda_{i\sigma}(1 - n_{i\bar{\sigma}})/\Xi_i = 1$. By solving the simultaneous equations for up and down spins, we obtain

$$\lambda_{i\sigma} \approx \frac{1 - n_{i\sigma}}{1 - n_i}, \quad \Xi_i \approx \frac{(1 - n_{i\uparrow})(1 - n_{i\downarrow})}{1 - n_i}. \tag{11}$$

The corrections to $\langle P^2 \rangle_0$ and $\langle n_{i\sigma} \rangle$ can be calculated by taking into account intersite contractions between site i and other sites $l \neq i$. Let us calculate terms proportional to $|n_{il\uparrow}|^2$. Such terms appear by the Wick decomposition of $\langle \hat{n}_{i\uparrow} P^2 \rangle_0$. We take on-site contractions for the sites other than i, l, and thus we only need to consider $\langle \hat{n}_{i\uparrow} P_l^2 \rangle_0$. The operators in $\hat{n}_{i\uparrow} = c_{i\uparrow}^\dagger c_{i\uparrow}$ are contracted with those in $c_{l\uparrow}^\dagger c_{l\uparrow}$ or $c_{l\uparrow} c_{l\uparrow}^\dagger$ in P_l^2. Then, the operators for the down spin are replaced by $n_{l\downarrow}$ or $1 - n_{l\downarrow}$. Namely, such contribution is written as

$$|n_{il\uparrow}|^2 [(1 - n_{l\downarrow}) - \lambda_{l\uparrow}(1 - n_{l\downarrow}) + \lambda_{l\downarrow} n_{l\downarrow}] = 0.$$

In other words, the terms proportional to $|n_{il\uparrow}|^2$ vanish when $\lambda_{i\sigma}$ is set as Eq. (11). Similarly, terms proportional to Δ_{il}^2 also vanish. Therefore, with Eq. (11), we have $\langle \hat{n}_{i\sigma} \rangle = n_{i\sigma} + O(n_{ij\sigma}^4) + O(\Delta_{ij}^4)$. Estimated corrections to $\lambda_{i\sigma}$ are also of the order of $n_{ij\sigma}^4$ or Δ_{ij}^4.

B. Hopping and pairing amplitude

For the hopping term, similar calculation can be carried out. Namely, for $i \neq j$,

$$\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle = \lambda_{i\uparrow}^{1/2} \lambda_{j\uparrow}^{1/2} \frac{\left\langle c_{i\uparrow}^\dagger c_{i\downarrow} c_{i\downarrow}^\dagger c_{j\uparrow} c_{j\downarrow} c_{j\downarrow}^\dagger \prod_{l \neq i,j} P_l^2 \right\rangle_0}{\langle P^2 \rangle_0} \tag{12}$$

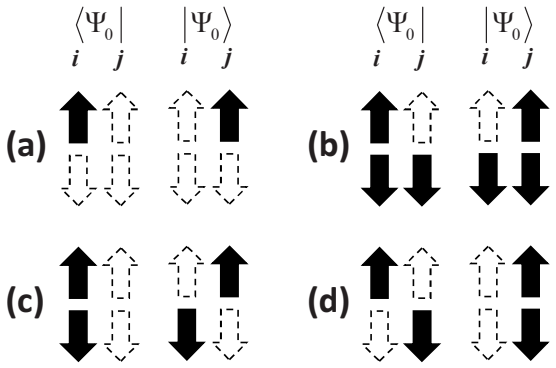

FIG. 1. Configurations contributing to $\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle_0$. Filled arrows represent occupied states, and open dashed arrows represent unoccupied states. Only (a) contributes to $\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle$.

$$\approx \frac{\lambda_{i\uparrow}^{1/2} \lambda_{j\uparrow}^{1/2} (1 - n_{i\downarrow})(1 - n_{j\downarrow})}{\Xi_i \Xi_j} \langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle_0, \tag{13}$$

where we took on-site contractions except one intersite contraction (that is necessary) in the numerator. Then, the Gutzwiller renormalization factor is given by[17]

$$\frac{\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle}{\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle_0} \approx \sqrt{\frac{1 - n_i}{1 - n_{i\sigma}}} \sqrt{\frac{1 - n_j}{1 - n_{j\sigma}}} \equiv g_{ij\sigma}^{t0}. \tag{14}$$

The next order in fact involves one more site other than i and j, but the second and the third order of the intersite contractions for such contribution vanish when $\lambda_{i\sigma}$ is set as Eq. (11). Therefore, the third order term involves only sites i and j. Namely, taking more contractions between i and j in Eq. (12),

$$\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle \approx g_{ij\uparrow}^{t0} \left(n_{ij\uparrow} - n_{ij\downarrow} \frac{n_{ij\uparrow} n_{ij\downarrow}^* + \Delta_{ij}^* \Delta_{ji}}{(1 - n_{i\downarrow})(1 - n_{j\downarrow})} \right). \tag{15}$$

The formula for $\langle c_{i\downarrow}^\dagger c_{j\downarrow} \rangle$ is obtained by replacing as $\uparrow \Leftrightarrow \downarrow$ and $\Delta_{ij} \Rightarrow -\Delta_{ji}$. The $n_{ij\uparrow} |n_{ij\downarrow}|^2$ term in Eq. (15) is from repulsive correlation between down-spin holes due to the Pauli principle: all of the four configurations in Fig. 1 contribute to $\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle_0$, but only Fig. 1(a) does to $\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle$. Then, taking into account repulsion between down-spin holes, Fig. 1(a) has less weight than the estimate by the conventional GA that neglects this correlation.

On the other hand, the $n_{ij\downarrow} \Delta_{ij}^* \Delta_{ji}$ term is from superconducting correlation; negative for $\Delta_{ij} = \Delta_{ji}$ (singlet), and positive for $\Delta_{ij} = -\Delta_{ji}$ (triplet). This term seems related to the phase difference between the four configurations in Fig. 2, which appear in $|\Psi\rangle_0$ (before the projection). Our rough ex-

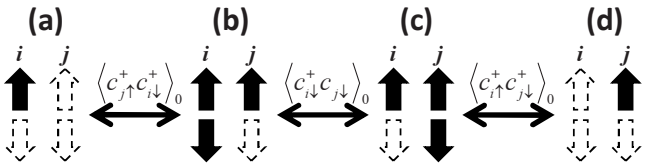

FIG. 2. Roundabout correlation between (a) and (d) via (b) and (c). These configurations in $|\Psi_0\rangle$ correlate in the presence of superconductivity.

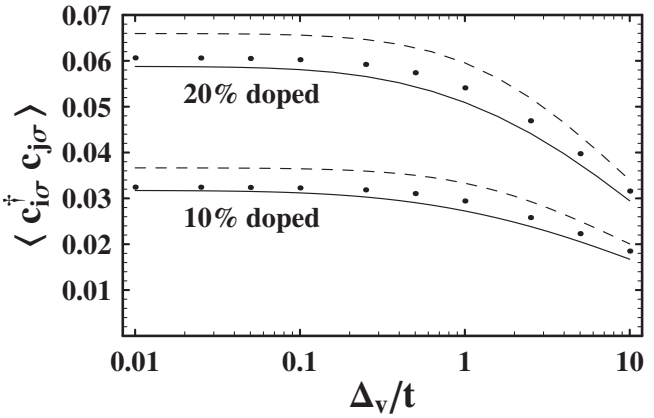

FIG. 3. The nearest-neighbor hopping amplitude $\langle c^{\dagger}_{i\sigma}c_{j\sigma}\rangle$ calculated by the conventional GA [Eq. (14), broken line], the generalized GA [Eq. (15), solid line], and the VMC [dots] for the projected uniform nonmagnetic BCS d-wave superconductor.

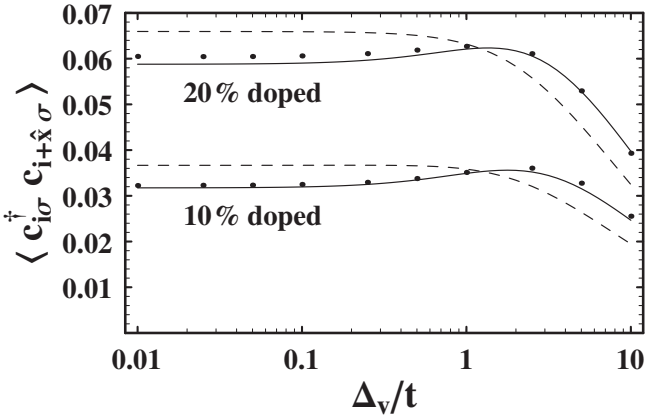

FIG. 4. The nearest-neighbor hopping amplitude of the projected "p-wave" superconductor calculated by the conventional GA [Eq. (14), broken line], the generalized GA [Eq. (15), solid line], and the VMC [dots].

planation in the case of $n_{ij\uparrow} \simeq n_{ij\downarrow}$ is as follows: Suppose ζ_a, ζ_b, ζ_c, and ζ_d are coefficients of the configuration (a, b, c, and d) in $|\Psi\rangle_0$, and assume they are real numbers. Then, $\zeta_a\zeta_d$ contributes to $n_{ij\uparrow}$, and $-\zeta_b\zeta_c$ contributes to $n_{ij\downarrow}$. Remember that the conventional GA can be derived by taking the ratio of the probability of configurations;[6,17] it implicitly assumes that $\zeta_a\zeta_d$ and $-\zeta_b\zeta_c$ have the same sign. Turning on the superconducting correlation, configurations (a) and (b), as well as (c) and (d), start to correlate. Then, their contribution to the singlet order parameter before the projection $\langle c^{\dagger}_{i\uparrow}c^{\dagger}_{j\downarrow} - c^{\dagger}_{i\downarrow}c^{\dagger}_{j\uparrow}\rangle_0$ is proportional to $\zeta_b\zeta_a + \zeta_c\zeta_d$. The magnitude of this quantity, however, is small if $\zeta_a\zeta_d$ and $-\zeta_b\zeta_c$ have the same sign. Therefore, to strengthen the singlet superconducting correlation, all of $\zeta_a\zeta_d, \zeta_b\zeta_c$ should be small. Accordingly, the weight of Fig. 1(a) should be smaller than the estimate by the conventional GA.

We test this formula for a simple case, i.e., the projected uniform nonmagnetic d-wave superconductor,

$$|\Psi_0\rangle = \prod_k (u_k + v_k c^{\dagger}_{k,\uparrow}c^{\dagger}_{k,\downarrow})|0\rangle,$$

$$u_k \equiv \sqrt{\frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right)}, \quad v_k \equiv \frac{\Delta_k}{|\Delta_k|}\sqrt{\frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right)},$$

$$E_k \equiv \sqrt{\xi_k^2 + \Delta_k^2}, \quad \Delta_k \equiv \Delta_v(\cos k_x - \cos k_y),$$

$$\xi_k \equiv -2t(\cos k_x + \cos k_y) - \mu. \tag{16}$$

The conventional GA as Eq. (14), the generalized GA as Eq. (15), and the VMC are compared in Fig. 3 for the nearest-neighbor hopping. Here, the generalized GA is done using 200×200 sites, and practically the finite-size effects are negligible; errors only come from neglect of the higher order of the intersite contractions. μ is adjusted to satisfy each hole concentration for each point. The VMC is carried out using 30×30 sites with x-antiperiodic y-periodic boundary condition. The hopping amplitude is averaged over every bond, and the statistical errors are negligible in the scale of this figure. For comparison with the GAs, μ is also adjusted to equalize the doping before the projection with that after. At small Δ_v, the generalized GA agrees with the VMC very well. As Δ_v increases, the deviation becomes larger. This is possibly because $O(\Delta_{ij}^4)$ term neglected in Eq. (9) may start to make an important contribution.

In inhomogeneous systems, there may be deviation from the d wave. Since it is rather difficult to force the local constraint for the VMC in inhomogeneous systems, let us test the formula using a simpler non-d wave, namely, a uniform p-wave superconductor by redefining

$$\Delta_k \equiv \Delta_v \sin k_x \tag{17}$$

in Eq. (16). The nearest-neighbor hopping amplitude in x direction is plotted in Fig. 4. The generalized GA shows a good overall agreement with the VMC. It especially reproduces characteristic peak at $\Delta_v \sim 2t$ caused by the $n_{ij\downarrow}\Delta^*_{ij}\Delta_{ji}$ term in contrast to the conventional GA.

The superconducting order parameters $\langle c^{\dagger}_{i\uparrow}c^{\dagger}_{j\downarrow}\rangle$ can be calculated similarly to the hopping term, i.e.,

$$\langle c^{\dagger}_{i\uparrow}c^{\dagger}_{j\downarrow}\rangle = \sqrt{g_{ii\uparrow}g_{jj\downarrow}}\left(\Delta^*_{ij} + \Delta^*_{ji}\frac{n_{ij\uparrow}n^*_{ij\downarrow} + \Delta^*_{ij}\Delta_{ji}}{(1-n_{i\downarrow})(1-n_{j\uparrow})}\right). \tag{18}$$

The Δ^*_{ij} term represents the direct correlation between the $i\uparrow, j\downarrow$ occupied state [Fig. 5(a)] and the empty state [Fig. 5(d)]. The $\Delta^*_{ij}|\Delta_{ji}|^2$ term contains the attractive correlation between holes of $i\downarrow$ and $j\uparrow$; if Δ_{ji} is finite, $i\downarrow$ and $j\uparrow$ tend to

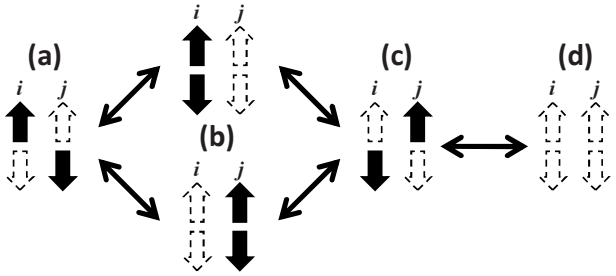

FIG. 5. Roundabout correlation between (a) and (d) via (b) and (c) in $|\Psi_0\rangle$.

be simultaneously occupied or unoccupied, and it is less likely that only one of them is occupied. Accordingly, this effect increases weight of the configurations in Figs. 5(a) and 5(d), and appears as the positive correction in Eq. (18). The $\Delta_{ij}^* n_{ij\uparrow} n_{ij\downarrow}^*$ term represents roundabout correlation between $i\uparrow$ and $j\downarrow$ through $i\downarrow$ and $j\uparrow$ as depicted in Fig. 5. Argument similar to what is used for the hopping amplitude (Fig. 2) leads to the conclusion that the singlet correlation enhances weight of configurations in Fig. 5 in this case.

Note that Eqs. (15) and (18) are mainly aimed at $|i-j|=1$. For next-nearest neighbors, $O(n_{ij}^4)$ of $|i-j|=1$ may be comparable to $O(n_{i'j'}^2)$ of $|i'-j'|=2$ and the former may be dominant especially in high dimensions. In general, as i and j separate from each other, the approximation by Eqs. (15) and (18) may lose accuracy.

C. Spin moment and exchange interaction

By definition, the local spin-z component at each site is not renormalized, i.e.,

$$\langle S_i^z \rangle = \langle S_i^z \rangle_0 = m_i. \tag{19}$$

For the exchange interaction term $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$, we take up to the second order of intersite contractions. Using symbols $\uparrow, \downarrow$, and $+1, -1$, interchangeably, it is written as

$$\langle S_i^z S_j^z \rangle = \frac{1}{4\langle P^2 \rangle_0} \sum_{\sigma,\tau=\pm 1} \sigma\tau \lambda_{i\sigma}\lambda_{j\tau} \left\langle c_{i\sigma}^\dagger c_{i\sigma} c_{i\bar{\sigma}}^\dagger c_{i\bar{\sigma}} c_{j\tau}^\dagger c_{j\tau} c_{j\bar{\tau}}^\dagger c_{j\bar{\tau}} \prod_{l\neq i,j} P_l^2 \right\rangle_0 \approx m_i m_j - \frac{1}{4}[(1-n_{i\uparrow})(1-n_{i\downarrow})(1-n_{j\uparrow})(1-n_{j\downarrow})]^{-1}$$
$$\times [|n_{ij\uparrow}|^2 (1-2m_i)(1-2m_j)(1-n_{i\downarrow})(1-n_{j\downarrow}) + |n_{ij\downarrow}|^2 (1+2m_i)(1+2m_j)(1-n_{i\uparrow})(1-n_{j\uparrow})$$
$$+ |\Delta_{ij}|^2 (1-2m_i)(1+2m_j)(1-n_{i\downarrow})(1-n_{j\uparrow}) + |\Delta_{ji}|^2 (1+2m_i)(1-2m_j)(1-n_{i\uparrow})(1-n_{j\downarrow})], \tag{20}$$

$$\langle S_i^x S_j^x + S_i^y S_j^y \rangle = \frac{\sqrt{\lambda_{i\uparrow}\lambda_{i\downarrow}\lambda_{j\uparrow}\lambda_{j\downarrow}}}{2\langle P^2 \rangle_0} \sum_\sigma \left\langle c_{i\sigma}^\dagger c_{i\bar{\sigma}} c_{j\bar{\sigma}}^\dagger c_{j\sigma} \prod_{l\neq i,j} P_l^2 \right\rangle_0 \approx \frac{-\mathrm{Re}[n_{ij\uparrow} n_{ij\downarrow}^* + \Delta_{ij}\Delta_{ji}^*]}{\sqrt{(1-n_{i\uparrow})(1-n_{i\downarrow})(1-n_{j\uparrow})(1-n_{j\downarrow})}} = g_{ij}^{sxy} \langle S_i^x S_j^x + S_i^y S_j^y \rangle_0, \tag{21}$$

with

$$g_{ij}^{sxy} \equiv \frac{1}{\sqrt{(1-n_{i\uparrow})(1-n_{i\downarrow})(1-n_{j\uparrow})(1-n_{j\downarrow})}}. \tag{22}$$

Here, Eq. (20) seems different from what is derived as a ratio of probabilities for the physical process using the canonical scheme with the fugacity factors by Ko *et al.*[17] We speculate that it possibly does not take into account all of the contractions above.

To compare with the result by $1/d$ expansion by Gebhard,[14] set $\Delta_{ij}=\Delta_{ji}=0$ and consider antiferromagnets. By setting $n_{i\sigma}=n_{j\bar{\sigma}}$ in Eqs. (20) and (21), these equations are reduced to

$$\langle S_i^z S_j^z \rangle \approx m_i m_j - \frac{(1-4m_i^2)(\langle S_i^z S_j^z \rangle_0 - m_i m_j)}{(1-n_{i\uparrow})(1-n_{i\downarrow})}, \tag{23}$$

$$\langle S_i^x S_j^x + S_i^y S_j^y \rangle \approx \frac{\langle S_i^x S_j^x + S_i^y S_j^y \rangle_0}{(1-n_{i\uparrow})(1-n_{i\downarrow})}, \tag{24}$$

which are equivalent to the formula by the $1/d$ expansion.[14] However, when $\Delta_{ij}\neq 0$, renormalization of $\langle S_i^z S_j^z \rangle$ is not reduced to such a simple form, and we need the original formula, Eq. (20). Note that Eqs. (23) and (24) can be used also for nonsuperconducting ferromagnets. Namely, the local constraint leads to the conclusion that antiferromagnets and ferromagnets are renormalized similarly. This is in distinct contrast to results of the GA with *global* constraint as will be discussed in Sec. IV F.

D. Systems with nonzero spin-*xy* components

This choice of fugacity factors encounters difficulties when $\langle S_i^x \rangle_0$ or $\langle S_i^y \rangle_0$ is finite. Let us redo the derivation including $\mathcal{S}_i^\pm \equiv \langle S_i^\pm \rangle_0$:

$$\langle \hat{n}_{i\sigma} \rangle \approx \frac{\lambda_{i\sigma}[n_{i\sigma}(1-n_{i\bar{\sigma}}) + \mathcal{S}_i^+ \mathcal{S}_i^-]}{\Xi_i}, \tag{25}$$

$$\Xi_i = (1-n_{i\uparrow})(1-n_{i\downarrow}) + \lambda_{i\uparrow} n_{i\uparrow}(1-n_{i\downarrow}) + \lambda_{i\downarrow} n_{i\downarrow}(1-n_{i\uparrow})$$
$$+ (\lambda_{i\uparrow} + \lambda_{i\downarrow} - 1)\mathcal{S}_i^+ \mathcal{S}_i^-. \tag{26}$$

The condition to determine $\lambda_{i\sigma}$ is

$$\lambda_{i\sigma} \frac{n_{i\sigma}(1-n_{i\bar{\sigma}}) + \mathcal{S}_i^+ \mathcal{S}_i^-}{\Xi_i} = n_{i\sigma}. \tag{27}$$

This is solved to give

$$\Xi_i \approx \frac{(1-n_{i\uparrow})(1-n_{i\downarrow}) - \mathcal{S}_i^+ \mathcal{S}_i^-}{1-n_i}, \tag{28}$$

$$\lambda_{i\sigma} \approx \frac{n_{i\sigma}}{n_{i\sigma}(1-n_{i\bar{\sigma}}) + \mathcal{S}_i^+ \mathcal{S}_i^-} \Xi_i. \tag{29}$$

For a spin moment, $\langle S_i^z \rangle = \langle S_i^z \rangle_0$, and

$$\langle S_i^{\pm}\rangle \approx \frac{\sqrt{\lambda_{i\uparrow}\lambda_{i\downarrow}}}{\Xi_i}\mathcal{S}_i^{\pm} = \mathcal{S}_i^{\pm}\sqrt{\frac{n_{i\uparrow}}{n_{i\uparrow}(1-n_{i\downarrow})+|\mathcal{S}_i^{+}|^2}}\sqrt{\frac{n_{i\downarrow}}{n_{i\downarrow}(1-n_{i\uparrow})+|\mathcal{S}_i^{+}|^2}}. \tag{30}$$

This renormalization factor for $\mathcal{S}_i^{\pm}$ is larger than unity because it is not bound by the local constraint. Since xy component is renormalized differently from z component, approximation depends on humans' choice of z axis. This asymmetry is probably related to what is discussed by Ko *et al.*[17] The most reasonable choice of z axis we think is making it parallel to $\langle \mathbf{S}_i\rangle_0$ at each site. Then, $\mathcal{S}_i^{\pm}=0$ for any i. It is equivalent to formulating a GA with constraints $\langle \hat{n}_{i\uparrow}+\hat{n}_{i\downarrow}\rangle = n_i$ and $\langle \mathbf{S}_i\rangle = \langle \mathbf{S}_i\rangle_0$. However, such a GA may yield very complicated renormalization factors for intersite terms. One way to avoid such a complexity is to use spin-independent constraint as shown in Sec. V A.

III. LOCAL CONSTRAINT: EXCITED STATES

The GA with the position- and spin-dependent constraint discussed in the previous section has an advantage in constructing plausible excited states which are approximately orthogonal to each other as shown below.

For shorthand notation, we use

$$c_i \equiv c_{i\uparrow}, \quad c_{N_L+i} \equiv c_{i\downarrow}^{\dagger}, \tag{31}$$

where N_L is the number of lattice sites. Then, the subscript of this new operator runs from 1 to $2N_L$, and we represent it by single Greek symbols as c_ρ. Furthermore, we define

$$\hat{\underline{n}}_{\rho\zeta} \equiv c_\rho^{\dagger}c_\zeta, \quad \underline{n}_{\rho\zeta} \equiv \langle \hat{\underline{n}}_{\rho\zeta}\rangle_0. \tag{32}$$

A. Bogoliubov–de Gennes equation

As a preparation, let us begin with deriving a Bogoliubov–de Gennes (BdG) equation by minimizing the Gutzwiller-approximated energy following the procedure by Wang *et al.*[16] In the following, we work more on general properties of a BdG equation with the Gutzwiller projection, and do not use any Hamiltonian explicitly. However, what we have in mind is inhomogeneous t-J–type models,

$$H_{tJ} \equiv P_G\left(-\sum_{ij\sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma} + \sum_{\langle i,j\rangle} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j\right)P_G, \tag{33}$$

where the t_{ij} term with $i=j$ may represent local impurity potentials. The zero-temperature grand potential $\Omega \equiv \langle H_{tJ} - \mu\Sigma_{i,\sigma}\hat{n}_{i\sigma}\rangle$ can be approximated by the GA, and represented by a function of $\underline{n}_{\rho\zeta}$, namely,

$$\Omega \approx \Omega_{GA}[\{\underline{n}_{\rho\zeta}\},\mu]. \tag{34}$$

We do not show the explicit form of Ω_{GA} because it can be derived straightforwardly by using the formulas in the previous section. In the derivation, one can choose the level of the approximation: If one takes only the leading order of the intersite contractions, formulas in the nonmagnetic case are equivalent to those derived by Wang *et al.*[16] and Li *et al.*[19] If an improved Gutzwiller approximation such as Eq. (15) is used, a more accurate solution can be obtained in principle, although it may be more difficult to find self-consistent solutions.

The chemical potential μ is determined to adjust the particle number N to satisfy $N=-\partial\Omega_{GA}/\partial\mu$. The other variables are functional of Ψ_0 and determined by minimizing Ω_{GA},

$$\frac{\delta\Omega_{GA}}{\delta\Psi_0} = \sum_{\rho\zeta}\frac{\partial\Omega_{GA}}{\partial\underline{n}_{\rho\zeta}}\frac{\delta\underline{n}_{\rho\zeta}}{\delta\Psi_0} = 0. \tag{35}$$

Assuming $\langle\Psi_0|\Psi_0\rangle = 1$, then

$$\delta\underline{n}_{\rho\zeta} = \langle\delta\Psi_0|\hat{\underline{n}}_{\rho\zeta}|\Psi_0\rangle + \langle\Psi_0|\hat{\underline{n}}_{\rho\zeta}|\delta\Psi_0\rangle. \tag{36}$$

By combining Eqs. (35) and (36),

$$\delta\Omega_{GA} = \langle\delta\Psi_0|H_{BdG}|\Psi_0\rangle + \langle\Psi_0|H_{BdG}|\delta\Psi_0\rangle, \tag{37}$$

where

$$H_{BdG} \equiv \sum_{\rho\zeta}\frac{\partial\Omega_{GA}}{\partial\underline{n}_{\rho\zeta}}\hat{\underline{n}}_{\rho\zeta}. \tag{38}$$

Then, Ω_{GA} takes an extremum when $|\Psi_0\rangle$ is an eigenstate of H_{BdG}, namely,

$$H_{BdG}|\Psi_0\rangle = E_{BdG}|\Psi_0\rangle, \tag{39}$$

$$\delta\Omega_{GA} = E_{BdG}(\langle\delta\Psi_0|\Psi_0\rangle + \langle\Psi_0|\delta\Psi_0\rangle) = 0. \tag{40}$$

The main differences from usual BdG Hamiltonian are the local renormalization factors in front of t_{ij} and J_{ij}, and the effective local chemical potential terms $-\Sigma_i\mu_{i\sigma}\hat{n}_{i\sigma}$ with $\mu_{i\sigma} = -\partial\Omega_{GA}/\partial n_{i\sigma} - \mu$, which come from the $n_{i\sigma}$ dependence of the renormalization factors. Local modulations of t_{ij} and J_{ij} tend to be enhanced by the local renormalization factors, and impurity potentials tend to be screened by the local chemical potentials.[20]

B. Quasiparticles

We rewrite H_{BdG} in a matrix form,

$$H_{BdG} = \sum_{\rho,\zeta=1}^{2N_L} c_\rho^{\dagger}H_{\rho\zeta}c_\zeta. \tag{41}$$

The $2N_L\times 2N_L$ matrix $H_{\rho\zeta}$ can be diagonalized using a unitary matrix U, namely,

$$H_{\rho\zeta} = \sum_n U_{\rho n}E_n(U^{\dagger})_{n\zeta}. \tag{42}$$

Then, using

$$\gamma_n \equiv \sum_\rho (U^{\dagger})_{n\rho}c_\rho \quad (E_n > 0),$$

$$\gamma_n^{\dagger} \equiv \sum_\rho (U^{\dagger})_{n\rho}c_\rho \quad (E_n < 0), \tag{43}$$

the Hamiltonian is diagonalized as

$$H_{\mathrm{BdG}} = \sum_n E_n \gamma_n^\dagger \gamma_n. \tag{44}$$

The ground state of this effective Hamiltonian is $|\Psi_0\rangle \equiv \Pi_n \gamma_n |0\rangle$. Suppose the ground state is well approximated by $P|\Psi_0\rangle$. Naively, one may assume that excited states are constructed by $P\gamma_n^\dagger|\Psi_0\rangle$. This form of excited states was first introduced for uniform systems by Zhang *et al.*[6] For fugacity factors in P, we use those in the ground state even for the excited states. It probably corresponds to assuming that the quasiparticles γ_n are not very localized and that the change of the particle distribution is negligible.

C. Orthogonality of the excited states

The orthogonality of these excited states can be checked by expanding γ_n using Eq. (43). For example, for $E_n > 0$, $E_m > 0$,

$$\langle\Psi_0|\gamma_n P P \gamma_m^\dagger|\Psi_0\rangle = \sum_{\rho\zeta} U_{\rho n}^* U_{\zeta m} \langle c_\rho P^2 c_\zeta^\dagger\rangle_0. \tag{45}$$

Here, we have to mind a discrepancy between creation and annihilation operators;

$$P_i^2 c_{i\sigma}^\dagger = c_{i\sigma}^\dagger \lambda_{i\sigma}(1-\hat{n}_{i\bar{\sigma}}), \tag{46}$$

$$P_i^2 c_{i\sigma} = c_{i\sigma}[(1-\hat{n}_{i\bar{\sigma}}) + \lambda_{i\bar{\sigma}}\hat{n}_{i\bar{\sigma}}]. \tag{47}$$

Then, as the leading-order theory, we take on-site contractions except one intersite contraction. Thanks to Eq. (11), renormalization factors are reduced to a simple form, i.e.,

$$\frac{\lambda_{i\sigma}(1-n_{i\bar{\sigma}})}{\Xi_i} = \frac{(1-n_{i\bar{\sigma}}) + \lambda_{i\bar{\sigma}} n_{i\bar{\sigma}}}{\Xi_i} = 1, \tag{48}$$

and we obtain simple results,

$$\frac{\langle c_{i\sigma}^\dagger P^2 c_{j\tau}\rangle_0}{\langle P^2\rangle_0} \approx \langle c_{i\sigma}^\dagger c_{j\tau}\rangle_0, \tag{49}$$

$$\frac{\langle c_{i\sigma} P^2 c_{j\tau}^\dagger\rangle_0}{\langle P^2\rangle_0} \approx \langle c_{i\sigma} c_{j\tau}^\dagger\rangle_0, \tag{50}$$

$$\frac{\langle c_{i\sigma}^\dagger P^2 c_{j\tau}^\dagger\rangle_0}{\langle P^2\rangle_0} \approx \langle c_{i\sigma}^\dagger c_{j\tau}^\dagger\rangle_0, \tag{51}$$

$$\frac{\langle c_{i\sigma} P^2 c_{j\tau}\rangle_0}{\langle P^2\rangle_0} \approx \langle c_{i\sigma} c_{j\tau}\rangle_0, \tag{52}$$

for any i,j,σ,τ including $i=j$. In general, $\langle c_{i\sigma}^\dagger P^2 c_{i\bar{\sigma}}^\dagger\rangle_0$ does not satisfy this relation, but we are lucky enough to use the off-site pairing assumption, $\langle c_{i\sigma}^\dagger c_{i\bar{\sigma}}^\dagger\rangle_0 = 0$, then $\langle c_{i\sigma}^\dagger P^2 c_{i\bar{\sigma}}^\dagger\rangle_0 \approx 0$, and can exclude such an exception. Our projected superconducting state includes the Fermi sea as a special case, and these relations look different at a sight from those derived for the Fermi sea by Fukushima *et al.*[21] In fact, however, these are identical if one remembers that P contains fugacity factors.

Using Eqs. (49)–(52), one can transform back from c_ρ to γ_n to yield

$$\frac{\langle\Psi_0|\gamma_n P^2 \gamma_m^\dagger|\Psi_0\rangle}{\langle\Psi_0|P^2|\Psi_0\rangle} \approx \langle\gamma_n \gamma_m^\dagger\rangle_0 = \delta_{nm}. \tag{53}$$

That is, the excited states are orthogonal to each other within the Gutzwiller approximation (GA).

D. Excitation energy

Let $|0\rangle$ and $|n\rangle$ denote the *normalized* ground and excited states,

$$|0\rangle \equiv \frac{P|\Psi_0\rangle}{\sqrt{\langle\Psi_0|P^2|\Psi_0\rangle}}, \quad |n\rangle \equiv \frac{P\gamma_n^\dagger|\Psi_0\rangle}{\sqrt{\langle\Psi_0|\gamma_n P^2 \gamma_n^\dagger|\Psi_0\rangle}}. \tag{54}$$

Neglecting the second order of the difference in $\underline{n}_{\rho\zeta}$,

$$\begin{aligned}\langle n|H_{tJ}|n\rangle - \langle 0|H_{tJ}|0\rangle &\approx \sum_{\rho\zeta} \frac{\partial\Omega_{\mathrm{GA}}}{\partial \underline{n}_{\rho\zeta}}(\langle n|\underline{n}_{\rho\zeta}|n\rangle - \langle 0|\underline{n}_{\rho\zeta}|0\rangle) \\ &= \langle n|H_{\mathrm{BdG}}|n\rangle - \langle 0|H_{\mathrm{BdG}}|0\rangle = E_n. \end{aligned} \tag{55}$$

Therefore, the excitation energies are approximately the same as eigenenergies of the effective Hamiltonian.

E. Density of states

To calculate the local density of states, we need matrix elements, $|\langle n|c_{i\sigma}^\dagger|0\rangle|^2$ and $|\langle n|c_{i\sigma}|0\rangle|^2$. First of all, using Eq. (53) with $n=m$, the normalization of the excited states can be replaced as

$$\langle\Psi_0|\gamma_n P^2 \gamma_n^\dagger|\Psi_0\rangle \approx \langle\Psi_0|P^2|\Psi_0\rangle. \tag{56}$$

Then, we expand γ_n in $|n\rangle$ using Eq. (43) and use simple relations similar to Eqs. (49)–(52), namely,

$$\frac{\langle c_{j\tau}^\dagger P c_{i\sigma} P\rangle_0}{\langle P^2\rangle_0} \approx \sqrt{g_{ii\sigma}^{t0}}\langle c_{j\tau}^\dagger c_{i\sigma}\rangle_0, \tag{57}$$

$$\frac{\langle c_{j\tau} P c_{i\sigma}^\dagger P\rangle_0}{\langle P^2\rangle_0} \approx \sqrt{g_{ii\sigma}^{t0}}\langle c_{j\tau} c_{i\sigma}^\dagger\rangle_0, \tag{58}$$

$$\frac{\langle c_{j\tau}^\dagger P c_{i\sigma}^\dagger P\rangle_0}{\langle P^2\rangle_0} \approx \sqrt{g_{ii\sigma}^{t0}}\langle c_{j\tau}^\dagger c_{i\sigma}^\dagger\rangle_0, \tag{59}$$

$$\frac{\langle c_{j\tau} P c_{i\sigma} P\rangle_0}{\langle P^2\rangle_0} \approx \sqrt{g_{ii\sigma}^{t0}}\langle c_{j\tau} c_{i\sigma}\rangle_0, \tag{60}$$

for any i,j,σ,τ. These formulas are true also for $i=j$, more explicitly,

$$\frac{\langle c_{i\sigma}^\dagger P c_{i\sigma} P\rangle_0}{\langle P^2\rangle_0} = \frac{1}{\sqrt{\lambda_{i\sigma}}} n_{i\sigma}, \tag{61}$$

$$\frac{\langle c_{i\sigma} P c_{i\sigma}^\dagger P\rangle_0}{\langle P^2\rangle_0} = \sqrt{\lambda_{i\sigma}}(1-n_{i\uparrow}-n_{i\downarrow}). \tag{62}$$

These relations are exact if exact $\lambda_{i\sigma}$ are used.

Since the indices of the renormalization factor are only from those of the operator between two P's, we can transform back to γ_n to yield

$$|\langle n|c_\rho^\dagger|0\rangle|^2 = g_{ii\sigma}^{t0}|\langle\Psi_0|\gamma_n c_\rho^\dagger|\Psi_0\rangle|^2 = g_{ii\sigma}^{t0}|U_{\rho n}|^2 \quad (E_n > 0), \tag{63}$$

$$|\langle n|c_\rho|0\rangle|^2 = g_{ii\sigma}^{t0}|\langle\Psi_0|\gamma_n c_\rho|\Psi_0\rangle|^2 = g_{ii\sigma}^{t0}|U_{\rho n}|^2 \quad (E_n < 0), \tag{64}$$

where $\rho=(i,\sigma)$ as Eq. (31). The common renormalization factor $g_{ii\sigma}^{t0}$ tells us that the positive and negative bias spectra are symmetric. This symmetric density of states is also obtained by the canonical-scheme GA.[21,22] We go one step further about this point in the next subsection.

For $A(k,\omega)$, we need matrix elements in k space, $|\langle n|c_{k,\sigma}^\dagger|0\rangle|^2$ and $|\langle n|c_{k,\sigma}|0\rangle|^2$, where $c_{k,\sigma} = N_L^{-1/2}\Sigma_i c_{i\sigma}\exp(ikR_i)$. These can be obtained by the Fourier transform of Eqs. (57)–(60).

F. Electron addition-removal asymmetry caused by higher-order terms

The conventional BCS theory tells us that the quasiparticle excitation spectra are symmetric between positive and negative bias. However, local density of states of high-T_c superconductors measured by the scanning tunnel microscope (STM) is highly asymmetric and there is an argument that attributes this asymmetry to strong electron correlation.[11] Namely, electron addition may be more difficult than electron removal because the injected electron may be repelled by the other electrons due to their strong Coulomb repulsion. It is controversial whether the projected quasiparticle states have symmetric spectra or not. The GA gives symmetric spectra[21,22] if only quasiparticle excitation is considered (incoherent excitations may cause asymmetry[22]). In contrast, the spectra calculated by the VMC show asymmetry.[10]

To discuss this point, here we calculate corrections to the results in the former sections. When these corrections are taken into account, the orthogonal relation, Eq. (53), may not be satisfied any more. Therefore, in the following, we assume that the systems are almost uniform; in the uniform limit the wave number is a good quantum number due to the translational symmetry, and thus excited states are orthogonal. The next order corrections contain only site i and j similarly to those in the hopping term. We put general formulas in Appendix B, and here only show a special case of $n_{i\uparrow}=n_{i\downarrow}=n_i/2$, $n_{ij\uparrow}=n_{ji\uparrow}=n_{ij\downarrow}=n_{ji\downarrow}\equiv n_{ij}$, $\Delta_{ij}=\Delta_{ji}=\Delta_{ij}^*=\Delta_{ji}^*$. Then, with

$$A_{ij} \equiv \begin{cases} \dfrac{n_{ij}^2+\Delta_{ij}^2}{\left(1-\frac{n_i}{2}\right)\left(1-\frac{n_j}{2}\right)} & (i\neq j) \\ 0 & (i=j), \end{cases} \tag{65}$$

$$\alpha_i \equiv \frac{\frac{n_i}{2}}{1-\frac{n_i}{2}}, \tag{66}$$

Eqs. (57)–(60) are rewritten as

$$\frac{\langle c_{j\uparrow}^\dagger P c_{i\uparrow} P\rangle_0}{\langle P^2\rangle_0} \approx \sqrt{g_{ii}^{t0}}\langle c_{j\uparrow}^\dagger c_{i\uparrow}\rangle_0(1+\alpha_j A_{ij}), \tag{67}$$

$$\frac{\langle c_{j\uparrow} P c_{i\uparrow}^\dagger P\rangle_0}{\langle P^2\rangle_0} \approx \sqrt{g_{ii}^{t0}}\langle c_{j\uparrow} c_{i\uparrow}^\dagger\rangle_0(1-A_{ij}), \tag{68}$$

$$\frac{\langle c_{j\downarrow}^\dagger P c_{i\uparrow}^\dagger P\rangle_0}{\langle P^2\rangle_0} \approx \sqrt{g_{ii}^{t0}}\langle c_{j\downarrow}^\dagger c_{i\uparrow}^\dagger\rangle_0(1-\alpha_j A_{ij}), \tag{69}$$

$$\frac{\langle c_{j\downarrow} P c_{i\uparrow} P\rangle_0}{\langle P^2\rangle_0} \approx \sqrt{g_{ii}^{t0}}\langle c_{j\downarrow} c_{i\uparrow}\rangle_0(1+A_{ij}). \tag{70}$$

Since $A_{ij}\geq 0$ and $\alpha_i \geq 0$, the corrections are positive for the electron removal, and negative for the addition. For more careful analysis, we also need to check the normalization. Including the corrections, Eqs. (49)–(52) are rewritten as

$$\frac{\langle c_{j\uparrow}^\dagger P^2 c_{i\uparrow}\rangle_0}{\langle P^2\rangle_0} \approx \langle c_{j\uparrow}^\dagger c_{i\uparrow}\rangle_0(1-\alpha_i\alpha_j A_{ij}), \tag{71}$$

$$\frac{\langle c_{j\uparrow} P^2 c_{i\uparrow}^\dagger\rangle_0}{\langle P^2\rangle_0} \approx \langle c_{j\uparrow} c_{i\uparrow}^\dagger\rangle_0(1-A_{ij}), \tag{72}$$

$$\frac{\langle c_{j\downarrow}^\dagger P^2 c_{i\uparrow}^\dagger\rangle_0}{\langle P^2\rangle_0} \approx \langle c_{j\downarrow}^\dagger c_{i\uparrow}^\dagger\rangle_0(1-\alpha_j A_{ij}), \tag{73}$$

$$\frac{\langle c_{j\downarrow} P^2 c_{i\uparrow}\rangle_0}{\langle P^2\rangle_0} \approx \langle c_{j\downarrow} c_{i\uparrow}\rangle_0(1-\alpha_i A_{ij}). \tag{74}$$

These corrections to the normalization are all negative, and they do not seem to cancel the asymmetry in Eqs. (67)–(70). Therefore, these results suggest that the higher-order GA exhibits asymmetric spectra whose electron addition spectra are smaller than the removal.

This asymmetry is consistent with the variational Monte Carlo (VMC) calculations for excitation spectra by Chou *et al.*,[10] and for spectral weights by Bieri and Ivanov[23] and Yang *et al.*[24] For more explicit comparison, we calculate the spectral weights,

$$Z^+(k) \equiv |\langle k\sigma|c_{k\sigma}^\dagger|0\rangle|^2 = \frac{\langle P^2\rangle_0}{\langle \gamma_{k\sigma} P^2 \gamma_{k\sigma}^\dagger\rangle_0}\left|\frac{\langle \gamma_{k\sigma} P c_{k\sigma}^\dagger P\rangle_0}{\langle P^2\rangle_0}\right|^2, \tag{75}$$

$$Z^-(k) \equiv |\langle k\sigma|c_{-k\bar{\sigma}}|0\rangle|^2 = \frac{\langle P^2\rangle_0}{\langle \gamma_{k\sigma} P^2 \gamma_{k\sigma}^\dagger\rangle_0}\left|\frac{\langle \gamma_{k\sigma} P c_{-k\bar{\sigma}} P\rangle_0}{\langle P^2\rangle_0}\right|^2, \tag{76}$$

and show them in Fig. 6 for both the conventional and the generalized GA. Here, we include t' and t'' in addition to Eq. (16) for a better correspondence to the high-T_c superconductors.

In the case of the standard BCS theory, $Z^+=|u_k|^2$, $Z^-=|v_k|^2$. Then, for each k point below the Fermi level, one can find a corresponding point k' above the Fermi level such that $E_{k'}=E_k$, $u_{k'}=v_k$, $v_{k'}=u_k$. Then, summation of the contribution from these two points to the spectra is unity for *both* addition and removal spectra[25] because $|u_k|^2+|u_{k'}|^2=|v_k|^2+|v_{k'}|^2=|u_k|^2+|v_k|^2=1$. Accordingly the excitation spectra are symmetric. The results of the conventional GA are Z^+

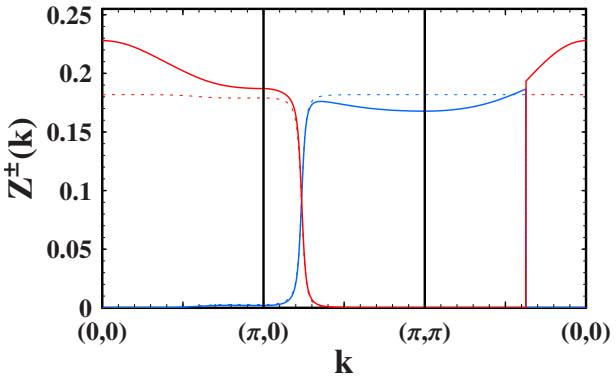

FIG. 6. (Color online) $Z^+(k)$ (blue lines) and $Z^-(k)$ (red lines) of a projected d-wave superconductor by the conventional (dotted lines) and the generalized (solid lines) GA with $t'=-0.3t$, $t''=0.2t$, $\Delta_v=0.15t$, and 10% hole concentration.

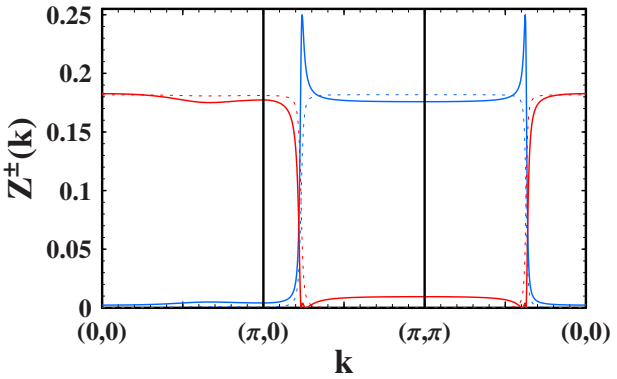

FIG. 7. (Color online) $Z^+(k)$ (blue lines) and $Z^-(k)$ (red lines) of a projected s-wave superconductor with $t'=-0.3t$, $t''=0.2t$, $\Delta_k=0.15t$, and 10% hole concentration.

$=g^t|u_k|^2$, $Z^-=g^t|v_k|^2$; namely, the spectra are just renormalized by g^t, and are symmetric as the standard BCS theory. In contrast, by including the corrections to them, Z^- decreases and Z^+ increases, which can cause the asymmetry in the spectra. These $Z^\pm$ are consistent with the VMC results.[23,24] Note that A_{ij} is finite even for $\Delta_{ij}=0$, i.e., the Fermi sea also has the asymmetry, which is also consistent.[24] Similarly to the hopping term, Eqs. (67)–(74) are more accurate for small $|i-j|$. Hence, the Fourier-transformed results may include errors from the summation over large $|i-j|$. It will be checked in the future studies by including higher-order terms. Since this asymmetry appears as a deviation from the conventional GA, it is rather small (especially near the Fermi level), and does not look like what is seen in the STM experiment.

G. Opposite asymmetry in projected s-wave superconductors

We speculate that the origin of the asymmetry may not be so simple as the intuition that *electron addition may be more difficult than removal because electrons repel each other*. Here, we show a counterexample against this simple scenario. That is to say, projected s-wave superconductors can have the opposite asymmetry; the electron addition spectra are larger than the removal. Such projected s-wave superconductors may be realized if the pairing interaction is spatially isotropic because d wave does not gain energy from diagonal J_{ij}. Even if J_{ij} is finite only for nearest neighbors, the mean-field approximation in very overdoped systems converges to extended s-wave solutions. To be more precise, this opposite asymmetry is related to finite on-site pairing *before* the projection, $\langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger\rangle_0 \neq 0$ and not really related to the symmetry of the gap. Then, even for d wave, inhomogeneity causes deviation from the d wave, and $\langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger\rangle_0$ can be nonzero in general. Therefore, strongly disordered d-wave superconductors could have similar properties.

To take $\Delta_{ii}\neq 0$ into account, we have to redo the derivation from the beginning. Then, Ξ_i and λ_i should be replaced by

$$\Xi_i \approx \frac{\left(1-\frac{n_i}{2}\right)^2+|\Delta_{ii}|^2}{1-n_i}, \tag{77}$$

$$\lambda_i \approx \frac{n_i\left[\left(1-\frac{n_i}{2}\right)^2+|\Delta_{ii}|^2\right]}{2(1-n_i)\left[\left(1-\frac{n_i}{2}\right)\frac{n_i}{2}-|\Delta_{ii}|^2\right]}. \tag{78}$$

In fact, this generalization makes analytical treatment very difficult, and in the following we take only the leading order of the intersite contractions. Accordingly, its $\Delta_{ii}\to 0$ limit corresponds to the conventional GA (not the generalized GA in Sec. III F).

The most important matrix elements are

$$\frac{\langle c_{i\downarrow}^\dagger P c_{i\uparrow}^\dagger P\rangle_0}{\langle P^2\rangle_0} \approx \frac{\sqrt{\lambda_i}}{\Xi_i}\langle c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger\rangle_0, \tag{79}$$

$$\langle c_{i\downarrow} P c_{i\uparrow} P\rangle_0 = 0. \tag{80}$$

Here, Eq. (80) is exact because of $P_G c_{i\uparrow} P_G = c_{i\uparrow} P_G$ and $P_G c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger = 0$. The renormalization factor in Eq. (79) is obviously larger than that in Eq. (80). Hence, these matrix elements suggest that the asymmetry is the opposite to that of d wave. We have also calculated other matrix elements, and after the Fourier transform, $Z^\pm$ for a uniform system are obtained as plotted in Fig. 7.

In comparing Figs. 6 and 7, we should keep in mind that a better approximation is used for Fig. 6, and the asymmetry as in Fig. 6 does not appear in Fig. 7. Nevertheless, the characteristic asymmetry near the Fermi surface in Fig. 7 is very strong, and may remain even in calculation with a better precision. Most likely, Eqs. (79) and (80) mainly contribute to the asymmetry because the vicinity of the Fermi level changes most dramatically.

H. Physical consideration for the asymmetries

For the projected s-wave superconductors, the physical origin of the asymmetry may be understood as follows. We have been using terms "addition" and "removal" but these are in fact named from the ground state's view. If one takes the complex conjugate, this addition (removal) matrix elements can be regarded as removal from (addition to) an excited state. Let us adopt the excited states' view for a while. In the s-wave BCS superconducting state (before the projection), a Cooper pair may be formed more or less on site,

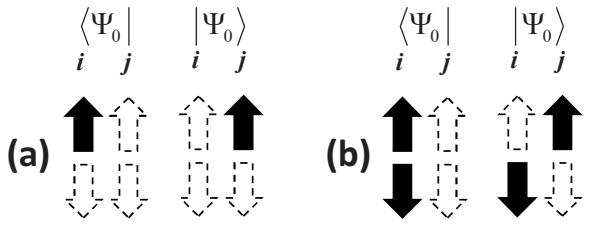

FIG. 8. Configurations in $|\Psi_0\rangle$.

which is a resonance of the doubly occupied state and the empty state. When $c_{i\sigma}$ is operated to this wave function, it chooses the "originally doubly occupied" state. Then, in $Pc_{i\sigma}|\Psi\rangle_0$, the opposite spin state, $i\bar{\sigma}$, is *occupied* with high probability. Accordingly, it is easy to remove $i\bar{\sigma}$ electron. In contrast, for $Pc^{\dagger}_{i\sigma}|\Psi\rangle_0$, it is impossible to add $i\bar{\sigma}$ electron. Finally, let us turn back to the ground state's view and review the arguments above. Then, *the removal is difficult, but the addition is easy*.

The asymmetry in the *d*-wave superconductors and the Fermi sea needs more consideration because it appears by higher-order correlations. Figure 8(a) shows a configuration in the ket $|\Psi\rangle_0$ contributing to $\langle c_{j\uparrow}Pc^{\dagger}_{i\uparrow}P\rangle_0$. The first term in Eq. (68) represents direct correlation between $c_{j\uparrow}$ and $c^{\dagger}_{i\uparrow}$. The second term comes from the repulsive correlation between down holes, which reduces weight of this configuration. On the other hand, for $\langle c^{\dagger}_{i\uparrow}Pc_{j\uparrow}P\rangle_0$, both configurations (a) and (b) in $|\Psi\rangle_0$ contribute. However, when electron density is high, configuration (b) is dominant because empty sites are rare. Then, correlation between down holes increases the weight of configuration (b). Since this effect appears only at high density, the second term in Eq. (67) accompanies the factor α_i.

IV. GLOBAL CONSTRAINT: QUASICANONICAL GA

In the former sections, we have used the local constraint. However, if one needs the GA as an approximate method of the VMC, it may be preferred to require the usual canonical constraint, i.e., the total particle number constraint for each of up and down spins,

$$\sum_i \langle \hat{n}_{i\sigma}\rangle = N^{\text{after}}_{\sigma}, \tag{81}$$

where $N^{\text{after}}_{\sigma}$ is the total number of σ electrons after the projection. Although one takes $N^{\text{after}}_{\sigma}=\Sigma_i n_{i\sigma}$ in the usual canonical GA, the particle numbers before and after the projection can be different in general. In fact, in the VMC, they are different; the particle number projection $P_{N^{\text{after}}_{\sigma}}$ is usually applied together with P_{G}, and the chemical potential of $|\Psi_0\rangle$ is more like a variational parameter and does *not* control the particle number *after* the projection. In the following we use the notation

$$n^{\text{after}}_{\sigma} \equiv N^{\text{after}}_{\sigma}/N_{\text{L}}, \quad n^{\text{after}} \equiv n^{\text{after}}_{\uparrow} + n^{\text{after}}_{\downarrow}, \tag{82}$$

with N_L the total number of sites. Our purpose here is formulating a grand canonical GA that gives results of the canonical scheme, by imposing Eq. (81).

If the total spin moment is nonzero, it must be reasonable to choose the spin-z axis parallel to the global moment so that $\Sigma_i\langle S^x_i\rangle_0=\Sigma_i\langle S^y_i\rangle_0=0$. In that case, local xy components, $\langle S^x_i\rangle_0$, $\langle S^y_i\rangle_0$, may be finite in general. Then, similarly to the local-constraint formulation in Sec. II D, xy components of the local spin moments are renormalized differently from their z components. The canonical-scheme condition for the total spin moment restricts the spin-z renormalization factor to the vicinity of unity, but the other directions are free from it. We expect that this spin-rotational asymmetric renormalization is a property from the canonical condition and should exist even in exact calculation. Furthermore, if the total spin moment is zero and local moments point to various directions, we have no idea how to choose the z axis. Here, to avoid such complexity, we assume $\langle S^x_i\rangle_0=\langle S^y_i\rangle_0=0$, and as in the former sections $\langle c^{\dagger}_{i\sigma}c_{j\bar{\sigma}}\rangle_0=\langle c^{\dagger}_{i\uparrow}c^{\dagger}_{i\downarrow}\rangle_0=\langle c^{\dagger}_{i\sigma}c^{\dagger}_{j\sigma}\rangle_0=0$.

A. Condition for fugacity factors

To control the total particle numbers, we need a factor in the form $\lambda_{\sigma}^{(1/2)\Sigma_i\hat{n}_{i\sigma}}$, namely, the fugacity factors λ_{σ} do not have the site index. Accordingly, the projected wave function is defined as $|\Psi\rangle=P|\Psi_0\rangle$ with $P\equiv\Pi_i\lambda_{\uparrow}^{(1/2)\hat{n}_{i\uparrow}}\lambda_{\downarrow}^{(1/2)\hat{n}_{i\downarrow}}(1-\hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$.

The formula for $\langle\hat{n}_{i\sigma}\rangle$ has the same form as Eq. (9), and only λ_{σ} is different, i.e.,

$$\langle\hat{n}_{i\sigma}\rangle \approx \frac{\lambda_{\sigma}(1-n_{i\bar{\sigma}})}{\Xi_i}n_{i\sigma}. \tag{83}$$

Note that Ξ_i is still site dependent because it contains local electron densities. By inserting it into Eq. (81), we obtain

$$\lambda_{\sigma}\sum_i \frac{1-n_{i\bar{\sigma}}}{\Xi_i}n_{i\sigma} = N^{\text{after}}_{\sigma}. \tag{84}$$

In inhomogeneous systems, λ_{σ} is solved numerically from Eq. (84) in general. An important point of this uniform fugacity approach is that the local electron density is also renormalized as in Eq. (83), and $\langle\hat{n}_{i\sigma}\rangle\neq\langle\hat{n}_{i\sigma}\rangle_0$ in general. When λ_{σ} is solved and inserted into Eq. (83), the corrections to $\langle\hat{n}_{i\sigma}\rangle$ are of the second order of intersite contractions as will be explicitly shown in Sec. IV D.

The local spin-z component is renormalized as

$$\langle S^z_i\rangle \approx \frac{1}{2}\sum_{\sigma=\pm1}\sigma\frac{\lambda_{\sigma}(1-n_{i\bar{\sigma}})}{\Xi_i}n_{i\sigma}, \tag{85}$$

where symbols $\uparrow,\downarrow$ and $+1,-1$ are interchangeably used.

B. Hopping term

The Gutzwiller renormalization factor of the hopping term is given by

$$\frac{\langle c^{\dagger}_{i\sigma}c_{j\sigma}\rangle}{\langle c^{\dagger}_{i\sigma}c_{j\sigma}\rangle_0} \approx \frac{\lambda_{\sigma}(1-n_{i\bar{\sigma}})(1-n_{j\bar{\sigma}})}{\Xi_i\Xi_j} \equiv g^{t0}_{ij\sigma}. \tag{86}$$

Next-order corrections to this formula involve another site, which may make important contribution for second or third

neighbor hopping in some systems. Using $a_{i\sigma}\equiv(1-\lambda_{\bar{\sigma}})(1-n_{i\sigma})+\lambda_\sigma n_{i\sigma}$, it is written as

$$\langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle \approx g_{ij\uparrow}^{t0}\left(n_{ij\uparrow}+\sum_l \frac{a_{l\downarrow}n_{il\uparrow}n_{lj\uparrow}-a_{l\uparrow}\Delta_{il}^*\Delta_{jl}}{\Xi_l}\right). \quad (87)$$

The corrections to $\lambda_{i\sigma}$ and Ξ_i affect only from third order and not relevant to the equation above. Note that $a_{i\sigma}$ goes to zero in the uniform limit with $n_\sigma^{\text{after}}=n_\sigma$.

In the uniform systems, by omitting irrelevant site indices and using $R_\sigma\equiv n_\sigma^{\text{after}}/n_\sigma$, we obtain

$$\lambda_\sigma \approx \frac{R_\sigma(1-n_\sigma)}{1-n^{\text{after}}}=\frac{R_\sigma(1-n_\sigma)}{1-R_\uparrow n_\uparrow-R_\downarrow n_\downarrow}, \quad (88)$$

$$g_\sigma^{t0}=\frac{R_\sigma(1-n^{\text{after}})}{1-n_\sigma}=\frac{R_\sigma^2}{\lambda_\sigma}. \quad (89)$$

C. Exchange term with zero total spin-z component and $\lambda_\uparrow=\lambda_\downarrow$

The general formulas for the exchange interaction term are too lengthy to present here. Our main interest is in systems with zero total spin-z component and $\lambda_\uparrow=\lambda_\downarrow$, which includes nonmagnetic systems, antiferromagnets, and stripes. Hence, for simplicity, we restrict ourselves to this case in the following except for Sec. IV F that treats ferromagnetic systems. The generalization to nonzero total spin-z component is straightforward but one has to work with more complexities.

When $\lambda_\uparrow=\lambda_\downarrow\equiv\lambda$, Eq. (85) is reduced to

$$\langle S_i^z\rangle \approx \frac{\lambda}{\Xi_i}m_i. \quad (90)$$

For the exchange interaction term $\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle$, we take up to the second order of intersite contractions. Assuming that m_i is small, namely, $m_i=O(n_{ij\sigma})=O(\Delta_{ij})$, we obtain

$$\langle S_i^zS_j^z\rangle \approx \frac{g_{ij}^s}{4}(4m_im_j-|n_{ij\uparrow}|^2-|n_{ij\downarrow}|^2-|\Delta_{ij}|^2-|\Delta_{ji}|^2)$$
$$=g_{ij}^s\langle S_i^zS_j^z\rangle_0, \quad (91)$$

$$\langle S_i^xS_j^x+S_i^yS_j^y\rangle \approx -g_{ij}^s\,\mathrm{Re}[n_{ij\uparrow}n_{ji\downarrow}+\Delta_{ij}^*\Delta_{ji}]=g_{ij}^s\langle S_i^xS_j^x+S_i^yS_j^y\rangle_0, \quad (92)$$

where $g_{ij}^s\equiv\lambda^2(\Xi_i\Xi_j)^{-1}$. This is the result of the conventional GA. However, note that if m_i is of the order of unity, terms such as $n_{ij\sigma}^2m_i$, $\Delta_{ij}^2m_i$ have about the same order of contribution as $n_{ij\sigma}^2$, Δ_{ij}^2, and formulas above should be modified as derived below.

D. Beyond the "conventional" GA

When $m_i\sim n_{i\sigma}$, terms neglected in the previous derivation may grow, and we need to redo the derivation from the beginning. It is known that expectation values by Gutzwiller-projected states can be written in the form of a linked-cluster expansion.[1] The terms we need here includes contribution from clusters one site larger than those in the previous derivation.

We relegate detailed derivation to Appendix A, and only show final results here. The renormalization of the particle densities is given by

$$\langle\hat{n}_{i\uparrow}\rangle \approx \frac{\lambda(1-n_{i\downarrow})}{\Xi_i}n_{i\uparrow}\left(1-\sum_{l\neq i}\frac{\Xi_{il}^{(2)}}{\Xi_i\Xi_l}\right)+\sum_{l\neq i}\frac{\lambda}{\Xi_i\Xi_l}\{a_{l\downarrow}[(1-n_{i\downarrow})\times|n_{il\uparrow}|^2+n_{i\uparrow}|\Delta_{li}|^2]-a_{l\uparrow}[n_{i\uparrow}|n_{il\downarrow}|^2+(1-n_{i\downarrow})|\Delta_{il}|^2]\}, \quad (93)$$

$$\Xi_{lm}^{(2)}\equiv -a_{l\uparrow}a_{m\uparrow}|n_{lm\downarrow}|^2-a_{l\downarrow}a_{m\downarrow}|n_{lm\uparrow}|^2+a_{l\downarrow}a_{m\uparrow}|\Delta_{lm}|^2+a_{l\uparrow}a_{m\downarrow}|\Delta_{ml}|^2, \quad (94)$$

where $a_{l\sigma}=(1-\lambda)(1-n_{l\sigma})+\lambda n_{l\sigma}$. The formula for $\langle\hat{n}_{i\sigma}\rangle$ is obtained by replacing as $\uparrow\Leftrightarrow\downarrow$ and $\Delta_{il}\Rightarrow-\Delta_{li}$. Then, the new equation to determine λ is given by $\Sigma_i\langle\hat{n}_{i\sigma}\rangle=N^{\text{after}}$. The solution can be written as $\lambda\approx\lambda^{(0)}+\lambda^{(2)}$, where $\lambda^{(0)}$ is λ determined by Eq. (84), and $\lambda^{(2)}$ is the correction to it represented by

$$\lambda^{(2)}=\left\{\sum_i\Xi_i^{-2}(1-n_{i\uparrow})(1-n_{i\downarrow})[n_{i\uparrow}(1-n_{i\downarrow})+n_{i\downarrow}(1-n_{i\uparrow})]\right\}^{-1}\times\sum_i\sum_{l\neq i}\frac{\lambda^{(0)}}{\Xi_i\Xi_l}\left\{\frac{n_{i\uparrow}(1-n_{i\downarrow})+n_{i\downarrow}(1-n_{i\uparrow})}{\Xi_i}\Xi_{il}^{(2)}-a_{l\downarrow}[(1-2n_{i\downarrow})|n_{il\uparrow}|^2-(1-2n_{i\uparrow})|\Delta_{li}|^2]-a_{l\uparrow}[(1-2n_{i\uparrow})|n_{il\downarrow}|^2-(1-2n_{i\downarrow})|\Delta_{il}|^2]\right\}. \quad (95)$$

Here, every λ is replaced by $\lambda^{(0)}$ in the right-hand side. Using this new λ, we can calculate spin terms,

$$\langle S_i^z\rangle \approx \frac{\lambda m_i}{\Xi_i}\left(1-\sum_{l\neq i}\frac{\Xi_{il}^{(2)}}{\Xi_i\Xi_l}\right)+\sum_{l\neq i}m_{il}^{(2)},$$
$$m_{il}^{(2)}\equiv\frac{\lambda}{2\Xi_i\Xi_l}[a_{l\downarrow}(|n_{il\uparrow}|^2+|\Delta_{li}|^2)-a_{l\uparrow}(|n_{il\downarrow}|^2+|\Delta_{il}|^2)], \quad (96)$$

$$\langle S_i^zS_j^z\rangle-\langle S_i^z\rangle\langle S_j^z\rangle \approx \frac{\lambda^2m_im_j}{\Xi_i\Xi_j}\left[1+\frac{\Xi_{ij}^{(2)}}{\Xi_i\Xi_j}\right]+\frac{\lambda^2}{\Xi_i\Xi_j}(\langle S_i^zS_j^z\rangle_0-m_im_j)-\frac{\lambda m_j}{\Xi_j}m_{ij}^{(2)}-\frac{\lambda m_i}{\Xi_i}m_{ji}^{(2)}. \quad (97)$$

Here, λ in the second-order terms can be replaced by $\lambda^{(0)}$. Note that the contribution that involves a third site l in $\langle S_i^z\rangle$ cancels that in $\langle S_i^zS_j^z\rangle$ by the subtraction of $\langle S_i^z\rangle\langle S_j^z\rangle$. There is no correction of this order for $\langle S_i^xS_j^x+S_i^yS_j^y\rangle$ in Eq. (92).

Although several authors[7–9] formulated improved canonical GAs by taking nearest-neighbor correlations similarly to ours, our result is different from any of them even if we neglect the second- and third-neighbor terms. The origin of this discrepancy is not clear at present.

E. Antiferromagnets

As an explicit example, we show the formulas for the square lattice antiferromagnet. For periodic systems, we can restrict the summation over the site index i to only inside of the unit cell. In the presence of the antiferromagnetic moments, n_{ij} between second- or third-neighbor pairs may be comparable to or larger than that of the nearest-neighbor pairs. To take into account these terms, we define $n_{ij\sigma}=\chi,\chi',\chi''$, $\Delta_{ij}=\Delta_{ji}=\Delta,\Delta',\Delta''$, for the nearest-, second-, and third-neighbor pairs, and assume these are real numbers. In addition, $n_{i\uparrow}=n_A$ and $n_{i\downarrow}=n_B$ for A sublattice, $n_{i\uparrow}=n_A$ and $n_{i\downarrow}=n_A$ for B sublattice, and then $m=(n_A-n_B)/2$. By omitting irrelevant site indices,

$$\lambda^{(0)}=\frac{n^{\text{after}}(1-n_A)(1-n_B)}{(1-n^{\text{after}})(n-2n_An_B)}, \tag{98}$$

$$a_A=(1-\lambda)(1-n_A)+\lambda n_A, \tag{99}$$

$$a_B=(1-\lambda)(1-n_B)+\lambda n_B, \tag{100}$$

$$g^{t0}=\frac{(1-n^{\text{after}})n^{\text{after}}}{n-2n_An_B}, \tag{101}$$

$$\Xi=(1-n_A)(1-n_B)+\lambda(n-2n_An_B), \tag{102}$$

$$\Xi^{(2)}_{\text{n.n.}}=-2a_Aa_B\chi^2+(a_A^2+a_B^2)\Delta^2, \tag{103}$$

$$\Xi^{(2)}_{\text{2nd}}=-(a_A^2+a_B^2)(\chi')^2+2a_Aa_B(\Delta')^2, \tag{104}$$

$$\Xi^{(2)}_{\text{3rd}}=-(a_A^2+a_B^2)(\chi'')^2+2a_Aa_B(\Delta'')^2, \tag{105}$$

$$\begin{aligned}\lambda^{(2)}=&\frac{4\lambda}{(1-n_A)(1-n_B)(n-2n_An_B)}\\&\times\left\{\frac{(n-2n_An_B)}{\Xi}(\Xi^{(2)}_{\text{n.n.}}+\Xi^{(2)}_{\text{2nd}}+\Xi^{(2)}_{\text{3rd}})+[a_A(1-2n_B)\right.\\&+a_B(1-2n_A)][-\chi^2+(\Delta')^2+(\Delta'')^2]+[a_A(1-2n_A)\\&\left.+a_B(1-2n_B)][\Delta^2-(\chi')^2-(\chi'')^2]\right\}|_{\lambda\to\lambda^{(0)}},\end{aligned} \tag{106}$$

$$\begin{aligned}\langle S_A^z\rangle=-\langle S_B^z\rangle\approx&\frac{\lambda m}{\Xi}\left(1-\frac{4\Xi^{(2)}_{\text{n.n.}}}{\Xi^2}-\frac{4\Xi^{(2)}_{\text{2nd}}}{\Xi^2}-\frac{4\Xi^{(2)}_{\text{3rd}}}{\Xi^2}\right)\\&+\frac{4\lambda(2\lambda-1)m}{\Xi^2}[\chi^2+\Delta^2-(\chi')^2-(\Delta')^2\\&-(\chi'')^2-(\Delta'')^2],\end{aligned} \tag{107}$$

$$\begin{aligned}\langle S_A^zS_B^z\rangle-\langle S_A^z\rangle\langle S_B^z\rangle\approx&\frac{-\lambda^2m^2}{\Xi^2}\left[1+\frac{\Xi^{(2)}_{\text{n.n.}}}{\Xi^2}\right]\\&-\frac{\lambda^2}{2\Xi^2}(\chi^2+\Delta^2)\left[1-\frac{4m^2}{\Xi}(2\lambda-1)\right],\end{aligned} \tag{108}$$

where Eq. (108) is for a nearest-neighbor pair. In general, $\Delta_{ij}\neq\Delta_{ji}$ may occur; in that case these equations need modification with a little more complexities.

F. Ferromagnets

Here, we show a remarkable difference from the local constraint. That is, ferromagnets are renormalized very differently from antiferromagnets in contrast to results by the local constraint in Sec. II C. For ferromagnetic wave functions without superconductivity, we can set $\Delta_{ij}=0$, and $N_\sigma^{\text{after}}=\Sigma_i\langle\hat{n}_{i\sigma}\rangle_0$. Then, in the uniform cases, this Gutzwiller approximation (GA) with the global constraint is equivalent to the one with the local constraint. Therefore, by setting $m_i=m$ in formulas in Sec. II, we obtain those for the ferromagnets,

$$\langle S_i^zS_j^z\rangle\approx m^2-\frac{1}{4}\left[|n_{ij\uparrow}|^2\frac{(1-2m)^2}{(1-n_\uparrow)^2}+|n_{ij\downarrow}|^2\frac{(1+2m)^2}{(1-n_\downarrow)^2}\right], \tag{109}$$

$$\langle S_i^xS_j^x+S_i^yS_j^y\rangle=g^s\langle S_i^xS_j^x+S_i^yS_j^y\rangle_0, \tag{110}$$

$$g^s\equiv\frac{1}{(1-n_\uparrow)(1-n_\downarrow)},\quad g^t_\sigma=\frac{1-n}{1-n_\sigma}. \tag{111}$$

Many of the formulas derived with the global constraint in this section contain a_σ, but it goes to zero in this ferromagnetic limit. It is consistent with no appearance of a_σ in the local-constraint formulation.

In fact, the renormalization for the spin-z component represented by Eq. (109) is different from the one derived by Zhang *et al.*[6] using a probability argument of the canonical GA, namely, $\langle S_i^zS_j^z\rangle=g^s\langle S_i^zS_j^z\rangle_0$ with g^s defined by Eq. (111). However, we speculate that our result is more reasonable because spin moment term m^2 is not renormalized; the canonical constraint prevents the spin-z component from growing larger, in contrast to the antiferromagnetic moments, which are not bound by the canonical constraint. It may be clearer if we take the limit of small m for Eq. (109),

$$\langle S_i^zS_j^z\rangle\approx m^2-\frac{g^s_{ij}}{4}(|n_{ij\uparrow}|^2+|n_{ij\downarrow}|^2)=m^2+g^s_{ij}(\langle S_i^zS_j^z\rangle_0-m^2), \tag{112}$$

and compare with Eq. (91) for antiferromagnets.

G. Effect of $N^{\text{after}}\neq N^{\text{before}}$

Projections reduce the Hilbert space. Hence, many wave functions may be equivalent to each other after the projection even if they are different before the projection. Here, we demonstrate it explicitly by the particle number projection. Let us start from uniform nonmagnetic cases. Define two BCS states,

$$|\Psi_0\rangle \equiv \prod_k (u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger)|0\rangle, \tag{113}$$

$$|\Psi_0'\rangle \equiv \tilde{\lambda}^{\hat{N}/2}|\Psi_0\rangle = \prod_k (u_k + v_k \tilde{\lambda} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger)|0\rangle, \tag{114}$$

where $\hat{N} \equiv \Sigma_{i\sigma} \hat{n}_{i\sigma}$. Under the particle number projection P_N,

$$P_N|\Psi_0'\rangle = \tilde{\lambda}^{N/2} P_N|\Psi_0\rangle \propto P_N|\Psi_0\rangle. \tag{115}$$

Namely, wave functions $P_N|\Psi_0\rangle$ and $P_N|\Psi_0'\rangle$ are equivalent whereas $|\Psi_0\rangle$ and $|\Psi_0'\rangle$ are nonequivalent. At a sight, the quasiparticle excited states of these two BCS states look different because $\gamma_{k\sigma}^\dagger$ does not commute with $\tilde{\lambda}^{\hat{N}/2}$. However, $c_{k\sigma}^\dagger$ and $c_{k-\sigma}$ in $\gamma_{k\sigma}^\dagger$ in fact yield the same state, and thus $P_N\gamma_{k\sigma}^\dagger|\Psi_0\rangle$ and $P_N\gamma_{k\sigma}'^\dagger|\Psi_0'\rangle$ are equivalent, where $\gamma_{k\sigma}'^\dagger$ is a quasiparticle operator for $|\Psi_0'\rangle$.

Therefore, even if the average particle number of $|\Psi_0\rangle$ is not N^{after}, one can make that of $|\Psi_0'\rangle$ equal to N^{after} by choosing $\tilde{\lambda}$ to satisfy

$$N^{\text{after}} = \sum_k \frac{2\tilde{\lambda}^2 |v_k|^2}{|u_k|^2 + \tilde{\lambda}^2 |v_k|^2}. \tag{116}$$

Then, using $|\Psi_0'\rangle$, the GA can be applied with the local constraint $\langle \hat{n}_{i\sigma}\rangle = \langle \hat{n}_{i\sigma}\rangle_0$. Accordingly, we can use convenient properties derived in Secs. II and III.

Such a transformation to relate the global constraint to the local one may be possible also for inhomogeneous systems, but there seems to be a problem. The particle numbers can be controlled by fugacity factors $\Pi_{i\sigma}\tilde{\lambda}_{i\sigma}^{\hat{n}_{i\sigma}/2}$ as Eq. (114). One can choose $\tilde{\lambda}_{i\sigma}$ in $|\Psi_0'\rangle$ to satisfy $\langle \hat{n}_{i\sigma}\rangle = \langle \hat{n}_{i\sigma}\rangle_0$. Then, $c_{i\sigma}^\dagger$ is replaced by $\tilde{\lambda}_{i\sigma}^{(1/2)} c_{i\sigma}^\dagger$, as well as $c_{i\sigma}$ is replaced by $\tilde{\lambda}_{i\sigma}^{-1/2} c_{i\sigma}$ (in annihilating the electron, the fugacity factor caused by the creation should be canceled). Accordingly, $|\Psi_0'\rangle$ is a rather strange wave function because the quasiparticles may not satisfy the fermion commutation relation. Then one may need to redefine a proper quasiparticle set for $|\Psi_0'\rangle$. Furthermore, since the quasiparticle operators do not commute with the fugacity's operator, definition of the excited states depends on their order, in contrast to the uniform cases.

We have originally speculated that the difference between the particle numbers before and after the projection may cause such asymmetry of the spectra as discussed in the latter part of Sec. III. Let us look again at Eqs. (61) and (62). Note that the electron removal matrix element is proportional to $n_{i\sigma}$ (density of the $i\sigma$ electrons), while the addition is to $1-n_i$ (density of the *empty* sites). Nevertheless, it is compensated by the fugacity factor and the renormalization factors for the removal and the addition are the same. Then, one may speculate that some asymmetry may appear if we destroy this balance by changing the fugacity factors. However, according to our analysis here, the particle number difference does not have much effect, and it does not cause any asymmetry at least in the uniform systems.

V. SPIN-INDEPENDENT CONSTRAINT

At present, our main interest is in the GAs with spin-dependent constraints in the former sections because they seem to be more convenient to investigate antiferromagnets, stripe state, impurity systems, and so on. However, in systems with a more complicated spin configuration, the GAs with spin-*independent* constraints may be useful. Therefore, here we work on it, but only take the leading order with respect to the intersite contractions.

A. Local constraint

A grand canonical GA with a spin-independent constraint,

$$\langle \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}\rangle = n_i, \tag{117}$$

was introduced by Wang *et al.*[16] In nonmagnetic cases ($n_{i\uparrow} = n_{i\downarrow}$), this is identical to the GA with the spin-dependent constraint in Secs. II and III. However, in magnetic cases, the results of these two GAs are different. Accordingly, the ferromagnetic homogeneous limit[17] with the spin-independent constraint is not equivalent to that of the canonical GA, but is reduced to the GA for charge-canonical spin-grand canonical functions explained in the next subsection.

Since the formulas for g^t and g^s have been already derived in Refs. 16 and 17, here we derive them in a slightly more general form by assuming that $\langle S_i^x\rangle$ and $\langle S_i^y\rangle$ are finite. By replacing $\lambda_{i\sigma}$ by λ_i in the derivation in Sec. II D and using $\mathcal{S}_i^\pm \equiv \langle S_i^\pm\rangle_0$, we obtain

$$\Xi_i \approx \frac{\xi_i}{1-n_i}, \quad \xi_i \equiv (1-n_{i\uparrow})(1-n_{i\downarrow}) - |\mathcal{S}_i^+|^2, \tag{118}$$

$$\lambda_i \approx \frac{n_i \xi_i}{(1-n_i)[n_i - 2n_{i\uparrow}n_{i\downarrow} + 2|\mathcal{S}_i^+|^2]}, \tag{119}$$

$$\frac{\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle}{\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle_0} \approx g_{ij\sigma}^t = \sqrt{g_{ii\sigma}^t g_{jj\sigma}^t}, \tag{120}$$

$$g_{ii\sigma}^t \equiv \frac{n_i(1-n_i)(1-n_{i\bar{\sigma}})^2}{\xi_i[n_i - 2n_{i\uparrow}n_{i\downarrow} + 2|\mathcal{S}_i^+|^2]}, \tag{121}$$

$$\langle \mathbf{S}_i\rangle \approx \frac{\lambda_i}{\Xi_i}\langle \mathbf{S}_i\rangle_0 = \sqrt{g_{ii}^s}\langle \mathbf{S}_i\rangle_0, \tag{122}$$

$$\sqrt{g_{ii}^s} \equiv \frac{n_i}{n_i - 2n_{i\uparrow}n_{i\downarrow} + 2|\mathcal{S}_i^+|^2}, \tag{123}$$

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j\rangle \approx \frac{\lambda_i}{\Xi_i}\frac{\lambda_j}{\Xi_j}\langle \mathbf{S}_i \cdot \mathbf{S}_j\rangle_0 = g_{ij}^s \langle \mathbf{S}_i \cdot \mathbf{S}_j\rangle_0, \tag{124}$$

$$g_{ij}^s \equiv \sqrt{g_{ii}^s g_{jj}^s}. \tag{125}$$

In this case, the derivation of g^s is rather simple because $\mathbf{S}_i$ is nonzero only when it is operated to states where site i is singly occupied.[16] Note that $\langle \mathbf{S}_i\rangle \| \langle \mathbf{S}_i\rangle_0$ is automatically satis-

fied, and there is no complexity appeared in Sec. II D. However, in this formulation, projected quasiparticle excited states are not orthogonal for magnetic systems in general.

B. Global constraint: charge-canonical spin-grand canonical GA

It is possible that a wave function before the projection is an eigenstate of the total particle number, but *not* any eigenstate of the total spin. One can formulate a GA also for such systems. In this case, the condition to impose is the canonical condition for the total particle number, $\Sigma_{i\sigma}\langle\hat{n}_{i\sigma}\rangle = N^{\text{after}}$, namely,

$$\lambda \sum_{i\sigma} \frac{n_{i\sigma}(1-n_{i\bar{\sigma}})}{\Xi_i} = N^{\text{after}}. \tag{126}$$

Here, λ does not depend on σ. The renormalization formulas for $\mathcal{S}_i^{\pm}=0$ are the same as those in Sec. IV if λ_σ is replaced by λ. The generalization to $\mathcal{S}_i^{\pm}\neq 0$ is straightforward.

The results for antiferromagnets are equivalent to those in Sec. IV. The limit to uniform ferromagnets without superconductivity can be taken by setting $\Delta_{ij}=0$, $N_\sigma^{\text{after}}=\Sigma_i\langle\hat{n}_{i\sigma}\rangle_0$, and dropping site indices,[17]

$$g_\sigma^t = \frac{(1-n_{\bar{\sigma}})(1-n)n}{(1-n_\sigma)(n-2n_\uparrow n_\downarrow)}, \quad g_\sigma^s = \left(\frac{n}{n-2n_\uparrow n_\downarrow}\right)^2. \tag{127}$$

These are different from our quasicanonical derivation in Eqs. (109) and (110). In fact, in this spin-grand canonical formulation, g^s for ferromagnets is the same as that for antiferromagnets. This discrepancy is explained as follows: If the wave function before the projection is an eigenstate of the total spin z, then the renormalization is represented by Eqs. (109) and (110). If not, by Eq. (127). The Gutzwiller projection tends to magnify spin moments as explained in Appendix A. However, in the canonical scheme, only xy components of the spins are allowed to be enhanced because of the canonical constraint. On the other hand, the spin-grand canonical case is free from this constraint, and spins are renormalized more isotropically.

VI. SUMMARY AND DISCUSSION

We have derived various formulas using the grand canonical Gutzwiller approximation with several different constraints imposed by the fugacity factors for inhomogeneous magnetic systems. The formulation with the local particle number conservation yields more simple formulas. On the other hand, the global particle number constraint is more convenient in comparing with the variational Monte Carlo (VMC).

In Secs. III, we have discussed the asymmetry of the density of states. Although the incoherent spectra are not taken into account in this paper, we speculate that they appear at much higher energy scale than the coherence peaks. The conventional BCS theory tells us that the quasiparticle excitation spectra are symmetric between positive and negative bias. In contrast, with the Gutzwiller projection, some asymmetry appears. One may think that electron addition is always more difficult than electron removal if repulsion between electrons is strong. However, we doubt if such simple intuition works, and speculate that the asymmetry depends on the Hamiltonian. As a counterexample, we have shown that the projected s-wave superconductor may have the opposite asymmetry. Namely, even with the strong repulsion, the addition spectra can be larger than the removal. We could be able to consider it in this way. Let us take two (normalized) Gutzwiller-projected wave functions, $|\psi\rangle$ and $|\phi\rangle$. Suppose they are the ground states of Hamiltonians, H_ψ and H_ϕ, respectively. Furthermore, we assume that $|\psi\rangle$ and $|\phi\rangle$ are also excited states of the other Hamiltonian, H_ϕ and H_ψ, respectively. Then, $\langle\phi|c_{i\sigma}^\dagger|\psi\rangle$ is an electron addition matrix element to the ground state of H_ψ. However, if one takes its complex conjugate, it is an electron removal matrix element to the ground state of H_ϕ. Note that $|\langle\psi|c_{i\sigma}|\phi\rangle| = |\langle\phi|c_{i\sigma}^\dagger|\psi\rangle|$. That is, if an electron addition matrix element for a Hamiltonian is small, an electron *removal* matrix element for a different Hamiltonian is also small. Therefore, the asymmetry is most likely determined not only by the projection, but also by the Hamiltonian.

Our ultimate purpose is to find good variational wave functions for systems with strong on-site Coulomb repulsion. Once the fugacity factors are introduced, one projected wave function can be related to a number of different *unprojected* wave functions, each of which is accompanied with fugacity factors of each definition. Therefore, one should probably choose a definition of fugacity factors that matches their purpose. We speculate that the projected optimized solution is similar in any choice of the fugacity factors if the calculation is done accurately enough.

There may be slight disagreement with the results by Ko *et al.* That is, their comparison between the VMC and the GA seems to say that the GA with the position- and spin-dependent constraint has larger errors than that with the global constraint. However, according to our estimation, the formulation with the position- and spin-dependent constraint has much smaller errors.

To improve the approximation, one can use techniques of the series expansion method such as the finite cluster method for calculating higher-order terms. One can also use the Padé approximation for extrapolation if necessary, but maybe it is enough just to neglect small terms without extrapolation. Since this linked-cluster expansion can be done analytically, there is a possibility to minimize the energy analytically in contrast to the VMC.

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APPENDIX A: DIFFERENCE BETWEEN CANONICAL AND GRAND CANONICAL SCHEME

Suppose $|\Psi_0^N\rangle$ is an eigenstate of the total particle number $\hat{N}\equiv\Sigma_{i\sigma}\hat{n}_{i\sigma}$ with $\hat{N}|\Psi_0^N\rangle = N|\Psi_0^N\rangle$. Then, since $[P_G,\hat{N}]=0$,

$$\hat{N}P_{\mathrm{G}}|\Psi_0^N\rangle = NP_{\mathrm{G}}|\Psi_0^N\rangle. \tag{A1}$$

Namely, in the canonical scheme, P_{G} does not change the particle number. On the other hand in the grand canonical scheme, a wave function $|\Psi_0\rangle$ is *not* an eigenstate of $\hat{N}$, and the particle number is distributed with the distribution function,

$$\rho_N^{(0)} \equiv \frac{\langle\Psi_0|P_N|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle},$$

where P_N is an operator which projects onto terms with particle number N. Suppose $\rho_N^{(0)}$ is sharply peaked at a mean value N, and fluctuation around it is of $O(\sqrt{1/N})$. Then, $|\Psi_0\rangle$ can be regarded as a wave function almost identical with $|\Psi_0^N\rangle$ in the thermodynamic limit. In contrast in the projected case, the average particle number of $P_{\mathrm{G}}|\Psi_0\rangle$ is in fact different from that of $P_{\mathrm{G}}|\Psi_0^N\rangle$. When N is large, an electron has more chance to meet another electron on a certain site. In other words, P_{G} excludes more states with large N, and thus the peak position of the N distribution is shifted to a smaller value. Such distribution change was explicitly estimated by Edegger *et al.*[12] as summarized below. The distribution function after the projection,

$$\rho_N \equiv \frac{\langle\Psi_0|P_{\mathrm{G}}P_NP_{\mathrm{G}}|\Psi_0\rangle}{\langle\Psi_0|P_{\mathrm{G}}P_{\mathrm{G}}|\Psi_0\rangle}, \tag{A2}$$

can be related to that before by $\rho_N = g_N\rho_N^0$ with

$$g_N \equiv C\frac{\langle\Psi_0|P_{\mathrm{G}}P_NP_{\mathrm{G}}|\Psi_0\rangle}{\langle\Psi_0|P_N|\Psi_0\rangle},$$

where C is a constant independent of N coming from the normalization of the wave functions. The GA can estimate g_N by the ratio of the relative sizes of the projected and unprojected Hilbert spaces as

$$g_N \approx C\frac{(N_L-N_\uparrow)!\,(N_L-N_\downarrow)!}{(N_L-N_\uparrow-N_\downarrow)!}, \tag{A3}$$

where N_L is the number of lattice sites and $N_\uparrow$ ($N_\downarrow$) is the number of up (down) spins.

We here discuss renormalization of spins using Eq. (A3). Since $[P_{\mathrm{G}},\mathbf{S}_i]=0$, if a wave function before the projection is an eigenstate of $(\Sigma_i\mathbf{S}_i)^2$ and/or $\Sigma_iS_i^z$ with eigenvalues $S(S+1),M$, respectively, then these quantities are not changed by P_{G}. If it is not such an eigenstate, P_{G} may change the distribution of S,M. If N is fixed, by changing M in Eq. (A3), one can see that P_{G} excludes more states with small M. As a result, the most "probable" M increases. In fact, Eq. (A3) correctly reproduce the limit of fully polarized states ($N_\sigma=0$), which are obviously not affected by P_{G}. By rotating spin axes, and repeating this argument for the x,y directions, we conclude that P_{G} excludes more states with small $\mathbf{S}^2$. Physically, this can be explained as follows: To make small $\mathbf{S}^2$, electrons have to cancel their spin moments, and then they have high chance to meet each other on a certain site. When $\mathbf{S}^2$ is large, the spin of an electron tend to orient the same direction as those of the other, then electrons prefer to stay at different sites, and not affected by the projection so much.

The Gutzwiller projection makes more singly occupied sites, and local spin moments also tend to be magnified (this is probably related to an increase in $\mathbf{S}^2$). In the canonical scheme, magnitude of uniform (ferromagnetic) moments are restricted by the canonical constraint, whereas nonuniform (e.g., antiferromagnetic, sinusoidal) moments are free from the canonical constraint and can be enhanced. On the other hand, in the spin-grand canonical scheme, the total spin-z component does not have such restriction, and ferromagnetic moments can be also enhanced (shown in Sec. V B).

APPENDIX B: ELECTRON ADDITION/REMOVAL MATRIX ELEMENTS

The general expressions of Eqs. (67)–(74) are written as follows using $\bar{n}_{i\sigma}\equiv 1-n_{i\sigma}$, $\alpha_{i\sigma}\equiv n_{i\sigma}(1-n_{i\sigma})^{-1}$, and $\tilde{A}_{ij}\equiv n_{ji\uparrow}n^*_{ji\downarrow}+\Delta^*_{ji}\Delta_{ij}$ $(i\neq j)$:

$$\frac{\langle c^\dagger_{j\uparrow}Pc_{i\uparrow}P\rangle_0}{\langle P^2\rangle_0} \approx \sqrt{g^{t0}_{ii\uparrow}}\left(n_{ji\uparrow}+\frac{n_{ji\downarrow}\alpha_{j\uparrow}\tilde{A}_{ij}}{\bar{n}_{i\downarrow}\bar{n}_{j\downarrow}}\right), \tag{B1}$$

$$\frac{\langle c_{j\uparrow}Pc^\dagger_{i\uparrow}P\rangle_0}{\langle P^2\rangle_0} \approx \sqrt{g^{t0}_{ii\uparrow}}\left(-n_{ij\uparrow}+\frac{n_{ij\downarrow}\tilde{A}^*_{ij}}{\bar{n}_{i\downarrow}\bar{n}_{j\downarrow}}\right), \tag{B2}$$

$$\frac{\langle c^\dagger_{j\downarrow}Pc^\dagger_{i\uparrow}P\rangle_0}{\langle P^2\rangle_0} \approx \sqrt{g^{t0}_{ii\uparrow}}\left(-\Delta^*_{ij}+\frac{\alpha_{j\downarrow}\Delta^*_{ji}\tilde{A}^*_{ij}}{\bar{n}_{i\downarrow}\bar{n}_{j\uparrow}}\right), \tag{B3}$$

$$\frac{\langle c_{j\downarrow}Pc_{i\uparrow}P\rangle_0}{\langle P^2\rangle_0} \approx \sqrt{g^{t0}_{ii\uparrow}}\left(\Delta_{ij}+\frac{\Delta_{ji}\tilde{A}_{ij}}{\bar{n}_{i\downarrow}\bar{n}_{j\uparrow}}\right), \tag{B4}$$

$$\frac{\langle c^\dagger_{j\uparrow}P^2c_{i\uparrow}\rangle_0}{\langle P^2\rangle_0} \approx n_{ji\uparrow}-\frac{n_{ji\downarrow}\alpha_{i\uparrow}\alpha_{j\uparrow}\tilde{A}_{ij}}{\bar{n}_{j\downarrow}\bar{n}_{i\downarrow}}, \tag{B5}$$

$$\frac{\langle c_{j\uparrow}P^2c^\dagger_{i\uparrow}\rangle_0}{\langle P^2\rangle_0} \approx -n_{ij\uparrow}+\frac{n_{ij\downarrow}\tilde{A}^*_{ij}}{\bar{n}_{j\downarrow}\bar{n}_{i\downarrow}}, \tag{B6}$$

$$\frac{\langle c^\dagger_{j\downarrow}P^2c^\dagger_{i\uparrow}\rangle_0}{\langle P^2\rangle_0} \approx -\Delta^*_{ij}+\frac{\alpha_{j\downarrow}\Delta^*_{ji}\tilde{A}^*_{ij}}{\bar{n}_{i\downarrow}\bar{n}_{j\uparrow}}, \tag{B7}$$

$$\frac{\langle c_{j\downarrow}P^2c_{i\uparrow}\rangle_0}{\langle P^2\rangle_0} \approx \Delta_{ij}-\frac{\alpha_{i\uparrow}\Delta_{ji}\tilde{A}_{ij}}{\bar{n}_{i\downarrow}\bar{n}_{j\uparrow}}. \tag{B8}$$

APPENDIX C: HIGHER-ORDER TERMS FOR THE GLOBAL CONSTRAINT

By taking up to the second order of the intersite contractions, $\langle P^2\rangle_0$ is represented by

$$\frac{\langle P^2\rangle_0}{\prod_l\Xi_l} \approx 1+\sum_{l<m}\frac{\Xi^{(2)}_{lm}}{\Xi_l\Xi_m}. \tag{C1}$$

Here, $\Xi^{(2)}_{lm}$ contains all the terms of the second order of intersite contractions in $\langle P^2\rangle_0$. The division by $\Pi_l\Xi_l$ cancels

single site contribution and simplifies the expression. For calculating $\langle n_{i\uparrow}\rangle$, we need

$$\frac{\langle n_{i\uparrow}P^2\rangle_0}{\prod_l \Xi_l} = \frac{\lambda(1-n_{i\downarrow})}{\Xi_i} n_{i\uparrow}\left(1+\sum_{l<m,l\neq i,m\neq i}\frac{\Xi^{(2)}_{lm}}{\Xi_l\Xi_m}\right)+\sum_{l\neq i}\frac{\lambda}{\Xi_i\Xi_l}\{a_{l\downarrow}[(1-n_{i\downarrow})|n_{il\uparrow}|^2+n_{i\uparrow}|\Delta_{li}|^2]-a_{l\uparrow}[n_{i\uparrow}|n_{il\downarrow}|^2+(1-n_{i\downarrow})|\Delta_{il}|^2]\}. \tag{C2}$$

By taking the ratio between Eqs. (C1) and (C2), and neglecting fourth order terms, contribution from disconnected clusters disappears. Then, we obtain renormalization of particle densities as Eq. (93).

To determine $\lambda^{(2)}$, we use the equation for $1-\langle \hat{n}_{i\uparrow}+\hat{n}_{i\downarrow}\rangle$, namely,

$$N_{\mathrm{L}}-N^{\mathrm{after}} = \sum_i \frac{(1-n_{i\uparrow})(1-n_{i\downarrow})}{\Xi_i}+\sum_i \lambda\frac{n_{i\uparrow}(1-n_{i\downarrow})+n_{i\downarrow}(1-n_{i\uparrow})}{\Xi_i}\sum_{l\neq i}\frac{\Xi^{(2)}_{il}}{\Xi_i\Xi_l}$$
$$-\sum_i\sum_{l\neq i}\frac{\lambda}{\Xi_i\Xi_l}\{a_{l\downarrow}[(1-2n_{i\downarrow})|n_{il\uparrow}|^2-(1-2n_{i\uparrow})|\Delta_{li}|^2]+a_{l\uparrow}[(1-2n_{i\uparrow})|n_{il\downarrow}|^2-(1-2n_{i\downarrow})|\Delta_{il}|^2]\}. \tag{C3}$$

By replacing λ by $\lambda^{(0)}+\lambda^{(2)}$, zeroth-order term cancels between the left-hand side and the first term of the right-hand side. The latter also contains $\lambda^{(2)}$; in fact, $\lambda^{(2)}$ in the other terms can be negligible because they are multiplied to other intersite contractions. Regarding $\lambda^{(2)}$ as the same order as $n^2_{ij\sigma}$ and Δ^2_{ij}, and neglecting high order terms, Eq. (95) is obtained.

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[1] M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963).
[2] M. C. Gutzwiller, Phys. Rev. **134**, A923 (1964).
[3] M. C. Gutzwiller, Phys. Rev. **137**, A1726 (1965).
[4] T. Ogawa, K. Kanda, and T. Matsubara, Prog. Theor. Phys. **53**, 614 (1975).
[5] D. Vollhardt, Rev. Mod. Phys. **56**, 99 (1984).
[6] F. C. Zhang, C. Gros, T. M. Rice, and H. Shiba, Supercond. Sci. Technol. **1**, 36 (1988).
[7] T. C. Hsu, Phys. Rev. B **41**, 11379 (1990).
[8] M. Sigrist, T. M. Rice, and F. C. Zhang, Phys. Rev. B **49**, 12058 (1994).
[9] M. Ogata and A. Himeda, J. Phys. Soc. Jpn. **72**, 374 (2003).
[10] C.-P. Chou, T. K. Lee, and C.-M. Ho, Phys. Rev. B **74**, 092503 (2006).
[11] P. W. Anderson and N. P. Ong, J. Phys. Chem. Solids **67**, 1 (2006).
[12] B. Edegger, N. Fukushima, C. Gros, and V. N. Muthukumar, Phys. Rev. B **72**, 134504 (2005).
[13] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **57**, 2482 (1988).
[14] F. Gebhard, Phys. Rev. B **41**, 9452 (1990).
[15] R. B. Laughlin, Philos. Mag. **86**, 1165 (2006).
[16] Q.-H. Wang, Z. D. Wang, Y. Chen, and F. C. Zhang, Phys. Rev. B **73**, 092507 (2006).
[17] W.-H. Ko, C. P. Nave, and P. A. Lee, Phys. Rev. B **76**, 245113 (2007).
[18] W. Metzner and D. Vollhardt, Phys. Rev. B **37**, 7382 (1988).
[19] C. Li, S. Zhou, and Z. Wang, Phys. Rev. B **73**, 060501(R) (2006).
[20] N. Fukushima, C.-P. Chou, and T. K. Lee, J. Phys. Chem. Solids (to be published).
[21] N. Fukushima, B. Edegger, V. N. Muthukumar, and C. Gros, Phys. Rev. B **72**, 144505 (2005).
[22] M. Randeria, R. Sensarma, N. Trivedi, and F. C. Zhang, Phys. Rev. Lett. **95**, 137001 (2005).
[23] S. Bieri and D. Ivanov, Phys. Rev. B **75**, 035104 (2007).
[24] H.-Y. Yang, F. Yang, Y.-J. Jiang, and T. Li, J. Phys.: Condens. Matter **19**, 016217 (2007).
[25] M. Tinkham, Phys. Rev. B **6**, 1747 (1972).