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

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Based on the Kotliar-Ruckenstein slave-boson scheme we develop a configuration-interaction (CI) approach which is suitable to improve the energy of 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 D prescription of the Gutzwiller method a CI approach does not improve the variational result since in the thermodynamic limit matrix elements between different inhomogeneous states vanish due to an 'orthogonality catastrophe'.

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I. INTRODUCTION

The Gutzwiller Ansatz is a variational wave function for correlated electronic models with purely local interaction. 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. 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 He (cf. Ref. 4) to the stripe phase of high-Tc cuprates.

The GA in its original formulation was restricted to homogeneous paramagnetic systems and only later on generalized to arbitrary Slater determinants by Gebhard and, more recently, by Attaccalite and Fabrizio. 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. Unconstrained minimization of the KR (or Gebhard) energy functional on finite clusters in general yields inhomogeneous solutions which break translational and spin-rotational invariance. This approach has been used for the investigation of electronic inhomogeneities, such as stripes and checkerboards, in the context of high-Tc superconductors.

Incorporation of fluctuations in the frame of the time-dependent Gutzwiller approximation tends to restore the original symmetry of the system. 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 one could envisage a superposition of solutions which are translated perpendicular to the stripe direction and also the corresponding solutions which are rotated by 90 degrees. In case of the unrestricted Hartree-Fock approximation such a configuration-interaction (CI) method has been proposed in Ref. and applied to the case of stripe textures in Ref. 7.

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. 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 Sr2CuO2Cl2.

In appendix A it is shown that the infinite D prescription of the Gutzwiller approximation 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' so that energy corrections and the dispersion of quasiparticles vanish.

II. MODEL AND FORMALISM

Our investigations are based on the one-band Hubbard model

\[ H = \sum_{ij,\sigma} t_{ij} c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \]  

(1)

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

Following KR we enlarge the original Hilbert space by introducing four subsidiary boson fields \( e_{i,\uparrow}^{(1)}, e_{i,\downarrow}^{(1)} \) and \( d_{i,\uparrow}^{(1)}, d_{i,\downarrow}^{(1)} \) 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
\[ \sum_{\sigma} s_{i,\sigma}^\dagger s_{i,\sigma} + d_{i}^\dagger d_i = 1 \]  

(2)

Furthermore
\[ n_{i,\sigma} = s_{i,\sigma}^\dagger s_{i,\sigma} + d_{i}^\dagger d_i \]  

(3)

Then, in the physical subspace defined by Eqs. (2,3) the Hamiltonian \( \hat{H} \) takes the form
\[ \hat{H} = \sum_{ij,\sigma} t_{ij} z_{i,\sigma}^\dagger f_{i,\sigma}^\dagger f_{j,\sigma} z_{j,\sigma} + U \sum_{i} d_{i}^\dagger d_i \]  

(4)

with
\[ z_{i,\sigma} = e_{i}^\dagger s_{i,\sigma} + s_{i,-\sigma}^\dagger d_i \]  

(5)

and has the same matrix elements than those calculated for \( \hat{H} \) in the original Hilbert space. The operators \( f_{i,\sigma} \) 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 \( \alpha \) as
\[ |\Psi^\alpha \rangle = |\Phi^\alpha_0 \rangle \otimes |B^\alpha_0 \rangle \]  

(6)

where \( |\Phi^\alpha_0 \rangle \) is a Slater determinant and the bosonic part \( |B^\alpha_0 \rangle \) is a coherent state
\[ |B^\alpha_0 \rangle = e_{\alpha}^{\dagger} \left( e_{\alpha} + \sum_{\sigma} (\tilde{s}_{i,\sigma}^\dagger s_{i,\sigma}^\dagger + e_{\alpha}^\dagger e_i^\dagger - 1/2) \right) |0 \rangle. \]  

(7)

Since a coherent state contains an arbitrary number of bosons the constraints Eqs. (2,3) are only fulfilled on average for a given inhomogeneous solution \( \alpha \) provided that
\[ 1 = (e_{\alpha}^{\dagger})^2 + \sum_{\sigma} (\tilde{s}_{i,\sigma}^\dagger s_{i,\sigma}^\dagger)^2 + (\tilde{d}_i^\dagger)^2 \]
\[ \langle n_{i,\sigma} \rangle^\alpha = (e_{\alpha}^\dagger)^2 + (\tilde{d}_i^\dagger)^2. \]

Note that here and in the following expectation values of fermion operators are denoted with respect to the Slater determinant of \( f \)-electron operators.

The problem with the Ansatz Eq. (3) is that one does not recover the correct non-interacting limit \( U \to 0 \) for which \( z_{i,\sigma} \to 1 \). Therefore KR introduced a unitary transformation in order to represent the \( z \)-operators in Eq. (5) as
\[ z_{i,\sigma} = \frac{1}{\sqrt{e_{i}^\dagger e_i + s_{i,-\sigma}^\dagger s_{i,-\sigma}^\dagger d_i}} \frac{1}{\sqrt{d_i^\dagger d_i + s_{i,\sigma}^\dagger s_{i,\sigma}^\dagger}} \]  

so that
\[ \langle \Psi^\alpha | z_{i,\sigma}^\dagger c_{i,\sigma}^\dagger c_{j,\sigma} z_{j,\sigma} | \Psi^\alpha \rangle = (q_{i,\sigma}^\alpha)^* q_{j,\sigma}^\alpha \langle \Phi^\alpha_0 | c_{i,\sigma}^\dagger c_{j,\sigma} | \Phi^\alpha_0 \rangle. \]  

(9)

The expectation values of the \( z \)-operators Eq. (8)
\[ q_{i,\sigma}^\alpha \]  

(10)

are equivalent to the renormalization factors derived within the infinite \( D \) prescription of the Gutzwiller approximation (cf. Eq. (10) in appendix A).

In previous works 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
\[ S_{\alpha\beta} = \langle \Psi^\alpha | \Psi^\beta \rangle \]
\[ = \langle \Phi^\alpha_0 | \Phi^\beta_0 \rangle \langle B^\alpha_0 | B^\beta_0 \rangle \]  

(11)

where the overlap between coherent states reads as
\[ \langle B^\alpha_0 | B^\beta_0 \rangle = e^{\sum_{i} (d_{i}^\dagger d_i + \sum_{\sigma} s_{i,\sigma}^\dagger s_{i,\sigma}^\dagger + e_{\alpha}^\dagger e_i^\dagger - 1)}. \]  

(12)

The fermionic overlap is given by
\[ \langle \Phi^\alpha_0 | \Phi^\beta_0 \rangle = \langle \Phi^\alpha_0 | \Phi^\beta_0 \rangle , \langle \Phi^\alpha_0 | \Phi^\beta_0 \rangle \]  

(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 Eq. (4) in the basis of the inhomogeneous wave-functions \( |\Psi^\alpha \rangle \). From the above definitions one obtains for the Hubbard interaction
\[ \langle \Psi^\alpha | U \sum_{i} d_{i}^\dagger d_i | \Psi^\beta \rangle = U \langle \Phi^\alpha_0 | \Phi^\beta_0 \rangle \langle B^\alpha_0 | B^\beta_0 \rangle \sum_{i} \hat{d}_i^\dagger \hat{d}_i. \]  

(14)

The kinetic term is evaluated in a similar way as
\[ \langle \Psi^\alpha | \hat{T} | \Psi^\beta \rangle = \sum_{ij,\sigma} \langle \Phi^\alpha_0 | c_{i,\sigma}^\dagger c_{j,\sigma} | \Phi^\beta_0 \rangle \langle B^\alpha_0 | B^\beta_0 \rangle \]  

(15)

with the fermionic part
\[ \langle \Phi^\alpha_0 | c_{i,\sigma}^\dagger c_{j,\sigma} | \Phi^\beta_0 \rangle = \left[ c_{i,\sigma}^\dagger c_{j,\sigma} \right]_{\alpha\beta} \langle \Phi^\alpha_0 | \Phi^\beta_0 \rangle \]  

(16)

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

The matrix elements of the 'bare' bosonic \( z \)-operators from Eq. (5) read as
\[ z_{i,\sigma}^\alpha = \frac{1}{\sqrt{e_{i}^\dagger e_i + s_{i,-\sigma}^\dagger s_{i,-\sigma}^\dagger d_i}} \frac{1}{\sqrt{d_i^\dagger d_i + s_{i,\sigma}^\dagger s_{i,\sigma}^\dagger}} \]  

(17)

Now we have to deal again with the problem that the \( z \)-factors as defined in Eqs. (17) do not yield the uncorrelated limit, i.e. \( z_{i,\sigma}^\alpha = z_{i,\sigma}^\alpha \to 1 \) for \( U \to 0 \). It is straightforward to prove that the representation of Eq. (5) does not work in this case since the above limit is only obeyed.
for homogeneous paramagnetic solutions. However, due to a non-symmetric 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 $U \to 0$.

A possible representation which yields $z_{i,\sigma}^{\alpha\beta} \to 1$ for $U \to 0$ is given by

$$z_{i,\sigma}^{\alpha\beta} = \frac{1}{\sqrt{1 - e_1 e_\sigma - s_{i,-\sigma} s_{i,\sigma}}} \left[ \frac{1}{\sqrt{1 - e_1 e_\sigma - s_{i,-\sigma} s_{i,\sigma}}} \right] \left[ \frac{1}{\sqrt{1 - e_1 e_\sigma - s_{i,-\sigma} s_{i,\sigma}}} \right]$$

Note that in the physical subspace defined by Eq. 2 the square root factors are identical 'one'. On the other hand, upon evaluating the matrix elements of Eq. 18 between coherent states $\alpha, \beta$ one obtains the hopping renormalization factors

$$z_{i,\sigma}^{\alpha\beta} = \langle B_0^{\alpha} | z_{i,\sigma}^{\dagger} | B_0^{\beta} \rangle = \frac{1}{\sqrt{1 - (n_{i,\sigma})_\alpha (1 - (n_{i,\sigma})_\beta)}}$$

$$\times \left\{ \frac{(n_{i,\sigma})_\alpha}{\sqrt{(n_{i,\sigma})_\beta}} \left( (d_{i,\sigma})^2 (n_{i,\sigma})_\beta^2 - (d_{i,\sigma})^2 \right) \right\}$$

where we have used the constraints Eqs. 19 to replace the boson fields but $d_{i,\sigma}$ by fermionic expectation values. The 'z-factors' Eq. 19 show the correct behavior $z_{i,\sigma}^{\alpha\beta} \to 1$ for $U \to 0$ and the diagonal elements reduce to the KR renormalization factors Eq. 10, i.e. $z_{i,\sigma}^{\alpha\alpha} = q_{i,\sigma}^\alpha$.

In appendix A it is shown that the renormalization factors Eq. 19 can be also motivated from the generalized Gutzwiller approach in the limit $D \to \infty$.

### III. Results

In the previous section we have calculated the matrix elements between different inhomogeneous states $|\Psi^\alpha\rangle$ of the Hubbard model. These results are now used for evaluating an improved ground state energy and wave-function similar than in the configuration interaction approach based on unrestricted HF wave-functions.22

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 $R_\alpha$ (cf. Ref. 1 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

$$|\Psi\rangle = \sum_\alpha v_\alpha |\Psi^\alpha\rangle$$

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 hamiltonian Eq. 1 to Eq. 20 one obtains the following eigenvalue problem

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

where the matrix $S_{\alpha\beta}$ is defined in Eq. 11.

#### A. One hole states in the 4x4 lattice

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

Table III A 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. 1) are also shown for comparison.

| U/t | exact | HF | GA | CHIF | CISB |
|-----|-------|----|----|------|------|
| 1   | 0.91658 | -0.83430 | -0.88815 | -0.83501 | -0.89091 |
| 2   | 0.74794 | -0.64222 | -0.70020 | -0.66214 | -0.70497 |
| 3   | 0.634203 | -0.52884 | -0.57518 | -0.54747 | -0.60295 |
| 5   | 0.42546 | -0.35869 | -0.37130 | -0.34664 | -0.38091 |
| 10  | 0.308473 | -0.25160 | -0.27209 | -0.23827 | -0.27685 |
| 20  | 0.206039 | -0.19335 | -0.20954 | -0.19617 | -0.23462 |

Table I: Energy per site for 15 particles on a 4 x 4 lattice. The values of the exact result, HF and CIHF method have been taken from Ref. 16.

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 $\approx 5\%$ whereas it is $\approx 13\%$ in case of the CIHF.

B. One hole states in the 16x16 lattice

We continue by evaluating the dispersion of the spin polaron in a 16 $\times$ 16 lattice. This problem has been extensively investigated within the tJ model, where for small $J/t$ one finds a bandwidth $\sim J$ which turns over into a $2t^2/J^4$ behavior for large $J/t$. Furthermore, the dispersion is characterized by a maximum at $(0,0)$ (and the analogous $(\pi,\pi)$ point) and displays a ‘hole pocket’ at $(\pi/2,\pi/2)$ which is slightly lower in energy than the $(\pi,0)$ point.

Fig. 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 $E_k \approx 4t' \cos(k_x) \cos(k_y) + 2t[\cos(2k_x) + \cos(2k_y)]$. There is a point $k = (\pi/2,\pi/2)$ which is slightly lower in energy than the $(\pi,0)$ point. For $U/t = 20$, the CISB differs from the exact result by $\approx 5\%$. 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 $E_k \approx 4t' \cos(k_x) \cos(k_y) + 2t[\cos(2k_x) + \cos(2k_y)]$. There is a point $k = (\pi/2,\pi/2)$ which is slightly lower in energy than the $(\pi,0)$ point. 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 $k = (\mp \pi/2, \pm \pi/2)$ whereas 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 $k = (\pm \pi, 0), (0, \pm \pi)$. This finding is also substantiated by exact diagonalization results of the same model on small clusters. Unfortunately, for the full Hubbard model there are no conclusive answers from Quantum Monte Carlo or exact methods yet available.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|}
\hline
 & SCBA & CIHF & CISB \\
\hline
$J$ & $E_{(\pi/2,\pi/2)}$ & $W$ & $E_{(\pi/2,\pi/2)}$ & $W$ & $E_{(\pi/2,\pi/2)}$ & $W$ \\
\hline
0.1 & -2.785 & 0.250 & -1.84 & 0.231 & -2.786 & 0.268 \\
0.2 & -2.540 & 0.400 & -1.703 & 0.518 & -2.604 & 0.521 \\
0.3 & -2.360 & 0.600 & -1.585 & 0.817 & -2.504 & 0.781 \\
0.4 & -2.200 & 0.747 & -1.508 & 1.118 & -1.95 & 1.084 \\
\hline
\end{tabular}
\caption{Binding energy $E_{\text{polaron}} - E_{\text{AF}}$ 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. [21]) and the CIHF and CISB method for the Hubbard model, respectively.}
\end{table}

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, 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 band 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 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 $k = (\pm \pi, 0), (0, \pm \pi)$. This finding is also substantiated by exact diagonalization results of the same model on small clusters. Unfortunately, for the full Hubbard model there are no conclusive answers from Quantum Monte Carlo or exact methods yet available.

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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 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 and the analysis of ARPES data that a next-nearest neighbor hopping $t'$ has to be considered in the model. In particular, it has been found 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 extended Hubbard model, which corresponds to Eq. 1 when the hopping $t_{ij}$ is restricted to nearest $\sim t$ and next-nearest $\sim t'$ hopping. In Fig. 2 we fit the resulting spin polaron dispersion to ARPES data on undoped Sr$_2$CuO$_2$Cl$_2$ obtained Wells et al. 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 $\Delta E_2 = E_{(\pi/2,\pi/2) - E_{(0,\pi)}}$ in order to fit two of the three parameters ($t$, $t'$, $U$). Therefore we additionally use our results from Ref. 36 where we have fitted the magnon dispersion of undoped La$_2$CuO$_4$ 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 on-site repulsion should not depend very much on the material we there also use the ratio $U/t$ in our present fit of the spin polaron dispersion for Sr$_2$CuO$_2$Cl$_2$. 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 formalism of the Hubbard model. 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. 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 wave-function in $D \rightarrow \infty$ 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/D corrections in order to construct a CI approach also within the Gutzwiller method.

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. In addition we have obtained a minimum of the spin polaron dispersion at $k = (\pm \pi,0),(0,\pi)$ 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 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 $18 \times 18$ or $20 \times 20$ Hubbard cluster which could substantiate the findings of Ref. 30. 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$_2$CuO$_2$Cl$_2$ from ARPES exper-
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APPENDIX A: GENERALIZED GUTZWILLER APPROXIMATION

Following Ref. [3] the Ansatz for a given inhomogeneous state $\alpha$ can be written as

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

(A1)

$$\hat{B}_i^\alpha = g^{K_i(\alpha)} = \hat{D}_i - \sum_\sigma \mu_{i,\sigma}^{\alpha} n_{i,\sigma} + \eta_{i,\sigma}^{\alpha}$$

(A2)

where the uncorrelated state $|\Phi_0^\alpha\rangle$ is a Slater-determinant with an inhomogeneous density matrix $\alpha$ 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 $\sigma$) and empty sites:

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

(A3)

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

(A4)

The parameters $\mu_{i,\sigma}^{\alpha}$ and $\eta_{i,\sigma}^{\alpha}$ have to be determined variationally. Gebhard [2] has shown that the requirement

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

(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 $|\Phi_0^\alpha\rangle$. Eq. (A5) yields a relation between the variational parameters $\mu_{i,\sigma}^{\alpha}$, $\eta_{i,\sigma}^{\alpha}$ and the variables $x_i^{\alpha}$ 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 $x_i^{\alpha}$ as

$$\hat{B}_i^\alpha = \hat{D}_i \sqrt{1 + x_i^{\alpha}(E_i)^{\alpha}} + \sum_\sigma \hat{S}_{i,\sigma} \sqrt{1 - x_i^{\alpha}(S_i^{1/2} - \alpha)}$$

and

$$\hat{E}_i \sqrt{1 + x_i^{\alpha}(D_i)^{\alpha}}.$$  

(A6)

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

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

(A7)

which will be used in the following.

First the double occupancy can be evaluated as

$$\langle \Psi^\alpha | \hat{D}_i | \Psi^\alpha \rangle = \langle \Phi_0^\alpha | \hat{D}_i | \Phi_0^\alpha \rangle$$

(A8)

which allows one to perform the variations with respect to the double occupancy $D_i^{\alpha}$ instead of $x_i^{\alpha}$ (or $q_{i,\sigma}^{\alpha}$, and $\eta_{i,\sigma}^{\alpha}$). Analogously the hopping term of Eq. (1) is given by

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

(A9)

with the hopping renormalization factors

$$q_{i,\sigma}^{\alpha} = \frac{1 - \langle \hat{n}_{i,-\sigma} \rangle^{\alpha}}{\langle \hat{E}_i \rangle^{\alpha}} \sqrt{\langle S_i^{\alpha} \rangle^{\alpha} \langle \hat{S}_{i,\sigma} \rangle^{\alpha}}$$

(A10)

Similar than in Eq. (A5) expectation values of a projection operator $P_i = \hat{D}_i$, $\hat{S}_{i,\sigma}$, $\hat{E}_i$ with regard to $|\Psi^\alpha\rangle$ have been denoted with calligraphic letters. The above representation of the hopping factors allows for a interpretation of the renormalized kinetic energy in terms of probability ratios [14]. Consider the term $q_{i,\sigma}^{\alpha} c_{i,\sigma} |\Phi_0^\alpha\rangle$ which is the sum of two processes: The contribution $\sim c_{i,\sigma} (1 - \langle \hat{n}_{i,-\sigma} \rangle^{\alpha})$ originates from the annihilation of a singly occupied (and thus creation of an empty) site and is weighted by the ratios between projected and unprojected probabilities of this process. The contribution $\sim c_{i,\sigma} \langle \hat{n}_{i,-\sigma} \rangle^{\alpha}$ weights in a similar way the annihilation of an electron on a doubly occupied site.

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

$$S_{\alpha,\beta} = \langle \Psi^{\beta} | \Psi^{\alpha} \rangle = \prod_i \langle \Phi_0^\alpha | \hat{B}_i^\alpha | \Phi_0^\alpha \rangle$$

(A11)

$$= \prod_i \left\{ \sum_\sigma \sqrt{\langle \hat{S}_{i,\sigma} \rangle^{\alpha} \langle \hat{S}_{i,\sigma} \rangle^{\beta}} \langle \Phi_0^\alpha | \hat{S}_{i,\sigma} | \Phi_0^\beta \rangle \right\}$$
where we have used Eqs. (A6, A7, A8) and the fact that only local contractions survive in infinite dimensions. Eq. (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

\[
\langle \Phi_0^\alpha | \hat{D}_i | \Phi_0^\beta \rangle = [\hat{n}_{i,\alpha}]_{\alpha\beta} \quad (A12)
\]

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

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

\[
\langle \Phi_0^\alpha | \hat{P}_i | \Phi_0^\beta \rangle \leq \sqrt{\langle \Phi_0^\alpha | \hat{P}_i | \Phi_0^\beta \rangle \langle \Phi_0^\beta | \hat{P}_i | \Phi_0^\alpha \rangle} \quad (A13)
\]

\[
\sqrt{\langle \Phi_0^\alpha | \hat{P}_i | \Phi_0^\beta \rangle} \leq \frac{\langle \Phi_0^\alpha | \hat{P}_i | \Phi_0^\beta \rangle + \langle \Phi_0^\beta | \hat{P}_i | \Phi_0^\alpha \rangle}{2} \quad (A14)
\]

yields

\[
\langle \Phi_0^\alpha | \hat{B}_i^\alpha c_{i,\sigma} \hat{B}_i^\beta | \Phi_0^\beta \rangle \leq 1 \quad (A15)
\]

where the equals sign holds for \( \alpha = \beta \).

Analogously to \( S \) one can evaluate the matrix elements of the hopping term Eq. (1). For the double occupancy operator one obtains

\[
\langle \Psi^{\alpha} | \hat{D}_i | \Psi^{\beta} \rangle = \frac{\langle \Phi_0^\alpha | \hat{B}_i^\alpha \hat{D}_i \hat{B}_i^\beta | \Phi_0^\beta \rangle}{\langle \Phi_0^\alpha | \hat{B}_i^\beta \hat{B}_i^\beta | \Phi_0^\beta \rangle} S_{\alpha\beta} \quad (A16)
\]

and the matrix elements of the hopping term are given by

\[
\langle \Psi^{\alpha} | c_{i,\sigma}^\dagger c_{j,\sigma} | \Psi^{\beta} \rangle = \frac{\langle \Phi_0^\alpha | \hat{B}_i^\alpha c_{i,\sigma}^\dagger \hat{B}_j^\beta c_{j,\sigma} | \Phi_0^\beta \rangle}{\langle \Phi_0^\alpha | \hat{B}_i^\beta \hat{B}_j^\beta | \Phi_0^\beta \rangle} S_{\alpha\beta} \quad (A17)
\]

Using Eqs. (A6, A7, A8), the projections of the creation and annihilation operators can be expressed as

\[
\hat{B}_i^\alpha c_{i,\sigma}^\dagger \hat{B}_i^\beta = \left[ (1 - n_{i,-\sigma}) \sqrt{\frac{S_{\alpha\sigma}^\beta g_i}{\langle E_i \rangle}} \right] c_{i,\sigma} \quad (A18)
\]

\[
\hat{B}_j^\beta c_{j,\sigma}^\dagger \hat{B}_j^\alpha = \left[ (1 - n_{j,-\sigma}) \sqrt{\frac{S_{\beta\sigma}^\alpha g_j}{\langle E_j \rangle}} \right] c_{j,\sigma} \quad (A19)
\]

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) by the following argument. With regard to the matrix element Eq. (A17) the projection Eq. (A18) describes the annihilation of a particle with spin \( \sigma \) in the Slater determinant \( |\Phi_0^\alpha \rangle \). The two contributions measure the probability whether site \( i \) in the state \( \alpha \) is singly or doubly occupied. Accordingly we replace the corresponding projections by their mean-values, e.g. \( 1 - n_{i,-\sigma} \rightarrow 1 - \langle n_{i,-\sigma} \rangle \). In the same way Eq. (A19) describes the annihilation of a particle with spin \( \sigma \) in the Slater-determinant \( |\Phi_0^\beta \rangle \) and we approximate in this case \( 1 - n_{i,-\sigma} \rightarrow 1 - \langle n_{i,-\sigma} \rangle \). Within this approximation one obtains for the projected creation and annihilation operators

\[
\hat{B}_i^\alpha c_{i,\sigma}^\dagger \hat{B}_i^\beta = q_{\alpha,\sigma}^i q_{\beta,\sigma}^i \quad (A20)
\]

\[
\hat{B}_j^\beta c_{j,\sigma}^\dagger \hat{B}_j^\alpha = q_{\beta,\sigma}^j q_{\alpha,\sigma}^j \quad (A21)
\]

where the \( q_{\alpha,\sigma}^i \) are equivalent to the renormalization factors Eq. (B9) 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’ and thus \( S_{\alpha\beta} = \delta_{\alpha\beta} \). Therefore we find that within the ‘infinite D’ prescription of the Gutzwiller approximation different inhomogeneous states are orthogonal to each other. As a consequence it turns out from Eqs. (A16, 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 non-interacting state \( |\Phi_0^\alpha \rangle \) as

\[
|\Phi_0^\alpha \rangle = |\varphi_1^\alpha \rangle \otimes |\varphi_2^\alpha \rangle \quad (B1)
\]

|\varphi_\sigma^\alpha \rangle = a_{i,\sigma}^\alpha a_{2,\sigma}^\alpha a_{3,\sigma}^\alpha \ldots a_{N,\sigma}^\alpha |0 \rangle \quad (B2)

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

\[
a_{i,\sigma}^\alpha = \sum_i \phi_{i,\sigma}(k) c_{i,\sigma} \quad (B3)
\]

which defines the specific inhomogeneous solution. Details for the calculation of the amplitudes \( \phi_{i,\sigma}(k) \) within the Gutzwiller approximation can be found in Ref. [4].
Within these definitions the evaluation of matrix elements between different Slater determinants is analogous to the scheme outlined in Ref. 16. Here we have defined the single-particle matrix elements as

\[ \langle k^\sigma_i | n^\sigma_i \rangle = \sum_k \phi^\sigma_i (k) \phi^\sigma_i (q) \quad (B4) \]

\[ \langle k^\sigma_i | n^\sigma_i \rangle = \phi^\sigma_i (k) \phi^\sigma_i (q). \quad (B5) \]

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

\[
\langle \Phi^\beta_0 | \Phi^\alpha_0 \rangle = \begin{vmatrix}
\langle 1^\alpha_1 | 1^\beta_1 \rangle & \langle 1^\alpha_1 | 2^\beta_1 \rangle & \cdots & \langle 1^\alpha_1 | N^\beta_1 \rangle \\
\langle 2^\alpha_1 | 1^\beta_1 \rangle & \langle 2^\alpha_1 | 2^\beta_1 \rangle & \cdots & \langle 2^\alpha_1 | N^\beta_1 \rangle \\
\vdots & \vdots & \ddots & \vdots \\
\langle N^\alpha_1 | 1^\beta_1 \rangle & \langle N^\alpha_1 | 2^\beta_1 \rangle & \cdots & \langle N^\alpha_1 | N^\beta_1 \rangle \\
\end{vmatrix}
\]

(B6)

\[
[\hat{n}_{i,\sigma}]_{\alpha,\beta} = \begin{vmatrix}
\langle 1^\alpha_i | n^\alpha_i \rangle | 1^\beta_{i,\sigma} \rangle & \langle 1^\alpha_i | n^\alpha_i \rangle | 2^\beta_{i,\sigma} \rangle & \cdots & \langle 1^\alpha_i | n^\alpha_i \rangle | N^\beta_{i,\sigma} \rangle \\
\langle 2^\alpha_i | n^\alpha_i \rangle | 1^\beta_{i,\sigma} \rangle & \langle 2^\alpha_i | n^\alpha_i \rangle | 2^\beta_{i,\sigma} \rangle & \cdots & \langle 2^\alpha_i | n^\alpha_i \rangle | N^\beta_{i,\sigma} \rangle \\
\vdots & \vdots & \ddots & \vdots \\
\langle N^\alpha_i | n^\alpha_i \rangle | 1^\beta_{i,\sigma} \rangle & \langle N^\alpha_i | n^\alpha_i \rangle | 2^\beta_{i,\sigma} \rangle & \cdots & \langle N^\alpha_i | n^\alpha_i \rangle | N^\beta_{i,\sigma} \rangle \\
\end{vmatrix}
\]

(B7)