

Time-Dependent Gutzwiller Approximation for the Hubbard Model

G. Seibold¹ and J. Lorenzana^{2,*}

¹*Institut für Physik, BTU Cottbus, P.O. Box 101344, 03013 Cottbus, Germany*

²*Istituto Nazionale di Fisica della Materia e Dipartimento di Fisica, Università di Roma "La Sapienza," Piazzale Aldo Moro 2, 00185 Roma, Italy*

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We develop a time-dependent Gutzwiller approximation (GA) for the Hubbard model analogous to the time-dependent Hartree-Fock (HF) method. This new formalism incorporates ground state correlations of the random phase approximation (RPA) type beyond the GA. Static quantities like ground state energy and double occupancy are in excellent agreement with exact results in one dimension up to moderate coupling and in two dimensions for all couplings. We find a substantial improvement over traditional GA and HF + RPA treatments. Dynamical correlation functions can be computed and are also substantially better than HF + RPA ones and obey well behaved sum rules.

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The Gutzwiller (GW) trial wave function [1] is probably the most popular variational approach to the Hubbard model which incorporates correlation effects beyond the Hartree-Fock (HF) approximation. Since the Hubbard model describes the competition between hopping and correlation induced localization of the charge carriers, the idea is to apply a projector to a Slater determinant (SD) which reduces the number of doubly occupied sites. The optimum double occupancy probability is determined variationally. Similar to HF best results are obtained if one allows for unrestricted charge and spin distributions which are also determined variationally. For example, for the half-filled Hubbard model a SD with long range antiferromagnetic order is favored [2] and prevents the occurrence of a Brinkmann-Rice transition up to infinite dimensions [3].

A formal diagrammatic solution of the GW variational problem has been given by Metzner and Vollhardt [4]; however, for the most part of practical purposes one approximates the corresponding expectation values using the so-called Gutzwiller approximation (GA) [1]. For this approach the computational effort is similar to the HF approximation, but results are superior due to a better treatment of correlations.

The GA can be derived using a variety of methods [1,4–6]. In particular, it is recovered at the mean-field level (saddle point) of the four-slave boson functional integral method introduced by Kotliar and Ruckenstein (KR) [6]. The latter offers the possibility of going beyond the Gutzwiller result as, for example, the inclusion of transversal spin degrees of freedom [7]. In addition it provides a scheme (at least in principle) to include fluctuations beyond the mean-field (MF) solution. This has made the KR method quite popular since the inclusion of fluctuations on top of the GA has been a long-standing goal. Expansions around the slave-boson saddle point have been performed for homogeneous systems in Ref. [8] in order to calculate correlation functions in the charge and longitudinal spin channels. However, the expansion of the KR hopping fac-

tor z^{SB} is a highly nontrivial task both with respect to the proper normal ordering of the bosons and also with respect to the correct continuum limit of the functional integral [9].

The complexity of the expansions around the slave boson saddle point has severely hampered practical computations of dynamical quantities within this formalism. One of the few serious attempts is the computation of the optical conductivity in the paramagnetic state in Ref. [10]. As far as we know this approach has not been pursued in broken symmetry states due to technical difficulties, including the fact that the KR choice for the z^{SB} hopping factor does not lead to controlled sum rules [11].

In this work we overcome the above mentioned difficulties within the functional integral formalism and introduce an alternative scheme to compute fluctuation corrections around the GA to dynamical and static correlation functions and the ground state energy. The method can be viewed as a time-dependent GA in the same way as the random phase approximation (RPA) method on top of a HF solution (HF + RPA) can be viewed as time-dependent HF approximation in the limit of small amplitude oscillations [12]. For this reason we label the method as GA + RPA. It is also a generalization of the method of Ref. [13] in order to describe the low temperature Fermi liquid regime. The method incorporates ground state correlations beyond the ones of the Gutzwiller type just as HF + RPA takes into account ground state correlations not present in the HF wave function. Moreover, we treat the double occupancy parameter as a dynamical variable in contrast to the conventional static interpretation and we show that an antiadiabatic approximation for the double occupancy works remarkably well. The GA + RPA ground state energy of the one-band Hubbard model is in excellent agreement with exact results up to moderate coupling in one dimension (1D) and for all couplings in a 2D system (Fig. 1). The optical conductivity of a Hubbard chain is in much better agreement with numerical results than HF + RPA (Fig. 2). In addition sum rules are well behaved in the HF + RPA sense [12,14].

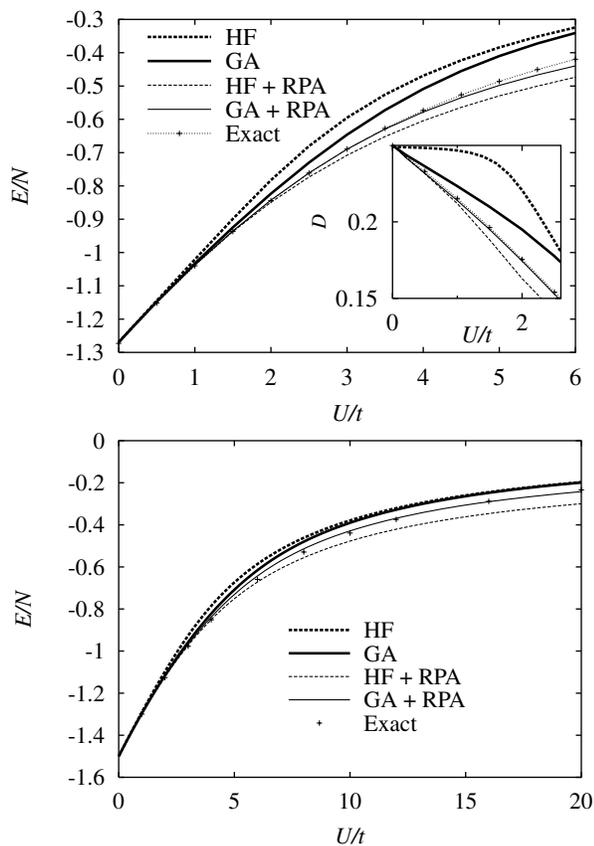


FIG. 1. Comparison of the exact ground state energy with the various approximate methods discussed in the text for the half-filled Hubbard model in 1D (upper panel) and 2D (lower panel). Exact results in the upper panel are for an infinite 1D system after Ref. [15], whereas approximate results are for a 32-site lattice. (Finite size errors are estimated to be of the order of line width.) Exact [16] and approximated results in the lower panel are for a 4×4 cluster. The insets show the corresponding curves for the 1D double occupancy (exact and GA + RPA are almost undistinguishable).

We consider the one-band Hubbard model

$$H = \sum_{ij,\sigma} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}, \quad (1)$$

and

$$z_{i\sigma} = \frac{\sqrt{(1 - \rho_{ii} + D_i)(\rho_{ii\sigma} - D_i)} + \sqrt{D_i(\rho_{ii,-\sigma} - D_i)}}{\sqrt{\rho_{ii\sigma}(1 - \rho_{ii\sigma})}}.$$

with $\rho_{ii} = \sum_{\sigma} \rho_{ii\sigma}$. The stationary solution $\rho^{(0)}$, $D^{(0)}$ is determined by minimizing the energy functional with respect to ρ and D .

The variation with respect to the density matrix has to be constrained to the subspace of Slater determinants by imposing the projector condition $\rho^2 = \rho$ [12]. Within this subspace we now consider small time-dependent amplitude fluctuations of the density matrix $\rho(t)$. We add a weak time-dependent field to Eq. (2) of the form $F(t) = \sum_{i\sigma,j\sigma'} (f_{i\sigma,j\sigma'} e^{-i\omega t} c_{i\sigma}^\dagger c_{j\sigma'} + \text{H.c.})$. This produces small

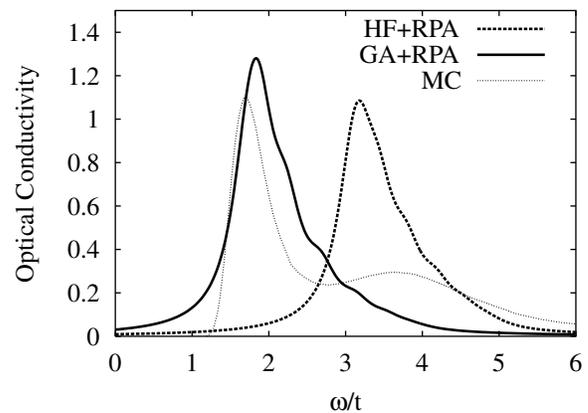


FIG. 2. Optical conductivity of a 32-site Hubbard ring for $U/t = 4$ in HF + RPA, GA + RPA, and Monte Carlo (MC) after Ref. [23]. The individual peaks of the GA + RPA and HF + RPA data have been broadened by a value of $0.25t$.

where $c_{i,\sigma}$ destroys an electron with spin σ at site i , and $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$. U is the on-site Hubbard repulsion and t_{ij} denotes the transfer parameter between sites i and j . In the numerical computations below we take only nearest neighbor matrix elements $t_{ij} = -t$ to be nonzero.

Our starting point is an energy functional $E[\rho, D]$ of the GA type [5]. Here ρ is the density matrix of an associated Slater determinant $|SD\rangle$, i.e., $\rho_{i\sigma,j\sigma'} = \langle SD | c_{i\sigma}^\dagger c_{j\sigma'} | SD \rangle$ and D is a vector of the GA double occupancy parameters D_i at site i . In order to consider arbitrary fluctuations the charge and spin distribution of ρ and the distribution of D should be completely unrestricted. For simplicity we consider only solutions where the associated SD is an eigenstate of the z component of the total spin operator ($\rho_{i\sigma,j\sigma'} \equiv \delta_{\sigma,\sigma'} \rho_{ij\sigma}$).

$E[\rho, D]$ can be obtained by exploiting the equivalence between the KR saddle point solution and the GA [5]. It is given by

$$E[\rho, D] = \sum_{ij\sigma} t_{ij} z_{i\sigma} z_{j\sigma} \rho_{ij\sigma} + U \sum_i D_i \quad (2)$$

amplitudes oscillations $\delta\rho(t)$ around the stationary density, i.e., $\delta\rho(t) \equiv \rho(t) - \rho^{(0)}$.

We assume that at each instant of time the double occupancy parameter is at the minimum of the energy functional compatible with the corresponding $\rho(t)$; i.e., the double occupancy parameters $\{D\}$ adjust antiadiabatically to the time evolution of the density matrix. This is reasonable since the double occupancy involves processes which are generally high in energy and hence fast. In

fact, using exact diagonalization on finite systems we have checked that the spectral function of the double occupancy operator has the main spectral features at energies much larger than the gap in the optical conductivity (Fig. 2) in agreement with our assumption. As the density varies the double occupancy shifts from $D^{(0)}$ to satisfy the antiadiabaticity constraint. We define $\delta D(t) = D(t) - D^{(0)}$ and $\delta\rho(t)$ and $\delta D(t)$ are linear in f .

The formal complication of the present approach as compared to the standard RPA has its origin in the proper adjustment of D to the time evolution of $\rho(t)$, i.e., the determination of $\delta D(t)$. This step is achieved by expanding the energy functional Eq. (2) up to second order in $\delta\rho$ and δD around the saddle point:

$$E[\rho, D] = E_0 + \bar{h}_0^\dagger \delta\bar{\rho} + \frac{1}{2} \delta\bar{\rho}^\dagger L_0 \delta\bar{\rho} + \delta D S_0 \delta\bar{\rho} + \frac{1}{2} \delta D^\dagger K_0 \delta D, \quad (3)$$

where the bar indicates that we are treating a matrix as a column vector and the subindex 0 indicates evaluation in the stationary state. Here we have defined an effective one-particle Gutzwiller Hamiltonian [12]:

$$h_{ji\sigma} = \frac{\partial E}{\partial \rho_{ij\sigma}}, \quad (4)$$

and the matrices

$$L_{ij\sigma,kl\sigma'} = \frac{\partial^2 E}{\partial \rho_{ij\sigma}^* \partial \rho_{kl\sigma'}}, \quad (5)$$

$$S_{k,ij\sigma} = \frac{\partial^2 E}{\partial D_k \partial \rho_{ij\sigma}}, \quad K_{k,l} = \frac{\partial^2 E}{\partial D_k \partial D_l}.$$

Using the condition of antiadiabaticity $\partial E / \partial \delta D = 0$ in Eq. (3) we obtain a linear relation between $\delta\rho$ and δD . Eliminating δD from Eq. (3) finally yields an expansion of the energy as a functional of $\delta\rho$ alone $\tilde{E}[\rho] \equiv E[\rho, D(\rho)]$,

$$\tilde{E}[\rho] = E_0 + \bar{h}_0^\dagger \delta\bar{\rho} + \frac{1}{2} \delta\bar{\rho}^\dagger (L_0 - S_0^\dagger K_0^{-1} S_0) \delta\bar{\rho}. \quad (6)$$

This can be regarded as the expansion of an effective interacting energy functional in which the interaction potential between particles is density dependent. This kind of functional often appears in the context of nuclear physics and a well-developed machinery exists to compute the RPA fluctuations induced by the interaction. We will only briefly outline here the corresponding formalism (for details, see Ref. [12]). The advantage of this method with respect to other methods (e.g., diagrammatic) is that the present derivation is solely based on the knowledge of an energy functional of a SD density matrix which is precisely what the GA provides.

At the saddle point h and ρ can be diagonalized simultaneously. As a result one obtains $(h_0)_{kl} = \delta_{kl} \epsilon_k$ and the density matrix has eigenvalue 1 below the Fermi level and eigenvalue 0 above the Fermi level. We will notate states

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

Up to linear order the density matrix obeys the equation of motion [12]:

$$i\hbar \delta\dot{\rho} = [\tilde{h}_0, \delta\rho] + \left[\frac{\partial \tilde{h}}{\partial \rho}, \delta\rho, \rho^{(0)} \right] + [f^{GA}, \rho^{(0)}], \quad (7)$$

where \tilde{h} is defined as in Eq. (4) but with \tilde{E} instead of E .

(Note that $\tilde{h}_0 = h_0$.) $\frac{\partial \tilde{h}}{\partial \rho} \cdot \delta\rho$ is a short hand notation for

$$\sum_{ph} \left(\frac{\partial \tilde{h}}{\partial \rho_{ph}} \Big|_{\rho=\rho^{(0)}} \delta\rho_{ph} + \frac{\partial \tilde{h}}{\partial \rho_{hp}} \Big|_{\rho=\rho^{(0)}} \delta\rho_{hp} \right). \quad (8)$$

f^{GA} is the GA version of f , i.e., it includes the z_0 factors for intersite matrix elements.

One can show that particle-particle and hole-hole matrix elements of Eq. (7) are zero and the particle-hole (ph) matrix elements of $\delta\rho$ satisfy the well-known RPA eigenvalue equation. The RPA dynamical matrix can be obtained from Eqs. (6) and (7). Upon diagonalizing the RPA matrix by a Bogoliubov transformation one obtains the eigenvectors $V^{(\lambda)} = [X_{ph}^{(\lambda)}, Y_{ph}^{(\lambda)}]$ and eigenvalues $E^{(\lambda)}$ where the latter correspond to the excitation energies of the system. An explicit expression for the response functions and a discussion of sum rules can be found in Ref. [12] which apply straightforwardly to our case.

The present formalism is well suited for the calculation of charge excitations in inhomogeneous doped systems [5,14,17,18] which will be presented elsewhere. In the following, we restrict ourselves to the half-filled Hubbard model in the antiferromagnetic Néel state [2]. The double occupancy at the RPA level is given by $D_{\text{RPA}} = \int d\omega \sum_{\lambda} \langle 0 | n_{i\uparrow} | \lambda \rangle \langle \lambda | n_{i\downarrow} | 0 \rangle \delta[\omega - E^{(\lambda)}]$ where the integrand is the Lehmann representation of an appropriately defined density-density correlation function. The matrix elements $\langle 0 | n_{\uparrow} | \lambda \rangle$ for $\lambda > 0$ can be computed in terms of the eigenvectors $V^{(\lambda)}$ [12].

In the inset of Fig. 1, we show the GA + RPA double occupancy compared with exact results and other approximations in a 1D system. For small U long range magnetic order is not enough to reduce substantially the HF double occupancy from the noninteracting value. RPA on top of HF corrects for this, but because the starting point is quite far from the exact result the correction is not so accurate and one gets that HF + RPA overstrikes the exact double occupancy and the energy [19]. On the contrary for the GA only a small correction is needed and RPA performs remarkably well. Note that $U(D_{\text{RPA}} - D_{\text{HF}})$ is a measure for the residual interaction in HF + RPA. In the GA + RPA approach such a simple relation is lost but clearly a smaller correction of the MF double occupancy suggests a smaller residual interaction.

Rigorously the residual interaction is given by the last term in Eq. (6). It is interesting to remark that this includes nonlocal terms which will affect long range correlations. This is in contrast to the HF + RPA method where the residual interaction is local.

From the interaction energy UD_{RPA} we compute the correction to the ground state energy using the coupling constant integration trick [20]. We find very good agreement with the exact results as shown in Fig. 1. This holds in 1D up to intermediate values of U/t and in a 4×4 2D cluster for all U/t . The improvement with dimensionality is expected as in any MF + RPA computation.

In order to examine the quality of dynamical correlation functions we have studied the optical conductivity in the GA + RPA approach. As in the HF + RPA method [12,14] the f -sum rule is exactly satisfied with the following prescription. The optical conductivity on one side of the equality should be computed at the GA + RPA (HF + RPA) level and the expectation value on the other side (essentially the kinetic energy in our case [21]) computed at GA (HF) level.

In this regard the f -sum rule provides also an encouraging argument that the GA + RPA dynamical correlation functions are much more accurate than those obtained via the corresponding HF + RPA method. We have compared the exact kinetic energy of a 4×4 lattice [22] with unrestricted GA and HF results for various hole concentrations and have found that over a wide range of doping and on-site correlation U there is almost perfect agreement between the GA method and exact results. On the other hand, the HF kinetic energy has an error that for example for $U = 4t$ is at least 40 times larger. This is not surprising since GA takes into account the correlation induced reduction of kinetic energy in a much better way than HF.

Figure 2 displays $\sigma(\omega)$ for a 32-site Hubbard ring and half-filling in case of $U/t = 4$. The onset of excitations across the Mott-Hubbard gap is signaled by the appearance of a large peak in $\sigma(\omega)$. We find excellent agreement between Monte Carlo (MC) and GA + RPA, whereas the excitation energy in HF is clearly overestimated. Note that the MC data display an additional hump at approximately twice the energy of the first peak. Processes in which a particle makes scattering with a particle-hole excitation (not included at RPA level) and the failure of the antiadiabaticity assumption for the double occupancy at high energies can explain the discrepancy. We see, however, that for energies of the order of the Hubbard band the method performs very well.

Regarding the computational effort, it is similar to the standard HF + RPA method [14,17]. For example, systems with 120 atoms can be solved in real space on a PC.

In conclusion, we have achieved the long standing goal of adding fluctuations to the GA. Our time dependent approach allows for the calculation of dynamical correlation functions and corrections to static quantities in Hubbard type models. The formalism is conceptually very simple and leads to much better agreement with exact results than previous approximations.

As in any computation of fluctuations we are dealing with the residual interaction between particles beyond the mean-field level. Roughly speaking since the GA contains

ground state correlations not included in a HF wave function the residual interaction is a smaller perturbation to the MF state and hence it is natural that RPA works much better in this case. In other words RPA fluctuations on top of a “correlated” mean field state (GW) converge much better to the exact result than fluctuations on top of an uncorrelated mean field state (HF), a concept which may be obvious *a posteriori* but by no means is obvious *a priori*.

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