

# Two-hole ground state wavefunction: A non-BCS pairing in a $t$ - $J$ system

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Superconductivity is usually described in the framework of the BCS wavefunction, which even includes the resonating-valence-bond (RVB) wavefunction proposed for the high-temperature superconductivity in the cuprate. A natural question is *if* any fundamental physics could be possibly missed by applying such a scheme to strongly correlated systems. Here we study the pairing wavefunction of two holes injected into a Mott insulator/antiferromagnet in a two-leg ladder using variational Monte Carlo (VMC) approach. By comparing with density matrix renormalization group (DMRG) calculation, we show that a conventional BCS or RVB pairing of the doped holes makes qualitatively wrong predictions and is incompatible with the fundamental pairing force in the  $t$ - $J$  model, which is kinetic-energy-driven by nature. By contrast, a non-BCS-like wavefunction incorporating such novel effect will result in a substantially enhanced pairing strength and improved ground state energy as compared to the DMRG results. We argue that the non-BCS form of such a new ground state wavefunction is essential to describe a doped Mott antiferromagnet at finite doping.

## I. INTRODUCTION

Three decades after the discovery of high-temperature superconductivity in the copper oxide materials<sup>1</sup>, it still remains a mystery whether the superconductivity can be described by a wavefunction of Bardeen-Cooper-Schrieffer (BCS) type<sup>2</sup>. For example, as a non-phonon mechanism, the resonating-valence-bonds (RVB) ground state proposed by Anderson<sup>3</sup> may be still regarded as the BCS-like, only subject to a Gutzwiller projection onto a restricted Hilbert space to enforce the no double occupancy of the electrons. Such a projection is due to the on-site Coulomb repulsion  $U$ , which will make the electrons form an insulating antiferromagnetic state (Mott insulator<sup>4,5</sup>) at half-filling, where the condensate of the Cooper pairs reduces to that of the neutral spin RVB pairing. The true Cooper pairing similar to a conventional superconductor is expected<sup>3</sup> to emerge by charging the neutral RVB background upon doping. Such an “RVB pairing mechanism” of superconductivity has been intensively studied<sup>6</sup> based on the variational RVB state<sup>3,7–10</sup>.

Taking an instructive limit of two holes injected into the half-filled spin background, one may examine the RVB origin of pairing by the following variational construction:

$$|\Psi_{\text{BCS}}\rangle_{2h} = \hat{\Delta}|\text{RVB}\rangle, \quad (1)$$

in which the two doped holes form a Cooper pair

$$\hat{\Delta} = \sum_{i,j} g(i,j) c_{i\uparrow} c_{j\downarrow}, \quad (2)$$

on a *half-filling* insulating ground state denoted by  $|\text{RVB}\rangle$ . Here  $|\text{RVB}\rangle$  is governed by the Heisenberg superexchange term with the coupling constant  $J$ , which is assumed<sup>3</sup> to be the main driving force for the Cooper

pairing of doped holes. Namely, the antiferromagnetic correlations in  $|\text{RVB}\rangle$  can provide a *bare* binding force for the two holes injected into such a spin background. Then Eq. (1) may serve as an important test of the RVB mechanism. To this end, the pair amplitude  $g(i,j)$  is taken as a c-number, which can be determined variationally by using the variational Monte Carlo (VMC) method<sup>8–11</sup> based on the  $t$ - $J$  model description of the doped Mott insulator.

However, the ansatz state in Eq. (1) does not necessarily capture the fundamental physics of two hole pairing<sup>12–14</sup>. The key assumption there is that the quantum fluctuation is negligible such that  $g(i,j)$  may be simulated by a “mean-field” in the variational approach. However, a recent density matrix renormalization group (DMRG) study on the ground state of two holes<sup>15,16</sup> has revealed a different nature of pairing other than Eq. (1). For such a strongly correlated model in which two holes are injected into two distinct Mott insulators of two-leg ladder systems, a strong *phase fluctuation* has been identified<sup>16</sup> in the pair-pair correlation functions. It suggests<sup>16</sup> that the pair amplitude  $g(i,j)$  in Eq. (2) should be replaced by

$$g(i,j) \rightarrow g(i,j) e^{-i(\hat{\Omega}_i + \hat{\Omega}_j)}, \quad (3)$$

where  $\hat{\Omega}_i$  represents a nonlocal phase shift produced by doping a hole into the system. Here  $\hat{\Omega}_i$  has been explicitly identified<sup>16</sup> as a pure spin string operator [cf. Eq. (11)] acting on the half-filling background  $|\text{RVB}\rangle$ , and is very sensitive to the spin-spin correlation in  $|\text{RVB}\rangle$ . In essence, it implies that the correct two-hole ground state should be properly characterized by

$$|\Psi_{\text{G}}\rangle_{2h} = \hat{D}|\text{RVB}\rangle, \quad (4)$$

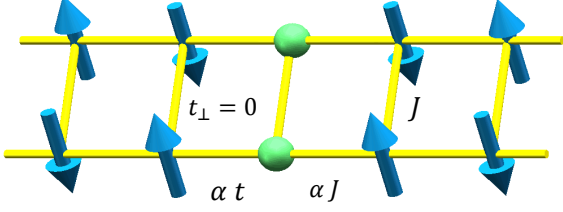


Fig. 1. (Color online.) The structure and parameters for a two-leg  $t$ - $J$  square ladder doped by two holes. Here, the intrachain hopping and superexchange coupling constants are denoted by  $\alpha t$  and  $\alpha J$ , respectively, with  $\alpha > 0$  as the anisotropic parameter and the interchain superexchange coupling defined by  $J$ . Note that the interchain hopping  $t_{\perp} = 0$  in the present work.

where

$$\hat{D} = \sum_{i,j} g(i,j) \tilde{c}_{i\uparrow} \tilde{c}_{j\downarrow}, \quad (5)$$

is equal to  $\hat{\Delta}$  in Eq. (2) with

$$c_{i\sigma} \rightarrow \tilde{c}_{i\sigma} \propto c_{i\sigma} e^{-i\hat{\Omega}_i}. \quad (6)$$

Namely, the Cooper pairing of two bare holes in the BCS-like ground state (1) should be replaced by the pairing of two new “twisted” quasiparticles, created by  $\tilde{c}_{i\uparrow}$  and  $\tilde{c}_{i\downarrow}$  on the “vacuum”  $|\text{RVB}\rangle$ . In other words, each doped hole has to change the spin background  $|\text{RVB}\rangle$  by a nonlocal phase shift  $\hat{\Omega}_i$  to become a true quasiparticle. Due to the spin-dependent many-body phase shift operator  $e^{-i\hat{\Omega}_i}$ , which is non-perturbative by nature<sup>16</sup>, the resulting new ground state (4) is obviously non-BCS-like in the original electron representation.

Similar novel quantum phase fluctuations have been also identified in a symmetry-protected topological phase of the two-leg system<sup>16</sup>, in which two spins at each rung are coupled by ferromagnetic instead of antiferromagnetic coupling. It implies that the pairing structure may be generally of non-BCS-type in a doped spin system enforced by the no-double-occupancy constraint. Recently, the pairing of holes at finite doping has been clearly found by DMRG in various generalized doped Mott insulators<sup>17–21</sup>. It is thus highly intriguing and motivated to understand the microscopic origin of the hole pairing state in the limit of two hole case, which should shed light on the superconducting mechanism and the wavefunction structure at finite doping, which are experimentally relevant.

In this paper, we comparably study the two variational ground states, Eq. (1) and Eq. (4), by the VMC approach based on the  $t$ - $J$  model. Specifically, the half-filling ground state  $|\text{RVB}\rangle$  will be first determined in a Heisenberg two-leg square ladder model as illustrated in

Fig. 1, which describes a short-range antiferromagnetic or RVB spin state. Then we examine the two-hole ground state with turning on the hopping integral along the chain direction (but without the inter-leg hopping along the rung direction for the simplicity in analytic analysis). We variationally determine the parameter  $g(i,j)$  by minimizing the two-hole ground state energies of Eq. (1) and Eq. (4), respectively. We find that the ground state energy and various pair-pair correlations of the ground state (4) are significantly and qualitatively improved over the BCS pairing state (1), in excellent agreement with the DMRG results. In particular, by using a unitary transformation, we show that the ground state (4) properly incorporates the kinetic-energy-driven pairing force hidden in the  $t$ - $J$ -type model, which is completely missed in the RVB-like description in Eq. (1). In fact, in the latter state, we show variationally that two holes do not form a bound state at all, even though  $|\text{RVB}\rangle$  as an RVB state possesses the same short-range antiferromagnetic correlation in the two-leg ladder. In other words, a new pairing mechanism distinct from the RVB mechanism can be explicitly identified in the strong binding state of Eq. (4), which is argued to be Amperean-like<sup>22,23</sup>. Generalizations to the  $t_{\perp} \neq 0$  or the two-dimensional case, as well as the finite doping case, will be also briefly discussed.

The rest of the paper is organized as follows. In Sec. II A, we first introduce a  $t$ - $J$  type model for the two-leg ladder illustrated in Fig. 1 and the corresponding  $\sigma \cdot t$ - $J$  model for the purpose of comparison. Then, in Sec. II B, we study the ground state properties of two different types of variational wavefunction,  $|\Psi_{\text{BCS}}\rangle_{2h}$  and  $|\Psi_{\text{G}}\rangle_{2h}$  outlined in the Introduction, by the VMC calculation. By making comparison with the DMRG results, we show that the latter ground state does capture the essential physics especially the non-BCS pairing in the  $t$ - $J$  type model, whose nature is further analyzed in Sec. II C. Finally, the summary and discussion of the main results, as well as some perspectives, are given in Sec. III.

## II. MODEL AND RESULTS

### A. The model

In this paper, we mainly focus on the ground state properties of the two-hole-doped Mott insulator on a two-leg-square-ladder illustrated in Fig. 1, which is described by the  $t$ - $J$  Hamiltonian<sup>16,24</sup>  $H_{t-J} = H_t + H_J$  as follows:

$$H_t = -\alpha t \sum_{i\sigma} \left( c_{1i\sigma}^\dagger c_{1i+1\sigma} + c_{2i\sigma}^\dagger c_{2i+1\sigma} + \text{H.c.} \right) \quad (7)$$

$$H_J = \alpha J \sum_i (\mathbf{S}_{1i} \cdot \mathbf{S}_{1i+1} + \mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1}) + J \sum_i \mathbf{S}_{1i} \cdot \mathbf{S}_{2i} \quad (8)$$

where the subscripts, 1 and 2, label the two legs and the anisotropic parameter  $\alpha > 0$  can continuously tune the spin-spin correlation length along the chain direction

in the quantum spin background.  $\mathbf{S}_i$  denotes the spin operator and  $c_{i\sigma}$  is the hole creation operator at site  $i$  with spin index  $\sigma$ . The Hilbert space should satisfy the no-double-occupancy constraint  $\sum_{\sigma} c_{1,2i\sigma}^{\dagger} c_{1,2i\sigma} \leq 1$ . We choose the typical ratio  $t/J = 3$ , while, for simplicity, the injected holes are only allowed to move along the chain (leg) direction with the rung hopping integral  $t_{\perp} = 0$  (cf. Fig. 1).

Previously the corresponding two-hole ground state has been studied numerically by DMRG in Ref. 16 for  $t_{\perp} = 0$ , and in Ref. 15 for the general case at  $t_{\perp} = t$ , respectively. In both cases, a strong binding between the two injected holes has been well established by DMRG<sup>15,16</sup>. By contrast, in these numerical studies, it has been shown that the pairing between the holes will get substantially weakened<sup>16</sup> or even disappear<sup>15</sup> if the hidden phase-string sign structure in the  $t$ - $J$  model is precisely removed in the so-called  $\sigma \cdot t$ - $J$  model defined by  $H_{\sigma \cdot t-J} = H_{\sigma \cdot t} + H_J$ , in which the superexchange Hamiltonian  $H_J$  remains the same, but the hopping term is changed to<sup>15,16</sup>

$$H_{\sigma \cdot t} = -\alpha t \sum_{\sigma i} \sigma \left( c_{1i\sigma}^{\dagger} c_{1i+1\sigma} + c_{2i\sigma}^{\dagger} c_{2i+1\sigma} + \text{h.c.} \right) \quad (9)$$

by inserting a spin-dependent sign factor  $\sigma = \pm 1$  in the original hopping term of Eq. (7). Then the novel non-BCS-pairing mechanism hidden in the  $t$ - $J$  model will lie in the distinction between the  $t$ - $J$  and  $\sigma \cdot t$ - $J$  model, which can be effectively revealed by using the  $\sigma \cdot t$ - $J$  model as a useful reference Hamiltonian in the following variational study.

## B. Ground state wavefunctions: Variational Monte Carlo calculation

As pointed out in the Introduction, the ground state (1) depicts the simplest pairing wavefunction of two holes doped into an RVB (short-ranged antiferromagnetic) background as envisaged originally by Anderson<sup>3</sup>. By contrast, the ground state (4) is modified non-perturbatively by that each doped hole induces a non-local phase shift as given by<sup>16</sup>

$$\tilde{c}_{\gamma i\sigma} = c_{\gamma i\sigma} e^{-i\hat{\Omega}_{\gamma i}} \quad (10)$$

and

$$\hat{\Omega}_{\gamma i} = \pi \sum_{l>i} n_{\gamma l}^{\downarrow}, \quad (11)$$

where the subscript  $\gamma = 1, 2$  labels the two legs of the square ladder shown in Fig. 1, and  $n_{\gamma l}^{\downarrow}$  denotes the number operator of a down spin at site  $l$  along the chain of leg  $\gamma$ <sup>16</sup>. Note that  $\hat{\Omega}_{\gamma i}$  is taken as purely one-dimensional here in Eq. (11) simply because the hopping integral  $t_{\perp} = 0$  along each rung of the ladder (cf. Fig. 1). In general with  $t_{\perp} \neq 0$ , the spins in another chain of the

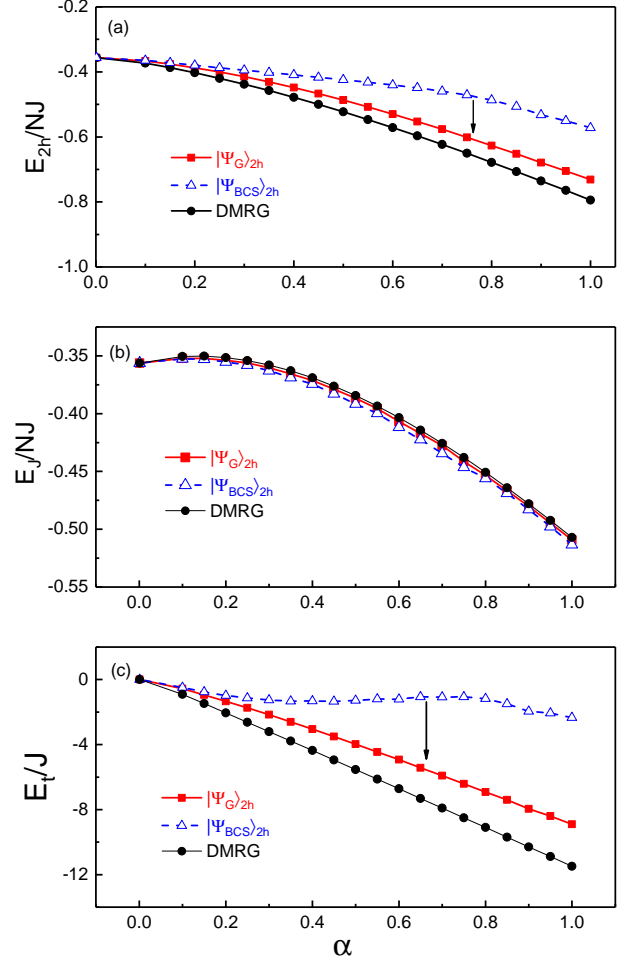


Fig. 2. (Color online.) The variational ground state energies of  $|\Psi_{\text{BCS}}\rangle_{2h}$  in Eq. (1) (blue triangle) and  $|\Psi_{\text{G}}\rangle_{2h}$  in Eq. (4) (red square) in comparison with the DMRG results (solid circle). (a) The total energies; (b) The superexchange energies; And (c), the kinetic energies. The ladder size is  $N = 20 \times 2$  under the open boundary condition.

two-leg ladder will also play a non-negligible role in  $\hat{\Omega}_{\gamma i}$  in general<sup>25</sup>.

Note that at half-filling, both the ground states of Eqs. (1) and (4) reduce to the same  $|\text{RVB}\rangle$ , which can be accurately determined based on the Liang-Doucot-Anderson bosonic RVB wavefunction<sup>26</sup> for the two-leg Heisenberg model<sup>25</sup>. As previously studied by DMRG and VMC calculations,  $|\text{RVB}\rangle$  describes a short-range antiferromagnetic ground state, with gapped low-lying spin excitations<sup>27</sup>. Based on such  $|\text{RVB}\rangle$ , we can then optimize the ground state energies of the RVB state in Eq. (1) and the non-BCS-like wavefunction of Eq. (4) with regard to the variational parameter  $g(i, j)$ . The details of the variational procedure are presented in the Appendix A, which has been developed based on the method firstly applying to the one-hole ground state in Ref. 25.

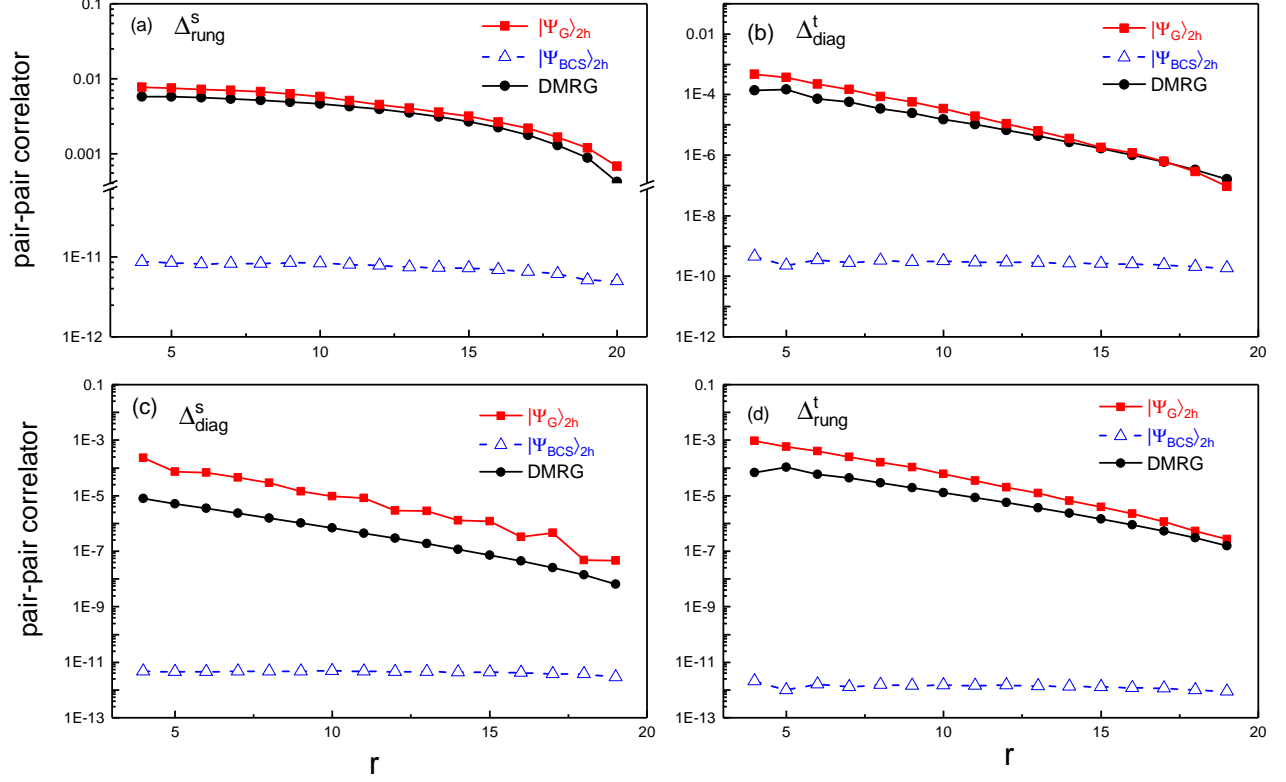


Fig. 3. (Color online.) Pair-pair correlators,  $C^{s,t}(r)$ , as a function of distance  $r$  calculated in the ground states  $|\Psi_{\text{BCS}}\rangle_{2h}$  (blue triangle) and  $|\Psi_{\text{G}}\rangle_{2h}$  (red square), respectively, in comparison with the DMRG results (solid circle), are shown for different channels in (a)-(d) as labeled by the pairing parameters defined in the text. While the present variational ground state  $|\Psi_{\text{G}}\rangle_{2h}$  in Eq. (4) has well captured the correct pair-pair correlations in all channels as compared with the DMRG results, the RVB type ground state  $|\Psi_{\text{BCS}}\rangle_{2h}$  in Eq. (1), however, does not show any meaningful pair-pair correlations in all channels. The ladder size is  $N = 40 \times 2$  with  $\alpha = 1$ .

Fig. 2 shows the variational ground state energies for the two ground states, Eqs. (1) and (4), respectively, as computed by the VMC method for a finite size ladder. As compared to the DMRG result, Fig. 2 (a) shows that the total energy of the “RVB wavefunction” in Eq. (1) is indeed much higher as compared to both the non-BCS wavefunction in Eq. (4) as well as the DMRG result, which are relatively much closer. In particular, as shown in Fig. 2 (b) and (c), the deviation between the two variational ground states mainly comes from the hopping energy  $E_t = \langle H_t \rangle$ , while they agree well with each other in the superexchange energy  $E_J = \langle H_J \rangle$ . In other words, by incorporating the non-perturbative phase shift effect in Eqs. (10) and (11), the kinetic energy does get substantially improved in the new ground state (4), while the superexchange energy remains approximately unchanged.

Furthermore, an interesting but surprising result is illustrated in Fig. 3, in which the pair-pair correlators in the two variational ground states are computed and compared with the DMRG simulation. For all the spin-singlet and -triplet channels with the two hole pairing

at the same rung or at the diagonal bond of a plaquette of the ladder in Fig. 1, the pair-pair correlations are all vanishingly small ( $< 10^{-11}$ ) in the “RVB variational wavefunction” (1). By comparison, the pair-pair correlations are much enhanced in the wavefunction (4) in all channels shown in Fig. 3 (a)-(d). Especially these pair-pair correlators of the ground state (4) are in excellent agreement with the DMRG results, which are also shown in Fig. 3 (a)-(d). Note that in Fig. 3, the pair-pair correlators are defined as  $C^{s,t}(r) = \langle \hat{\Delta}_{1i'2j'}^{s,t} (\hat{\Delta}_{1i2j}^{s,t})^\dagger \rangle$  where the singlet and triplet channels are

$$\begin{aligned} \hat{\Delta}_{ij}^s &= \frac{1}{\sqrt{2}} \sum_{\sigma} \sigma c_{1i\sigma} c_{2j-\sigma}, \\ \hat{\Delta}_{ij}^t &= \frac{1}{\sqrt{2}} \sum_{\sigma} c_{1i\sigma} c_{2j-\sigma}. \end{aligned} \quad (12)$$

Here we only focus on the local rung pairing  $\hat{\Delta}_{\text{rung}}^{s,t}$  ( $i = j$ ) with  $r = |i - i'|$  and local diagonal pairing  $\hat{\Delta}_{\text{diag}}^{s,t}$  ( $i = j + 1$ ),

which represent the dominant pairings in the present two-leg ladder system<sup>16</sup>.

Therefore, in contrast to the conventional wisdom, the “RVB ground state” of Eq. (1) actually is not in favor of pairing between two holes upon doping, even though the half-filling  $|\text{RVB}\rangle$  state has already exhibited a short-range antiferromagnetism (an RVB state). On the other hand, in the new ground state of Eq. (4), two doped holes do form a strong bound pair, accompanied by the fact that its kinetic energy is significantly lowered as compared with the variational energy of Eq. (1). The overall ground state variational energy of  $|\Psi_G\rangle_{2h}$  is in qualitative agreement with the corresponding DMRG result. In particular, the pair-pair correlations calculated based on  $|\Psi_G\rangle_{2h}$  is in excellent agreement with the precise results. It thus clearly indicates that a *kinetic energy driven mechanism* must be at play in the  $t$ - $J$  model. This is in sharp contrast to a conventional BCS theory or Anderson’s RVB theory, in which the pairing strength is usually gained from the potential (superexchange) energy, whereas it causes the further *increase* of the kinetic energy in forming a bound state. In the following, we further explore the underlying pairing mechanism.

### C. Non-BCS pairing mechanism

The above variational calculations demonstrate that two doped holes injected into the short-range antiferromagnet  $|\text{RVB}\rangle$  can indeed form a tightly bound state. However, it is not described by Eq. (1) but by Eq. (4). The latter is non-BCS-like as each hole has to simultaneously induce a nonlocal spin “twist” via the phase string factor  $e^{-i\hat{\Omega}_i}$  in the spin background  $|\text{RVB}\rangle$ , which is in favor of pairing once two holes are present. By contrast, the pairing between the two holes vanishes in Eq. (4) once  $\hat{\Omega}_i$  is turned off, which results in Eq. (1).

In order to further understand the underlying physics, let us note that the two variational states in Eqs. (1) and (4) can be connected by the following unitary transformation:

$$|\Psi_G\rangle_{2h} = e^{i\hat{\Theta}} |\Psi_{\text{BCS}}\rangle_{2h}, \quad (13)$$

where

$$e^{i\hat{\Theta}} \equiv e^{-i \sum_{\gamma i} n_{\gamma i}^h \hat{\Omega}_{\gamma i}} \quad (14)$$

with  $n_{\gamma i}^h$  denoting the hole number operator at the site  $i$  of the leg  $\gamma$  (clearly this unitary transformation can be generalized to arbitrary dopings).

Then, given the fact that  $|\Psi_G\rangle_{2h}$  is an excellent variational ground state for the  $t$ - $J$  model, the “RVB ground state”  $|\Psi_{\text{BCS}}\rangle_{2h}$  in Eq. (1) can be taken as the *correct* trial wavefunction only if the target Hamiltonian is transformed from the  $t$ - $J$  type Hamiltonian  $H_{t-J}$  in Eq. (7) by  $\tilde{H}_{t-J} \equiv e^{-i\hat{\Theta}} H_{t-J} e^{i\hat{\Theta}}$ , which has the following form

$$\tilde{H}_{t-J} = H_{\sigma \cdot t-J} + H_1^{\text{string}}. \quad (15)$$

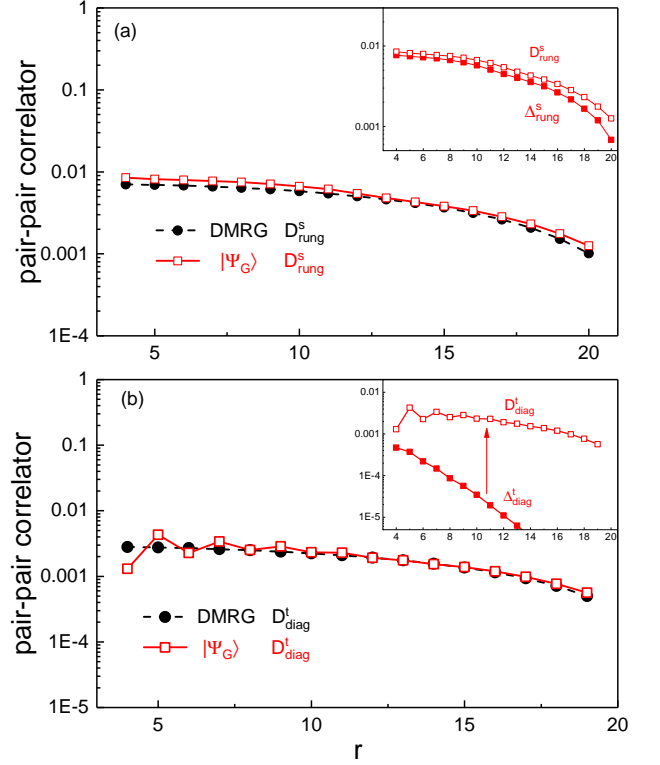


Fig. 4. (Color online.) The correlations of  $\hat{D}_{\text{diag/rung}}^{s/t}$  defined in Eqs. (19) and (20) calculated by VMC (open square) and DMRG (solid circle) in the singlet (a) and triplet (b) channels. Here  $\hat{D}_{\text{diag/rung}}^{s/t}$  may be regarded as the pair amplitude of the Cooper pair operator  $\hat{\Delta}_{\text{diag/rung}}^{s/t}$ , and the correlations of both operators are presented in the insets of (a) and (b), which indicate the strengths of the phase fluctuations in the Cooper pair correlators<sup>16</sup>. The system size is  $N = 40 \times 2$  with  $\alpha = 1$ .

Here the first term on the right-hand-side (rhs) is the  $\sigma \cdot t$ - $J$  model defined in Sec. II A, in which the hopping term is changed to  $H_{\sigma \cdot t}$  in Eq. (9), which is free from the frustration caused by the phase-string sign structure in the original  $t$ - $J$  model<sup>12–14</sup>. It has been previously shown by DMRG<sup>16</sup> that such  $\sigma \cdot t$ - $J$  model with  $t_{\perp} = 0$  would only lead to a weakly bound state of two holes, which may be regarded as the RVB mechanism for pairing due to  $H_J$ . By contrast, the pairing is absent in the two-leg  $\sigma \cdot t$ - $J$  ladder model for the isotropic case with  $t_{\perp} = t$ <sup>15</sup>. However, as pointed out in the above, in either case of  $t_{\perp} = 0$  or  $t_{\perp} = t$ , a strong binding between the two doped holes has been clearly identified in the  $t$ - $J$  model by DMRG<sup>15,16</sup>.

Thus, the last term  $H_1^{\text{string}}$  on the rhs of Eq. (15) in the transformed representation must play a dominant role in

the pairing mechanism of the  $t$ - $J$  model. It reads<sup>16</sup>

$$H_I^{\text{string}} = \frac{1}{2}J \sum_i (S_{1i}^+ S_{2i}^- + S_{1i}^- S_{2i}^+) (\Delta\Lambda_i^h - 1), \quad (16)$$

where the summation over  $i$  is along the chain direction, in which

$$\Delta\Lambda_i^h = e^{-i\pi \sum_{l<i} (n_{1l}^h - n_{2l}^h)} \quad (17)$$

describes the nonlocal phase shift effect created by the doped holes at both chains (legs) of  $\gamma = 1, 2$ . Since  $\langle S_{1i}^+ S_{2i}^- + S_{1i}^- S_{2i}^+ \rangle < 0$  at half-filling, one finds that two doped holes will generally acquire a string-like pairing potential as follows:

- If both holes lie on the right hand or left hand of the rung  $1i, 2i$ , the factor  $\Delta\Lambda_i^h = 1$  makes a vanishing contribution in Eq. (16).
- Only when the rung  $1i, 2i$  is sandwiched by the two holes along the chain direction, the factor  $\Delta\Lambda_i^h = -1$  makes a finite contribution in Eq. (16).

Consequently, an effective potential given by Eq. (16) for two holes can be found

$$V(h_1, h_2) \propto J |x_{h_1} - x_{h_2}|, \quad (18)$$

where  $|x_{h_1} - x_{h_2}|$  denotes the distance between the two holes at site  $h_1$  and  $h_2$  along the chain ( $x$ ) direction.

Namely, if one insists on using the BCS-type wavefunction of Eq. (1) to describe the hole pairing ground state, then the original  $t$ - $J$  Hamiltonian has to be transformed into a new Hamiltonian  $\tilde{H}_{t-J}$  in Eq. (15), in which the hopping term is replaced by that of the  $\sigma$ - $t$ - $J$  that is free from the phase string effect. Nevertheless, there emerges an additional nonlocal string-like pairing potential besides the original superexchange term. It is this new string-like potential  $H_I^{\text{string}}$  that will lead to the strong binding between the two doped holes in  $\tilde{H}_{t-J}$  rather than the superexchange term  $H_J$  in the  $\sigma$ - $t$ - $J$  term in Eq. (15).

Let us further examine the pair-pair correlators in such a transformed representation. Note that in the new Hamiltonian (15) the pair operators  $\hat{\Delta}_{ij}^{s,t}$  defined in Eq. (12) will correspond to the following operators  $\hat{D}_{ij}^{s,t}$  in the original  $t$ - $J$  model:

$$\begin{aligned} \hat{D}_{ij}^{s,t} &\equiv e^{i\hat{\Theta}} \hat{\Delta}_{ij}^{s,t} e^{-i\hat{\Theta}} \\ &= \hat{\Delta}_{ij}^{s,t} e^{-i(\hat{\Omega}_i + \hat{\Omega}_j)}, \end{aligned} \quad (19)$$

or

$$\begin{aligned} \hat{D}_{ij}^s &= \frac{1}{\sqrt{2}} \sum_{\sigma} \sigma \tilde{c}_{1i\sigma} \tilde{c}_{2j-\sigma}, \\ \hat{D}_{ij}^t &= \frac{1}{\sqrt{2}} \sum_{\sigma} \tilde{c}_{1i\sigma} \tilde{c}_{2j-\sigma}. \end{aligned} \quad (20)$$

One may then calculate the pair-pair correlators of  $\hat{D}_{ij}^{s,t}$  based on Eq. (19) in the original representation of  $H_{t-J}$  and  $|\Psi_G\rangle_{2h}$ . As shown in Fig. 4, the VMC calculations are in excellent agreement with the DMRG simulation, indicating that the two-hole ground state in the transformed representation governed by the new Hamiltonian (15) is indeed described by a BCS-like ‘‘Cooper pairing’’ in the wavefunction (1). Equivalently in the original representation, it is the operator  $\tilde{c}$  instead of the bare hole creation operator  $c$  that plays the central role in ‘‘Cooper pairing’’.

As indicated in the insets of Figs. 4 (a) and (b), the strengths of the  $\hat{D}$  correlators generally get enhanced as compared with those of the true Cooper pairs characterized by  $\hat{\Delta}$  in the original  $t$ - $J$  model. It indicates that the *true* Cooper pair operator  $\hat{\Delta}$  must possess a composite structure including both a pairing amplitude (mean-field-like)  $\hat{D}_{ij}^{s,t}$  and a phase fluctuation as shown in Eq. (19), which has already been established by the DMRG calculation in Ref. 16.

### III. DISCUSSION

In this work, the pairing of two holes doped into a Mott insulator has been studied by the VMC calculation. Specifically, we have explored a non-BCS-type wavefunction [Eq. (4)] with incorporating an intrinsic phase fluctuation discovered in a previous DMRG approach<sup>15,16</sup>. Such a new variational wavefunction has been shown to give rise to the correct behavior of the two-hole ground state in comparison with the DMRG results<sup>16</sup>. By contrast, the conventional BCS (RVB) like wavefunction [Eq. (1)] leads to the qualitatively wrong behavior in both the ground state energy and the pair-pair correlations. Especially it predicts the absence of any meaningful pairing as opposed to a strong binding between the holes as revealed by DMRG<sup>16</sup> as well as by the present variational wavefunction.

It means that the so-called RVB mechanism<sup>3</sup> is not sufficient at least in the present two-leg ladder case in describing the hole pairing, even though the spin-spin correlation is already short-ranged here as envisaged originally by Anderson<sup>3</sup> for an RVB state. Rather than the conventional RVB pairing potential contributed by the superexchange term  $H_J$ , the strong pairing state for the two holes is found to be due to a distinct mechanism, which is of ‘‘kinetic energy driven’’ by nature. Namely, each doped hole will have to induce an irreparable phase string effect in the spin background<sup>12-14</sup>, which strongly frustrates its kinetic energy<sup>15,16</sup>. The bare hole is then renormalized by a nonlocal phase shift to form a ‘‘twisted’’ quasiparticle as given in Eqs. (10) and (11). What we have found in this work is that two of the twisted holes can indeed form a tightly bound pair as described by Eq. (4), and by doing so the strong frustration on the kinetic energy can be effectively released.

Thus, the Cooper pairing of two doped holes can no

longer be simply attributed to exchanging a “bosonic mode” nor via an RVB pairing of the spins. Instead, the dominant pairing force is originated from the phase string effect of the  $t$ - $J$  model. Such a non-BCS pairing force can be explicitly revealed by utilizing a unitary transformation to “gauge away” the phase string effect from the hopping term, which results in an effective string-like pairing potential in Eq. (16) that is nonlocal and of non-perturbative nature. Physically, the phase string effect can be also interpreted in terms of the spin current back-flow produced by the hopping of the doped holes<sup>28</sup>. In this sense, the string-like force shown in Eqs. (16) and (18) may be also regarded as a special type of the Amperean pairing potential<sup>22,23</sup>.

We point out that both the ansatz states given in Eqs. (4) and (1) have omitted the usual “spin-polaron”<sup>29–32</sup> or “spin bag” effect<sup>33,34</sup>, which arises from the “amplitude” distortion in the spin background around the doped hole, in contrast to the “phase” or the “transverse” (spin current) distortion given in Eq. (10). The former should improve further the variational ground state energy shown in Fig. 2, and renormalize the effective mass of the doped hole. But we do not think such an effect will violate the Landau’s one-to-one correspondence, as the present phase shift in Eq. (10) does, to result in a qualitative change in the ground state properties, including the pairing mechanism. Nevertheless, properly including such an effect is expected to further lower the variational energy of Eq. (4) in comparison with the DMGR results, even though the pair-pair correlations should not be improved much according to Fig. 3.

The present study of the hole pairing in the  $t$ - $J$  model has been carried out in one of the simplest limits. Namely, we have considered two holes doped into a spin gapped two-leg Heisenberg ladder, in which two holes are only allowed to hop along the chain direction of the ladder with  $t_{\perp} = 0$ . As the consequence, the phase shift operator  $\hat{\Omega}_i$  takes the simple one-dimensional form given in Eq. (11). On the other hand, with  $t_{\perp} \neq 0$ ,  $\hat{\Omega}_i$  associated with one hole doping will generally involve both two chains of the two-leg ladder as previously shown in Ref. 25. The pairing of the two twisted holes should remain the same as in Eq. (4) in the variational approach, with  $\hat{\Omega}_i$  being modified. Similar approach may be further generalized to the two-dimensional case, where the phase shift operator  $\hat{\Omega}_i$  will take an isotropic form<sup>12–14</sup>.

Finally, a natural generalization of the ground state ansatz in Eq. (4) for the two-hole case to the finite doping may be straightforwardly written down as follows,

$$|\Psi_G\rangle = e^{\hat{D}}|\text{RVB}\rangle, \quad (21)$$

which has been previously constructed in Ref. 12, where  $|\text{RVB}\rangle$  still denotes a spin “vacuum” state and the “twisted” Cooper pair  $\hat{D}$  is defined in Eq. (5). As a technical remark, we note here that the compact form in Eq. (21) should be correctly understood as an abbreviation expression for a truly fractionalized state<sup>12,13</sup>. That

is, the phase shift operator  $\hat{\Omega}_i$  in  $\hat{D}$  [Eq.(5)] should always act on the half-filling vacuum state  $|\text{RVB}\rangle$  *before* the annihilations of the electrons at the hole sites by  $\hat{D}$ , which can only be precisely implemented by introducing a specific fractionalization<sup>12,13</sup>. By such a construction, the pairing amplitude  $g(i, j)$  in Eq. (11) and the RVB pairing in  $|\text{RVB}\rangle$  can still remain mean-field-like to give rise to a nontrivial/non-BCS superconducting ground state at finite doping, which is to be further investigated variationally elsewhere.

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## Appendix A: Variational Monte Carlo procedure

For the sake of self-consistence, we first present the VMC procedures for the half-filled RVB state. Subsequently, we derive the two-hole variational wavefunctions and some formulas used in the VMC procedure.

### 1. VMC for Half-filling wavefunctions

At half-filling both the  $t$ - $J$  and  $\sigma \cdot t$ - $J$  model reduce to a pure Heisenberg spin ladder whose ground state  $|\text{RVB}\rangle$  is an anti-ferromagnetic gapped system. A pure Heisenberg model can have a good simulation by the Liang-Doucot-Anderson type bosonic RVB variational wavefunction<sup>26</sup> :

$$|\text{RVB}\rangle = \sum_v \omega_v |v\rangle, \quad (\text{A1})$$

where  $|v\rangle$  is a singlet pairing valence bond (VB) state where spins on sites  $i$  and  $j$  from different sublattices form a singlet pairing, which enables  $|\text{RVB}\rangle$  obey the Marshall sign rule<sup>35</sup>. The amplitude of each VB state  $|v\rangle$  can be factorized by  $\omega_v = \prod_{(ij) \in v} h_{ij}$ . Here  $h_{ij}$  is a non-negative function with respect to sites  $i$  and  $j$ . Such a scheme will tremendously decrease the number of variational parameters.

The norm of the RVB state in Eq. (A1) is given as

$$\langle \text{RVB} | \text{RVB} \rangle = \sum_{v, v'} \omega_v \omega_{v'} \langle v' | v \rangle. \quad (\text{A2})$$

The positiveness of  $\omega_v \omega_{v'} \langle v' | v \rangle$  allows an explanation as a distribution function. The sampling of  $\langle v' | v \rangle$  is time-consuming. We can introduce the Ising configuration  $\sigma$  (simply use  $\sigma$  for  $\{\sigma\}$ ), whose relation to the VB state is

$$|\sigma\rangle \langle \sigma | v \rangle = \delta_{v, \sigma} |v, \sigma\rangle, \quad (\text{A3})$$

in which  $\delta_{v, \sigma} = |\langle \sigma | v \rangle|$  and  $\langle \sigma | v \rangle$  is zero or the Marshall sign for the RVB state. Then the RVB state in Eq. (A1) can be rewritten as

$$|\text{RVB}\rangle = \sum_v \omega_v |v\rangle = \sum_{v, \sigma} \delta_{v, \sigma} |v, \sigma\rangle. \quad (\text{A4})$$

The summation is constrained in the space where the VB state  $|v\rangle$  is compatible with the Ising basis  $|\sigma\rangle$ . With the fact

$$\begin{aligned} \langle v' | v \rangle &= 2^{N_{v, v'}^{\text{loop}}}, \\ \langle v', \sigma' | v, \sigma \rangle &= \delta_{\sigma, \sigma'}, \end{aligned}$$

the norm in Eq. (A2) has more explicit form

$$\langle \text{RVB} | \text{RVB} \rangle = \sum_{v, v', \sigma} \omega_v \omega_{v'} \delta_{v', \sigma} \delta_{v, \sigma}. \quad (\text{A5})$$

Here  $N_{v, v'}^{\text{loop}}$  is the number of loops in the transposition-graph covers  $(v, v')$ .

The formulas for averaging physical operators can be found in Ref. 25. Whereafter, we will generalize the same trick to two-hole wavefunctions.

### 2. Two-hole ground state

We can construct a two-hole VB state by removing two electrons with opposite spin indexes from the half-filled VB state:

$$|h_1, h_2, v\rangle \equiv \text{sign}(h_1 - h_2) c_{h_1 \uparrow} c_{h_2 \downarrow} |v\rangle = \sum_{\sigma_h} \delta_{v, \sigma_h} |h_1, h_2, \sigma_h\rangle, \quad (\text{A6})$$



where  $|v\rangle$  is a half-filled VB state and  $|h_1, h_2, \sigma_h\rangle \equiv \text{sign}(h_1 - h_2)c_{h_1\uparrow}c_{h_2\downarrow}|\sigma_h\rangle$  with  $|\sigma_h\rangle$  denoting a half-filled Ising basis. The function  $\text{sign}(h_1 - h_2)$  is the sign function i.e if  $h_1 > h_2$ ,  $\text{sign}(h_1 - h_2) = 1$ ; if  $h_1 = h_2$ ,  $\text{sign}(h_1 - h_2) = 0$  and if  $h_1 < h_2$ ,  $\text{sign}(h_1 - h_2) = -1$ . If  $v$  and  $\sigma_h$  are not compatible,  $\delta_{v, \sigma_h} = 0$ , namely for some dimer  $(i, j)$ ,  $\sigma_h(i) = \sigma_h(j)$ ,  $(\sigma_h(i))$  is the spin index on the site  $i$  in the Ising basis  $|\sigma_h\rangle$  or  $\sigma_h(h_1) = \uparrow$  or  $\sigma_h(h_2) = \downarrow$ .

The two-hole variational wavefunction is obtained from removing two anti-directed spins on the RVB state in Eq. (A1) accompanied with a unitary transformation  $\hat{\Lambda}$

$$\begin{aligned} |\Psi\rangle_G &= \hat{\Lambda} \sum_{\substack{h_1, h_2 \\ h_1 \neq h_2}} g(h_1, h_2) \text{sign}(h_1 - h_2) c_{h_1\uparrow} c_{h_2\downarrow} |\text{RVB}\rangle \\ &= \sum_{\substack{h_1, h_2 \\ h_1 \neq h_2}} \sum_{\sigma_h, v} g(h_1, h_2) \hat{\Lambda}(h, \sigma_h) \delta_{v, \sigma_h} \omega_v |h_1, h_2, \sigma_h\rangle \end{aligned} \quad (\text{A7})$$

in which  $g(h_1, h_2)$  is the hole wavefunction that only depend on holes' position and it will entangle with antiferromagnetic background through the phase operator  $\hat{\Lambda}$ . The phase  $\Lambda(h, \sigma_h)$  generally is the function of the two hole positions  $h_1$  and  $h_2$  and spin configuration  $\sigma_h$  and is defined by

$$\hat{\Lambda}(h, \sigma_h) |h_1, h_2, \sigma_h\rangle = \prod_{h \in \{h_1, h_2\}} \prod_{l \neq h_1, h_2} \Lambda(h, l, \sigma_h(l)) |h_1, h_2, \sigma_h\rangle \quad (\text{A8})$$

We factorize  $\hat{\Lambda}(h, \sigma_h)$  via  $\Lambda(h, l, \sigma_h(l))$ , which is a phase factor felt by a hole from the spin at the site  $l$ . Specifically, it has different forms for different variational assumptions:

- 1) If we take  $\Lambda(h, l, \sigma_h(l)) = 1$ , then  $\hat{\Lambda} = 1$  and we get the BCS-type wavefunction in Eq. (1),
- 2) For the non-BCS type wavefunction in Eq. (4) in the  $t$ - $J$  ladder system with  $t_\perp = 0$  in the main body,

$$\Lambda(h, l, \sigma_h(l)) = \begin{cases} 1 & h, l \text{ lie in different legs} \\ e^{-i\pi \delta_{\sigma_h(l), \downarrow}} & h, l \text{ lie in the same leg and } x_l > x_h \\ 1 & h, l \text{ lie in the same leg and } x_l < x_h \end{cases} \quad (\text{A9})$$

where  $x_l$  is the coordinate of site  $l$  along the chain ( $x$ ) direction.

- 3) For  $t$ - $J$  model with  $t_\perp \neq 0$  ladder systems or 2D systems, the expression of  $\Lambda(h, l, \sigma_h(l))$  can be found in Ref. 25.

With the inner product formulas

$$\langle h'_1, h'_2, \sigma'_h | h_1, h_2, \sigma_h \rangle = \delta_{h'_1, h_1} \delta_{h'_2, h_2} \delta_{\sigma_h, \sigma'_h} \delta_{\sigma_h(h_1), -\sigma_h(h_2)}, \quad (\text{A10})$$

$$\langle h'_1, h'_2, v' | h_1, h_2, v \rangle = \begin{cases} \delta_{h'_1, h_1} \delta_{h'_2, h_2} 2^{N_{v, v'}^{\text{loop}} - 1} (1 - \delta_{h_1 h_2}^{\text{sublatt}}) & h_1, h_2 \in \text{s.l.} \\ \delta_{h'_1, h_1} \delta_{h'_2, h_2} 2^{N_{v, v'}^{\text{loop}} - 2} & h_1, h_2 \notin \text{s.l.} \end{cases} \quad (\text{A11})$$

where  $h_1, h_2 \in \text{s.l.}$  means that sites  $h_1$  and  $h_2$  belong to the same close loop in the transposition graph  $(v, v')$  and  $\delta_{h'_1, h_1} = 1$  if  $h'_1 = h_1$ , and otherwise  $\delta_{h'_1, h_1} = 0$ .  $\delta_{h_1 h_2}^{\text{sublatt}} = 1$  if sites  $h_1, h_2$  are in the same sublattice, and otherwise,  $\delta_{h_1 h_2}^{\text{sublatt}} = 0$ , we can express the norm of  $|\Psi\rangle_G$  as :

$$\langle \Psi | \Psi \rangle_G = \frac{1}{4} \sum_{v, v', \sigma^0} \delta_{v, \sigma^0} \delta_{v', \sigma^0} \omega_v \omega_{v'} \left[ \sum_{\substack{h_1, h_2 \\ h_1, h_2 \in \text{s.l.}}} 2 (1 - \delta_{h_1 h_2}^{\text{sublatt}}) + \sum_{\substack{h_1, h_2 \\ h_1, h_2 \notin \text{s.l.}}} 1 \right] |g(h_1, h_2)|^2, \quad (\text{A12})$$

where  $\sigma^0$  is a compatible spin configuration with a transposition graph  $(v, v')$ . Note that the norm of  $|\Psi\rangle_G$  depends on different VB configuration  $(v, v')$ . To overcome it, we have to employ a similar trick as Gutzwiller projection<sup>9</sup>: using

average values of  $\left[ \sum_{\substack{h_1, h_2, \\ h_1, h_2 \in \text{s.l.}}} 2(1 - \delta_{h_1 h_2}^{\text{sublatt}}) + \sum_{\substack{h_1, h_2, \\ h_1, h_2 \notin \text{s.l.}}} 1 \right] |g(h_1, h_2)|^2$  under the half-filled RVB state instead:

$$\begin{aligned}
& \left\langle \left[ \sum_{\substack{h_1, h_2, \\ h_1, h_2 \in \text{s.l.}}} 2(1 - \delta_{h_1 h_2}^{\text{sublatt}}) + \sum_{\substack{h_1, h_2, \\ h_1, h_2 \notin \text{s.l.}}} 1 \right] |g(h_1, h_2)|^2 \right\rangle_{\text{RVB}} \\
&= \sum_{h_1, h_2} [2(1 - \delta_{h_1 h_2}^{\text{sublatt}}) P_{h_1 h_2} + (1 - P_{h_1 h_2})] |g(h_1, h_2)|^2 \\
&\equiv \sum_{h_1, h_2} a(h_1, h_2)^2 |g(h_1, h_2)|^2, \tag{A13}
\end{aligned}$$

where  $P_{h_1 h_2}$  describes possibility of two sites  $h_1, h_2$  belonging to the same loop in all the transposition graphs  $(v, v')$ . The factor  $a(h_1, h_2)^2 \equiv 2(1 - \delta_{h_1 h_2}^{\text{sublatt}}) P_{h_1 h_2} + (1 - P_{h_1 h_2})$  will regularize the norm that relates  $|\Psi\rangle_{\text{G}}$  to  $|\text{RVB}\rangle$ :

$$\sum_{\substack{h_1, h_2 \\ h_1 \neq h_2}} a(h_1, h_2)^2 |g(h_1, h_2)|^2 = 1. \tag{A14}$$

$$\langle \Psi | \Psi \rangle_{\text{G}} = \frac{1}{4} \sum_{v, v', \sigma^0} \delta_{v, \sigma^0} \delta_{v', \sigma^0} \omega_{v'} \omega_v = \frac{1}{4} \langle \text{RVB} | \text{RVB} \rangle \tag{A15}$$

In Sec A 3, we will describe the procedures for variational optimization on the wavefunction  $g(h_1, h_2)$ . Together with Eq. (A7) and the identity  $\langle v | v' \rangle = \sum_{\sigma^0} \delta_{v, \sigma^0} \delta_{v', \sigma^0}$ , the expectation value of an operator  $\hat{O}$  can be generally expressed as

$$\begin{aligned}
\langle \hat{O} \rangle &= \frac{\langle \Psi | \hat{O} | \Psi \rangle_{\text{G}}}{\langle \Psi | \Psi \rangle_{\text{G}}} \\
&= \frac{4 \left( \sum_{v, v', \sigma^0} \delta_{v, \sigma^0} \delta_{v', \sigma^0} \right) \omega_{v'} \omega_v \sum_{h'_1 \neq h'_2, \sigma'_{h'}, \sigma_h} \delta_{v', \sigma'_{h'}} \delta_{v, \sigma_h} E(\hat{O})}{\left( \sum_{v, v', \sigma^0} \delta_{v, \sigma^0} \delta_{v', \sigma^0} \right) \omega_{v'} \omega_v} \tag{A16}
\end{aligned}$$

where

$$E(\hat{O}) = \text{Re}(\Delta\Lambda) \frac{\langle h'_1, h'_2, \sigma'_{h'} | \hat{O} | h_1, h_2, \sigma_h \rangle}{\langle v' | v \rangle} \tag{A17}$$

and

$$\text{Re}(\Delta\Lambda) = \text{Re} [\Lambda^*(h'_1, h'_2, \sigma'_{h'}) \Lambda(h_1, h_2, \sigma_h) g^*(h'_1, h'_2) g(h_1, h_2)]. \tag{A18}$$

Here  $\text{Re}(\Delta\Lambda)$  denotes the real part of  $\Delta\Lambda$ . We interpret  $\omega_{v'} \omega_v / \langle \Psi | \Psi \rangle_{\text{G}}$  as a distribution function in the space of compatible spin configurations  $(v, v', \sigma^0)$ .

### 3. VMC Procedure

We have to optimize parameters  $h_{ij}$  of the background RVB<sup>36</sup> and the wavefunction  $g(h_1, h_2)$  with respect to the total energy  $E_{\text{total}}$ . The total energy of system reads

$$E_{\text{total}} = \langle \Psi | H_t + H_J | \Psi \rangle_{\text{G}} = \sum_{j_1 j_2, i_1 i_2} H_{j_1 j_2, i_1 i_2}^{\text{eff}} g^*(j_1, j_2) g(i_1, i_2), \tag{A19}$$

where  $H^{\text{eff}}$  is an effective Hamiltonian for the hole wavefunction  $g$

$$H^{\text{eff}} = H_t^{\text{eff}} + H_J^{\text{eff}}. \tag{A20}$$

We introduce a renormalized wavefunction  $\tilde{g}$  to incorporate with its normalization condition (A15),

$$\tilde{g}(h_1, h_2) = a(h_1, h_2) g(h_1, h_2) .$$

Consistently,  $H^{\text{eff}}$  will be transformed into  $\tilde{H}^{\text{eff}}$  whose elements are

$$\tilde{H}_{j_1 j_2, i_1 i_2}^{\text{eff}} = a^{-1}(j_1, j_2) H_{j_1 j_2, i_1 i_2}^{\text{eff}} a^{-1}(i_1, i_2) . \quad (\text{A21})$$

Thus the total energy is expressed as

$$E_{\text{total}} = \sum_{j_1 j_2, i_1 i_2} \tilde{H}_{j_1 j_2, i_1 i_2}^{\text{eff}} \tilde{g}^*(j_1, j_2) \tilde{g}(i_1, i_2) , \quad (\text{A22})$$

with the normalization condition for  $\tilde{g}(i_1, i_2)$ :

$$\sum_{i_1, i_2} |\tilde{g}(i_1, i_2)|^2 = 1 . \quad (\text{A23})$$

Diagonalize  $\tilde{H}^{\text{eff}}$  and the minimal eigenvalue and the corresponding eigenvector are the variational energy and renormalized wavefunction respectively. All remained are to simulate elements of  $H_t^{\text{eff}}$  and  $H_f^{\text{eff}}$ . In the following, we provide some explicit formulas used in the Monte Carlo simulation.

#### 4. Superexchange Energy

Superexchange terms  $H_J$  only affect spin configuration with the positions of holes unchanged, which will simplify calculation processes. The average value of superexchange energy of two sites  $i, j$  with fixed positions of holes is

$$\langle H_{ij}^J \rangle = \frac{(\sum_{v, v', \sigma^0} \delta_{v, \sigma^0} \delta_{v', \sigma^0}) \omega_{v'} \omega_v E_{ij}^J(v, v')}{(\sum_{v, v', \sigma^0} \delta_{v, \sigma^0} \delta_{v', \sigma^0}) \omega_{v'} \omega_v} , \quad (\text{A24})$$

where

$$E_{ij}^J(v, v') = |g(h_1, h_2)|^2 E_{ij}^J(h, v, v') , \quad (\text{A25})$$

$$E_{ij}^J(h, v, v') = \sum_{\sigma'_h, \sigma_h} \delta_{v', \sigma'_h} \delta_{v, \sigma_h} \text{Re}(\Lambda^*(h_1, h_2, \sigma'_h) \Lambda(h_1, h_2, \sigma_h)) \frac{4 \langle h_1, h_2, \sigma'_h | \mathbf{S}_i \cdot \mathbf{S}_j | h_1, h_2, \sigma_h \rangle}{\langle v' | v \rangle} . \quad (\text{A26})$$

Given a transposition graph  $(v, v')$ , we categorize  $E_{ij}^J(h, v, v')$  in a list below.

- $h_1$  and  $h_2$  belong to the same loop  $L_{h_1 h_2}$  in a given transposition graph  $(v, v')$  .
- 1) One of the two holes coincides with the site  $i$  or  $j$ , which gives  $E_{ij}^J(h, v, v') = 0$  .
- 2) Sites  $i$  and  $j$  belong to the different loops of the transposition graph  $(v, v')$ . The contributions from terms  $S_i^+ S_j^- + S_i^- S_j^+$  always vanish since a closed loop can not have a single antiferromagnetic domain. Although the expectation value of diagonal terms  $S_i^z S_j^z$  for a fixed spin configuration is not zero, their contributions vanish after summation of all compatible spin configurations.
- 3) Sites  $i, j$  belong to the same loop  $L_{ij}$  that contains no holes,  $L_{ij} \neq L_{h_1 h_2}$ . If the two holes belong to different sublattices  $\delta_{h_1 h_2}^{\text{sublatt}} = 0$  (to satisfy compatibility), the contribution  $E_{ij}^J(h, v, v')$  reads

$$\begin{aligned} E_{ij}^J(h, v, v') &= 2 \times 2^{N_{v, v'}^{\text{loop}} - 2} \cdot \text{Re}(\Delta \Lambda_{ij}^J) \cdot \frac{-J/2}{2^{N_{v, v'}^{\text{loop}} - 2}} + 2^{N_{v, v'}^{\text{loop}} - 1} \cdot 1 \cdot \frac{-J/4}{2^{N_{v, v'}^{\text{loop}} - 2}} \\ &= 2 \left( -\frac{J}{2} \text{Re}(\Delta \Lambda_{ij}^J(h)) - \frac{J}{4} \right) . \end{aligned} \quad (\text{A27})$$

Otherwise,  $E_{ij}^J(h, v, v') = 0$ .

- 4) Sites  $i, j$  belong to the loop  $L_{h_1 h_2}$ . This is more complicated. If and only if holes  $h_1$  and  $h_2$  belong to different sublattices, terms  $S_i^z S_j^z$  contribute nonvanishingly to  $E_{ij}^J(h, v, v')$ . Terms  $S_i^+ S_j^- + S_i^- S_j^+$  depend on relative positions of sites  $i, j$  and holes. For the sake of clarity, we introduce an auxiliary loop  $L'_{h_1 h_2}$ , which is obtained from the loop  $L_{h_1 h_2}$  by setting  $v(v(i)) = j, v(v(j)) = i$  in loop  $L_{h_1 h_2}$ . We also introduce an auxiliary dimmer configuration  $|h_1, h_2, v''\rangle = (S_i^+ S_j^- + S_i^- S_j^+) |h_1, h_2, v\rangle$ , and spin configuration  $|h_1, h_2, \sigma_h''\rangle = (S_i^+ S_j^- + S_i^- S_j^+) |h_1, h_2, \sigma_h\rangle$  ( $\sigma_h''$  is compatible with transposition graph  $(v', v'')$ ). Note that the auxiliary loop  $L'_{h_1 h_2}$  and dimmer configuration  $|h_1, h_2, v''\rangle$  do not satisfy original rules of construction. If the spin configuration  $\sigma_h''$  satisfies  $\sigma_h''(h_1) = -\sigma_h''(h_2)$ ,

$$E_{ij}^J(h, v, v') = 2 \left[ -\frac{J}{2} \text{Re}(\Delta \Lambda_{ij}^J(h)) \delta_{\sigma_h''(h_1), -\sigma_h''(h_2)} - \frac{J}{4} (1 - \delta_{h_1 h_2}^{\text{sublatt}}) \right], \quad (\text{A28})$$

where  $(1 - \delta_{h_1 h_2}^{\text{sublatt}}) = 1$  if the two holes  $h_1, h_2$  belong to the different sublattices.

- Holes  $h_1$  and  $h_2$  belong to different loops  $L_{h_1}, L_{h_2}$  in a given transposition graph  $(v, v')$ 
  - 1) If one of  $h_1$  and  $h_2$  coincides to site  $i$  or  $j$ ,  $E_{ij}^J(h, v, v') = 0$ .
  - 2) Sites  $i, j$  belong to different loops of  $(v, v')$ . Contributions from terms  $S_i^+ S_j^- + S_i^- S_j^+$  vanish for there exists no compatible spin configuration with a VB state. Only when  $i \in L_{h_1}, j \in L_{h_2}$  or  $i \in L_{h_2}, j \in L_{h_1}$ , the diagonal terms  $S_i^z S_j^z$  contributes to  $E_{ij}^J(h, v, v')$ ,

$$E_{ij}^J(h, v, v') = \frac{J}{4} \frac{2^{N_{v, v'}^{\text{loop}} - 2}}{2^{N_{v, v'}^{\text{loop}} - 2}} (\delta_{\sigma_h(i), \sigma_h(j)} - \delta_{-\sigma_h(i), \sigma_h(j)}) = \frac{J}{4} (\delta_{\sigma_h(i), \sigma_h(j)} - \delta_{-\sigma_h(i), \sigma_h(j)}) . \quad (\text{A29})$$

- 3) Site  $i, j$  belong to the same loop  $L_{ij}$  of the transposition graph  $(v, v')$ . If  $L_{ij}$  does not contain holes, we obtain

$$\begin{aligned} E_{ij}^J(h, v, v') &= 2 \times 2^{N_{v, v'}^{\text{loop}} - 3} \cdot \text{Re}(\Delta \Lambda_{ij}^J) \cdot \frac{-J/2}{2^{N_{v, v'}^{\text{loop}} - 2}} + 2^{N_{v, v'}^{\text{loop}} - 2} \cdot 1 \cdot \frac{-J/4}{2^{N_{v, v'}^{\text{loop}} - 2}} \\ &= -\frac{J}{2} \text{Re}(\Delta \Lambda_{ij}^J(h)) - \frac{J}{4} . \end{aligned} \quad (\text{A30})$$

The case that  $L_{ij}$  contains one or two holes shows the same result, but only one term of  $S_i^+ S_j^-$  and  $S_i^- S_j^+$  helps.

## 5. Hopping Energy

In this section, we turn to calculation of  $\langle H^t \rangle$

$$\langle H^t \rangle = \frac{(\sum_{v, v', \sigma^0} \delta_{v, \sigma^0} \delta_{v', \sigma^0}) \omega_{v'} \omega_v E(v, v')}{(\sum_{v, v', \sigma^0} \delta_{v, \sigma^0} \delta_{v', \sigma^0})} , \quad (\text{A31})$$

where

$$E(v, v') = \sum_{\substack{h_1, h_2, \\ h_1 \neq h_2}} \sum_{\substack{h'_1, h'_2 \\ h'_1 \neq h'_2}} E(h, h', v, v') , \quad (\text{A32})$$

$$E(h, h', v, v') = 4 \sum_{\sigma_{h'}, \sigma_h} \delta_{v', \sigma_{h'}} \delta_{v, \sigma_h} g^*(h'_1, h'_2) g(h_1, h_2) \frac{\langle h'_1, h'_2, \sigma_{h'} | e^{i\hat{\Theta}} H^t e^{-i\hat{\Theta}} | h_1, h_2, \sigma_h \rangle}{\langle v' | v \rangle} . \quad (\text{A33})$$

where we take  $h$  ( $h'$ ) in  $E(h, h', v, v')$  as a shorthand for  $h_1$  and  $h_2$  ( $h'_1$  and  $h'_2$ ). Each hopping term only moves one hole within a single action. Without loss of generality, we can assume the position of hole  $h_1$  unchanged, i.e.  $h_1 = h'_1$ . Furthermore, similar to the trick upon terms  $S_i^+ S_j^- + S_i^- S_j^+$  in the superexchange energy, we introduce an auxiliary spin and VB configuration:

$$|h_1, h'_2, \sigma_h''\rangle = c_{h'_2 \uparrow} c_{h_2 \uparrow}^\dagger |h_1, h_2, \sigma_h\rangle , \quad (\text{A34})$$

$$|h_1, h'_2, v''\rangle = c_{h'_2 \uparrow} c_{h_2 \uparrow}^\dagger |h_1, h_2, v\rangle . \quad (\text{A35})$$

The auxiliary VB configuration  $|h_1, h'_2, v''\rangle$  requires  $v''(h'_2) = v(h_2)$  and other dimmers stay the same. The non-vanishing contributions require compatibility between spin configuration  $|h'_1, h'_2, \sigma_h''\rangle$  and a new transposition graph  $\langle h_1, h'_2, v' | h_1, h'_2, v'' \rangle$ . The expression of  $E(h, h', v, v')$  can be decomposed into several factors

$$E(h, h', v, v') = - \sum_{\sigma_h, \sigma_h'} \Delta(\sigma_h, \sigma_h') \cdot g^*(h'_1, h'_2) g(h_1, h_2) \cdot \frac{4}{2^n} \cdot \Delta\Lambda, \quad (\text{A36})$$

where  $n$  is the number of loops including sites  $h_1, h_2$  and  $h'_2$  in  $\langle v' | v \rangle$ , and  $\Delta(\sigma_h, \sigma_h')$  is the Marshall sign difference between the initial  $\sigma_h$  and final states  $\sigma_h'$ . The minus sign comes from the permutation of Fermions. The phase difference  $\Delta\Lambda$ , induced by phase string effect, can be divided into four parts:

$$\Delta\Lambda = \Delta\Lambda_0 \cdot \Delta\Lambda_1 \cdot \Delta\Lambda_2 \cdot \Delta\Lambda_3. \quad (\text{A37})$$

- $\Delta\Lambda_0$  comes from sites  $h_1, h_2$  and  $h'_2$ :

$$\Delta\Lambda_0 = \Lambda^*(h'_2, h_2, \sigma_h(h'_2)) \Lambda(h_2, h'_2, \sigma_h(h'_2)) \Lambda^*(h_1, h_2, \sigma_h(h'_2)) \Lambda(h_1, h'_2, \sigma_h(h'_2)), \quad (\text{A38})$$

with  $\Lambda(h, l, \sigma_h(l))$  defined in (A8).

- $\Delta\Lambda_1$  comes from sites in the VB configuration  $\langle h_1, h'_2, v' | h_1, h'_2, v'' \rangle$  loops  $L$  that contain sites  $h'_1 (= h_1)$  or  $h'_2$  but except sites that coincide with  $h_1 (= h'_1)$ ,  $h_2$  or  $h'_2$ .

$$\Delta\Lambda_1 = \prod_{\substack{l \in L_{h'_1}, L_{h'_2} \\ l \neq h_1, h_2, h'_1, h'_2}} \Lambda^*(h'_2, l, \sigma_h(l)) \Lambda(h_2, l, \sigma_h(l)), \quad (\text{A39})$$

where  $L_{h'_1}$  ( $L_{h'_2}$ ) is the loop containing  $h'_1$  ( $h'_2$ ).

- If neither of the loops  $L_{h_1}$  nor  $L_{h'_2}$  of the VB configuration  $\langle h_1, h'_2, v' | h_1, h'_2, v'' \rangle$  contain the site  $h_2$ , that is  $L_{h_2} \neq L_{h_1}$  and  $L_{h_2} \neq L_{h'_2}$ , There are two different spin configurations that are compatible with the loop  $L_{h_2}$ , which account for the phase factor  $\Delta\Lambda_2$ .

$$\Delta\Lambda_2 = \sum_{\sigma_l = \pm} \prod_{l \in L_{h_1}} \Lambda^*(h'_2, l, \sigma_h(l)) \Lambda(h_2, l, \sigma_h(l)). \quad (\text{A40})$$

Otherwise,  $\Delta\Lambda_2 = 1$ .

- $\Delta\Lambda_3$  comes from the rest loops of VB configuration  $\langle h_1, h'_2, v' | h_1, h'_2, v'' \rangle$

$$\Delta\Lambda_3 = \prod_{L \neq L_{h_1}, L_{h_2}, L_{h'_2}} \left[ \frac{1}{2} \sum_{\{\sigma_l\}} \prod_{l \in L} \Lambda^*(h'_2, l, \sigma_h(l)) \Lambda(h_2, l, \sigma_h(l)) \right]. \quad (\text{A41})$$

## 6. Pair-Pair correlation

One may examine the pair-pair correlators,  $\langle \Delta_{ij}^{s,t} (\Delta_{ij}^{s,t})^\dagger \rangle$  where the singlet/triplet channels are defined as follows

$$\Delta_{ij}^s = \frac{1}{\sqrt{2}} \sum_{\sigma} \sigma c_{1i\sigma} c_{2j-\sigma}, \quad (\text{A42})$$

$$\Delta_{ij}^t = \frac{1}{\sqrt{2}} \sum_{\sigma} c_{1i\sigma} c_{2j-\sigma}. \quad (\text{A43})$$

Expand the correlators,

$$C(i, j) = \langle \Delta_{ij}^{s,t} (\Delta_{ij}^{s,t})^\dagger \rangle = \langle c_{1i\downarrow} c_{2j\uparrow} c_{2j\uparrow}^\dagger c_{1i\downarrow}^\dagger \mp c_{1i\uparrow\downarrow} c_{2j\downarrow} c_{2j\uparrow}^\dagger c_{1i\downarrow}^\dagger \rangle. \quad (\text{A44})$$

For the simulation of the pair-pair correlators, we only have to deal with terms like

$$C(h', h) = \langle c_{h'_1\downarrow} c_{h'_2\uparrow} c_{h_2\uparrow}^\dagger c_{h_1\downarrow}^\dagger \rangle. \quad (\text{A45})$$

Here  $h'_1$  and  $h'_2$  correspond to the hole  $h_1$  and  $h_2$  with the same spin index respectively. Some simple operations give

$$C(h', h) = \frac{(\sum_{v, v', \sigma^0} \delta_{v, \sigma^0} \delta_{v', \sigma^0}) \omega_{v'} \omega_v \mathcal{C}_{h'h}}{(\sum_{v, v', \sigma^0} \delta_{v, \sigma^0} \delta_{v', \sigma^0}) \omega_{v'} \omega_v}, \quad (\text{A46})$$

where

$$\mathcal{C}_{h'h} = \frac{4 \left\langle h'_1, h'_2, v' \left| e^{i\Theta} c_{h'_1 \downarrow} c_{h'_2 \uparrow} c_{h_2 \uparrow}^\dagger c_{h_1 \downarrow}^\dagger e^{-i\Theta} \right| h_1, h_2, v \right\rangle g^*(h'_1, h'_2) g(h_1, h_2)}{\langle v' | v \rangle}. \quad (\text{A47})$$

Introduce an auxiliary spin and VB configuration:

$$|h'_1, h'_2, \sigma_h''\rangle = c_{h'_1 \downarrow} c_{h'_2 \uparrow} c_{h_2 \uparrow}^\dagger c_{h_1 \downarrow}^\dagger |h_1, h_2, \sigma_h\rangle \quad (\text{A48})$$

$$|h'_1, h'_2, v''\rangle = c_{h'_1 \downarrow} c_{h'_2 \uparrow} c_{h_2 \uparrow}^\dagger c_{h_1 \downarrow}^\dagger |h_1, h_2, v\rangle. \quad (\text{A49})$$

The auxiliary VB configuration  $|h'_1, h'_2, v''\rangle$  requires  $v''(h'_1) = v(h_1), v''(h'_2) = v(h_2)$  and other dimmers stay the same. The nonvanishing contributions require compatibility of spin configuration  $|h'_1, h'_2, \sigma_h''\rangle$  with a new transposition graph  $\langle h'_1, h'_2, v' | h'_1, h'_2, v'' \rangle$ .

The factor  $C$  can be decomposed into several parts:

$$\mathcal{C}_{h'h} = \sum_{\sigma_h, \sigma_h'} \Delta(\sigma_h, \sigma_h') \cdot g^*(h'_1, h'_2) g(h_1, h_2) \cdot \frac{4}{2^n} \cdot \Delta\Lambda, \quad (\text{A50})$$

where

$$\Delta(\sigma_h, \sigma_h'): \text{Marshall sign difference between initial } \sigma_h \text{ and final states } \sigma_h' \quad (\text{A51})$$

$$n: \text{the number of loops including sites } h_1, h_2, h'_1 \text{ and } h'_2 \text{ in } \langle v' | v \rangle. \quad (\text{A52})$$

The phase difference  $\Delta\Lambda$  induced by phase string effect can be divided into four parts:

$$\Delta\Lambda = \Delta\Lambda_0 \cdot \Delta\Lambda_1 \cdot \Delta\Lambda_2 \cdot \Delta\Lambda_3. \quad (\text{A53})$$

- $\Delta\Lambda_0$  comes from sites  $h_1, h_2, h'_1$  and  $h'_2$ :

$$\Delta\Lambda_0 = \prod_{l=1,2} \Lambda^*(h'_l, h_2, \sigma_l) \Lambda^*(h'_l, h_2, \sigma_l) \Lambda(h_l, h'_1, \sigma_l) \Lambda(h_l, h'_2, \sigma_l), \quad (\text{A54})$$

where  $\sigma_1 = \sigma_h(h'_1)$  and  $\sigma_2 = \sigma_h(h'_2)$ .

- $\Delta\Lambda_1$  comes from sites in the VB configuration  $\langle v' | v'' \rangle$  loops that contains sites  $h'_1$  and  $h'_2$ , except sites  $h_1, h_2, h'_1, h'_2$ .

$$\Delta\Lambda_1 = \prod_{\substack{l \in L_{h'_1}, L_{h'_2} \\ l \neq h_1, h_2, h'_1, h'_2}} \Lambda^*(h'_1, l, \sigma_l) \Lambda^*(h'_2, l, \sigma_l) \Lambda(h_1, l, \sigma_l) \Lambda(h_2, l, \sigma_l). \quad (\text{A55})$$

where  $\sigma_l = \sigma_h(l)$ .

- Similar to the discussion in Sec A 5, we list cases for  $\Delta\Lambda_2$ .

- 1)  $h_1 \notin L_{h'_1} \cup L_{h'_2}$  and  $h_2 \in L_{h_1}$  in  $\langle v' | v'' \rangle$ ; Or  $h_1 \notin L_{h'_1} \cup L_{h'_2}$  and  $h_2 \notin L_{h_1}, h_2 \in L_{h'_1} \cup L_{h'_2}$  in  $\langle h'_1, h'_2, v' | h'_1, h'_2, v'' \rangle$

$$\Delta\Lambda_2 = \sum_{\sigma_l} \prod_{\substack{l \in L_{h_1} \\ l \neq h_1, h_2}} \Lambda^*(h'_1, l, \sigma_l) \Lambda^*(h'_2, l, \sigma_l) \Lambda(h_1, l, \sigma_l) \Lambda(h_2, l, \sigma_l); \quad (\text{A56})$$

- 2)  $h_2 \notin L_{h'_1} \cup L_{h'_2}$  and  $h_1 \notin L_{h_2}$  in  $\langle h'_1, h'_2, v' | h'_1, h'_2, v'' \rangle$

$$\Delta\Lambda_2 = \sum_{\sigma_l} \prod_{\substack{l \in L_{h_2} \\ l \neq h_2}} \Lambda^*(h'_1, l, \sigma_l) \Lambda^*(h'_2, l, \sigma_l) \Lambda(h_1, l, \sigma_l) \Lambda(h_2, l, \sigma_l); \quad (\text{A57})$$

3)  $h_1 \notin L_{h'_1} \cup L_{h'_2}, h_2 \notin L_{h'_1} \cup L_{h'_2}$  and  $L_{h_1} \neq L_{h_2}$  in  $\langle h'_1, h'_2, v' | h'_1, h'_2, v'' \rangle$

$$\Delta\Lambda_2 = \prod_{L=L_{h_1}, L_{h_2}} \sum_{\sigma_l} \prod_{\substack{l \in L \\ l \neq h_1, h_1}} \Lambda^*(h'_1, l, \sigma_l) \Lambda^*(h'_2, l, \sigma_l) \Lambda(h_1, l, \sigma_l) \Lambda(h_2, l, \sigma_l) ; \quad (\text{A58})$$

4) Otherwise

$$\Delta\Lambda_2 = 1 . \quad (\text{A59})$$

Here, the notation  $L_{h'_1} \cup L_{h'_2}$  represents the set containing all sites from  $L_{h'_1}$  and  $L_{h'_2}$  in  $\langle v' | v'' \rangle$ .

- $\Delta\Lambda_3$  comes from the rest parts of VB configuration  $\langle h'_1, h'_2, v' | h'_1, h'_2, v'' \rangle$

$$\Delta\Lambda_3 = \prod_{L \neq L_{h_1}, L_{h_2}, L_{h'_1}, L_{h'_2}} \left[ \frac{1}{2} \sum_{\{\sigma_l\}} \prod_{l \in L} \Lambda^*(h'_1, l, \sigma_l) \Lambda^*(h'_2, l, \sigma_l) \Lambda(h_1, l, \sigma_l) \Lambda(h_2, l, \sigma_l) \right] , \quad (\text{A60})$$

where  $\sigma_l = \sigma_h(l)$ .



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