Slave-boson based configuration-interaction approach for the Hubbard model

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(Received 31 January 2008; revised manuscript received 18 April 2008; published 12 June 2008)

Based on the Kotliar–Ruckenstein slave-boson scheme, we develop a configuration-interaction (CI) approach that is suitable to evaluate energy corrections for symmetry-broken saddle-point solutions. The theory is applied to spin-polaron states in the Hubbard model and compared with analogous results obtained within the Hartree–Fock approximation. In addition, we show that within the infinite $\mathcal{D}$ prescription of the Gutzwiller method a CI approach does not correct the variational result since in the thermodynamic limit matrix elements between different inhomogeneous states vanish due to an "orthogonality catastrophe."

DOI: 10.1103/PhysRevB.77.235109 PACS number(s): 71.10.Fd, 75.10.Lp, 71.27.+a

I. INTRODUCTION

The Gutzwiller Ansatz is a variational wave function for correlated electronic models with purely local interaction.[1,2] The basic idea to treat these Hubbard-type Hamiltonians is to partially project out configurations with doubly-occupied sites from the Fermi sea in order to optimize the contributions from kinetic and potential energy. As a consequence, in contrast to the conventional Hartree–Fock (HF) theory, the Gutzwiller wave function captures correlation effects like the band narrowing already on the variational level. However, the exact evaluation of the ground-state energy within the Gutzwiller wave function is fairly difficult and up to now has only been achieved in one and infinite dimensions.[3] In the latter case, the solution is equivalent to the so-called Gutzwiller approximation (GA), which has been applied to describe a variety of finite-dimensional systems ranging from the properties of normal ^{3}He (cf. Ref. 4) to the stripe phase of high-T_c cuprates.[5–7]

The GA in its original formulation was restricted to homogeneous paramagnetic systems and only later on generalized to arbitrary Slater determinants by Gebhard[8] and more recently by Attaccalite and Fabrizio.[9] The same energy functional was obtained from the Kotliar–Ruckenstein (KR) slave-boson formulation of the Hubbard model when the bosons are replaced by their mean values.[10] Unconstrained minimization of the KR (or Gebhards) energy functional in general yields inhomogeneous solutions that break translational and spin-rotational invariance.[11,12] This approach has been used e.g., for the investigation of electronic inhomogeneities, such as stripes and checkerboards,[7,13–15] in the context of high-T_c superconductors, and for interface controlled electronic charge inhomogenities in correlated heterostructures.[16,17]

For local observables, the good agreement between inhomogeneous slave-boson and quantum Monte Carlo methods has been demonstrated in Ref. 18.

Incorporation of fluctuations in the frame of the time-dependent Gutzwiller approximation tends to restore the original symmetry of the system.[19] An alternative would be the construction of a wave function, which is a linear superposition of equivalent symmetry-broken states. In case of stripe states,[7,13,14] one could e.g., envisage a superposition of solutions that are translated perpendicular to the stripe direction and also the corresponding solutions which are rotated by 90°. In case of the unrestricted Hartree–Fock approximation, such a configuration-interaction (CI) method has been proposed in Ref. 20 and applied to the case of stripe textures in Ref. 21.

The present paper investigates the possibility whether an improvement of the inhomogeneous Gutzwiller approximation is possible within an analogous framework. In Sec. II, we evaluate the matrix elements of the Hubbard Hamiltonian between different inhomogeneous solutions obtained from the saddle-point approximation of the KR slave-boson scheme.[10] Based on these results, we construct a CI method which in Sec. III is applied to spin-polaron states. We compare ground-state energies with exact diagonalization results and for larger lattices evaluate the dispersion relation of the spin-polaron states which can be compared with analogous solutions obtained in the tJ-model. In this context we also compare our results with angle-resolved photoemission (ARPES) experiments on $Sr_2CuO_2Cl_2$.

In Appendix A it is shown that the infinite $\mathcal{D}$ prescription of the Gutzwiller approximation[8] cannot be used for an analogous construction of a CI approach. The reason is that in the thermodynamic limit this scheme leads to an "orthogonality catastrophe"[22] so that energy corrections and the dispersion of quasiparticles vanish.

II. MODEL AND FORMALISM

Our investigations are based on the one-band Hubbard model

$$H = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} \tag{1}$$

where $c^{(\dagger)}_{i,\sigma}$ destroys (creates) an electron with spin σ at site i, and $n_{i,\sigma}=c^{\dagger}_{i,\sigma}c_{i,\sigma}$. U is the on-site Hubbard repulsion.

Following KR,[10] we enlarge the original Hilbert space by introducing four subsidiary boson fields $e^{(\dagger)}_i$, $s^{(\dagger)}_{i,\uparrow}$, $s^{(\dagger)}_{i,\downarrow}$, and $d^{(\dagger)}_i$ for each site i. These operators stand for the annihilation (creation) of empty, singly occupied states with spin up or down, and doubly-occupied sites, respectively. Since there are only four possible states per site, these boson projection operators must satisfy the completeness condition

$$e_i^\dagger e_i + \sum_\sigma s_{i,\sigma}^\dagger s_{i,\sigma} + d_i^\dagger d_i = 1. \tag{2}$$

Furthermore

$$n_{i,\sigma} = s_{i,\sigma}^\dagger s_{i,\sigma} + d_i^\dagger d_i. \tag{3}$$

Then, in the physical subspace defined by Eqs. (2) and (3), the Hamiltonian (1) takes the form

$$\tilde{H} = \sum_{ij,\sigma} t_{ij} z_{i,\sigma}^\dagger f_{i,\sigma}^\dagger f_{j,\sigma} z_{j,\sigma} + U \sum_i d_i^\dagger d_i \tag{4}$$

with

$$z_{i,\sigma} = e_i^\dagger s_{i,\sigma} + s_{i,-\sigma}^\dagger d_i \tag{5}$$

and has the same matrix elements than those calculated for Eq. (1) in the original Hilbert space. The operators $f_{i,\sigma}^{(\dagger)}$ are the electron annihilation (creation) operators in the new Hilbert space.

In the saddle-point approximation, we can represent the wave function for a specific inhomogeneous solution α as

$$|\Psi^\alpha\rangle = |\Phi_0^\alpha\rangle \otimes |B_0^\alpha\rangle \tag{6}$$

where $|\Phi_0^\alpha\rangle$ is a Slater determinant and the bosonic part $|B_0^\alpha\rangle$ is a coherent state

$$|B_0^\alpha\rangle = e^{\sum_i (\bar{d}_i^\alpha d_i^\dagger + \sum_\sigma \bar{s}_{i,\sigma}^\alpha s_{i,\sigma}^\dagger + \bar{e}_i^\alpha e_i^\dagger - 1/2)} |0\rangle, \tag{7}$$

Since a coherent state contains an arbitrary number of bosons the constraints Eq. (2) and (3) are only fulfilled on average for a given inhomogeneous solution α provided that

$$1 = (\bar{e}_i^\alpha)^2 + \sum_\sigma (\bar{s}_{i,\sigma}^\alpha)^2 + (\bar{d}_i^\alpha)^2,$$

$$\langle n_{i,\sigma}\rangle^\alpha \equiv \langle \Phi_0^\alpha | n_{i,\sigma} | \Phi_0^\alpha \rangle = (\bar{s}_{i,\sigma}^\alpha)^2 + (\bar{d}_i^\alpha)^2.$$

Note that here and in the following, expectation values of fermion operators are denoted with respect to the Slater determinant of f-electron operators. For completeness it should be mentioned that the assumption of "condensed" bosons has been criticized since phase fluctuations may prevent the boson fields to acquire a finite value. On the other hand, it has been shown recently[23] that a radial decomposition of the bosonic field may be a way out of this problem.

Another problem with the Ansatz Eq. (6) is that one does not recover the correct noninteracting limit $U \to 0$ for which $z_{i,\sigma} \to 1$. Therefore, KR[10] introduced a unitary transformation in order to represent the z operators in Eq. (5) as

$$z_{i,\sigma} = \frac{1}{\sqrt{e_i^\dagger e_i + s_{i,-\sigma}^\dagger s_{i,-\sigma}}} (e_i^\dagger s_{i,\sigma} + s_{i,-\sigma}^\dagger d_i) \frac{1}{\sqrt{d_i^\dagger d_i + s_{i,\sigma}^\dagger s_{i,\sigma}}} \tag{8}$$

so that

$$\langle \Psi^\alpha | z_{i,\sigma}^\dagger f_{i,\sigma}^\dagger f_{j,\sigma} z_{j,\sigma} | \Psi^\alpha \rangle = (q_i^\alpha)^* q_j^\alpha \langle \Phi_0^\alpha | f_{i,\sigma}^\dagger f_{j,\sigma} | \Phi_0^\alpha \rangle. \tag{9}$$

The expectation values of the z-operators Eq. (8)

$$q_{i,\sigma}^\alpha = \langle B_0^\alpha | z_{i,\sigma} | B_0^\alpha \rangle \tag{10}$$

are equivalent to the renormalization factors derived within the infinite $\mathcal{D}$ prescription of the Gutzwiller approximation[8] (cf. Eq. (A10) in Appendix A).

In previous works,[11,12] we have proposed a method for minimizing the KR energy functional $E^\alpha = \langle \Psi^\alpha | H | \Psi^\alpha \rangle$ on finite clusters without imposing constraints with respect to translational and spin-rotational invariance. In the remainder of this section, we evaluate the matrix elements of the Hubbard model between two different inhomogeneous solutions $|\Psi^\alpha\rangle$, which then will be used in order to partially restore these symmetries.

We start with the overlap between wave functions belonging to different inhomogeneous solutions

$$S_{\alpha\beta} = \langle \Psi^\alpha | \Psi^\beta \rangle = \langle \Phi_0^\alpha | \Phi_0^\beta \rangle \langle B_0^\alpha | B_0^\beta \rangle \tag{11}$$

where the overlap between coherent states reads as

$$\langle B_0^\alpha | B_0^\beta \rangle = e^{\Sigma_i (\bar{d}_i^\alpha \bar{d}_i^\beta + \Sigma_\sigma \bar{s}_{i,\sigma}^\alpha \bar{s}_{i,\sigma}^\beta + \bar{e}_i^\alpha \bar{e}_i^\beta - 1)}. \tag{12}$$

The fermionic overlap is given by

$$\langle \Phi_0^\alpha | \Phi_0^\beta \rangle = \langle \Phi_0^\alpha | \Phi_0^\beta \rangle_\uparrow \langle \Phi_0^\alpha | \Phi_0^\beta \rangle_\downarrow \tag{13}$$

and the evaluation of the spin-dependent factors is outlined in Appendix B.

We now proceed by calculating the matrix elements of the Hamiltonian (4) in the basis of the inhomogeneous wave functions $|\Psi^\alpha\rangle$. From the above definitions, one obtains for the Hubbard interaction

$$\langle \Psi^\alpha | U \sum_i d_i^\dagger d_i | \Psi^\beta \rangle = U \langle \Phi_0^\alpha | \Phi_0^\beta \rangle \langle B_0^\alpha | B_0^\beta \rangle \sum_i \bar{d}_i^\alpha \bar{d}_i^\beta. \tag{14}$$

The kinetic term is evaluated in a similar way as

$$\langle \Psi^\alpha | \hat{T} | \Psi^\beta \rangle = \sum_{ij,\sigma} t_{ij} z_{i,\sigma}^{\alpha\beta} z_{j,\sigma}^{\beta\alpha} \langle \Phi_0^\alpha | f_{i,\sigma}^\dagger f_{j,\sigma} | \Phi_0^\beta \rangle \langle B_0^\alpha | B_0^\beta \rangle \tag{15}$$

with the fermionic part

$$\langle \Phi_0^\alpha | f_{i,\sigma}^\dagger f_{j,\sigma} | \Phi_0^\beta \rangle = [f_{i,\sigma}^\dagger f_{j,\sigma}]_{\alpha\beta} \langle \Phi_0^\alpha | \Phi_0^\beta \rangle_{-\sigma} \tag{16}$$

and the brackets are defined in Eq. (B7) of Appendix B.

The matrix elements of the "bare" bosonic "z" operators from Eq. (5) read as

$$z_{i,\sigma}^{\alpha\beta} \equiv \langle B_0^\alpha | z_{i,\sigma}^\dagger | B_0^\beta \rangle = \bar{d}_i^\alpha \bar{s}_{i,-\sigma}^\beta + \bar{s}_{i,\sigma}^\alpha \bar{e}_i^\beta. \tag{17}$$

Now we have to deal again with the problem that the z factors as defined in Eq. (17) do not yield the uncorrelated limit, i.e., $z_{i,\sigma}^{\alpha\beta} \to 1$ for $U \to 0$. It is straightforward to proof that the representation of Eq. (8) does not work in this case since the above limit is only obeyed for homogeneous paramagnetic solutions. However, due to a nonsymmetric population of momentum states on finite clusters or in case of inclusion of an electron-phonon coupling, the charge and spin structure in general is inhomogeneous even in the limit $U \to 0$.

In order to overcome these difficulties, it is helpful to adopt the interpretation of the z factors in terms of "probability ratios,"[4,24] which leads us to the following representation:

TABLE I. Energy per site for 15 particles on a 4×4 lattice. The values of the exact result, HF and CIHF method have been taken from Ref. 20.

U/t	exact	HF	GA	CIHF	CISB
4	−0.91658	−0.83139	−0.88815	−0.83501	−0.89091
6	−0.74794	−0.64222	−0.70020	−0.66214	−0.70497
8	−0.634203	−0.52884	−0.57518	−0.54767	−0.60295
16	−0.42546	−0.33589	−0.37130	−0.34604	−0.38091
32	−0.308473	−0.23160	−0.27209	−0.23627	−0.27685
50	−0.266039	−0.19335	−0.23954	−0.19617	−0.24362

$$z_{i,\sigma}^{\alpha\beta}=\langle n_{i,-\sigma}\rangle_\alpha\frac{\bar{d}_i^\alpha\bar{s}_{i,-\sigma}^\beta}{\sqrt{\langle n_{i,\uparrow}\rangle_\alpha\langle n_{i,\downarrow}\rangle_\alpha}\sqrt{\langle n_{i,-\sigma}\rangle_\beta(1-\langle n_{i,\sigma}\rangle_\beta)}}+(1-\langle n_{i,-\sigma}\rangle_\alpha)\times\frac{\bar{s}_{i,\sigma}^\alpha\bar{e}_i^\beta}{\sqrt{\langle n_{i,\sigma}\rangle_\alpha(1-\langle n_{i,-\sigma}\rangle_\alpha)}\sqrt{(1-\langle n_{i,\uparrow}\rangle_\beta)(1-\langle n_{i,\downarrow}\rangle_\beta)}}. \tag{18}$$

Then the state $\langle\Phi_0^\alpha|f_{i,\sigma}^\dagger z_{i,\sigma}^{\alpha\beta}$ that enters Eq. (15) can be considered as the sum of two processes: The contribution $\sim f_{i\sigma}^\dagger(1-\langle n_{i,-\sigma}\rangle_\alpha)$ originates from the annihilation of a singly occupied (and thus creation of an empty) site in the Slater determinant $\langle\Phi_0^\alpha|$ and is weighted by the ratios between projected and unprojected probabilities of this process. The contribution $\sim f_{i\sigma}^\dagger\langle n_{i,-\sigma}\rangle^\alpha$ weights in a similar way the annihilation of an electron on a doubly-occupied site. The "z factors" Eq. (18) thus show the correct behavior $z_{i,\sigma}^{\alpha\beta}\to1$ for $U\to0$ and the diagonal elements reduce to the KR renormalization factors Eq. (10), i.e., $z_{i,\sigma}^{\alpha\alpha}=q_{i,\sigma}^\alpha$. An open problem remains in deriving Eq. (18) from a unitary transformation of the boson operators, similar to the transformation from Eq. (5) to Eq. (8). A straightforward construction of $z_{i,\sigma}^\dagger$ which yields $z_{i,\sigma}^{\alpha\beta}$ in the saddle-point approximation suffers from the fact that it is not gauge invariant.

In Appendix A it is shown that the renormalization factors Eq. (18) can be also motivated from the generalized Gutzwiller approach in the limit $\mathcal{D}\to\infty$.

III. RESULTS

In Sec. II, we have calculated the matrix elements between different inhomogeneous states $|\Psi^\alpha\rangle$ of the Hubbard model. These results are now used for evaluating ground-state energy and wave-function corrections similar to the configuration-interaction approach based on unrestricted HF wave-functions.[21]

We apply the method to the investigation of spin-polaron states on a square lattice, i.e., we have one hole with respect to half filling. Minimization of the KR (or GA) energy functional leads to the localization of this hole at a given site R_α (cf. Ref. 11 for a method of performing the unrestricted variation) and we denote the corresponding projected or fermion-boson wave-function with $|\Psi^\alpha\rangle$.

Now we generate all translations of this solution within the same sublattice since solutions belonging to different sublattices are orthogonal. The superposition

$$|\Psi\rangle=\sum_\alpha v_\alpha|\Psi^\alpha\rangle \tag{19}$$

thus only includes states $|\Psi^\alpha\rangle$ with the same energy $E=E^\alpha$. In principle, one could systematically improve the approach by including also excited states of the underlying fermionic Slater determinant.

If we apply the slave-boson transformed Hamiltonian (4) to Eq. (19), one obtains the following eigenvalue problem:

$$\langle\Psi^\alpha|\tilde{H}|\Psi^\beta\rangle v_\beta=\varepsilon S_{\alpha\beta}v_\beta \tag{20}$$

where the matrix $S_{\alpha\beta}$ is defined in Eq. (11). Note that the Hamiltonian entering Eq. (20) does not contain the constraints Eqs. (2) and (3) but only the slave-boson transformed kinetic and potential energy. The constraints establish a relation between the boson and fermion parts of each individual wave function $|\Psi^\alpha\rangle$ but not between different wave functions $|\Psi^\alpha\rangle$ and $|\Psi^\beta\rangle$ so that the corresponding matrix elements have no physical significance.

A. One hole states in the 4×4 lattice

We start by investigating the quality of the present approach with regard to exact results and the HF configuration-interaction method (CIHF).

Table I reports the energy correction obtained with our slave-boson configuration-interaction approach (CISB) as compared to the unrestricted GA. The values for the exact result, the CIHF and the unrestricted HF (from Ref. 20) are also shown for comparison.

It turns out that the CISB leads to an energy correction to the GA result which is of the same order of magnitude than the CIHF correction to the HF energy. However, this improvement is on top of the GA which itself provides a much better estimate for the ground-state energy than the HF approximation. For example, one finds that for $U/t=8$ the CISB differs from the exact result by $\approx5\%$ whereas it is $\approx13\%$ in case of the CIHF.

B. One hole states in the 16×16 lattice

We continue by evaluating the dispersion of the spin polaron on a 16×16 lattice. This problem has been extensively investigated within the tJ model,[25–33] where for small J/t one finds a bandwidth $\sim J$ which turns over into a $2t^2/J^4$ behavior for large J/t. Further on, the dispersion is characterized

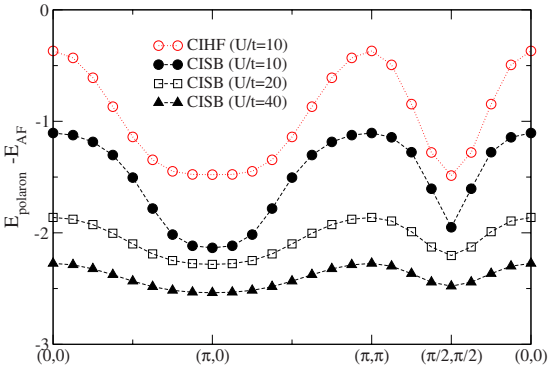

FIG. 1. (Color online) Dispersion of the spin polaron in the Hubbard model evaluated within the CISB ($U/t=10,20,40$) and CIHF ($U/t=10$) method. Energies are with respect to the half-filled antiferromagnet.

by a maximum at (0,0) (and the analogous (π,π) point) and displays a "hole pocket" at $(\pi/2,\pi/2)$ which is slightly lower in energy than the $(\pi,0)$ point.

Figure 1 displays the polaron dispersion obtained within the SBCI method for $U/t=10,20,40$. For comparison, we also show the $U/t=10$ result obtained from the CIHF method. Since the wave function incorporates only polaron states localized on the same sublattice the dominant contribution to the dispersion is given by $E_k \approx 4t' \cos(k_x)\cos(k_y) + 2t[\cos(2k_x)+\cos(2k_y)]$. Therefore at the point $k=(\pi,\pi/2)$ the energy difference between CIHF and CISB corresponds to the difference between GA and HF energies for the spin polaron. Since within the CISB approach, the matrix elements which enter Eq. (20) are additionally scaled by the bosonic exponential overlap Eq. (12) the corresponding long-range contributions to the dispersion are in generally smaller than for the CIHF method. On the other hand, this scaling affects also the matrix $S_{m\alpha\beta}$ in Eq. (20) so that due to partial cancellation the overall effect on the bandwidth is less pronounced as one might expect (see below).

From analogous investigations in the tJ-model,[25–33] it is known that the dispersion of a single hole has a saddle-point at $k=(\pi,0)$ and $k=(\pi/2,\pi/2)$, where the latter corresponds to the minimum of the band. From Fig. 1, it turns out that the CIHF spin-polaron dispersion also displays the minimum at $k=(\pm\pi/2,\pm\pi/2)$ whereas within the CISB method the state at $k=(\pm\pi,0),(0,\pm\pi)$ is slightly lower in energy. However, a direct comparison of results between tJ and Hubbard model is hampered by the fact that the strong-coupling expansion of the Hubbard model generates a three-site term of order J in addition to the "conventional" tJ model. Since we find that the energy difference between $k=(\pm\pi/2,\pm\pi/2)$ and $k=(\pm\pi,0),(0,\pm\pi)$ states is always smaller than $J=4t^2/U$ there appears no inconsistency with results from the tJ model. In fact, calculations of a single hole in the antiferromagnet based on an expanded tJ model (including the three-site term) provide evidence that the minimum of the band may be at $k=(\pm\pi,0),(0,\pm\pi)$.[34] This finding is also substantiated by exact diagonalization results of the same model on small clusters.[35] Unfortunately, for the full Hubbard model, there are no conclusive answers from quantum Monte Carlo or exact methods yet available.[36,37]

Table II reports the bandwidth, and the energy at $k=(\pm\pi/2,\pm\pi/2)$ of the spin-polaron dispersion obtained within the SCBA,[25] CIHF, and CISB method, respectively. Note that for the latter approach the bandwidth is $W=E_{(0,0)}-E_{(\pi,0)}$ whereas for the SCBA and CIHF methods it is given by $W=E_{(0,0)}-E_{(\pi/2,0)}$. Despite this difference we find that the CISB bandwidth scales as $W\approx 2.2J$ up to $J\approx 0.3$ in agreement with analogous considerations in the tJ model. It also turns out that (at least for $J>0.1$) the CISB bandwidth is smaller than that of the CIHF approach. Formally, this is again due to the additional renormalization of the matrix elements by the bosonic exponential overlap Eq. (12). On the other hand, it is quite natural that the CISB approach leads to "heavier" spin polarons than the CIHF method due to the incorporation of correlation effects already on the Gutzwiller level. Similar to the case of the 4×4 lattice the CISB leads to a significant energy correction with regard to the CIHF as exemplified by the value of $E_{(\pi/2,\pi/2)}$ in Table II.

C. Comparison with experiment

Undoped cuprate superconductors are antiferromagnetic Mott insulators. Within a angle-resolved photoemission (ARPES) experiment, one can in principle observe the dispersion of the created hole in the antiferromagnetic background of these compounds and compare with that of the spin-polaron quasiparticle concept from the previous section. On the basis of the single-band description, it is now well established from LDA[38] and the analysis of ARPES data[39] that a next-nearest-neighbor hopping t' has to be considered in the model. In particular, it has been found[39] that the quasiparticle dispersion from $(\pi,0)$ to $(\pi/2,\pi/2)$, which is determined by t', is characteristic for the different cuprate families. Our analysis below is therefore based on the ex-

TABLE II. Binding energy $E_{polaron}-E_{AF}$ taken at momentum $q=(\pi/2,\pi/2)$ and the bandwidth W for various values of $J=4t^2/U$. Shown are results for the self-consistent Born approximation (SCBA) of the tJ-model (from Ref. 25) and the CIHF and CISB method for the Hubbard model, respectively.

	SCBA		CIHF		CISB	
J	$E_{(\pi/2,\pi/2)}$	W	$E_{(\pi/2,\pi/2)}$	W	$E_{(\pi/2,\pi/2)}$	W
0.1	−2.785	0.239	−1.84	0.231	−2.4786	0.263
0.2	−2.540	0.430	−1.703	0.513	−2.204	0.421
0.3	−2.360	0.600	−1.588	0.817	−2.036	0.68
0.4	−2.209	0.741	−1.487	1.118	−1.95	1.031

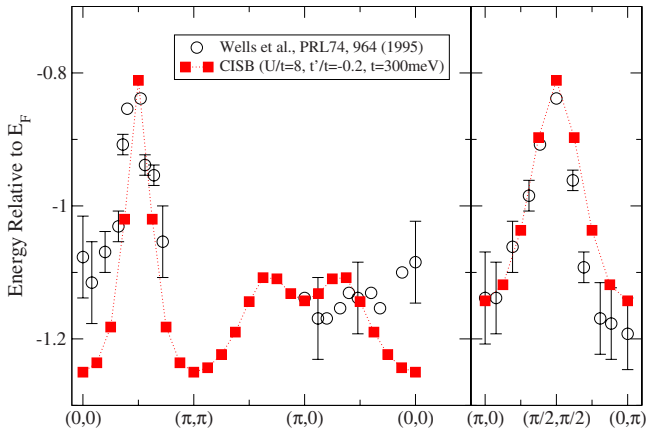

FIG. 2. (Color online) Dispersion of the spin polaron in the extended Hubbard model evaluated within the CISB ($U/t=8$, $t'/t=-0.2$, $t=300$ meV). The right panel shows the direction along the boundary of the magnetic Brillouin zone. Experimental data are from Ref. 40.

tended Hubbard model, which corresponds to Eq. (1) when the hopping t_{ij} is restricted to nearest $\sim t$ and next-nearest $\sim t'$ neighbors. In Fig. 2, we fit the resulting spin-polaron dispersion to ARPES data on undoped $Sr_2CuO_2Cl_2$ obtained by Wells *et al.*[40] Since the experiment measures the single-particle Green's function for electrons the dispersion in Fig. 2 is "reversed" with respect to those shown in Fig. 1 which were obtained for holes.

We can use the experimental energy differences $\Delta E_1 = E_{(\pi/2,\pi/2)} - E_{(0,0)}$ and $\Delta E_2 = E_{(\pi/2,\pi/2)} - E_{(\pi,0)}$ in order to fit two of the three parameters (t, t', U). Therefore, we additionally use our results from Ref. 41 where we have fitted the magnon dispersion of undoped La_2CuO_4 within the time-dependent Gutzwiller approximation. In this case, the value of the Hubbard repulsion $U/t \approx 8$ could be accurately determined from the dispersion of spin excitations along the magnetic Brillouin zone whereas this dispersion is rather unsensitive to t'. Given that the Cu onsite repulsion should not depend very much on the material we also use the ratio U/t in our present fit of the spin-polaron dispersion for $Sr_2CuO_2Cl_2$. As a result we find that the ratio $t'/t=-0.2$ yields an overall good agreement with the data and the nearest-neighbor hopping $t=300$ meV is set by the absolute energy scale. The ARPES data in addition allow for an accurate determination of t' so that a combination of both approaches in principle can be used to obtain parameter sets for the Hubbard model in order to describe different materials.

IV. CONCLUSIONS

We have developed a configuration-interaction approach based on the KR slave-boson mean-field formulation of the Hubbard model.[10] In principle, this method provides a controlled scheme for including fluctuations beyond the mean-field solution. Formally this has been achieved by several authors within the functional-integral formalism.[42–50] Here we have discussed an alternative extension which is based on the observation that unrestricted variation of the KR energy functional in general leads to a class of degenerate solutions which are connected by symmetry transformations. The CISB method discussed in this paper allows for a tunneling between these degenerate solutions and thus for a construction of eigenstates with well defined momentum.

Although the KR mean-field energy functional is identical to the that obtained with the generalized Gutzwiller wavefunction in $\mathcal{D} \to \infty$ [8] the considerations in Appendix A show that the latter approach leads to an "orthogonality catastrophe" for matrix elements between *different* inhomogeneous states. Therefore, one would have to invoke $1/\mathcal{D}$ corrections in order to construct a CI approach also within the Gutzwiller method. It should be noted that a similar orthogonality catastrophe occurs in the large N limit of the KR representation[51,52] where the individual "mean-field" solutions become exact. It is therefore a consistent result that the configuration interaction does not induce corrections to the saddle-point solutions in this limit, i.e., that the overlap between these solutions vanishes for large N.

Application of the CISB to the spin-polaron problem for the Hubbard model leads to a significant energy gain with respect to the CIHF method. Of course this result has to be treated with the usual reserve that the present approach is not variational and therefore does not necessarily yield an upper bound for the total energy. This is similar to the RPA or to the evaluation of fluctuation corrections to the KR energy functional[48] which can easily overshoot energy corrections. In addition, we have obtained a minimum of the spin-polaron dispersion at $k=(\pm\pi,0),(0,\pm\pi)$ in contrast to analogous calculations in the tJ-model but also in contrast to the CIHF method. However, calculations based on the full strong-coupling expansion of the Hubbard model,[34,35] which take into account the three-site terms of order t^2/U, neglected in the conventional tJ model, indicate the occurrence of dispersion minima around the corners of the magnetic Brillouin zone. To our knowledge, there are no recent exact diagonalization studies of one hole in a $\sqrt{18}\times\sqrt{18}$ or $\sqrt{20}\times\sqrt{20}$ Hubbard cluster which could substantiate the findings of Ref. 35. However, since on the mean-field level, the KR slave-boson formulation of the Hubbard model takes into account correlations beyond HF we expect that the CISB is more accurate concerning fine details of the spin-polaron dispersion as compared to the CIHF method. Further investigations are needed in order to confirm the finding of one hole dispersion minima at $k=(\pm\pi,0),(0,\pm\pi)$ in the Hubbard model.

Finally, we have included a next-nearest-neighbor hopping $t'/t<0$ in the bare Hamiltonian in order to fit the low energy dispersion of $Sr_2CuO_2Cl_2$ from ARPES experiments.[40] The parameter t' is essential in order to obtain the measured dispersion along the border of the magnetic Brillouin zone. More recent ARPES experiments[53] have also revealed a strong dispersion along the $(0,0)\to(\pi,0)$ direction. Within a one-band description modeling of these data requires inclusion of a significant third nearest-neighbor hopping. However, since our CISB approach can be implemented also on the more realistic three-band model, it would be interesting to study the spin-polaron dispersion within this Hamiltonian. The comparison with ARPES experiments would then allow to elucidate the parameters of this Hamiltonian for different cuprate materials. Moreover, since the

superposition in Eq. (19) can be extended to include also excited states, it should be possible to calculate also the incoherent part of the ARPES spectrum and thus to provide a more detailed description of the data. Work in this direction is in progress.

ACKNOWLEDGMENTS

I'm indebted to J. Lorenzana for a critical reading of the manuscript any many valuable comments. I also thank V. Hizhnyakov for helpful discussions.

APPENDIX A: GENERALIZED GUTZWILLER APPROXIMATION

Following Ref. 8, the Ansatz for a given inhomogeneous state α can be written as

$$|\Psi^\alpha\rangle = g^{\hat{K}(\alpha)}|\Phi_0^\alpha\rangle = \prod_i \hat{B}_i^\alpha |\Phi_0^\alpha\rangle, \tag{A1}$$

$$\hat{B}_i^\alpha = g^{\hat{K}_i(\alpha)} = g^{\hat{D}_i - \Sigma_\sigma \mu_{i,\sigma}^\alpha \hat{n}_{i,\sigma} + \eta_i^\alpha} \tag{A2}$$

where the uncorrelated state $|\Phi_0^\alpha\rangle$ is a Slater determinant with an inhomogeneous density matrix α and $\hat{D}_i = n_{i,\uparrow} n_{i,\downarrow}$ is the double occupancy operator. For later purposes we also define the operators for single occupied (with spin σ) and empty sites:

$$\hat{S}_{i,\sigma} = \hat{n}_{i,\sigma}(1 - \hat{n}_{i,-\sigma}), \tag{A3}$$

$$\hat{E}_i = (1 - \hat{n}_{i,\sigma})(1 - \hat{n}_{i,-\sigma}). \tag{A4}$$

The parameters $\mu_{i,\sigma}^\alpha$ and η_i^α have to be determined variationally. Gebhard[8] has shown that the requirement

$$g^{2\hat{K}(\alpha)} \equiv \sum_i \ln[1 + x_i^\alpha (\hat{D}_i - D_i^{HF,\alpha})] \tag{A5}$$

leads to the same energy functional than the Kotliar–Ruckenstein slave-boson approach in the mean-field approximation when the expectation values are formally evaluated in the limit of infinite dimensions. Here, $D_i^{HF,\alpha}$ denotes the Hartree–Fock decoupled double occupancy operator in the basis of the Slater determinant $|\Phi_0^\alpha\rangle$. Equation (A5) yields a relation between the variational parameters g, $\mu_{i,\sigma}^\alpha$, η_i^α and the variables x_i^α which turn out to be the relevant parameters when one evaluates expectation values in infinite dimensions. The essential step in this direction is to express the operator $\hat{B}_i^\alpha$ defined in Eq. (A2) in terms of the x_i^α as

$$\hat{B}_i^\alpha = \hat{D}_i \sqrt{1 + x_i^\alpha \langle E_i\rangle^\alpha} + \sum_\sigma \hat{S}_{i,\sigma} \sqrt{1 - x_i^\alpha \langle S_{i,-\sigma}\rangle^\alpha} + \hat{E}_i \sqrt{1 + x_i^\alpha \langle D_i\rangle^\alpha} \tag{A6}$$

and the expectation values are defined with regard to $|\Phi_0^\alpha\rangle$. An important result of the $d \to \infty$ description is the equivalence of local densities in the projected and unprojected states

$$\langle \Psi^\alpha | c_{i,\sigma}^\dagger c_{i,\sigma} | \Psi^\alpha \rangle = \langle \Phi_0^\alpha | c_{i,\sigma}^\dagger c_{i,\sigma} | \Phi_0^\alpha \rangle \tag{A7}$$

which will be used in the following.

First the double occupancy can be evaluated as

$$\langle \Psi^\alpha | \hat{D}_i | \Psi^\alpha \rangle \equiv \mathcal{D}_i^\alpha = \langle D_i \rangle^\alpha (1 + x_i^\alpha \langle E_i \rangle^\alpha) \tag{A8}$$

which allows one to perform the variations with respect to the double occupancy $\mathcal{D}_i^\alpha$ instead of x_i^α (or g, $\mu_{i,\sigma}^\alpha$, and η_i^α). Analogously the hopping term of Eq. (1) is given by

$$\langle \Psi^\alpha | c_{i,\sigma}^\dagger c_{j,\sigma} | \Psi^\alpha \rangle = q_{i,\sigma}^\alpha q_{j,\sigma}^\alpha \langle \Phi_0^\alpha | c_{i,\sigma}^\dagger c_{j,\sigma} | \Phi_0^\alpha \rangle \tag{A9}$$

with the hopping renormalization factors

$$q_{i,\sigma}^\alpha = \frac{1 - \langle n_{i,-\sigma}\rangle^\alpha}{\sqrt{\langle E_i\rangle^\alpha \langle S_{i,\sigma}\rangle^\alpha}} \sqrt{\mathcal{S}_{i,\sigma}^\alpha \mathcal{E}_i^\alpha} + \frac{\langle n_{i,-\sigma}\rangle^\alpha}{\sqrt{\langle D_i\rangle^\alpha \langle S_{i,-\sigma}\rangle^\alpha}} \sqrt{\mathcal{D}_i^\alpha \mathcal{S}_{i,-\sigma}^\alpha}. \tag{A10}$$

Similar than in Eq. (A8) expectation values of a projection operator $\hat{P}_i = \hat{D}_i$, $\hat{S}_{i,\sigma}$, $\hat{E}_i$ with regard to $|\Psi^\alpha\rangle$ have been denoted with calligraphic letters.

We now proceed by evaluating the matrix $\mathbf{S}$ which contains the overlap elements of wave-functions belonging to different inhomogeneous states

$$\begin{aligned} S_{\alpha\beta} = \langle \Psi^\alpha | \Psi^\beta \rangle &= \prod_i \langle \Phi_0^\alpha | \hat{B}_i^\alpha \hat{B}_i^\beta | \Phi_0^\beta \rangle \\ &= \prod_i \left\{ \sum_\sigma \sqrt{\frac{\mathcal{S}_{i,\sigma}^\alpha \mathcal{S}_{i,\sigma}^\beta}{\langle S_{i,\sigma}\rangle^\alpha \langle S_{i,\sigma}\rangle^\beta}} \langle \Phi_0^\alpha | \hat{S}_{i,\sigma} | \Phi_0^\beta \rangle \right. \\ &\quad + \sqrt{\frac{\mathcal{E}_i^\alpha \mathcal{E}_i^\beta}{\langle E_i\rangle^\alpha \langle E_i\rangle^\beta}} \langle \Phi_0^\alpha | \hat{E}_i | \Phi_0^\beta \rangle \\ &\quad \left. + \sqrt{\frac{\mathcal{D}_i^\alpha \mathcal{D}_i^\beta}{\langle D_i\rangle^\alpha \langle D_i\rangle^\beta}} \langle \Phi_0^\alpha | \hat{D}_i | \Phi_0^\beta \rangle \right\} \end{aligned} \tag{A11}$$

where we have used Eqs. (A6)–(A8) and the fact that only local contractions survive in infinite dimensions. Equation (A11) also requires the evaluation of matrix elements of $\hat{P}_i$ between different Slater determinants $\langle \Phi_0^\alpha | \hat{P}_i | \Phi_0^\beta \rangle$. For example, one finds for the double occupancy operator

$$\langle \Phi_0^\alpha | \hat{D}_i | \Phi_0^\beta \rangle = [\hat{n}_{i,\uparrow}]_{\alpha\beta} [\hat{n}_{i,\downarrow}]_{\alpha\beta} \tag{A12}$$

and the brackets are defined in Eq. (B7).

Schwartz's inequality together with the relation between harmonic and geometric mean

$$\langle \Phi_0^\alpha | \hat{P}_i | \Phi_0^\beta \rangle \le \sqrt{\langle P_i\rangle^\alpha \langle P_i\rangle^\beta}, \tag{A13}$$

$$\sqrt{\mathcal{P}_i^\alpha \mathcal{P}_i^\beta} \le (\mathcal{P}_i^\alpha + \mathcal{P}_i^\beta)/2, \tag{A14}$$

yields

$$\langle \Phi_0^\alpha | \hat{B}_i^\alpha \hat{B}_i^\beta | \Phi_0^\beta \rangle \le 1 \tag{A15}$$

where the equals sign holds for $\alpha = \beta$. Therefore in the thermodynamic limit, the overlap Eq. (A11) is a product of an infinite number of factors <1 which yields an orthogonality catastrophe $S_{\alpha \neq \beta} = 0$. The difference to the analogous slave-

boson expression Eq. (12), where this orthogonality catastrophe does not occur in general, can be understood from the spin-polaron example investigated in Sec. III. In this case the doped charge is confined to approximately five sites (central site and four adjacent sites) and spin and charge densities on sites further apart from the polaron core coincide practically with those of the undoped AF solution. The exponent of Eq. (12) then equals "zero" when site "i" belongs to an AF region of both solutions $|\Psi^\alpha\rangle$, $|\Psi^\beta\rangle$. In case site i belongs to a polaron site of $|\Psi^\alpha\rangle$ or $|\Psi^\beta\rangle$ (there are at most ten such sites) the exponent is smaller than zero. The value of Eq. (12) is therefore mainly determined from the contributions where i belongs to a polaron site and hence the overlap Eq. (12) can be small but remains finite. In contrast, the analogous expression for the GA in Eq. (A11) depend on the matrix elements Eqs. (B4) and (B5) which decay with the distance between the polaron cores of solutions $|\Psi^\alpha\rangle$, $|\Psi^\beta\rangle$. For this reason the '=' sign in Eqs. (A13) and (A14) only holds for $\alpha=\beta$. Otherwise for $\alpha\neq\beta$ all factors in Eq. (12) are smaller "one" whereas for the bosonic overlap this is only the case when the site i belongs to the polaron core of $|\Psi^\alpha\rangle$ and (or) $|\Psi^\beta\rangle$..

Analogously to **S**, one can evaluate the matrix elements of the Hubbard Hamiltonian Eq. (1). For the double occupancy operator one obtains

$$\langle\Psi^\alpha|\hat{D}_i|\Psi^\beta\rangle = \frac{\langle\Phi_0^\alpha|\hat{B}_i^\alpha\hat{D}_i\hat{B}_i^\beta|\Phi_0^\beta\rangle}{\langle\Phi_0^\alpha|\hat{B}_i^\alpha\hat{B}_i^\beta|\Phi_0^\beta\rangle}S_{\alpha\beta} = \sqrt{\frac{\mathcal{D}_i^\alpha\mathcal{D}_i^\beta}{\langle D_i\rangle^\alpha\langle D_i\rangle^\beta}}\frac{\langle\Phi_0^\alpha|\hat{D}_i|\Phi_0^\beta\rangle}{\langle\Phi_0^\alpha|\hat{B}_i^\alpha\hat{B}_i^\beta|\Phi_0^\beta\rangle}S_{\alpha\beta} \tag{A16}$$

and the matrix elements of the hopping term are given by

$$\langle\Psi^\alpha|c_{i,\sigma}^\dagger c_{j,\sigma}|\Psi^\beta\rangle = \frac{\langle\Phi_0^\alpha|\hat{B}_i^\alpha c_{i,\sigma}^\dagger\hat{B}_i^\beta\hat{B}_j^\alpha c_{j,\sigma}\hat{B}_j^\beta|\Phi_0^\beta\rangle}{\langle\Phi_0^\alpha|\hat{B}_i^\alpha\hat{B}_i^\beta|\Phi_0^\beta\rangle\langle\Phi_0^\alpha|\hat{B}_j^\alpha\hat{B}_j^\beta|\Phi_0^\beta\rangle}S_{\alpha\beta}. \tag{A17}$$

Using Eqs. (A6)–(A8), the projections of the creation and annihilation operators can be expressed as

$$\hat{B}_i^\alpha c_{i,\sigma}^\dagger\hat{B}_i^\beta = \left[(1-n_{i,-\sigma})\sqrt{\frac{\mathcal{S}_{i\sigma}^\alpha\mathcal{E}_i^\beta}{\langle S_{i\sigma}\rangle^\alpha\langle E_i\rangle^\beta}} + n_{i,-\sigma}\sqrt{\frac{\mathcal{D}_i^\alpha\mathcal{S}_{i,-\sigma}^\beta}{\langle D_i\rangle^\alpha\langle S_{i,-\sigma}\rangle^\beta}}\right]c_{i,\sigma}^\dagger, \tag{A18}$$

$$\hat{B}_j^\alpha c_{j,\sigma}\hat{B}_j^\beta = \left[(1-n_{j,-\sigma})\sqrt{\frac{\mathcal{E}_j^\alpha\mathcal{S}_{j\sigma}^\beta}{\langle E_j\rangle^\alpha\langle S_{j\sigma}\rangle^\beta}} + n_{j,-\sigma}\sqrt{\frac{\mathcal{S}_{j,-\sigma}^\alpha\mathcal{D}_j^\beta}{\langle S_{j,-\sigma}\rangle^\alpha\langle D_j\rangle^\beta}}\right]c_{j,\sigma}. \tag{A19}$$

In principle, it is possible to evaluate the matrix elements from Eqs. (A17) in terms of the Slater determinants $|\Phi_0^\alpha\rangle$, however, the calculation of contributions which involve density correlations of the form $\langle\Phi_0^\alpha|n_{i,-\sigma}n_{j,-\sigma}|\Phi_0^\beta\rangle$ are rather time consuming. We therefore simplify the expression of the projections Eqs. (A18) and (A19) by the following argument. With regard to the matrix element Eq. (A17) the projection Eq. (A18) describes the annihilation of a particle with spin σ in the Slater determinant $\langle\Phi_0^\alpha|$. The two contributions measure the probabilty whether site i in the state α is singly or doubly occupied. Accordingly, we replace the corresponding projections by their mean values, e.g., $1-n_{i,-\sigma}\rightarrow 1-\langle n_{i,-\sigma}\rangle^\alpha$. In the same way Eq. (A19) describes the annihilation of a particle with spin σ in the Slater determinant $|\Phi_0^\beta\rangle^\beta$ and we approximate in this case $1-n_{i,-\sigma}\rightarrow 1-\langle n_{i,-\sigma}\rangle^\beta$. Within this approximation one obtains for the projected creation and annihilation operators

$$\hat{B}_i^\alpha c_{i,\sigma}^\dagger\hat{B}_i^\beta = q_{i,\sigma}^{\alpha\beta}c_{i,\sigma}^\dagger, \tag{A20}$$

$$\hat{B}_j^\alpha c_{j,\sigma}\hat{B}_j^\beta = q_{j,\sigma}^{\beta\alpha}c_{j,\sigma} \tag{A21}$$

where the $q_{i,\sigma}^{\alpha\beta}$ are equivalent to the renormalization factors [Eq. (18)] derived with the KR slave-boson method.

In case of the GA, we observe from Eq. (A11) that $S_{\alpha\neq\beta}$ is a product over lattice sites of terms less than one which in the thermodynamic limit leads to an orthogonality catastrophe[22] and thus $S_{\alpha\beta}=\delta_{\alpha\beta}$. Therefore we find that within the "infinite D" prescription of the Gutzwiller approximation[8] different inhomogeneous states are orthogonal to each other. As a consequence it turns out from Eqs. (A16) and (A17) that these states are not connected by matrix elements of the Hubbard Hamiltonian so that a CI approach does not yields any correction to the symmetry-broken solutions.

APPENDIX B: FERMIONIC MATRIX ELEMENTS

When we restrict to collinear inhomogeneous Gutzwiller solutions, i.e., where the associated density matrix is diagonal in spin space, we can represent the noninteracting state $|\Phi_0^\alpha\rangle$ as

$$|\Phi_0^\alpha\rangle = |\varphi_\uparrow^\alpha\rangle\otimes|\varphi_\downarrow^\alpha\rangle, \tag{B1}$$

$$|\varphi_\sigma^\alpha\rangle = a_{1,\sigma}^{\alpha,\dagger}a_{2,\sigma}^{\alpha,\dagger}a_{3,\sigma}^{\alpha,\dagger}\ldots a_{N\sigma,\sigma}^{\alpha,\dagger}|0\rangle \tag{B2}$$

and the operators $a_{k,\sigma}^\alpha$ are related to the real-space operators $c_{i,\sigma}$ by the linear transformation

$$a_{k,\sigma}^\alpha = \sum_i \phi_{i,\sigma}^\alpha(k)c_{i,\sigma} \tag{B3}$$

which defines the specific inhomogeneous solution. Details for the calculation of the amplitudes $\phi_{i,\sigma}^\alpha(k)$ within the Gutzwiller approximation can be found in Ref. 11. Within these definitions, the evaluation of matrix elements between different Slater determinants is analogous to the scheme outlined in Ref. 20. Here, we have defined the single-particle matrix elements as

$$\langle k_\sigma^\alpha | q_\sigma^\beta \rangle = \sum_i \phi_{i,\sigma}^\alpha(k) \phi_{i,\sigma}^\beta(q), \tag{B4}$$

$$\langle k_\sigma^\alpha | n_{i,\sigma} | q_\sigma^\beta \rangle = \phi_{i,\sigma}^\alpha(k) \phi_{i,\sigma}^\beta(q). \tag{B5}$$

The matrix elements between Slater determinant and also those of single-particle operators between different Slater determinants as used e.g., in Eq. (A12) are given by

$$\langle \Phi_0^\alpha | \Phi_0^\beta \rangle_\sigma = \begin{vmatrix} \langle 1_\sigma^\alpha | 1_\sigma^\beta \rangle & \langle 1_\sigma^\alpha | 2_\sigma^\beta \rangle & \cdots & \langle 1_\sigma^\alpha | N_\sigma^\beta \rangle \\ \langle 2_\sigma^\alpha | 1_\sigma^\beta \rangle & \langle 2_\sigma^\alpha | 2_\sigma^\beta \rangle & \cdots & \langle 2_\sigma^\alpha | N_\sigma^\beta \rangle \\ \cdots & \cdots & \cdots & \cdots \\ \langle N_\sigma^\alpha | 1_\sigma^\beta \rangle & \langle N_\sigma^\alpha | 2_\sigma^\beta \rangle & \cdots & \langle N_\sigma^\alpha | N_\sigma^\beta \rangle \end{vmatrix}, \tag{B6}$$

$$[\hat{n}_{i,\sigma}]_{\alpha\beta} = \begin{vmatrix} \langle 1_\sigma^\alpha | n_{i,\sigma} | 1_\sigma^\beta \rangle & \langle 1_\sigma^\alpha | 2_\sigma^\beta \rangle & \cdots & \langle 1_\sigma^\alpha | N_\sigma^\beta \rangle \\ \langle 2_\sigma^\alpha | n_{i,\sigma} | 1_\sigma^\beta \rangle & \langle 2_\sigma^\alpha | 2_\sigma^\beta \rangle & \cdots & \langle 2_\sigma^\alpha | N_\sigma^\beta \rangle \\ \cdots & \cdots & \cdots & \cdots \\ \langle N_\sigma^\alpha | n_{i,\sigma} | 1_\sigma^\beta \rangle & \langle N_\sigma^\alpha | 2_\sigma^\beta \rangle & \cdots & \langle N_\sigma^\alpha | N_\sigma^\beta \rangle \end{vmatrix} + \begin{vmatrix} \langle 1_\sigma^\alpha | 1_\sigma^\beta \rangle & \langle 1_\sigma^\alpha | n_{i,\sigma} | 2_\sigma^\beta \rangle & \cdots & \langle 1_\sigma^\alpha | N_\sigma^\beta \rangle \\ \langle 2_\sigma^\alpha | 1_\sigma^\beta \rangle & \langle 2_\sigma^\alpha | n_{i,\sigma} | 2_\sigma^\beta \rangle & \cdots & \langle 2_\sigma^\alpha | N_\sigma^\beta \rangle \\ \cdots & \cdots & \cdots & \cdots \\ \langle N_\sigma^\alpha | 1_\sigma^\beta \rangle & \langle N_\sigma^\alpha | n_{i,\sigma} | 2_\sigma^\beta \rangle & \cdots & \langle N_\sigma^\alpha | N_\sigma^\beta \rangle \end{vmatrix} + + \cdots$$
$$+ \begin{vmatrix} \langle 1_\sigma^\alpha | 1_\sigma^\beta \rangle & \langle 1_\sigma^\alpha | 2_\sigma^\beta \rangle & \cdots & \langle 1_\sigma^\alpha | n_{i,\sigma} | N_\sigma^\beta \rangle \\ \langle 2_\sigma^\alpha | 1_\sigma^\beta \rangle & \langle 2_\sigma^\alpha | 2_\sigma^\beta \rangle & \cdots & \langle 2_\sigma^\alpha | n_{i,\sigma} | N_\sigma^\beta \rangle \\ \cdots & \cdots & \cdots & \cdots \\ \langle N_\sigma^\alpha | 1_\sigma^\beta \rangle & \langle N_\sigma^\alpha | 2_\sigma^\beta \rangle & \cdots & \langle N_\sigma^\alpha | n_{i,\sigma} | N_\sigma^\beta \rangle \end{vmatrix}. \tag{B7}$$

[1] M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963).
[2] M. C. Gutzwiller, Phys. Rev. **134**, A923 (1964); **137**, A1726 (1965).
[3] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **59**, 121 (1987); Phys. Rev. B **37**, 7382 (1988).
[4] D. Vollhardt, Rev. Mod. Phys. **56**, 99 (1984).
[5] G. Seibold, C. Castellani, C. Di Castro, and M. Grilli, Phys. Rev. B **58**, 13506 (1998).
[6] J. Lorenzana and G. Seibold, Phys. Rev. Lett. **89**, 136401 (2002).
[7] M. Raczkowski, R. Frésard, and A. M. Oleś, Phys. Rev. B **73**, 174525 (2006).
[8] F. Gebhard, Phys. Rev. B **41**, 9452 (1990).
[9] C. Attaccalite and M. Fabrizio, Phys. Rev. B **68**, 155117 (2003).
[10] G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986).
[11] G. Seibold, E. Sigmund, and V. Hizhnyakov, Phys. Rev. B **57**, 6937 (1998).
[12] G. Seibold, Phys. Rev. B **58**, 15520 (1998).
[13] J. Lorenzana and G. Seibold, Phys. Rev. Lett. **89**, 136401 (2002).
[14] G. Seibold and J. Lorenzana, Phys. Rev. B **69**, 134513 (2004).
[15] G. Seibold, J. Lorenzana, and M. Grilli, Phys. Rev. B **75**, 100505(R) (2007).
[16] N. Pavlenko and T. Kopp, Phys. Rev. Lett. **97**, 187001 (2006).
[17] A. Rüegg, S. Pilgram, and M. Sigrist, Phys. Rev. B **75**, 195117 (2007).
[18] L. Lilly, A. Muramatsu, and W. Hanke, Phys. Rev. Lett. **65**, 1379 (1990).
[19] G. Seibold and J. Lorenzana, Phys. Rev. Lett. **86**, 2605 (2001).
[20] E. Louis, F. Guinea, M. P. López Sancho, and J. A. Vergés, Phys. Rev. B **59**, 14005 (1999).
[21] E. Louis, F. Guinea, M. P. López Sancho, and J. A. Vergés, Phys. Rev. B **64**, 205108 (2001).
[22] P. W. Anderson, Phys. Rev. Lett. **18**, 1049 (1967).
[23] R. Frésard, H. Ouerdane, and T. Kopp, Nucl. Phys. B **785**, 286 (2007).
[24] F. C. Zhang, C. Gros, T. M. Rice, and H. Shiba, Supercond. Sci. Technol. **1**, 36 (1988).
[25] G. Martinez and P. Horsch, Phys. Rev. B **44**, 317 (1991).
[26] J. Bonca, S. Maekawa, and T. Tohyama, Phys. Rev. B **76**, 035121 (2007).
[27] Z. Liu and E. Manousakis, Phys. Rev. B **45**, 2425 (1992).
[28] M. Vojta and K. W. Becker, Phys. Rev. B **57**, 3099 (1998).
[29] G. F. Reiter, Phys. Rev. B **49**, 1536 (1994).
[30] P. W. Leung and R. J. Gooding, Phys. Rev. B **52**, R15711 (1995).
[31] S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. **60**, 2793 (1988).
[32] F. Marsiglio, A. E. Ruckenstein, S. Schmitt-Rink, and C. M. Varma, Phys. Rev. B **43**, 10882 (1991).
[33] C. L. Kane, P. A. Lee, and N. Read, Phys. Rev. B **39**, 6880 (1989).
[34] B. M. Elrick and A. E. Jacobs, Phys. Rev. B **52**, 10369 (1995).
[35] H. Fehske, V. Waas, H. Röder, and H. Büttner, Phys. Rev. B **44**, 8473 (1991).
[36] S. Sorella, Phys. Rev. B **46**, 11670 (1992).
[37] E. Dagotto, A. Moreo, F. Ortolani, D. Poilblanc, and J. Riera,

Phys. Rev. B **45**, 10741 (1992).
[38] E. Pavarini, I. Dasgupta, T. Saha-Dasgupta, O. Jepsen, and O. K. Andersen, Phys. Rev. Lett. **87**, 047003 (2001).
[39] K. Tanaka, T. Yoshida, A. Fujimori, D. H. Lu, Z.-X. Shen, X.-J. Zhou, H. Eisaki, Z. Hussain, S. Uchida, Y. Aiura, K. Ono, T. Sugaya, T. Mizuno, and I. Terasaki, Phys. Rev. B **70**, 092503 (2004).
[40] B. O. Wells, Z.-X. Shen, A. Matsuura, D. M. King, M. A. Kastner, M. Greven, and R. J. Birgeneau, Phys. Rev. Lett. **74**, 964 (1995).
[41] G. Seibold and J. Lorenzana, Phys. Rev. Lett. **94**, 107006 (2005).
[42] E. Arrigoni and G. C. Strinati, Phys. Rev. Lett. **71**, 3178 (1993); Phys. Rev. B **52**, 2428 (1995).
[43] M. Lavagna, Phys. Rev. B **41**, 142 (1990).
[44] J. W. Rasul and T. Li, J. Phys. C **21**, 5119 (1988).
[45] Th. Jolicoeur and J. C. Le Guillou, Phys. Rev. B **44**, 2403 (1991).
[46] W. Zimmermann, R. Frésard, and P. Wölfle, Phys. Rev. B **56**, 10097 (1997).
[47] E. Koch, Phys. Rev. B **64**, 165113 (2001).
[48] E. Arrigoni, C. Castellani, M. Grilli, R. Raimondi, and C. Castellani, Phys. Rep. **241**, 291 (1994).
[49] R. Raimondi and C. Castellani, Phys. Rev. B **48**, R11453 (1993).
[50] R. Raimondi, Phys. Rev. B **51**, 10154 (1995).
[51] R. Frésard and P. Wölfle, Int. J. Mod. Phys. B **6**, 237 (1992).
[52] S. Florens, A. Georges, G. Kotliar, and O. Parcollet, Phys. Rev. B **66**, 205102 (2002).
[53] C. Dürr, S. Legner, R. Hayn, S. V. Borisenko, Z. Hu, A. Theresiak, M. Knupfer, M. S. Golden, J. Fink, F. Ronning, Z.-X. Shen, H. Eisaki, S. Uchida, C. Janowitz, R. Müller, R. L. Johnson, K. Rossnagel, L. Kipp, and G. Reichardt, Phys. Rev. B **63**, 014505 (2000).