I. INTRODUCTION

The Gutzwiller variational wave function together with the Gutzwiller approximation (GA) 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. 1 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 been also used for realistic band structure computations.\textsuperscript{2,3,4} 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), 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 HF 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.\textsuperscript{6} This method maps the physical hole (or particle) into products of fermion and boson 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.

We present a detailed study of the time-dependent Gutzwiller approximation for the Hubbard model. The formalism, labelled 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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In this paper we use the GA+RPA to compute various correlation functions in the one-band Hubbard model and compare 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 demonstrate 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
\[ H = \sum_{ij} t_{ij} c_{i\uparrow}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \] (1)
where \( c_{i\sigma} \) destroys (creates) an electron with spin \( \sigma \) at site \( i \), and \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \). \( U \) 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. 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. The same unrestricted Gutzwiller energy functional has been obtained by Gebhard exploiting the fact that the GA becomes the exact solution of the Gutzwiller variational problem in the limit of infinite spatial dimensions.

In Gebhard’s formulation the variational wave function is written as
\[ |\Psi\rangle = \prod_i \frac{\tilde{U}_i}{K_i^{1/2}} |SD\rangle, \] (2)
\[ \tilde{U}_i = \exp \left( -\gamma_i n_{i\uparrow} n_{i\downarrow} - \sum_{\sigma} \mu_{i,\sigma} n_{i,\sigma} \right) \] (3)
where \( K_i = \langle \Psi | \tilde{U}_i \tilde{U}_i^\dagger |\Psi\rangle \). In Eq. (2) \( |SD\rangle \) 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 for 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:
\[ \langle \Psi | n_{i,\sigma} |\Psi\rangle = \langle SD | n_{i,\sigma} |SD\rangle. \]

As a result one obtains for the GA energy functional
\[ E^{GA}[\rho, D] = \sum_{ij,\sigma} t_{ij} z_{ij,\sigma} z_{ji,\sigma} \rho_{ij,\sigma} + U \sum_i D_i, \] (4)
\[ z_{ij,\sigma} = \sqrt{(1 - \rho_{ii} + D_i)(\rho_{ii,\sigma} - D_i)} + \sqrt{D_i(\rho_{ii,\sigma} - D_i)}, \]
which is a functional of the density matrix \( \rho_{ij,\sigma} \equiv \langle SD | c_{j\sigma}^\dagger c_{i\sigma} |SD\rangle \) and the double occupancy parameters \( D_i \). We denote the set of all matrix elements \( \{ \rho_{ij,\sigma} \} \) and \( \{ D_i \} \) by \( \rho \) and \( D \). Notice that in this paper we do not consider spin-canted solutions which would have density matrix elements \( \langle SD | c_{j\sigma}^\dagger c_{i\sigma} |SD\rangle \neq 0 \) for \( \sigma \neq \sigma' \). However, transverse spin degrees of freedom can be straightforwardly incorporated within the spin-rotationally invariant slave boson formulation.

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

\[ \delta\{ E^{GA}[\rho, D] - \text{tr}[A(\rho^2 - \rho)] \} = 0, \] (5)
where \( A \) denotes the Lagrange parameter matrix. It is convenient to define a Gutzwiller Hamiltonian,
\[ h_{ij,\sigma}[\rho, D] = \frac{\partial E^{GA}}{\partial \rho_{ij,\sigma}}, \] (6)
which is also a functional of \( \rho \) and \( D \). Variation of Eq. (5) with respect to the density matrix leads to:
\[ h - \rho \Lambda - \Lambda \rho + \Lambda = 0. \] (7)
The Lagrange parameters can be eliminated and together with the variation with respect to \( D \) we obtain the self consistent GA equations:
\[ [h, \rho] = 0, \] (8)
\[ \frac{\partial E^{GA}}{\partial D_i} = 0. \] (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:
\[ c_{i,\sigma} = \sum_{\nu} \psi_{i,\sigma}^{(\nu)} a_\nu, \] (10)
leading to \( h_{\mu\nu}^0 = \delta_{\mu\nu} \epsilon_{\mu} \). Moreover, the diagonalized density matrix \( \rho = \rho^{(0)} \) has eigenvalue 1 below the Fermi level and eigenvalue 0 above it. We use Greek letters to denote any state of this particular basis and the nought indicates evaluation in the saddle-point. Additionally we denote states below 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 \( \sigma^{(0)} = 1 - \rho^{(0)} \) corresponds to the projector onto particle states.

The diagonalization of Eq. (8) has to be supplemented by the minimization of the Gutzwiller energy with respect to the double occupancy parameters of Eq. (9). A convenient method for this purpose in order to obtain inhomogeneous GA solutions has been discussed in Ref. 24. Notice that the unrestricted variational procedure with respect to charge and (or) spin degrees of freedom prevents the occurrence of the Brinkmann-Rice transition towards localization which has already been 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:

\[
O^{GA} = \sum_{ij\sigma} (\delta_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma} + h.c.),
\]

where \( \delta_{ij\sigma} = q_{ij\sigma} a_{ij\sigma} \) and \( q_{ij\sigma} = 1 \) if \( i = j \) and \( q_{ij\sigma} = z_{i,\sigma}^GA a_{ij\sigma}^GA \) otherwise.

In order to derive the RPA equation we introduce a small time-dependent external field added to Eq. (11):

\[
F(t) = \sum_{ij\sigma} (f_{ij\sigma}(t) c_{i\sigma}^\dagger c_{j\sigma} + h.c.),
\]

with \( f_{ij\sigma}(t) = f_{ij\sigma}(0) e^{-i\omega t} \). As a consequence \( |\Psi\rangle \), \( |SD\rangle \), and the variational parameters acquire a time dependence and an additional term appears in the energy functional Eq. (11):

\[
E_f^{GA}[\rho, D](t) = \langle \Psi(t)| H_f(t) |\Psi(t)\rangle = \sum_{ij\sigma} (f_{ij\sigma}\rho_{ji\sigma} e^{-i\omega t} + h.c.),
\]

where \( f_{ij\sigma} = q_{ij\sigma} f_{ij\sigma} \).

The time dependent field induces small amplitude oscillations of \( D \) and \( \rho \) around the GA saddle-point:

\[
D = D^{(0)} + \delta D(t),
\]

\[
\rho = \rho^{(0)} + \delta \rho(t).
\]

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

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

\[
\rho = \rho^2.
\]

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, \( \delta D \) adjusts instantaneously to the evolution of the density matrix via the condition

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

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. (8) and (11)] around the saddle-point. The first part, Eq. (8), is needed up to second order in the density and double occupancy deviations:

\[
E^{GA}[\rho, D] = E_0 + \text{tr}(h^0 \delta \rho) + \sum_{ij\sigma} t_{ij\sigma} [z_{i,\sigma}^{GA} \delta_1 z_{j,\sigma}^{GA} + z_{j,\sigma}^{GA} \delta_1 z_{i,\sigma}^{GA}] \rho_{ji,\sigma} + \sum_{ij\sigma} \delta_2 [z_{i,\sigma}^{GA} \delta_2 z_{j,\sigma}^{GA} + z_{j,\sigma}^{GA} \delta_2 z_{i,\sigma}^{GA}].
\]

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

\[
\delta_1 z_{i,\sigma}^{GA} = \frac{\partial z_{i,\sigma}^{GA}}{\partial D_i} \delta D_i + \sum_{\sigma'} \frac{\partial z_{i,\sigma}^{GA}}{\partial \rho_{i,\sigma'}} \delta \rho_{i,\sigma'},
\]

\[
\delta_2 z_{i,\sigma}^{GA} = \frac{1}{2} \frac{\partial^2 z_{i,\sigma}^{GA}}{\partial D_i^2} (\delta D_i)^2 + \sum_{\sigma,\sigma'} \frac{\partial^2 z_{i,\sigma}^{GA}}{\partial D_i \partial \rho_{i,\sigma'}} \delta D_i \delta \rho_{i,\sigma'} + \frac{1}{2} \sum_{\sigma,\sigma',\sigma''} \frac{\partial^2 z_{i,\sigma}^{GA}}{\partial \rho_{i,\sigma'} \partial \rho_{i,\sigma''}} \delta \rho_{i,\sigma'} \delta \rho_{i,\sigma''}.
\]

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

\[
E^{GA}[\rho, D] = E_0 + \text{tr}(h^0 \delta \rho) + \frac{1}{2} \delta \rho_{i,\sigma'} L_{ijkl}^{\sigma\sigma'} \delta \rho_{k,l},
\]

\[
+ \frac{1}{2} \delta D_i K_{ij} \delta D_j + \delta D_i S_{i,k\sigma} \delta \rho_{k,\sigma},
\]

\[
(14)
\]

\[
(15)
\]

\[
(16)
\]

\[
(17)
\]

\[
(18)
\]

\[
(19)
\]

\[
(20)
\]

\[
(21)
\]
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:

$$
L^\sigma_{ij,i'i''} = \sum_{j'\sigma'} t_{ij} \partial^2 z_{i,\sigma''} \partial p_{i',\sigma}\partial p_{i'',\sigma'} (\rho_{ij,\sigma''} + \rho_{ji,\sigma''}) ,
$$

$$
L^\sigma_{ij,ij} = \sum_{j'\sigma'} t_{ij} \partial z_{i,\sigma''} \partial p_{i',\sigma} (\rho_{ij,\sigma''} + \rho_{ji,\sigma''}) i \neq j ,
$$

$$
L^\sigma_{ii,ij} = L^\sigma_{ij,ii} = t_{ij} \partial z_{i,\sigma''} \partial p_{i,\sigma} (\rho_{ij,\sigma''} + \rho_{ji,\sigma''}) i \neq j ,
$$

$$
K^\sigma_{ii} = \sum_{j'\sigma'} t_{ij} \frac{\partial^2 z_{i,\sigma}}{\partial D^2} z_{i',\sigma'} (\rho_{ij,\sigma} + \rho_{ji,\sigma}) ,
$$

$$
K_{ij} = \sum_{\sigma'} t_{ij} \partial z_{i,\sigma} \partial z_{i',\sigma'} (\rho_{ij,\sigma} + \rho_{ji,\sigma}) i \neq j ,
$$

$$
S^\sigma_{i,i\sigma} = \sum_{j'\sigma'} t_{ij} \frac{\partial^2 z_{i,\sigma}}{\partial D^2} \partial p_{i',\sigma} z_{i',\sigma'} (\rho_{ij,\sigma'} + \rho_{ji,\sigma'}) ,
$$

$$
S_{i,ij\sigma} = t_{ij} \sum_{\sigma'} \partial z_{i,\sigma'} \partial z_{i',\sigma} (\rho_{ij,\sigma'} + \rho_{ji,\sigma'}) i \neq j ,
$$

$$
S_{i,ij\sigma} = t_{ij} \frac{\partial z_{i,\sigma}}{\partial D^2} z_{i',\sigma'} i \neq j .
$$

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

We can integrate out the $D$ fluctuations using the antiadiabaticity condition Eq. (17). First, we express $\delta D_i$ in terms of the density fluctuations via

$$
\delta D_i = -(K^{-1})_{ij} S_{j,k\alpha\sigma} \delta \rho_{k,\alpha\sigma} ,
$$

(23)

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

$$
\tilde{E}[\rho] = E_0 + \text{tr}(\hbar^2 \delta \rho)
$$

+ $\frac{1}{2} \delta \rho_{ij,\sigma} [L_0 - S_0^{-1} K_0^{-1} S_0]_{ij kl}^{\sigma\sigma'} \delta \rho_{k,\sigma'} .
$$

(24)

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

The matrix $(L_0 - S_0^{-1} K_0^{-1} S_0)$ 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.

Interestingly, the off-diagonal elements of the matrices $K_{ij}$, $L^\sigma_{ij,kl}$, and $S_{i,kl\sigma\sigma'}$ can induce intersite interactions between the GA quasiparticles. This is in contrast with conventional HF theory of the Hubbard model which is purely local.

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

$$
E^{GA}_f[\rho, D] = F_0 + \text{tr}(f^{GA}_0 \delta \rho)
$$

+ $\sum_{ijkl\sigma\kappa\sigma'} \rho^0_{ij,\sigma} f_{ij,\sigma} \frac{\partial q_{ij,\sigma}}{\partial \rho_{k,\kappa\sigma'}} \delta \rho_{k,\kappa\sigma'}
$$

+ $\sum_{ijkl\sigma} \rho^0_{ij,\sigma} f_{ij,\sigma} \frac{\partial q_{ij,\sigma}}{\partial D_k} \delta D_k .
$$

(25)

Here $F_0 = f^{GA}_0 \rho^{(0)}$ 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 $E^{GA}_f[\rho] = E^{GA}_f[\rho, D(\rho)]$ and

$$
\tilde{f}_{ij,\sigma} = \frac{\partial E^{GA}_f[\rho]}{\partial \rho_{ij,\sigma}} .
$$

(26)

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

$$
\mathbf{J} = \sum_{(ij)} \mathbf{j}_{ij} ,
$$

(27)

and

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

(28)

When only densities are involved $f_{ij,\sigma}$ is diagonal in the site index, only $q_{ij,\sigma} = 1$ is present and the last two terms in Eq. (21) vanish. If currents are involved it is easy to show directly from Eq. (23) that the last two terms also vanish in the absence of currents in the ground state, i.e. $\tilde{f}_0 = f^{GA}_0$.

Now, we proceed in analogy with the nuclear physics treatment of effective mean-field theories in which the interaction potential is density dependent.

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:

$$
\mathbf{h}\partial \rho = \tilde{\mathcal{H}}[\rho] + \tilde{f}(t), \rho ,
$$

(28)

where we have defined an effective Gutzwiller Hamiltonian

$$
\tilde{\mathcal{H}}_{ij,\sigma}[\rho] = \frac{\partial \tilde{E}}{\partial \rho_{ij,\sigma}} .
$$

(29)
which depends on densities only. At the saddle-point, we have $\hat{h}_0 = \hat{h}[\rho(0) = \rho_0$. The RPA is obtained 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:

\[
\begin{align*}
\delta \rho_{hh} &\equiv \rho(0) \delta \rho_{hh}(0), \\
\delta \rho_{pp} &\equiv \sigma(0) \delta \rho_{pp}(0), \\
\delta \rho_{hp} &\equiv \rho(0) \delta \rho_{hp}(0), \\
\delta \rho_{ph} &\equiv \sigma(0) \delta \rho_{ph}(0).
\end{align*}
\]

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:

\[
\delta \rho = \rho(0) \delta \rho + \delta \rho_{hh}(0) + (\delta \rho)^2.
\]

Projecting Eq. (24) onto the $hh$ and $pp$ sector of the saddle point Slater determinant yields

\[
\begin{align*}
\delta \rho_{hh} &= -(1 + \delta \rho_{hh})^{-1} \delta \rho_{hp} \delta \rho_{ph} \approx -\delta \rho_{hp} \delta \rho_{ph}, \\
\delta \rho_{pp} &= (1 - \delta \rho_{pp})^{-1} \delta \rho_{hp} \delta \rho_{ph} \approx \delta \rho_{hp} \delta \rho_{ph},
\end{align*}
\]

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

\[
tr(h^0 \delta \rho) = \sum_p \epsilon_p \delta \rho_{pp} + \sum_h \epsilon_h \delta \rho_{hh} = \sum_{ph} (\epsilon_p - \epsilon_h) \rho_{ph} \rho_{hp}.
\]

In addition one can neglect the $pp$ and $hh$ matrix element 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)

\[
\tilde{E}[\rho] = E_0 + \frac{1}{2} (\delta \rho_{hp}, \delta \rho_{ph}) \left( \begin{array}{cc} A & B \\ B^* & A^* \end{array} \right) \left( \begin{array}{c} \delta \rho_{hp} \\ \delta \rho_{ph} \end{array} \right).
\]

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

\[
\begin{align*}
A_{ph,p'h'} &= (\epsilon_p - \epsilon_h) \delta_{pp'} \delta_{hh'} + \frac{\partial \tilde{h}_{ph}}{\partial \rho_{pp'}}, \\
B_{ph,p'h'} &= \frac{\partial \tilde{h}_{ph}}{\partial \rho_{pp'}}.
\end{align*}
\]

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 $M \equiv (L_0 - S^0_1 K^{-1}_0 S_0)$ via

\[
\begin{align*}
A_{ph,p'h'} &= (\epsilon_p - \epsilon_h) \delta_{pp'} \delta_{hh'} + \sum_{ij\sigma, nm\sigma'} \psi_{ij,\sigma}^* (p) \psi_{ij,\sigma} (h) M_{ij, nm} \psi_{nm, \sigma'}^* (h') \psi_{nm, \sigma'} (p'), \\
B_{ph,p'h'} &= \sum_{ij\sigma, nm\sigma'} \psi_{ij,\sigma}^* (h) \psi_{ij,\sigma} (p) M_{ij, nm} \psi_{nm, \sigma'}^* (h') \psi_{nm, \sigma'} (p'),
\end{align*}
\]

and the transformation amplitudes $\psi_{i,\sigma}(\nu)$ have been defined in Eq. (14).

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

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

where we use the shorthand notation

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

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

\[
\left( \begin{array}{cc} A & B \\ B^* & A^* \end{array} \right) - \hbar \omega \left( \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right) \left( \begin{array}{c} \delta \rho_{ph} \\ \delta \rho_{hp} \end{array} \right) = -\left( \begin{array}{c} \tilde{f}_{ph} \\ \tilde{f}_{hp} \end{array} \right).
\]

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

\[
\delta \rho = R(\omega) \tilde{f}.
\]

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

\[
O = \sum_{ij\sigma} (\epsilon_{ij,\sigma} c^\dagger_{ij} c_{i\sigma} + h.c.),
\]

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

\[
\langle \Psi(t)|O|\Psi(t) \rangle = \sum_{ij\sigma} (\epsilon_{ij,\sigma} c^\dagger_{ij} c_{i\sigma}(t) + h.c.),
\]

and the time evolution of $\rho$ is known from Eq. (44).

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

\[
\left( \begin{array}{cc} A & B \\ B^* & A^* \end{array} \right) - \hbar \Omega_n \left( \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right) \left( \begin{array}{c} X(n) \\ Y(n) \end{array} \right) = 0.
\]

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:

\[
R(\omega)_{\phi\phi'} = \sum_{n>0} \left[ \frac{X_{\rho\rho'}^n X_{\rho\rho'}^{*n}}{\omega - \Omega_n + i\epsilon} - \frac{Y_{\rho\rho'}^n Y_{\rho\rho'}^{*n}}{\omega + \Omega_n + i\epsilon} \right].
\] (47)

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

\[
\langle 0 | a_{\phi}^\dagger a_\rho | n \rangle = X_{\phi\rho}^n,
\]

(48)

\[
\langle 0 | a_{\phi}^\dagger a_{\rho h} | n \rangle = Y_{\phi h}^n.
\]

(49)

The states \( |n\rangle \) are not true excitations of the system but represent auxiliary notational 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 \( |SD\rangle \) but at RPA level (it contains RPA ground-state correlations but lacks Gutzwiller correlations). We will call them unprojected RPA states. The eigenvector \( (X_{\phi\rho}^n, Y_{\phi h}^n) \) 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:

\[
|SD\rangle \xrightarrow{P} |\Psi_0\rangle,
\]

RPA ↓ ↓ RPA

\[
|0\rangle \xrightarrow{P} |\Phi_0\rangle,
\]

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 \( \omega > 0 \):

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

(50)

With the above approximations and notations

\[
\langle \Phi_n | j_\alpha | \Phi_0 \rangle = \langle n | \phi_\alpha^{GA} | 0 \rangle,
\]

where the matrix element on the right 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 next section)

\[
\int_0^\infty d\omega \sigma(\omega) = -\frac{1}{2} \pi \langle T_n \rangle_{GA},
\]

(51)

where the kinetic energy in \( \alpha \)-direction \( \langle T_n \rangle_{GA} \) is evaluated within the GA.

In practice, for computational purposes one can use all the standard formulas of the HF+RPA scheme by substituting true operators with GA effective operators and excitations by the 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

\[
\delta n_i^m \equiv \langle 0 | \hat{n}_i | m \rangle,
\]

(52)

and the transition current

\[
\delta j_i^m \equiv \langle 0 | j_i^{GA} | m \rangle,
\]

(53)

which can be interpreted as follows. Consider a wave packet

\[
\langle \psi(t) | \hat{n}_i | \psi(t) \rangle = \langle 0 | \hat{n}_i | 0 \rangle + \eta \delta n_i^m e^{-\Omega_i m t} + h.c.,
\]

and an analogous expression holds also for the current. Here \( \langle 0 | \hat{n}_i | 0 \rangle = \langle SD | \hat{n}_i | SD \rangle \) 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 \( \Omega_i m \) if the state \( m \) is excited by a weak perturbation (see also 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 \( k \)-th moment of the excitation strength distribution produced by a single-particle operator \( O \) (see e.g., Ref. [24]):

\[
S^k \equiv \sum_n (E_n - E_0)^k |\langle \Phi_n | O | \Phi_0 \rangle|^2.
\]

(54)

Within the present scheme we have:

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

(55)

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

\[
S^1 = \sum_{n=1} (E_n - E_0)|\langle \Psi_n | O | \Phi_0 \rangle|^2 = \frac{1}{2} \langle \Psi_0 | [O, [H, O]] | \Phi_0 \rangle.
\]

(56)
In analogy with the derivation by Thouless, 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 in case of the optical conductivity discussed above corresponds to the f-sum rule.

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

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

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 ($4 \times 4$ lattice) with nearest neighbor hopping $t_{ij} = -t$. The GA Slater determinants have been obtained using the method described in Ref. 20. Notice 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 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 element $t_{ij}$. On the other hand, for $U/t = 8$ the large HF onsite renormalization (corresponding to an overestimate of the spin-polarization) is the origin for the kinetic energy to be lower than the exact result. In contrast, the values of $\langle -T \rangle$ in the GA approximation correctly reproduce the exact result, especially in 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 GA+RPA than in the HF+RPA approximation. The same holds for the $S^{-1}$-sum rule for 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. Since the GA provides a much better initial saddle-point than HF one can expect that the fluctuation corrections within

![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.](image)

**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

$$\langle n_{i\uparrow}n_{i\downarrow} \rangle = \frac{E_0^2}{24t^2 + E_0^2},$$

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

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

and a Neél-type state with \( m_i^0 = -m_j^0 \) where

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

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

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

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

\[ \text{tr}(h_0 \rho) = t(1 - u^2) \sum_\sigma (\rho_{pp,\sigma} - \rho_{hh,\sigma}), \]

which defines the diagonal Gutzwiller Hamiltonian in Eq. (4). The hole (particle) state is the bonding (antibonding) state and \( u = U/(8t) \).

The GA kinetic energy reads as

\[ E_{\text{kin}} = -2t(1 - u^2), \]

and the expansion of the GA energy functional leads to the same spin \( \langle L_{ii,i,i}^{\sigma\sigma} \rangle \neq 0 \). 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. Notice also 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 help of the antiadiabatic condition Eq. (17), the following interaction matrix is obtained:

\[ M_{ii,i,i}^{\sigma\sigma} = \frac{4tu^2 (3 - u^2)}{1 - u^2}, \]

\[ M_{ii,i,i}^{\sigma,-\sigma} = \frac{8tu}{1 - u^2}, \]

\[ M_{ii,j,j}^{\sigma\sigma'} = 0 \quad i \neq j, \]

\[ M_{ii,j,j}^{\sigma\sigma'} = 0 \quad i \neq j, \]

\[ M_{ij,i,j}^{\sigma\sigma'} = M_{ij,j,i}^{\sigma\sigma'} = -tu^2 \quad i \neq j. \]

Remarkably, intersite interactions vanish except for the appearance of a new interaction term between off-diagonal charges \( \langle M_{ij,j,i}^{\sigma\sigma'} \rangle \). Using Eqs. (58) and (59) one can show that these new off-diagonal interactions do not contribute to the RPA matrices and the expansion of the energy reads as:

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

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

\[ U^c = u \frac{(2 - u)(1 + u)}{1 - u} t, \]

\[ U^s = -u \frac{(2 + u)(1 - u)}{1 - u} t, \]

and naturally coincide with the Landau parameters \( F_0^c \), \( F_0^s \) derived by Vollhardt in Ref. 15.

The RPA-matrices read as

\[ A = \begin{pmatrix} \Delta E + U^+ & U^- \\ U^- & \Delta E + U^+ \end{pmatrix}, \]

\[ B = \begin{pmatrix} U^+ & U^- \\ U^- & U^+ \end{pmatrix}, \]

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:

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

which correspond to a singlet \( (\omega_+) \) and a magnetic excitation \( (\omega_-) \), 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 \( U_{\text{crit}}^{HF}/t = 2 \) as stated above.

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

\[
\omega^2_+ = 2t(2t + U) + \frac{1}{4}U^2 + O(U^3) \quad (GW + RPA),
\]

and the expansion partially includes higher order contributions in \( U \) which are not contained in the HF+RPA approach.

Thus the RPA corrections to the Gutzwiller approximation includes higher order contributions in \( U \) which are not contained in the HF+RPA approach.

The eigenvectors of Eq. (46) are given by

\[
X_\pm^t = \frac{1}{2}\alpha_\pm(1 + \omega_+/\Delta E),
\]

\[
X_\pm^t = \pm 1/2\alpha_\pm(1 + \omega_+/\Delta E),
\]

\[
Y_\pm^t = 1/2\alpha_\pm(1 - \omega_+/\Delta E),
\]

\[
Y_\pm^t = \pm 1/2\alpha_\pm(1 - \omega_+/\Delta E),
\]

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 \( \sum_{m=\pm}(|0\rangle\langle m|\langle m|n_j|0\rangle \) leading to

\[
D_{\text{GA}}^{\text{RPA}} = \frac{1}{4} + \frac{1}{8}\Delta E \left( 1/\omega_+ - 1/\omega_- \right).
\]

Approaching the SDW transition leads to an increase of spin fluctuations which leads to a divergent D_{\text{RPA}} at the transition point due to the Goldstone mode \( \omega_- \rightarrow 0 \) (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, i.e. \( E_{\text{int}} = \int_U dx D_{\text{RPA}}(x) \) which yields

\[
E_{\text{int}}^{\text{GA} + \text{RPA}} = -2t + U/2 + 2t \left( -2 + \sqrt{2 - (1-u)^2} + \sqrt{2 - (1+u)^2} \right).
\]

We thus obtain the GA+RPA ground-state energy which is displayed in Fig. 3 together with the corresponding HF+RPA and the exact result.

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 model. In the first part, we show that already on the saddle-point level, the GA yields rather accurate excitation energies as compared to HF. Inclusion of RPA corrections then lead to an additional redistribution of spectral weight in the correlation functions, which is demonstrated in the second part by a detailed comparison of exact diagonalization results with GA+RPA and HF+RPA. Especially this comparative study is 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. [3] 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 GA in comparison to HF, with respect to the one-particle excitation energies. For this purpose, we compare in the following 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 GA+RPA introduces non trivial corrections to the dynamical response functions.

Fig. 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, the ground state is characterized by long-range SDW order and the regular part of \( \sigma(\omega) \) is given by

\[
\sigma(\omega) = \frac{\Delta^2}{2\omega^2} \Re \sqrt{\frac{16t^2_{\text{eff}}}{\omega^2 - \Delta^2}} - 1, \tag{90}
\]

where \( t_{\text{eff}} \) contains the z-factor renormalization in case of the GA \( t_{\text{eff}}^{\text{GA}} = tz_1z_2 \), \( t_{\text{eff}}^{\text{HF}} = t \) and \( \Re \) denotes the real part. The SDW gap in HF is related to the onsite magnetization \( \Delta^{\text{HF}} = 2U|S_1| \), whereas within the Kotliar-Ruckenstein formulation of the GA it is determined by the difference in the local spin-dependent Lagrange multipliers \( \Delta^{\text{GA}} = \lambda_2 - \lambda_1 \). It is quite interesting to observe that the onset of excitations coincides rather well in the DDMRG[27] and GA approaches, whereas the HF gives a gap which is by far to 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 shows a much broader spectrum. We have checked the breadth of the exact spectrum by performing exact diagonalization in small clusters. In fact from Eq. (90) one obtains that the large frequency tail for GA and HF behaves as \( \sigma(\omega \gg \Delta) \sim 1/\omega^3 \) whereas the correct field theoretical result is \( \sigma(\omega \gg \Delta) \sim 1/\omega^2 \).

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, GA performs much better than HF since it reproduces the onset of excitations with a better accuracy.

B. Comparison with exact results

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

\[
S_{z}(\omega) = \sum_{m > 0} \left| \langle \Psi_{m}|n_{\downarrow}\Psi_{0} \rangle \right|^2 \delta(\omega - (E_{m} - E_{0})). \tag{91}
\]

In this case GA and GA+RPA solutions are different since the pathology discussed in the previous subsection is not present.

The following sum rule is obeyed [see Eq. (57)]:

\[
\int d\omega S_{z}(\omega) = -\langle T \rangle_{\text{GA}}. \tag{92}
\]

In Fig. 3 we show \( S_{z}(\omega) \) for a half-filled Hubbard chain with 14 sites calculated with exact diagonalization, GA+RPA, and 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 GA+RPA is much more accurate than the standard HF+RPA approach. Also the higher energy excitations computed with 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, GA+RPA slightly overestimates the intensity between $\omega \sim 3t$ 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 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 (GA) corresponds to a SDW state, whereas the exact solution in 1D 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 one expects disagreement due to this problem and since excitations in the system under consideration are gapped this discrepancy does not really show up.

Fig. 4(b) reveals that GA+RPA provides a better description of the low-energy excitations than HF+RPA, even at larger values of $U/t$. In addition, we show in Fig. 4(b) the charge-charge correlations for the bare GA. In this case, the corresponding excitations are located in a narrow energy window on the low-energy side of the exact spectrum with rather incorrect oscillator strength. Thus RPA corrections induce the broadening and shift of excitations to higher energies with a simultaneous redistribution of intensity. This can also be deduced from the inset to Fig. 4(b) which shows the evolution of the integrated spectrum $\int_0^\infty S_c(\nu) d\nu$ for GA and GA+RPA. From the sum rule Eq. (92) it is obvious that both GA and 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. Fig. 5 displays $S_c(\omega)$ for a half-filled $4 \times 4$ system (i.e. 16 particles) with $U/t = 10$. The lowest prominent energy peak in the exact solution occurs at $\omega_{min}^{exact} = 8.4t$ and a second bunch of excitations starts at $U/t \approx 10t \ldots 11t$ decaying in intensity towards higher energy. The lowest energy excitation within GA+RPA ($\omega_{min}^{GA+RPA} = 8.7t$) is remarkably close to the exact value in contrast to 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 energy within 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 HF+RPA despite the expected failure of the antiadiabaticity condition Eq. (17) for energies larger than the Mott-Hubbard gap.

We finally 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
satisfy a sum rule which involves the kinetic energy on the right hand side [Eqs. (15) and (17)], 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 $\omega$ factor. Therefore, the high-energy part of $S_c(\omega)$ is much more constrained to be accurate than the high-energy part of $\sigma$. 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. 3(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 render difficult due to the hopping factor expansion.

Compared to numerical methods\cite{28,29} our approach can be pushed to much larger systems. Our experience on modeling real data\cite{30,31} is that often finite size effects are much severer 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\cite{32} This has enormously increased our understanding of these systems. However, on making the limit of

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig6}
\caption{Charge correlation function $S_c(\omega)$ for the $4 \times 4$ Hubbard model and 10 particles in case of $U/t = 4$ (a) and $U/t = 10$ (b).}
\end{figure}
large dimensions important parts of the physics are lost. For example all acoustic like collective behavior, like spin waves disappears. On the other hand, these collective effects are naturally captured in our approach.

The GA+RPA formalism can be also applied to multiband Hubbard models, which are relevant for a more quantitative analysis of excitations in the cuprate high-Tc 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. In this context it is very important to make an 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 A: RELATIONSHIP TO KOTLIAR-RUCKENSTEIN SLAVE BOSON APPROACH

In the Kotliar-Ruckenstein slave-boson approach to the Hubbard model[1] the original Hilbert space is enlarged by introducing four subsidiary boson fields $c_i$, $s_{i,\uparrow}$, $s_{i,\downarrow}$, 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:

$$\epsilon_i^\dagger \epsilon_i + \sum_{\sigma} s_{i,\sigma}^\dagger s_{i,\sigma} + d_i^\dagger d_i = 1, \quad (A1)$$

and

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

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 $i,\sigma$ and $j,\sigma$ is renormalized by a factor $z_{i,\sigma} z_{j,\sigma}^*$ with

$$z_{i,\sigma} = (\epsilon_i^2 + s_{i,\sigma}^2)^{-1/2} (\epsilon_i s_{i,\sigma} + s_{i,\sigma} \rho_{ij}^* d_i) (d_i^2 + s_{i,\sigma}^2)^{-1/2}. \quad (A3)$$

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

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

which has to be minimized (i) with respect to the bosonic fields within the constraints Eqs. (A1) and (A2) and (ii) with respect to $\rho$ 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 Eqs. (A1) and (A2) one can eliminate 3N of them which leads to the Gutzwiller energy $E^{GA}$ when one keeps the double occupancy variable $D = d_i^2$ for each lattice site. Thus the expansions of $E^{SB}$ and $E^{GA}$ are connected via the transformation

$$\frac{\partial z_{i,\sigma}}{\partial D} = \frac{\partial z_{i,\sigma}^{SB}}{\partial d_i^2} = \frac{\partial z_{i,\sigma}^{SB}}{\partial s_{\sigma}^z} - \frac{\partial z_{i,\sigma}^G}{\partial \rho_{i,\sigma}}, \quad (A5)$$

and the derivatives have to be taken at the saddle-point. Upon inserting this transformation in Eqs. (14) 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. [20].

1. M. C. Gutzwiller, Phys. Rev. 137, A1726 (1965).
2. J. Bünnemann, F. Gebhard, and W. Weber, cond-mat/0006283.
3. J. Bünnemann, W. Weber and F. Gebhard, Phys. Rev. B 57, 6896 (1998).
4. N. E. Zein, Phys. Rev. B 52, 11813 (1995).
5. D. Pines and P. Nozieres, The Theory of Quantum Liquids, Vol. 1, Addison-Wesley (1989).
6. G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. 57, 1362 (1986).
7. T. Li, P. Wölfle, and P. J. Hirschfeld, Phys. Rev. B 40, 6817 (1989); R. Frésard and P. Wölfle, Int. J. Mod. Phys. B 6, 237 (1992).
8. E. Arrigoni and G. C. Strinati, Phys. Rev. Lett. 71, 3178 (1993); Phys. Rev. B 52, 2428 (1995).
9. J. W. Rasul and T. Li, J. Phys. C 21, 5119 (1988).
10. M. Lavagna, Phys. Rev. B 51, 142 (1990).
11. R. Raimondi and C. Castellani, Phys. Rev. B 48, 11453 (1993); R. Raimondi, Phys. Rev. B 51, 10154 (1995).
12. R. Raimondi, private communication.
13. G. Seibold and J. Lorenzana, Phys. Rev. Lett. 86, 2605 (2001).
14. D. J. Thouless, Nucl. Phys. 22, 78 (1961).
15. D. Vollhardt, Rev. Mod. Phys. 56, 99 (1984).
16. F. Gebhard, Phys. Rev. B 41, 9452 (1990).
17. W. Metzner and D. Vollhardt, Phys. Rev. Lett. 59, 121 (1987); Phys. Rev. B 37, 7382 (1988).
18. P. Ring and P. Schuck, The Nuclear Many-Body Problem, Springer-Verlag, New York, 1980.
19. J.-P. Blaizot and G. Ripka, Quantum Theory of Finite Systems, MIT Press, 1986.
20. G. Seibold, E. Sigmund, and V. Hizhnyakov, Phys. Rev. B 57, 6937 (1998).
21. W. F. Brinkman and T. M. Rice, Phys. Rev. B 2, 4302 (1970).
22. H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. 56, 3582 (1987).
23. J. Lorenzana, M. D. Grynberg, L. Yu, K. Yonemitsu, and A. R. Bishop, Phys. Rev. B 47, 13156 (1993).
24. G. D. Mahan, Many Particle Physics, Plenum, New York, 1990.
25. K. Yonemitsu, I. Batistić, and A. R. Bishop, Phys. Rev. B 44, 2652 (1991); K. Yonemitsu and A. R. Bishop, Phys. Rev. B 45, 5530 (1992).
26. A. L. Fetter and J. D. Walecka, Quantum Theory of Many-Particle Systems, McGraw-Hill, New York, 1971.
27. E. Jeckelmann, F. Gebhard, and F. H. L. Essler, Phys. Rev. Lett. 85, 3910 (2000).
28. E. Dagotto, Rev. Mod. Phys. 66, 763 (1994).
29. K. Binder and D. W. Heermann, Monte Carlo Simulations in Statistical Physics. An Introduction, Springer Series in Solid State Sciences Vol. 80, Springer-Verlag, Berlin/Heidelberg/New York, 1992.
30. J. Lorenzana and L. Yu, Phys. Rev. Lett. 70, 861 (1993).
31. G. Seibold, C. Castellani, C. Di Castro, and M. Grilli, Phys. Rev. B 58, 13506 (1998).
32. A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).
33. J. Lorenzana and G. Seibold, Phys. Rev. Lett. 89, 136401 (2002).