Inhomogeneous Gutzwiller approximation with random phase fluctuations for the Hubbard model

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We present a detailed study of the time-dependent Gutzwiller approximation for the Hubbard model. The formalism, labeled GA+RPA, allows us to compute random-phase-approximation-like (RPA) fluctuations on top of the Gutzwiller approximation (GA). No restrictions are imposed on the charge and spin configurations which makes the method suitable for the calculation of linear excitations around symmetry-broken solutions. Well-behaved sum rules are obeyed as in the Hartree-Fock (HF) plus RPA approach. Analytical results for a two-site model and numerical results for charge-charge and current-current dynamical correlation functions in one and two dimensions are compared with exact and HF+RPA results, supporting the much better performance of GA+RPA with respect to conventional HF+RPA theory.

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I. INTRODUCTION

The Gutzwiller variational wave function, together with the Gutzwiller approximation (GA),[1] is a widely used approach in order to deal with Hubbard-type models. Originally introduced in order to explore the possibility of ferromagnetism within the Hubbard model (see, e.g., Ref. 2, and references therein) its popularity resides in the fact that it captures correlation effects like the band narrowing already on the variational level. More recently the GA has also been used for realistic band structure computations.[2–4] Since in the Hubbard model one has a competition between delocalization, from the hopping of the charge carriers, and localization, from the onsite interaction U, the idea is to apply a projector to a given Slater determinant which reduces the number of doubly occupied sites. Within the GA, one has to minimize an energy functional which is composed of a renormalized kinetic term and the interaction energy UD, where D denotes the concentration of doubly occupied sites.

On the other hand, mean-field theories, like Hartree-Fock (HF) theory, are usually only the first step in a many-body computation and it is often desirable to include the effect of fluctuations within the random-phase approximation (RPA). In case of the HF approach this has been achieved by numerous techniques (for an overview see, e.g., Ref. 5), however, the development of a similar scheme in the GA has been a long-standing problem of the condensed-matter many-body community. The major step in this direction was the reformulation of the GA by Kotliar and Ruckenstein (KR) within the so-called four slave-boson approach.[6] This method maps the physical hole (or particle) into products of fermionic and bosonic operators where the latter additionally label the occupancy of the site. At the saddle-point level the bosons are replaced by their mean-field values and one recovers the GA energy functional showing its underlying mean-field character.

The KR slave-boson formulation offers the possibility of going beyond the Gutzwiller result by the inclusion of transversal spin degrees of freedom.[7] Moreover, in principle, it provides a controlled scheme of including fluctuations beyond the mean-field solution. However, the expansion of the KR hopping factor z^{SB} is a highly nontrivial task, both with respect to the proper normal ordering of the bosons and with respect to the correct continuum limit of the functional integral.[8] Expansions around the slave-boson saddle point were performed for homogeneous systems in Refs. 9 and 10 in order to calculate correlation functions in the charge and longitudinal spin channels. Furthermore, the optical conductivity in the paramagnetic regime of the Hubbard model was calculated in Ref. 11. A severe difficulty in this approach is the fact that the KR choice for the hopping factor does not lead to controlled sum rules.[12] Moreover, to our knowledge, this approach has not been extended to symmetry broken states due to the complexity of the computation.

Recently, two of us have presented a computation of RPA fluctuations on top of GA states (GA+RPA).[13] Our approach borrows ideas from well developed techniques in nuclear physics,[14] and RPA fluctuations are obtained in the small oscillation limit of a time-dependent Gutzwiller approximation. Since response functions are derived for systems with completely unrestricted charge and spin distributions, GA+RPA is also suitable for the calculation of charge excitations of inhomogeneous textures. A key point of the GA+RPA approach is the proper determination of the time dependence of the variational double occupancy parameter. We have adopted an antiadiabatic approximation in the sense that the double occupancy adjusts instantaneously to the time evolution of the single particle densities. In this context our approach can be viewed as a generalization of the Fermi liquid analysis of Vollhardt.[15] In this paper we use the GA+RPA to compute various correlation functions in the one-band Hubbard model and compare them with exact diagonalization and HF+RPA results.

This paper is organized as follows. In Sec. II we present the formalism. We concentrate on the case of the one-band Hubbard model although generalization to more complicated

models is straightforward. From the expansion of the GA energy functional up to second order in the densities, we demonstrate how the RPA response functions can be calculated and show that standard sum rules are obeyed. The method is illustrated in Sec. III for the two-site Hubbard model, which can be treated analytically. Finally, in Sec. IV we compare the GA+RPA excitation spectra with exact diagonalization and HF+RPA results respectively.

II. MODEL AND FORMALISM

We consider 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 onsite Hubbard repulsion and t_{ij} denotes the hopping parameter between sites i and j.

A. Gutzwiller approximation

In its original formulation, the GA yields an approximation for the energy of a uniform paramagnetic system.[1] Only in the late 80's this approach has been consistently generalized to an unrestricted Slater determinant within the Kotliar and Ruckenstein slave-boson approach.[6] The same unrestricted Gutzwiller energy functional was obtained by Gebhard,[16] exploiting the fact that the GA becomes the exact solution of the Gutzwiller variational problem in the limit of infinite spatial dimensions.[17]

In Gebhard's formulation the variational wave function is written as[4,16]

$$|\Psi\rangle=\prod_{i}\frac{\hat{U}_i}{K_i^{1/2}}|\mathrm{SD}\rangle, \tag{2}$$

$$\hat{U}_i=\exp\left(-\gamma_i n_{i,\uparrow}n_{i,\downarrow}-\sum_{\sigma}\mu_{i,\sigma}n_{i,\sigma}\right) \tag{3}$$

where $K_i=\langle\Psi|\hat{U}_i\hat{U}_i|\Psi\rangle$. In Eq. (2) $|\mathrm{SD}\rangle$ denotes a Slater determinant which already incorporates the Hartree contribution of the local interactions and which has to be determined variationally. The solution of the variational problem in the limit of infinite dimensions turns out to be the GA generalized to an arbitrary charge and spin distribution of the SD. The $\mu_{i,\sigma}$ act as local chemical potentials and are determined within the GA by the infinite dimension prescription that the diagonal charges are not renormalized:

$$\langle\Psi|n_{i,\sigma}|\Psi\rangle=\langle\mathrm{SD}|n_{i,\sigma}|\mathrm{SD}\rangle.$$

As a result one obtains, for the GA energy functional,[6,16]

$$E^{GA}[\rho,D]=\sum_{ij,\sigma} t_{ij}z^{GA}_{i,\sigma}z^{GA}_{j,\sigma}\rho_{ji,\sigma}+U\sum_{i} D_i,$$

$$z^{GA}_{i,\sigma}=\frac{\sqrt{(1-\rho_{ii}+D_i)(\rho_{ii,\sigma}-D_i)}+\sqrt{D_i(\rho_{ii,-\sigma}-D_i)}}{\sqrt{\rho_{ii,\sigma}(1-\rho_{ii,\sigma})}}, \tag{4}$$

which is a functional of the density matrix $\rho_{ij,\sigma}\equiv\langle\mathrm{SD}|c^{\dagger}_{j,\sigma}c_{i,\sigma}|\mathrm{SD}\rangle$ and the double occupancy parameters D_i. We denote the set of all matrix elements $\{\rho_{ij,\sigma}\}$ and $\{D_i\}$ by ρ and D. Note that in this paper we do not consider spin-canted solutions which would have density matrix elements $\langle\mathrm{SD}|c^{\dagger}_{j,\sigma}c_{i,\sigma'}|\mathrm{SD}\rangle\neq 0$ for $\sigma\neq\sigma'$. However, transverse spin degrees of freedom can be straightforwardly incorporated within the spin-rotationally invariant slave-boson formulation.[7]

We will denote by $|\Psi_0\rangle$ the particular wave function of form [Eq. (2)] that minimizes the energy. In order to obtain the corresponding stationary solution $\rho^{(0)},D^{(0)}$ one has to minimize E^{GA} with respect to the double occupancy parameters D and the density matrix ρ, where the latter variation has to be constrained to the subspace of Slater determinants by imposing the projector condition $\rho^2=\rho$,[18,19]

$$\delta\{E^{GA}[\rho,D]-\mathrm{tr}[\Lambda(\rho^2-\rho)]\}=0, \tag{5}$$

where Λ denotes the Lagrange parameter matrix. It is convenient to define a Gutzwiller Hamiltonian[18,19]

$$h_{ij\sigma}[\rho,D]=\frac{\partial E^{GA}}{\partial\rho_{ji\sigma}}, \tag{6}$$

which is also a functional of ρ and D. Variation of Eq. (5) with respect to the density matrix leads to

$$h-\rho\Lambda-\Lambda\rho+\Lambda=0. \tag{7}$$

The Lagrange parameters can be eliminated[19] and together with the variation with respect to D we obtain the self-consistent GA equations

$$[h,\rho]=0, \tag{8}$$

$$\frac{\partial E^{GA}}{\partial D_i}=0. \tag{9}$$

The first equation can be solved by diagonalizing both the Gutzwiller Hamiltonian and the density matrix by a linear transformation of the single-particle orbital basis,

$$c_{i,\sigma}=\sum_{\nu}\psi_{i,\sigma}(\nu)a_{\nu}, \tag{10}$$

leading to $h^0_{\mu\nu}=\delta_{\mu\nu}\epsilon_{\nu}$. Moreover, the diagonalized density matrix $\rho\equiv\rho^{(0)}$ has an eigenvalue 1 below the Fermi level, and an eigenvalue 0 above it. We use Greek letters to denote any state of this particular basis, and the zero indicates evaluation in the saddle point. Additionally, we denote states be-

low the Fermi level as hole (h) states and the states above the Fermi level as particle states (p).

Notice that in this base $(\rho^{(0)})^2=\rho^{(0)}$ is trivially satisfied. $\rho^{(0)}$ acts as a projector onto the hole states of the saddle-point Slater determinant in the space of the density matrices whereas $\sigma^{(0)}\equiv 1-\rho^{(0)}$ corresponds to the projector onto particle states.

The diagonalization of Eq. (8) has to be supplemented by a minimization of the Gutzwiller energy with respect to the double occupancy parameters of Eq. (9). For this purpose, a convenient method in order to obtain inhomogeneous GA solutions was discussed in Ref. 20. Note that the unrestricted variational procedure with respect to charge and (or) spin degrees of freedom prevents the occurrence of the Brinkmann-Rice transition toward localization,[21] which was already shown in Ref. 22 for Neél-type antiferromagnetism.

B. Derivation of the RPA equation

Before starting our analysis it is convenient for later use to define the GA effective operator

$$O^{GA}=\sum_{ij\sigma}\ (o^{GA}_{ij,\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}+\text{H.c.}), \tag{11}$$

where $o^{GA}_{ij\sigma}=q_{ij\sigma}o_{ij,\sigma}$ and $q_{ij\sigma}=1$ if $i=j$ and $q_{ij\sigma}=z^{GA}_{i,\sigma}z^{GA}_{j,\sigma}$ otherwise. In order to derive the RPA equation we introduce a small time-dependent external field added to Eq. (1),

$$F(t)=\sum_{ij\sigma}\ (f_{ij,\sigma}(t)c^{\dagger}_{i\sigma}c_{j\sigma}+\text{H.c.}), \tag{12}$$

with $f_{ij,\sigma}(t)=f_{ij,\sigma}(0)e^{-i\omega t}$. As a consequence $|\Psi\rangle$, $|\text{SD}\rangle$, and the variational parameters acquire a time dependence and an additional term appears in the energy functional [Eq. (4)],

$$E^{GA}_f[\rho,D](t)=\langle\Psi(t)|H_f(t)|\Psi(t)\rangle$$

$$=\sum_{ij\sigma}\ (f^{GA}_{ij\sigma}\rho_{ji,\sigma}e^{-i\omega t}+\text{H.c.}), \tag{13}$$

where $f^{GA}_{ij\sigma}=q_{ij\sigma}f_{ij,\sigma}$.

The time-dependent field induces small amplitude oscillations of D and ρ around the GA saddle point:

$$D=D^{(0)}+\delta D(t), \tag{14}$$

$$\rho=\rho^{(0)}+\delta\rho(t). \tag{15}$$

The density and double occupancy fluctuations are constrained by the following requirements:

(i) At all times ρ is constrained to be the one-body density matrix associated with a Slater determinant. This can be achieved by imposing

$$\rho=\rho^2. \tag{16}$$

(ii) The double occupancy is assumed to have a much faster dynamics than the density matrix so that it can be treated antiadiabatically. As a consequence, δD adjusts instantaneously to the evolution of the density matrix via the condition

$$\frac{\partial E^{GA}[\rho,D]}{\partial\delta D_i}=0. \tag{17}$$

In fact Eq. (17) constitutes the basic hypothesis of the present formalism which is necessary in order to derive an effective *Gutzwiller interaction* between particles (see below). We expect this approximation to be accurate for sufficiently low-energy excitations. At high energies one can check the accuracy and the limits of validity of this approximation by comparing with exact diagonalization, as done in the following sections. Surprisingly, it turns out to be accurate at least up to energies of the order of the Mott-Hubbard gap.

As in any small amplitude approximation, we start by expanding the GA energy [Eqs. (4) and (13)] around the saddle point. The first part [Eq. (4)], is needed up to second order in the density and double occupancy deviations:

$$E^{GA}[\rho,D]=E_0+\text{tr}(h^0\delta\rho)+\sum_{ij,\sigma}\ t_{ij}[z^{GA}_{i,\sigma}\delta_1 z^{GA}_{j,\sigma}$$

$$+z^{GA}_{j,\sigma}\delta_1 z^{GA}_{i,\sigma}]\delta\rho_{ji,\sigma}+\sum_{ij,\sigma}\ t_{ij}\rho_{ji,\sigma}\delta_1 z^{GA}_{i,\sigma}\delta_1 z^{GA}_{j,\sigma}$$

$$+\sum_{ij,\sigma}\ t_{ij}\rho_{ji,\sigma}[z^{GA}_{i,\sigma}\delta_2 z^{GA}_{j,\sigma}+z^{GA}_{j,\sigma}\delta_2 z^{GA}_{i,\sigma}]. \tag{18}$$

Here E_0 denotes the saddle-point (mean-field) energy, and the trace includes sum over spins. We have used the following abbreviations for the z-factor expansion:

$$\delta_1 z^{GA}_{i,\sigma}\equiv\frac{\partial z^{GA}_{i,\sigma}}{\partial D_i}\delta D_i+\sum_{\sigma'}\ \frac{\partial z^{GA}_{i,\sigma}}{\partial\rho_{ii,\sigma'}}\delta\rho_{ii,\sigma'}, \tag{19}$$

$$\delta_2 z^{GA}_{i,\sigma}\equiv\frac{1}{2}\frac{\partial^2 z^{GA}_{i,\sigma}}{\partial D_i^2}(\delta D_i)^2+\sum_{\sigma'}\ \frac{\partial^2 z^{GA}_{i,\sigma}}{\partial D_i\partial\rho_{ii,\sigma'}}\delta D_i\delta\rho_{ii,\sigma'}$$

$$+\frac{1}{2}\sum_{\sigma'\sigma''}\ \frac{\partial^2 z^{GA}_{i,\sigma}}{\partial\rho_{ii,\sigma'}\partial\rho_{ii,\sigma''}}\delta\rho_{ii,\sigma'}\delta\rho_{ii,\sigma''}. \tag{20}$$

To proceed further it is convenient to cast the second order expression in matrix form

$$E^{GA}[\rho,D]=E_0+\text{tr}(h^0\delta\rho)+\frac{1}{2}\delta\rho_{ji,\sigma}L^{\sigma\sigma'}_{ijkl}\delta\rho_{lk,\sigma'}$$

$$+\frac{1}{2}\delta D_i K_{ij}\delta D_j+\delta D_i S_{i,kl\sigma}\delta\rho_{lk\sigma}, \tag{21}$$

where the matrix multiplications imply the Einstein sum convention and the definitions for the matrices L, K, and S follow immediately from Eqs. (18), (19), and (20). The nonzero matrix elements are given by

$$
\begin{aligned}
L^{\sigma\sigma'}_{ii,ii} &= \sum_{j\sigma''} t_{ij} \frac{\partial^2 z_{i,\sigma''}}{\partial\rho_{ii,\sigma}\partial\rho_{ii,\sigma'}} z_{j,\sigma''}(\rho_{ij,\sigma''}+\rho_{ji,\sigma''}),\\
L^{\sigma\sigma'}_{ii,jj} &= \sum_{\sigma''} t_{ij} \frac{\partial z_{i,\sigma''}}{\partial\rho_{ii,\sigma}} \frac{\partial z_{j,\sigma''}}{\partial\rho_{jj,\sigma}}(\rho_{ij,\sigma''}+\rho_{ji,\sigma''}), \quad i\neq j,\\
L^{\sigma\sigma'}_{ii,ij} &= L^{\sigma'\sigma}_{ij,ii} = t_{ij}\frac{\partial z_{i,\sigma'}}{\partial\rho_{ii,\sigma}} z_{j,\sigma'}, \quad i\neq j,\\
K_{ii} &= \sum_{j\sigma} t_{ij} \frac{\partial^2 z_{i,\sigma}}{D_i^2} z_{j,\sigma}(\rho_{ij,\sigma}+\rho_{ji,\sigma}),\\
K_{ij} &= \sum_{\sigma} t_{ij} \frac{\partial z_{i,\sigma}}{\partial D_i}\frac{\partial z_{j,\sigma}}{\partial D_j}(\rho_{ij,\sigma}+\rho_{ji,\sigma}), \quad i\neq j,\\
S_{i,ii\sigma} &= \sum_{j\sigma'} t_{ij} \frac{\partial^2 z_{i,\sigma'}}{\partial D_i\partial\rho_{ii,\sigma}} z_{j,\sigma'}(\rho_{ij,\sigma'}+\rho_{ji,\sigma'}),\\
S_{i,jj\sigma} &= t_{ij}\sum_{\sigma'} \frac{\partial z_{i,\sigma'}}{\partial D_i}\frac{\partial z_{j,\sigma'}}{\partial\rho_{jj,\sigma}}(\rho_{ij,\sigma'}+\rho_{ji,\sigma'}), \quad i\neq j,\\
S_{i,ij\sigma} &= t_{ij}\frac{\partial z_{i,\sigma}}{\partial D_i} z_{j,\sigma}, \quad i\neq j.
\end{aligned}
\tag{22}
$$

Note the formal similarity between Eq. (21) and an electron-boson problem where particle-hole excitations interact with a bosonic degree of freedom in place of D. The matrix K plays the role of a double occupancy stiffness, and S that of a double occupancy-electron interaction.

We can integrate out the D fluctuations using the antiadiabaticity condition [Eq. (17)]. First, we express δD_i in terms of the density fluctuations via

$$
\delta D_i = -(K^{-1})_{ij} S_{j,kl\sigma}\delta\rho_{lk,\sigma}, \tag{23}
$$

which finally yields an expansion of the energy as a functional of $\delta\rho$ alone $\tilde{E}[\rho]\equiv E^{GA}[\rho,D(\rho)]$:

$$
\tilde{E}[\rho] = E_0 + \mathrm{tr}(h^0\delta\rho) + \frac{1}{2}\delta\rho_{ji,\sigma}[L_0 - S_0^\dagger K_0^{-1} S_0]^{\sigma\sigma'}_{ijkl}\delta\rho_{lk,\sigma'}. \tag{24}
$$

Note that we could also have derived Eq. (24) within the KR slave-boson approach. The corresponding transformations for the derivatives are given in the Appendix.

The matrix $(L_0 - S_0^\dagger K_0^{-1} S_0)$ can be considered as an effective interaction kernel between particle-hole excitations in the GA. For the paramagnetic regime this kernel reduces to the quasiparticle kernel of Vollhardt's Fermi liquid analysis.[15] Interestingly, the off-diagonal elements of the matrices K_{ij}, $L^{\sigma\sigma'}_{ijkl}$, and $S_{i,kl\sigma}$ can induce intersite interactions between the GA quasiparticles. This is in contrast to conventional HF theory of the Hubbard model which is purely local.

The expansion of $E_f^{GA}[\rho,D]$ [Eq. (13)], is needed up to first order only, since it is linear in the external field:

$$
\begin{aligned}
E_f^{GA}[\rho,D] = F_0 + \mathrm{tr}(f_0^{GA}\delta\rho) &+ \sum_{ijk\sigma\sigma'} \rho^0_{ji,\sigma} f_{ij,\sigma}\frac{\partial q_{ij\sigma}}{\partial\rho_{kk\sigma'}}\delta\rho_{kk\sigma'}\\
&+ \sum_{ijk\sigma} \rho^0_{ji,\sigma} f_{ij,\sigma}\frac{\partial q_{ij\sigma}}{\partial D_k}\delta D_k .
\end{aligned}
\tag{25}
$$

Here $F_0 = f_0^{GA}\rho^{(0)}$ describes the energy contribution when the system would be frozen at the saddle-point level and we used the fact that $q_{ij\sigma}$ does not depend on off-diagonal densities. As before, the double occupancy fluctuations can be eliminated through Eq. (23). We define $\tilde{E}_f^{GA}[\rho] \equiv E_f^{GA}[\rho,D(\rho)]$ and

$$
\tilde{f}_{ij\sigma} \equiv \frac{\partial\tilde{E}_f^{GA}[\rho]}{\partial\rho_{ji\sigma}}. \tag{26}
$$

In this paper we will restrict ourselves to density-density and current-current response functions, with the current operator given by

$$
\mathbf{J} = \sum_{\langle ij\rangle} \mathbf{j}_{ij}, \tag{27}
$$

and

$$
\mathbf{j}_{ij} = -i\sum_{\sigma} t_{ij}(c^\dagger_{i\sigma}c_{j\sigma} - c^\dagger_{j\sigma}c_{i\sigma}).
$$

When only densities are involved $f_{ij\sigma}$ is diagonal in the site index, only $q_{ii\sigma}=1$ is present and the last two terms in Eq. (25) vanish. If currents are involved it is easy to show directly from Eq. (25) that the last two terms also vanish in the absence of currents in the ground state, i.e., $\tilde{f}_0 = f_0^{GA}$.

Now, we proceed in analogy with the nuclear physics treatment of effective mean-field theories in which the interaction potential is density dependent.[18,19] Indeed Eq. (24) can be viewed as the energy expansion of an effective mean-field theory with the only difference that part of the density dependence is due to the GA hopping renormalization factors in the *kinetic* part of the Hamiltonian. The advantage of this method with respect to other methods (e.g., equation of motion or diagrammatic methods) is that the present derivation is solely based on the knowledge of an energy functional associated with a Slater determinant which is precisely what the Gutzwiller approximation provides.

The density matrix of an effective mean-field theory of this kind obeys the equation of motion[18,19]

$$
i\hbar\dot{\rho} = [\tilde{h}[\rho] + \tilde{f}(t), \rho], \tag{28}
$$

where we have defined an effective Gutzwiller Hamiltonian

$$
\tilde{h}_{ij\sigma}[\rho] = \frac{\partial\tilde{E}}{\partial\rho_{ji\sigma}}, \tag{29}
$$

which depends on densities only. At the saddle-point, we have $\tilde{h}_0 = \tilde{h}[\rho^{(0)}] = h_0$. The RPA is obtain by considering the limit of small amplitude fluctuations in Eq. (28).

It is convenient to define the four sub-sectors of the fluctuations of the density matrix using the projector properties of the density matrix discussed above:

$$\delta\rho^{hh} \equiv \rho^{(0)}\delta\rho\rho^{(0)}, \tag{30}$$

$$\delta\rho^{pp} \equiv \sigma^{(0)}\delta\rho\sigma^{(0)}, \tag{31}$$

$$\delta\rho^{hp} \equiv \rho^{(0)}\delta\rho\sigma^{(0)}, \tag{32}$$

$$\delta\rho^{ph} \equiv \sigma^{(0)}\delta\rho\rho^{(0)}. \tag{33}$$

The Slater determinant condition [Eq. (16)] implies that the fluctuations [Eqs. (30)–(33)], are not independent. In fact, in terms of the fluctuations, Eq. (16) reads

$$\delta\rho = \rho^{(0)}\delta\rho + \delta\rho\rho^{(0)} + (\delta\rho)^2. \tag{34}$$

Projecting Eq. (34) onto the hh and pp sector of the saddle point Slater determinant yields

$$\delta\rho^{hh} = -(1+\delta\rho^{hh})^{-1}\delta\rho^{hp}\delta\rho^{ph} \approx -\delta\rho^{hp}\delta\rho^{ph}, \tag{35}$$

$$\delta\rho^{pp} = (1-\delta\rho^{pp})^{-1}\delta\rho^{ph}\delta\rho^{hp} \approx \delta\rho^{ph}\delta\rho^{hp}, \tag{36}$$

where the right-hand equality is valid in the small amplitude limit. Thus it turns out that pp and hh density projections are quadratic in the ph and hp matrix elements. Therefore, when computing $\tilde{h}$ from Eqs. (24) and (29) one should be aware of the fact that the term $\mathrm{tr}(h^0\delta\rho) = \Sigma_\mu \epsilon_\mu \rho_{\mu\mu}$ (which is first order in the pp and hh density projections) yields a quadratic contribution in the ph and hp matrix elements:

$$\mathrm{tr}(h^0\delta\rho) = \sum_p \epsilon_p \delta\rho_{pp} + \sum_h \epsilon_h \delta\rho_{hh}$$

$$= \sum_{ph} (\epsilon_p - \epsilon_h)\rho_{ph}\rho_{hp}. \tag{37}$$

In addition, one can neglect the pp and hh matrix elements in the last term of Eq. (24). Thus, up to second order in the particle-hole density fluctuations, one obtains, for the energy expansion [Eq. (24)],

$$\tilde{E}[\rho] = E_0 + \frac{1}{2}(\delta\rho^{hp}, \delta\rho^{ph}) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \delta\rho^{ph} \\ \delta\rho^{hp} \end{pmatrix}. \tag{38}$$

Here the so called RPA matrices A and B are given by:

$$A_{ph,p'h'} = (\epsilon_p - \epsilon_h)\delta_{pp'}\delta_{hh'} + \frac{\partial\tilde{h}_{ph}}{\partial\rho_{p'h'}}, \tag{39}$$

$$B_{ph,p'h'} = \frac{\partial\tilde{h}_{ph}}{\partial\rho_{h'p'}}, \tag{40}$$

where the matrix A contains matrix elements between particle-hole excitations, whereas the matrix B is composed of matrix elements between the ground state and two particle-hole excitations. A and B are related to $M \equiv (L_0 - S_0^\dagger K_0^{-1} S_0)$ via

$$A_{ph,p'h'} = (\epsilon_p - \epsilon_h)\delta_{pp'}\delta_{hh'} + \sum_{ij\sigma,nm\sigma'} \psi^*_{i,\sigma}(p)\psi_{j,\sigma}(h) \times M^{\sigma\sigma'}_{ij,nm}\psi^*_{n,\sigma'}(h')\psi_{m,\sigma'}(p'),$$

$$B_{ph,p'h'} = \sum_{ij\sigma,nm\sigma'} \psi^*_{i,\sigma}(h)\psi_{j,\sigma}(p)M^{\sigma\sigma'}_{ij,nm}\psi^*_{n,\sigma'}(h')\psi_{m,\sigma'}(p'),$$

and the transformation amplitudes $\psi_{i,\sigma}(\nu)$ have been defined in Eq. (10).

To lowest order, we can now linearize Eq. (28) retaining only ph and hp matrix elements,

$$i\hbar\,\delta\dot{\rho} = [h_0, \delta\rho] + \left[\frac{\partial\tilde{h}}{\partial\rho}\delta\rho + \tilde{f}, \rho^{(0)}\right], \tag{41}$$

where we use the shorthand notation

$$\frac{\partial\tilde{h}}{\partial\rho}\delta\rho = \sum_{ph}\left(\frac{\partial\tilde{h}}{\partial\rho_{hp}}\delta\rho_{hp} + \frac{\partial\tilde{h}}{\partial\rho_{ph}}\delta\rho_{ph}\right). \tag{42}$$

Then from Eqs. (29), (38), and (41) one obtains the following linear response equation:

$$\left\{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \hbar\omega\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}\begin{pmatrix} \delta\rho^{ph} \\ \delta\rho^{hp} \end{pmatrix} = -\begin{pmatrix} \tilde{f}_{ph} \\ \tilde{f}_{hp} \end{pmatrix}. \tag{43}$$

This inhomogeneous equation can be solved by inverting the matrix on the left-hand side, yielding a linear relation between the external field and the change in the density:

$$\delta\rho = R(\omega)\tilde{f}. \tag{44}$$

We are now in a position to compute the response of a one particle observable

$$O = \sum_{ij\sigma}(o_{ij,\sigma}c^\dagger_{i\sigma}c_{j\sigma} + \mathrm{H.c.}),$$

since, in analogy with Eqs. (12) and (13) its time evolution is given by

$$\langle\Psi(t)|O|\Psi(t)\rangle = \sum_{ij\sigma}[o^{GA}_{ij\sigma}\rho_{ji,\sigma}(t) + \mathrm{H.c.}], \tag{45}$$

and the time evolution of ρ is known from Eq. (44).

The linear response matrix $R(\omega)$ has poles at the eigenfrequencies of the eigenvalue problem corresponding to Eq. (43) with $\tilde{f} = 0$:

$$\left\{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \hbar\Omega_n\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}\begin{pmatrix} X^{(n)} \\ Y^{(n)} \end{pmatrix} = 0. \tag{46}$$

Here $\hbar\Omega_n \equiv E_n - E_0$ denote the excitation energies of the system. In analogy with the HF+RPA approximation the vacuum of these excitations is not the old starting GA state $|\Psi_0\rangle$ but a new state with both Gutzwiller-type correlations

and RPA ground-state correlations. We denote this state by $|\Phi_0\rangle$ and the corresponding exited states by $|\Phi_n\rangle$.

The matrix R can be written in the following Lehmann representation:

$$R(\omega)_{ph,p'h'}=\sum_{n>0}\left[\frac{X^n_{ph}X^{n*}_{p'h'}}{\omega-\Omega_n+i\epsilon}-\frac{Y^n_{p'h'}Y^{n*}_{ph}}{\omega+\Omega_n+i\epsilon}\right]. \quad (47)$$

In analogy with the HF+RPA method, we introduce the following notations:

$$\langle 0|a^\dagger_h a_p|n\rangle\equiv X^n_{ph}, \quad (48)$$

$$\langle 0|a^\dagger_p a_h|n\rangle\equiv Y^n_{hp}. \quad (49)$$

The states $|n\rangle$ are not true excitations of the system but represent auxiliary objects. Roughly speaking, they can be thought of as RPA states without the Gutzwiller projector. For example $|0\rangle$ is the analog of the state $|\mathrm{SD}\rangle$ but at the RPA level (it contains RPA ground-state correlations but lacks Gutzwiller correlations). We will call them unprojected RPA states. The eigenvector $(X^{(n)}_{ph},Y^{(n)}_{hp})$ can be identified with the particle-hole and hole-particle components of the unprojected RPA excited state $|n\rangle$ with respect to the unprojected RPA ground state $|0\rangle$.

Schematically the four states are related in the following way:

$$\begin{array}{ccc} |\mathrm{SD}\rangle & \overset{P}{\rightarrow} & |\Psi_0\rangle \\ \mathrm{RPA}\downarrow & & \downarrow\mathrm{RPA} \\ |0\rangle & \overset{P}{\rightarrow} & |\Phi_0\rangle, \end{array}$$

where P indicates Gutzwiller projection.

Within the above formalism, it is straightforward to evaluate the current-current correlation function. The real part of the optical conductivity consists of a Drude part at $\omega=0$ and a regular part for $\omega>0$:

$$\sigma(\omega)=D\,\delta(\omega)+\pi\sum_{n>0}\frac{|\langle\Phi_n|j_\alpha|\Phi_0\rangle|^2}{E_n-E_0}\delta(\omega-(E_n-E_0)). \quad (50)$$

With the above approximations and notations

$$\langle\Phi_n|j_\alpha|\Phi_0\rangle=\langle n|j^{GA}_\alpha|0\rangle,$$

where the matrix element on the right-hand side can be evaluated using Eqs. (10), (11), (48), and (49). Obviously, the matrix elements within $\sigma(\omega)$ are renormalized by the GA hopping factors whereas $R(\omega)$ does not contain such renormalization. Thus, the latter quantity does not correspond to a physical response function within the GA+RPA approach.

The Drude weight D can be obtained from the f-sum rule (see S^{-1} in Sec. II C)

$$\int_0^\infty d\omega\sigma(\omega)=-\frac{1}{2}\pi\langle T_\alpha\rangle_{GA}, \quad (51)$$

where the kinetic energy in the α-direction $\langle T_\alpha\rangle_{GA}$ is evaluated within the GA.

In practice, for computational purposes, one can use all the standard formulas of the HF+RPA scheme by substituting GA effective operators and excitations for true operators and unprojected excitations $|n\rangle$.

The matrix elements $\langle\Phi_0|O|\Phi_n\rangle=\langle 0|O^{GA}|n\rangle$ can be used to characterize a given RPA excitation. Specific examples which will be considered below are the transition density

$$\delta n^m_i\equiv\langle 0|\hat{n}_i|m\rangle \quad (52)$$

and the transition current

$$\delta\mathbf{j}^n_{ij}\equiv\langle 0|\mathbf{j}^{GA}_{ij}|n\rangle, \quad (53)$$

which can be interpreted as follows. Consider a wave packet

$$|\psi(t)\rangle=\exp(-iE_0t)|\Phi_0\rangle+\eta\exp(-iE_mt)|\Phi_m\rangle,$$

consisting of a small admixture η of an exited state m to the ground state. For example this can be the result of an excitation of the mode m by an appropriate weak external perturbation. The time-dependent expectation value of the charge is then given by

$$\langle\psi(t)|\hat{n}_i|\psi(t)\rangle=\langle 0|\hat{n}_i|0\rangle+\eta\delta n^m_i e^{-i\Omega_m t}+\mathrm{H.c.},$$

and an analogous expression holds for the current. Here $\langle 0|\hat{n}_i|0\rangle=\langle\mathrm{SD}|\hat{n}_i|\mathrm{SD}\rangle$, since one-particle densities are not renormalized by the RPA. We see that the transition charges and currents are proportional to the amplitude of the time-dependent fluctuation that would occur at frequency Ω_m if the state m is excited by a weak perturbation[18] (also see Ref. 23).

C. Sum rules

Sum rules form a very important tool in the theory of collective excitations. In many cases they allow us to calculate global properties in a simple way and therefore they are useful in testing different approximation schemes. In general, a sum rule is related to the kth moment of the excitation strength distribution produced by a single-particle operator O (see, e.g., Ref. 24):

$$S^k\equiv\sum_n(E_n-E_0)^k|\langle\Psi_n|O|\Psi_0\rangle|^2. \quad (54)$$

Within the present scheme we have

$$S^k=\sum_n(E_n-E_0)^k|\langle n|O^{GA}|0\rangle|^2, \quad (55)$$

and we restrict ourselves ourselves to current or density operators for O. The energy sum rule S^1 can be written as a double commutator

$$S^1=\sum_{n=1}(E_n-E_0)|\langle\Psi_n|O|\Psi_0\rangle|^2=\frac{1}{2}\langle\Psi_0|[O,[H,O]|\Psi_0\rangle. \quad (56)$$

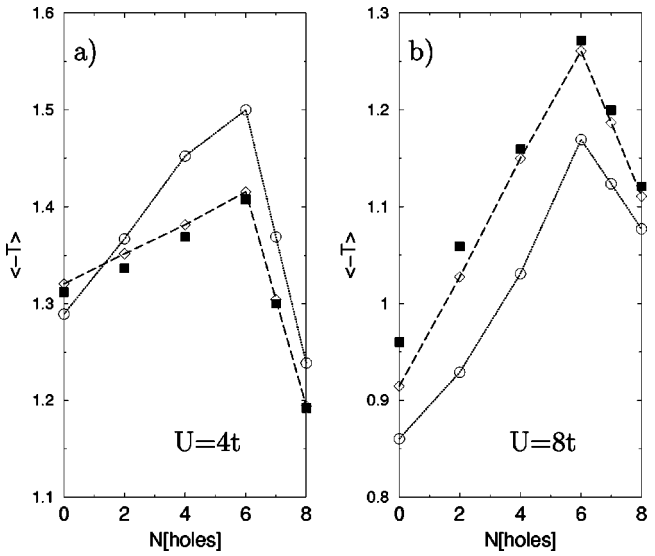

FIG. 1. Kinetic energy per site of a 4×4 Hubbard model for $U/t=4$ (a) and $U/t=8$ (b) with periodic boundary conditions as a function of hole doping. Filled squares: exact result; circles: unrestricted HF approximation; diamonds: unrestricted GA.

In analogy with the derivation by Thouless,[14] one can show that the sum rule Eq. (56) is satisfied if the left-hand side is evaluated at the GA+RPA level and the right-hand side is calculated using the GA ground-state wave function. The same applies for the S^{-1} sum rule, which corresponds to the *f*-sum rule in the case of the optical conductivity discussed above.

In the following, we consider as an example the first moment of the charge-charge correlation function by setting $O \equiv n_i = \Sigma_\sigma n_{i\sigma}$ for some lattice site $\mathbf{R}_i$. It is straightforward to evaluate the double commutator and we find for the corresponding sum rule

$$S_n^1 = -2\sum_{m,i} (E_m - E_0)|\langle 0|n_i|m\rangle|^2 = 2\langle T\rangle_{GA}, \qquad (57)$$

where $\langle T\rangle_{GA}$ denotes the kinetic energy evaluated within the GA.

The sum rules of Eqs. (51) and (57) provide a first encouraging argument that the unrestricted GA could improve the description of charge fluctuation with respect to the corresponding HF method. This is based on the fact that the GA kinetic energy is already renormalized on the mean-field level. In Fig. 1 we compare the exact kinetic energy with unrestricted GA and HF results for various hole concentrations in a Hubbard model (4×4 lattice) with nearest neighbor hopping $t_{ij}=-t$. The GA Slater determinants have been obtained using the method described in Ref. 20. Note that for this small system it is in general not a problem to find the true mean-field ground state via the variational procedure. We usually performed several runs starting from different initial configurations and checked the stability of the resulting states by adding some noise to the solutions. These are in general characterized by an inhomogeneous charge distribution except for the closed shell configurations.

For small values of U/t there is almost perfect agreement between the GA method and the exact results. In this limit, where kinetic effects dominate the correlation part, HF overestimates the value of $\langle -T\rangle$ since the corresponding quasiparticle hopping between sites *i* and *j* is described by the bare matrix elements t_{ij}. On the other hand, for $U/t=8$ the large HF on-site renormalization (corresponding to an overestimate of the spin polarization) is the reason kinetic energy is lower than the exact result. In contrast, the values of $\langle -T\rangle$ in the GA approximation correctly reproduce the exact result, especially in the high-doping regime, where the spin density is reduced in large parts of the lattice. It follows that the first moment of a density-density correlation function will be more accurate in the GA+RPA approximation than in the HF+RPA approximation. The same holds for the S^{-1}-sum rule of the optical conductivity.

To summarize this section, the idea of our method is to supplement the Gutzwiller approximation with RPA fluctuations analogous to the HF+RPA approach.[25] Since the GA provides a much better initial saddle-point than the HF approach one can expect that the fluctuation corrections within the GA+RPA will allow a more accurate description of correlation effects than the HF+RPA approach. In the remaining sections we analyze in detail small data cases to test the domain of applicability of the method, and we finally show some applications in larger systems.

III. TWO-SITE HUBBARD MODEL

In order to demonstrate the method developed above, we consider in the following the two-site Hubbard model which can be solved exactly and can be studied analytically in both the GA+RPA and HF+RPA approximations.

Exact ground-state energy and double occupancy at half-filling (i.e., two particles) are given by

$$E_0 = \frac{U}{2}[1-\sqrt{1+(4t/U)^2}]$$

and

$$\langle n_\uparrow n_\downarrow\rangle = \frac{1}{2}\frac{E_0^2}{4t^2+E_0^2},$$

respectively. The exact optical conductivity displays one transition between the ground state and an excited state with energy $E_U=U$ resulting in the excitation energy

$$E_U - E_0 = \frac{U}{2}[1+\sqrt{1+(4t/U)^2}].$$

The corresponding matrix element of the current operator is

$$|\langle 0|j|U\rangle|^2 = \frac{16t^4}{(E_0^2+4t^2)}.$$

Upon minimizating the GA energy functional of the half-filled two-site model one finds a paramagnetic solution below

$$U_{crit}^{GA}/t = 8(\sqrt{2}-1) \approx 3.31,$$

and a Neél-type state with $m_1^0 = -m_2^0$, where

$$m_i = \langle n_{i,\uparrow} \rangle - \langle n_{i,\downarrow} \rangle \neq 0$$

for $U > U_{crit}^{GA}$. Within the HF theory the corresponding critical value is $U_{crit}^{HF}/t = 2$.

Clearly the transition in either case is nonphysical since it does not occur in the exact solution. In this sense the increase of U_{crit}^{GA} with respect to U_{crit}^{HF} is in favor of the GA since it extends the parameter range of the right singlet paramagnetic solution. At large U, disregarding the nonphysical broken symmetry, the Neél-type state in the GA allows the system to reduce the double occupancy and at the same time prevents the occurrence of the Brinkmann-Rice (BR) transition toward localization at $U_{BR} = 8t$.

Since the analytic expressions for the symmetry-broken regime become quite lengthy we restrict the derivation below to the paramagnetic case. In this limit the mean-field part of the energy is given by

$$\mathrm{tr}(h_0 \rho) = t(1-u^2) \sum_{\sigma} (\rho_{pp,\sigma} - \rho_{hh,\sigma}), \tag{58}$$

which defines the diagonal Gutzwiller Hamiltonian in Eq. (6). The hole (particle) state is the bonding (antibonding) state and $u = U/(8t)$.

The GA kinetic energy reads

$$E_{kin} = -2t(1-u^2),$$

and the expansion of the GA energy functional leads to [see Eqs. (22)]

$$L_{ii,ii}^{\sigma\sigma} = \frac{4t(2+3u^2-u^4)}{1-u^2}, \tag{59}$$

$$L_{ii,ii}^{\sigma,-\sigma} = \frac{8t}{1-u}, \tag{60}$$

$$L_{ii,jj}^{\sigma\sigma'} = -\frac{8tu^2}{1-u^2}, \quad i \neq j, \tag{61}$$

$$L_{ii,ij}^{\sigma\sigma'} = 2tu, \quad i \neq j, \tag{62}$$

$$K_{ii} = \frac{32t}{1-u^2}, \tag{63}$$

$$K_{ij} = -\frac{32tu^2}{1-u^2}, \quad i \neq j, \tag{64}$$

$$S_{i,ii\sigma} = -\frac{16t}{1-u^2}, \tag{65}$$

$$S_{i,jj\sigma} = \frac{16tu^2}{1-u^2}, \quad i \neq j, \tag{66}$$

$$S_{i,ij\sigma} = -4tu, \quad i \neq j. \tag{67}$$

One of the peculiarities of the present approach is the appearance of onsite interactions for quasiparticles with the same spin ($L_{ii,ii}^{\sigma\sigma} \neq 0$). These interactions do not occur in the standard RPA since they would violate the Pauli exclusion principle but appear here because of the density dependence of the effective interaction between particles. Also notice that many of the matrix elements would diverge at the BR transition if it were not hidden by the spin-density-wave (SDW) transition.

Eliminating the double occupancy fluctuations with the help of the antiadiabatic condition [Eq. (17)], the following interaction matrix is obtained:

$$M_{ii,ii}^{\sigma\sigma} = \frac{4tu^2(3-u^2)}{1-u^2}, \tag{68}$$

$$M_{ii,ii}^{\sigma,-\sigma} = \frac{8tu}{1-u^2}, \tag{69}$$

$$M_{ii,jj}^{\sigma\sigma'} = 0, \quad i \neq j, \tag{70}$$

$$M_{ii,ij}^{\sigma\sigma'} = 0, \quad i \neq j, \tag{71}$$

$$M_{ij,ij}^{\sigma\sigma'} = M_{ij,ji}^{\sigma\sigma'} = -tu^2, \quad i \neq j. \tag{72}$$

Remarkably, intersite interactions vanish except for the appearance of a new interaction term between off-diagonal charges ($M_{ij,ij}^{\sigma\sigma'}$). Using Eqs. (35) and (36) one can show that these new off-diagonal interactions do not contribute to the RPA matrices and the expansion of the energy reads

$$E = E_{GA} + \sum_{i=1}^{2} [U^s (\delta m_i)^2 + U^c (\delta \rho_i)^2], \tag{73}$$

where the charge- and spin-interaction coefficients are given by

$$U^c = u \frac{(2-u)(1+u)}{1-u} t, \tag{74}$$

$$U^s = -u \frac{(2+u)(1-u)}{1+u} t, \tag{75}$$

and naturally coincide with the Landau parameters F_0^s and F_0^a derived by Vollhardt in Ref. 15.

The RPA matrices read

$$A = \begin{pmatrix} \Delta E + U^+ & U^- \\ U^- & \Delta E + U^+ \end{pmatrix}, \tag{76}$$

$$B = \begin{pmatrix} U^+ & U^- \\ U^- & U^+ \end{pmatrix}, \tag{77}$$

with the GA particle-hole excitation energy $\Delta E = 2t(1-u^2)$ and $U^{\pm} = U^c \pm U^s$.

Upon diagonalizing the RPA problem one obtains the eigenvalues

$$\omega_{\pm}^2 = \Delta E[\Delta E + 2(U^+ \pm U^-)], \tag{78}$$

which correspond to a singlet (ω_+) and a magnetic excitation (ω_-), respectively. The former is the charge excitation which contributes to the optical conductivity, whereas the latter can be identified with the Goldstone mode driving the transition from the paramagnetic to the SDW state. This transition occurs at $\omega_-^2 = 0 = \Delta E + 4U^s$, so that the transition to the symmetry-broken state is only determined by the spin interaction U^s. Notice that for the HF approximation we have $U^c = U/4 = -U^s$, so that in this case the transition occurs at $U_{crit}^{HF}/t = 2$, as stated above.

When we expand the RPA charge excitation energy of the GA approach for small U/t we obtain

$$\omega_+^2 = 2t(2t+U) + \frac{1}{4}U^2 + \mathcal{O}(U^4) \quad \text{(GW+RPA)}, \tag{79}$$

$$\omega_+^2 = 2t(2t+U) \quad \text{(HF+RPA)}, \tag{80}$$

which has to be compared with the expansion of the exact excitation:

$$\omega_{exact}^2 = 2t(2t+U) + \frac{1}{2}U^2 + \mathcal{O}(U^3). \tag{81}$$

Thus the RPA corrections to the Gutzwiller approximation partially include higher order contributions in U which are not contained in the HF+RPA approach.

The eigenvectors of Eq. (46) are given by

$$X_{\uparrow}^{\pm} = 1/2\alpha_{\pm}[1 + \omega_{\pm}/(\Delta E)], \tag{82}$$

$$X_{\downarrow}^{\pm} = \pm 1/2\alpha_{\pm}[1 + \omega_{\pm}/(\Delta E)], \tag{83}$$

$$Y_{\uparrow}^{\pm} = 1/2\alpha_{\pm}[1 - \omega_{\pm}/(\Delta E)], \tag{84}$$

$$Y_{\downarrow}^{\pm} = \pm 1/2\alpha_{\pm}[1 - \omega_{\pm}/(\Delta E)], \tag{85}$$

and the normalization factor is $\alpha_{\pm}^2 = \Delta E/(2\omega_{\pm})$.

We are now able to compute the RPA double occupancy by evaluating the corresponding correlation function as $\Sigma_{m=\pm}\langle 0|n_{\uparrow}|m\rangle\langle m|n_{\downarrow}|0\rangle$ leading to

$$D_{GA}^{RPA} = \frac{1}{4} + \frac{1}{8}\Delta E(1/\omega_+ - 1/\omega_-). \tag{86}$$

Approaching the SDW transition leads to an increase of spin fluctuations to a divergent D^{RPA} at the transition point due to the Goldstone mode $\omega_- \to 0$ (see inset of Fig. 2). From the double occupancy we can compute the corrections to the ground state energy using the coupling constant integration trick,[24,26] i.e., $E_{int} = \int_0^U dx D^{RPA}(x)$ which yields

$$E_{int}^{GA+RPA} = -2t + U/2 + 2t[-2 + \sqrt{2-(1-u)^2} + \sqrt{2-(1+u)^2}]. \tag{87}$$

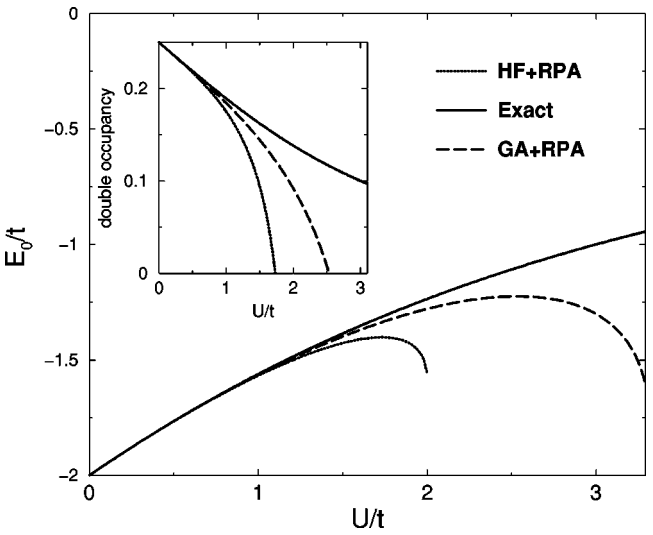

FIG. 2. Comparison of the GA+RPA, HF+RPA, and exact results for the ground-state energy E_0 of the two-site Hubbard model. The inset shows the double occupancy as a function of U/t within the same approaches.

We thus obtain the GA+RPA ground-state energy which is displayed in Fig. 2 together with the corresponding HF+RPA and the exact result.

Naturally for such a small system any mean-field treatment would result in large errors, however, due to the increased value of U_{crit}^{GA} and the extra contributions in U discussed above, GA+RPA performs much better than HF +RPA. In general, RPA corrections overshoot the exact energy, which becomes significant when one approaches the nonphysical SDW transition.

For larger systems, where the broken symmetry mean field can correspond to long-range order or quasi-long-range order in the exact solution, the agreement is much better, as shown in Ref. 13. In addition the performance improves with increasing dimensionality as in any mean-field+RPA theory.

Finally it is straightforward to check that standard sum rules are obeyed. For example the current operator matrix elements between ground state and the charge (+) and the magnetic (−) excitation are given by

$$|\langle 0|j^{GA}|-\rangle|^2 = 0, \tag{88}$$

$$|\langle 0|j^{GA}|+\rangle|^2 = t(1-u^2)\omega_+ . \tag{89}$$

As a result one thus obtains that the f-sum rule $|\langle 0|j^{GA}|+\rangle|^2/\omega_+ + (1/2)E_{kin}^{GA} = 0$ is satisfied within the GA +RPA approach.

IV. RESPONSE FUNCTIONS IN THE 1D AND 2D HUBBARD MODEL

In this section we apply our method to the calculation of response functions in the 1D and 2D Hubbard models. In the first part, we show that already on the saddle-point level, the GA yields rather accurate excitation energies as compared to the HF approach. Inclusion of RPA corrections then leads to an additional redistribution of spectral weight in the correla-

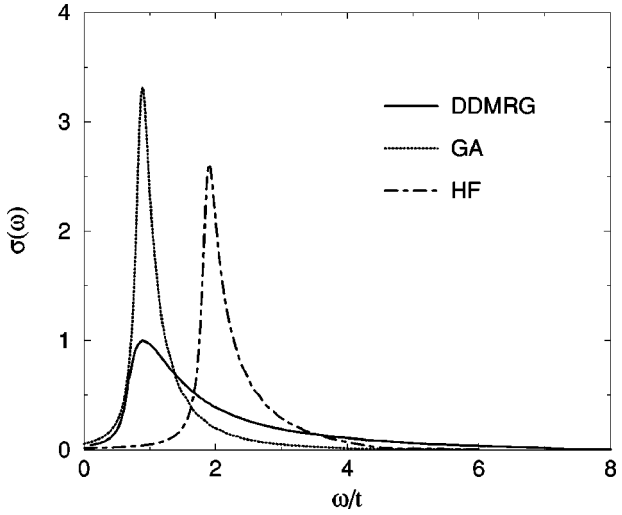

FIG. 3. Optical conductivity of the 1D Hubbard chain (120 sites) for $U/t=3$. Solid: DDMRG; dotted: GA; dash-dotted: HF. DDMRG data by courtesy of E. Jeckelmann. $\sigma(\omega)$ has been convoluted with a Lorentzian with a width $\varepsilon=0.1t$.

tion functions, which is demonstrated in the second part by a detailed comparison of exact diagonalization results with the GA+RPA and HF+RPA. This comparative study is especially intended for an *a posteriori* justification of the antiadiabaticity assumption [Eq. (17)].

A. Optical conductivity of the half-filled Hubbard model in the Gutzwiller approximation

After Ref. 13 was published we became aware that the RPA residual interaction for the SDW vanishes in the channel relevant for the optical conductivity (zero momentum and odd parity). This is a pathology of the Hubbard model at half-filling, and occurs both in the HF+RPA and in the GA +RPA, whereas it does not occur for more complicated models (like multiband Hubbard) or symmetry-broken ground states, like polarons or stripes. As a consequence the optical conductivity $\sigma(\omega)$ is the same on the GA+RPA and GA level. It is nevertheless quite instructive to examine $\sigma(\omega)$ within the mean-field approximation since this demonstrates the better starting saddle-point of the GA in comparison to the HF approach, with respect to the one-particle excitation energies. For this purpose, in the following we compare the GA and HF optical conductivity with numerical results, and present the results for charge-charge correlation functions where the mentioned pathology does not occur and instead the GA+RPA introduces nontrivial corrections to the dynamical response functions.

Figure 3 displays $\sigma(\omega)$ for a half-filled Hubbard chain and $U/t=3$ convoluted with a Lorentzian $L(\omega)=\varepsilon/[\pi(\varepsilon^2+\omega^2)]$ and $\varepsilon=0.1t$. For both GA and HF approaches, the ground state is characterized by long-range SDW order, and the regular part of $\sigma(\omega)$ is given by

$$\sigma(\omega)=\frac{\Delta^2}{2\omega^2}\Re\sqrt{\frac{16t_{eff}^2}{\omega^2-\Delta^2}-1}, \tag{90}$$

where t_{eff} contains the z-factor renormalization in the case of the GA ($t_{eff}^{GA}=tz_\uparrow z_\downarrow$), $t_{eff}^{HF}=t$ and $\Re$ denotes the real part. The SDW gap in the HF approach is related to the onsite magnetization $\Delta^{HF}=2U|S_z|$, whereas within the Kotliar-Ruckenstein formulation of the GA (Ref. 6) it is determined by the difference in the local spin-dependent Lagrange multipliers $\Delta^{GA}=\lambda_\uparrow-\lambda_\downarrow$. It is quite interesting to observe that the onset of excitations coincides rather well in the DDMRG (Ref. 27), and GA approaches, whereas the HF approach gives a gap which is by far too large. However, although GA leads to excellent results for the gap energies it turns out that the corresponding intensity is overestimated. This has the consequence that most of the high-frequency evolution of $\sigma(\omega)$ is compressed close to the threshold, whereas the DDMRG approach shows a much broader spectrum. We have checked the broadness of the exact spectrum by performing exact diagonalization in small clusters. From Eq. (90) one obtains that the large frequency tail for GA and HF approaches behaves as $\sigma(\omega\gg\Delta)\sim 1/\omega^3$, whereas the correct field theoretical result is $\sigma(\omega\gg\Delta)\sim 1/\omega$.[27]

To summarize, the optical conductivity results are the same at mean field or mean field plus RPA, and, therefore, no corrections are introduced by our method in this (rather pathological) case. As compared to the DDMRG results, the GA performs much better than the HF approach since it reproduces the onset of excitations with a better accuracy. However, the width of the spectrum is underestimated in both mean-field approaches.

B. Comparison with exact results

In order to compare the GA+RPA approach with exact results, we investigate the on-site density-density response function

$$S_c(\omega)=\sum_i\sum_{m>0}|\langle\Psi_m|n_i|\Psi_0\rangle|^2\delta[\omega-(E_m-E_0)]. \tag{91}$$

In this case, GA and GA+RPA solutions are different, since the pathology discussed in Sec. IV A is not present. The following sum rule is obeyed [see Eq. (57)]:

$$\int \mathrm{d}\omega\,\omega S_c(\omega)=-\langle T\rangle_{GA}. \tag{92}$$

In Fig. 4 we show $S_c(\omega)$ for a half-filled Hubbard chain with 14 sites calculated with exact diagonalization, the GA +RPA, and the HF+RPA. For $U/t=3$ the lowest energy excitation is at $\omega\sim 1.4t$ (exact), $\omega\sim 1.3t$ (GA+RPA) and $\omega\sim 2.1t$ (HF+RPA), respectively, so that the GA+RPA approach is much more accurate than the standard HF+RPA approach. Also the higher energy excitations computed with the GA+RPA are in remarkable agreement with the exact results. Moreover, the oscillator strength of the two lowest excitations coincides rather well with the intensity obtained with exact diagonalization. The small high-energy features between $\omega\sim 5t$ and $\omega\sim 7t$ present in the exact result do not show up in the GA+RPA correlations. As a consequence, the GA+RPA slightly overestimates the intensity between ω

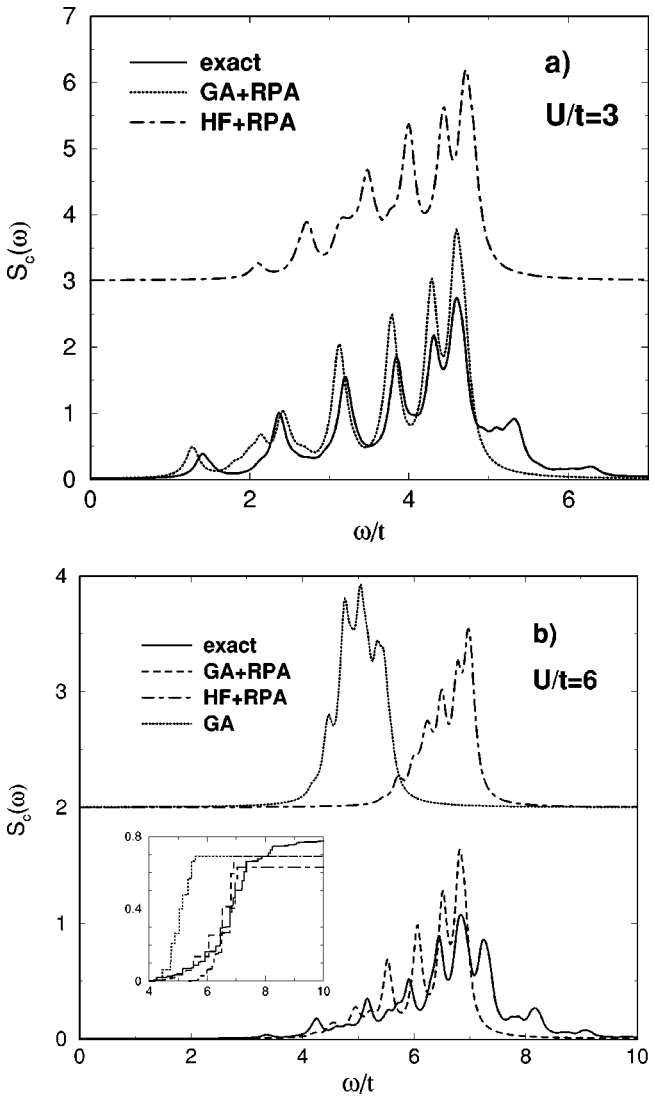

FIG. 4. Charge correlation function $S_c(\omega)$ for a half-filled Hubbard chain (14 site) in cases of $U/t=3$ (a) and $U/t=6$ (b). For clarity the curves for HF+RPA and GA [in (b)] have been shifted upwards. The inset in (b) shows the integrated weight as a function of frequency for GA and GA+RPA, respectively.

$\sim 3t$ and $\omega \sim 5t$, since from $\langle T\rangle_{GA} \approx \langle T\rangle_{exact}$, the sum rule requires the integrated spectral weight to be approximately the same in both the GA and the exact result.

The accuracy of the GA+RPA approach is also remarkable with respect to the fact that the underlying mean-field solution (the GA) corresponds to a SDW state, whereas the exact solution in one dimension does not show long-range order. However, it is well known that correlation functions decay slowly and thus are quasi-long-ranged. Hence only for very low energies does one expects disagreement due to this problem, and since excitations in the system under consideration are gapped this discrepancy does not really show up.

Figure 4(b) reveals that GA+RPA provides a better description of the low-energy excitations than the HF+RPA, even at larger values of U/t. In addition, in Fig. 4(b) we show the charge-charge correlations for the bare GA. In this case, the corresponding excitations are located in a narrow

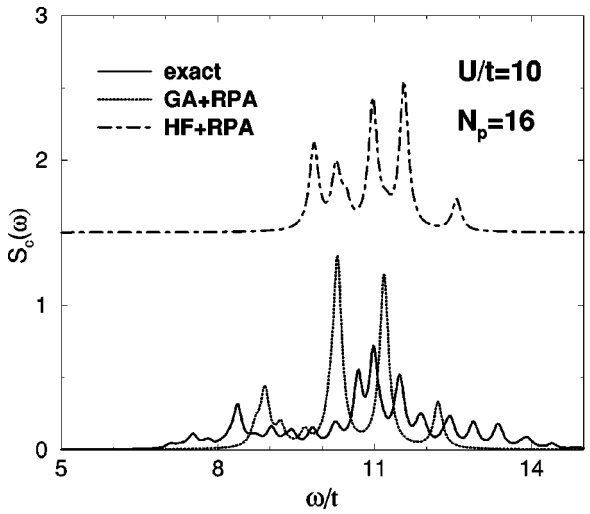

FIG. 5. Charge correlation function $S_c(\omega)$ for the half-filled 4 $\times$4 Hubbard model (16 particles) in the case of $U/t=10$.

energy window on the low-energy side of the exact spectrum with rather incorrect oscillator strength. Thus, RPA corrections induce a broadening and shift of excitations to higher energies with a simultaneous redistribution of intensity. This can also be deduced from the inset of Fig. 4(b), which shows the evolution of the integrated spectrum $\int_0^\omega S_c(\nu)d\nu$ for the GA and GA+RPA. From the sum rule [Eq. (92)] it is obvious that both the GA and the GA+RPA approach the same integrated spectral intensity but with the GA+RPA spectral evolution broadened and shifted to higher energies with respect to the bare GA.

In systems with large dimensionality we expect our approach to improve, since the GA is an exact solution of the Gutzwiller variational problem in infinite dimensions. Furthermore, quite generally mean-field theories become better as the dimensionality is increased. Figure 5 displays $S_c(\omega)$ for a half-filled 4×4 system (i.e., 16 particles) with $U/t=10$. The lowest prominent energy peak in the exact solution occurs at $\omega_{min}^{ex}=8.4t$ and a second bunch of excitations starts at $U/t \approx 10t \ldots 11t$ decaying in intensity toward higher energies. The lowest energy excitation within the GA+RPA ($\omega_{min}^{GA+RPA}=8.7t$) is remarkably close to the exact value in contrast to the HF+RPA where the lowest peak appears at $\omega_{min}^{HF}=9.8t$. Moreover, the center of high energy excitations in the exact solution is represented by two peaks in the GA +RPA spectrum at $9.7t$ and $11.2t$, whereas they are shifted to slightly higher energies within the HF+RPA. It is interesting to observe that also in this energy range the GA+RPA method gives a better (although rather crude) approximation than the HF+RPA method despite the expected failure of the antiadiabaticity condition Eq. (17) for energies larger than the Mott-Hubbard gap.

Finally we would like to demonstrate the importance of an accurate mean-field solution for the quality of the RPA excitation spectrum. For this purpose Fig. 6 shows $S_c(\omega)$ for a 4×4 system and ten particles. In the case $U/t=4$ [Fig. 6(a)] the HF+RPA and the GA+RPA give a good approximation to the lowest excitation, both with respect to the oscillator strength and the energy. For $U/t=4$ and 10 particles

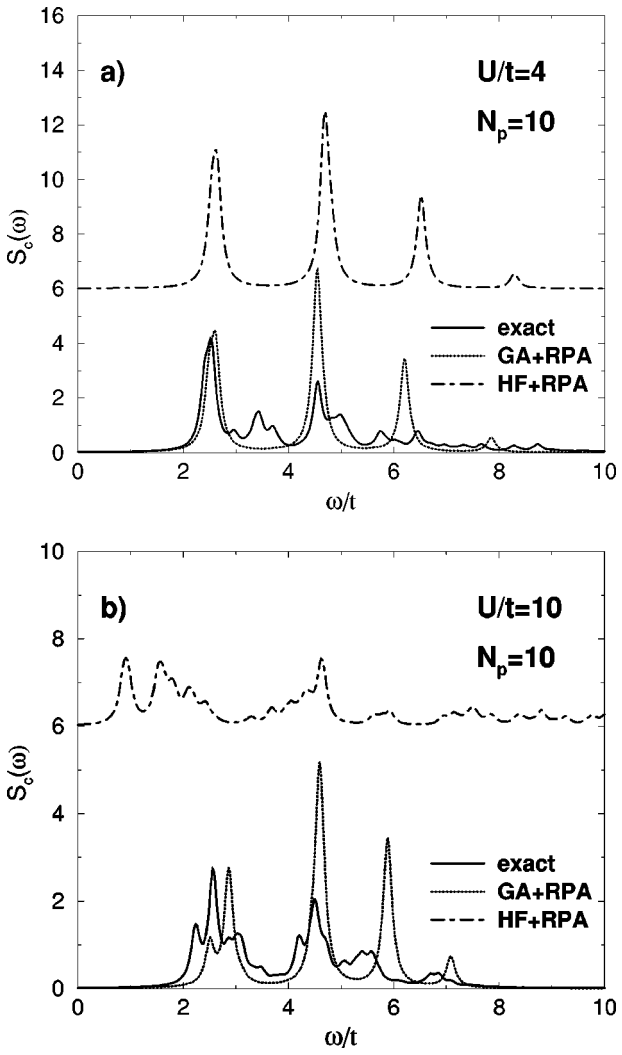

FIG. 6. Charge correlation function $S_c(\omega)$ for the 4×4 Hubbard model and ten particles in the case of $U/t=4$ (a) and $U/t=10$ (b).

(corresponding to a closed shell configuration) the underlying mean-field solutions are homogeneous with respect to the charge and do not show a SDW order. However, whereas the homogeneous GA solution also remains a stable saddle point for large values of U/t, the HF solution becomes instable with respect to a disordered charge and spin texture. This obviously has dramatic consequences for the dynamical properties as shown in Fig. 6(b). In fact, the GA+RPA spectrum still shows a remarkable agreement with the exact solution in contrast to the RPA on top of the inhomogeneous HF solution.

Notice that the GA+RPA oscillator strength for the charge-charge correlations is distributed in a much better way than for the optical conductivity (see Fig. 3). To some extent, this can be attributed to the constraints imposed by the sum rules. Both correlation functions satisfy a sum rule which involves the kinetic energy on the right-hand side [Eqs. (51) and (57)]; however, in case of the optical conductivity the high-energy states contribute much less to the sum rule than in the case of $S_c(\omega)$ due to the ω factor. Therefore, the high-energy part of $S_c(\omega)$ is much more constrained to be accurate than the high-energy part of σ. This argument assumes that at least the excitation energies are approximately correct; otherwise one can satisfy the sum rule by a compensation between the incorrect excitation energies and the incorrect matrix elements as it occurs within the bare GA for the charge correlation function [Fig. 4(b)].

Finally, it is remarkable that the GA+RPA dynamical correlation functions perform rather well even at energies much larger than the charge gap (Figs. 4, 5, and 6) where the antiadiabatic condition [Eq. (17)] is not expected to hold. To some extent this may be due to the constraints imposed by sum rules. It shows that at least for some correlation functions (charge-charge) the domain of applicability of our theory may be much wider than expected.

V. CONCLUSION

In summary, we have presented a method for the calculation of dynamical correlation functions in the Hubbard model, based on the Gutzwiller approximation. Our method obeys well-behaved sum rules and we have demonstrated that it is suitable for practical computations: excitation energies compare remarkably better with exact diagonalization results than the related HF+RPA approach. Moreover, since the performance of any RPA computation crucially depends on the quality of the underlying mean-field solution, we conclude from our analysis that the GA provides a much better starting point for this purpose than HF.

The dynamical matrix has been calculated as a quadratic expansion of the GA energy functional in the densities, which allows us to construct the RPA eigenvectors and eigenvalues. Essential assumption for carrying out this expansion is the antiadiabaticity condition [Eq. (17)]. Despite the fact that charge and double occupancy dynamics seem to be governed by different time scales, it would be desirable to relax the antiadiabatic approximation and to treat the double occupancy dynamics explicitly. This is in principle possible via the Kotliar-Ruckenstein slave-boson scheme; however, attempts in this direction are rendered difficult due to the hopping factor expansion.

Compared to numerical methods[28,29] our approach can be pushed to much larger systems. Our experience in modeling real data[30,31] is that often finite-size effects are more severe than the inaccuracies introduced by mean-field+RPA approaches. A more recent approach for dynamical properties consists of mapping the problem onto quantum impurity models (dynamical mean-field theory) which becomes exact in the limit of large dimensions.[32] This has enormously increased our understanding of these systems. However, when making the limit of large dimensions important parts of the physics are lost. For example, all acousticlike collective behavior, like spin waves, disappears. On the other hand, these collective effects are naturally captured in our approach.

The GA+RPA formalism can also be applied to multiband Hubbard models, which are relevant for a more quantitative analysis of excitations in the cuprate high-T_c superconductors. It has been shown recently that the GA provides an excellent starting point to describe the physics of stripes in cuprates including the behavior of incommensurability,

chemical potential and some transport experiments with doping.[33] In this context it is very important to make a RPA analysis on top of GA states, since within the HF approximation one obtains a ground state which does not correspond to experiment. Work in this direction is in progress.

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APPENDIX: RELATIONSHIP TO THE KOTLIAR-RUCKENSTEIN SLAVE-BOSON APPROACH

In the Kotliar-Ruckenstein slave-boson approach to the Hubbard model[6] the original Hilbert space is enlarged by introducing four subsidiary boson fields e_i, $s_{i,\uparrow}$, $s_{i,\downarrow}$, and d_i for each site $\mathbf{R}_i$. These operators stand for the annihilation 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 constraints

$$e_i^\dagger e_i + \sum_\sigma s_{i,\sigma}^\dagger s_{i,\sigma} + d_i^\dagger d_i = 1 \tag{A1}$$

and

$$n_{i,\sigma} = s_{i,\sigma}^\dagger s_{i,\sigma} + d_i^\dagger d_i . \tag{A2}$$

In the saddle-point approximation, all bosonic operators are treated as numbers, and the resulting effective one-particle Hamiltonian H^{KR} describes the dynamics of particles where the hopping amplitude between states (i,σ) and (j,σ) is renormalized by a factor $z_{i,\sigma}^{SB} z_{j,\sigma}^{SB}$ with

$$z_{i,\sigma}^{SB} = (e_i^2 + s_{i,-\sigma}^2)^{-1/2} (e_i s_{i,\sigma} + s_{i,-\sigma} d_i)(d_i^2 + s_{i,\sigma}^2)^{-1/2}. \tag{A3}$$

The total energy of H^{KR} is given by

$$E^{SB} = \sum_{ij,\sigma} t_{ij} z_{i,\sigma}^{SB} z_{j,\sigma}^{SB} \rho_{ij} + U \sum_i d_i^2 , \tag{A4}$$

which has to be minimized (i) with respect to the bosonic fields within constraints (A1) and (A2) and (ii) with respect to ρ within the subspace of Slater determinants.

The slave-boson energy functional E^{SB} is a function of $4N$ boson variables where N is the number of lattice sites. Since these bosons obey the constraints (A1) and (A2) one can eliminate 3N of them which leads to the Gutzwiller energy E^{GA} when one keeps the double occupancy variable $D = d^2$ for each lattice site. Thus the expansions of E^{SB} and E^{GA} are connected via the transformations

$$\frac{\partial z_{i,\sigma}^{GA}}{\partial D} = \frac{\partial z_{i,\sigma}^{SB}}{\partial d^2} - \frac{\partial z_{i,\sigma}^{SB}}{\partial s_\sigma^2} - \frac{\partial z_{i,\sigma}^{SB}}{\partial s_{-\sigma}^2} + \frac{\partial z_{i,\sigma}^{SB}}{\partial e^2},$$

$$\frac{\partial z_{i,\sigma}^{GA}}{\partial \rho_{ii,\sigma}} = \frac{\partial z_{i,\sigma}^{SB}}{\partial s_\sigma^2} - \frac{\partial z_{i,\sigma}^{SB}}{\partial e^2},$$

$$\frac{\partial z_{i,\sigma}^{GA}}{\partial \rho_{ii,-\sigma}} = \frac{\partial z_{i,\sigma}^{SB}}{\partial s_{-\sigma}^2} - \frac{\partial z_{i,\sigma}^{SB}}{\partial e^2}, \tag{A5}$$

and the derivatives have to be taken at the saddle point. Upon inserting this transformation in Eqs. (19) and (20) leads to an analogous energy expansion than Eq. (24), but now within the KR scheme. For paramagnetic solutions this corresponds to the analysis done in Ref. 10.

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