Equivalence of Gutzwiller and slave-boson mean-field theories for multiband Hubbard models

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We demonstrate that a recently introduced slave-boson mean-field theory is equivalent to our Gutzwiller theory for multiband Hubbard models with general onsite interactions. We relate the different objects that appear in both approaches at zero temperature and discuss the limitations of both methods.

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I. INTRODUCTION

Over the past few years the Gutzwiller variational theory has developed into a useful tool for correlated multiband systems.[1–4,6,5,7–9] Gutzwiller introduced his wave function to study ferromagnetism in the one-band Hubbard model.[10] For the evaluation of expectation values he used a classical counting scheme, the so-called "Gutzwiller approximation"; see also Ref. 11 for the discussion of its physical content and Ref. 12 for its mathematical formulation. It was found later that this somewhat ad hoc approximation is equivalent to an exact evaluation of expectation values in the limit of infinite spatial dimensions or lattice coordination number.[13,14] An evaluation of Gutzwiller wave-functions in this limit will be denoted the "Gutzwiller theory" throughout this work. The limit of infinite spatial dimensions is also the central assumption in the dynamical mean-field theory (DMFT).[15] The solution of the DMFT equations is quite challenging even for the one-band Hubbard model. In contrast, the corresponding Gutzwiller variational space is just one-dimensional and its minimization is a trivial numerical task. Of course, the study of the electronic properties of real materials requires the treatment of multiband Hubbard models. This task was accomplished some years ago in Refs. 1, 2, and 4.

An alternative scheme to derive the Gutzwiller energy functional for a single band is based on the slave-boson mean-field theory (SBMFT) of Kotliar and Ruckenstein.[16] A generalization of this approach which reproduces the results of the multiband Gutzwiller theory is straightforward for systems with only density-density interaction.[1,17,18] It was only recently, however, that Lechermann *et al.*[19] succeeded to develop a SBMFT scheme that allows to investigate systems with general multi-band interactions. The authors interpret their approach as a generalization of the Gutzwiller theory. In fact, as we will show in this work, both theories are completely equivalent.

Our article is structured as follows. In Sec. II we introduce the multiband Hamiltonian and the general class of Gutzwiller wave functions. The equivalence of the SBMFT, as derived in Ref. 19, and the Gutzwiller theory is demonstrated in Sec. III. Finally, we critically discuss the limitations of both methods in Sec. IV.

II. HUBBARD MODELS AND GUTZWILLER WAVE FUNCTIONS

We investigate multiband Hubbard models, described by the general class of Hamiltonians

$$\hat{H} = \sum_{i \neq j;\sigma,\sigma'} t_{i,j}^{\sigma,\sigma'} \hat{c}_{i,\sigma}^{\dagger} \hat{c}_{j,\sigma'} + \sum_{i} \hat{H}_{\mathrm{loc},i} = \hat{H}_0 + \hat{H}_{\mathrm{loc}}. \tag{1}$$

Here, the first term describes the hopping of electrons between spin-orbital states σ, σ' on lattice sites i, j, respectively. The Hamiltonian $\hat{H}_{\mathrm{loc},i}$ contains all local terms, i.e., the two-particle Coulomb interactions and the orbital onsite-energies. For any lattice site i one introduces the Fock-states $|I\rangle_i$, in which certain sets of spin-orbital states σ are occupied.[2,4] These states form a basis of the local atomic Hilbert space and can be used to write any other local multiplet state as

$$|\Gamma\rangle_i = \sum_I T_{I,\Gamma}^{(i)} |I\rangle_i. \tag{2}$$

The most general ansatz for a multiband Gutzwiller wave function has the form

$$|\Psi_G\rangle = \hat{P}_G |\Psi_0\rangle = \prod_i \hat{P}_i |\Psi_0\rangle, \tag{3}$$

where $|\Psi_0\rangle$ is a normalized single-particle product state and the local Gutzwiller correlator is defined as

$$\hat{P}_i = \sum_{\Gamma,\Gamma'} \lambda_{\Gamma,\Gamma'}^{(i)} |\Gamma\rangle_{ii}\langle\Gamma'|. \tag{4}$$

Here, the states $|\Gamma\rangle_i$ can be an arbitrary atomic basis and the numbers $\lambda_{\Gamma,\Gamma'}^{(i)}$ are variational parameters. In our first work, Ref. 2, we assumed that the multiplets $|\Gamma\rangle_i$ are the eigenstates of $\hat{H}_{\mathrm{loc},i}$ and $\lambda_{\Gamma,\Gamma'}^{(i)} \sim \delta_{\Gamma,\Gamma'}$. The more general ansatz (4) was first evaluated in Ref. 4 for Hermitian operators $\hat{P}_{G,i}$. The non-Hermitian case has been studied in Ref. 8. In the following, we drop the site index when we deal with purely local quantities.

In general, the uncorrelated local density matrix

$$C_{\sigma,\sigma'}^0 \equiv \langle \hat{c}_{\sigma}^{\dagger} \hat{c}_{\sigma'} \rangle_{\Psi_0} \tag{5}$$

is not diagonal. It is then useful to introduce a second orbital basis, defined by the operators $\hat{h}_{\gamma}^{(\dagger)}$, which, by construction, have a diagonal local density matrix,

$$\hat{h}_{\gamma}^{(\dagger)} = \sum_{\sigma} u_{\gamma,\sigma}^{(*)} \hat{c}_{\sigma}^{(\dagger)}, \quad \langle \hat{h}_{\gamma}^{\dagger} \hat{h}_{\gamma'} \rangle_{\Psi_0} = \delta_{\gamma,\gamma'} n_{\gamma}^0. \tag{6}$$

Within the Gutzwiller theory one usually works in the new "*h* representation" because all formulae have a much simpler

form than in the original "c representation." However, in order to show the equivalence of the Gutzwiller theory with the slave-boson results in Sec. III, we have to work with both representations simultaneously. The operators $\hat{h}^\dagger_\gamma$ define Fock states $|H\rangle$ which can also be used to write the multiplet states (2) as

$$|\Gamma\rangle = \sum_H T_{H,\Gamma}|H\rangle, \tag{7}$$

where the coefficients $T_{H,\Gamma}$ and $T_{I,\Gamma}$ are related through

$$T_{H,\Gamma} = \sum_I \Omega_{H,I} T_{I,\Gamma}, \quad \Omega_{H,I} \equiv \langle H|I\rangle. \tag{8}$$

III. COMPARISON

The calculation of expectation values for Gutzwiller wave functions is a straightforward task, once the basic structure of diagrams in infinite dimensions is understood.[1,2,4] In contrast, the derivation of the generalized slave-boson mean-field theory in Ref. 19 requires a number of subtle ideas. Furthermore, there is not a clear correspondence of all the mathematical objects that appear in both approaches. Therefore, we are not going to compare any particular steps of the two quite different derivations, but focus on the final energy functional at zero temperature in order to show the equivalence of both approaches. For all details of the derivations we refer the reader to Refs. 1, 2, 4, and 19.

A. Local energy

In infinite dimensions, the expectation value of the local Hamiltonian $\hat{H}_{\mathrm{loc},i}$ in the Gutzwiller wave function reads

$$\langle \hat{H}_{\mathrm{loc},i}\rangle_{\Psi_G} = \sum_{\Gamma_1\ldots\Gamma_4} \lambda^*_{\Gamma_2,\Gamma_1}\lambda_{\Gamma_3,\Gamma_4} E^{\mathrm{loc}}_{\Gamma_2,\Gamma_3} m^0_{\Gamma_1,\Gamma_4}, \tag{9}$$

where

$$E^{\mathrm{loc}}_{\Gamma_2,\Gamma_3} \equiv \langle \Gamma_2|\hat{H}_{\mathrm{loc},i}|\Gamma_3\rangle, \tag{10}$$

$$m^0_{\Gamma_1,\Gamma_4} \equiv \langle (|\Gamma_1\rangle\langle\Gamma_4|)\rangle_{\Psi_0}. \tag{11}$$

The expectation value (11) can be written as

$$m^0_{\Gamma_1,\Gamma_4} = \sum_{H_1,H_4} T_{H_1,\Gamma_1} T^*_{H_4,\Gamma_4} m^0_{H_1,H_4} \tag{12}$$

$$= \sum_H T_{H,\Gamma_1} T^*_{H,\Gamma_4} m^0_H \tag{13}$$

because, for a diagonal local density-matrix in the h representation, one readily finds

$$m^0_{H,H'} = \delta_{H,H'} m^0_H, \tag{14}$$

$$m^0_H \equiv \prod_{\gamma(\mathrm{occ})} n^0_\gamma \prod_{\gamma'(\mathrm{unocc})} (1 - n^0_{\gamma'}). \tag{15}$$

In order to make contact with the results in Ref. 19 we need to bring Eq. (13) in the slightly more complicated form

$$m^0_{\Gamma_1,\Gamma_4} = \sum_{H,H',I} T_{H,\Gamma_1} \Omega^*_{H,I} \sqrt{m^0_H} T^*_{H',\Gamma_4} \Omega_{H',I} \sqrt{m^0_{H'}} \tag{16}$$

which is equivalent to Eq. (13) because of the completeness relation

$$\sum_I \Omega_{H',I}\Omega^*_{H,I} = \delta_{H,H'}. \tag{17}$$

We now introduce the new variational parameters

$$\varphi_{\Gamma,I} \equiv \sum_{\Gamma',H} \lambda_{\Gamma,\Gamma'} T^*_{H,\Gamma'} \Omega_{H,I} \sqrt{m^0_H} \tag{18}$$

which allow us to write the expectation value (9) as

$$\langle \hat{H}_{\mathrm{loc},i}\rangle_{\Psi_G} = \sum_{\Gamma,\Gamma'} \sum_I \varphi^*_{\Gamma,I}\varphi_{\Gamma',I} E^{\mathrm{loc}}_{\Gamma,\Gamma'} \tag{19}$$

This equation has exactly the same form as Eq. (47) in Ref. 19, after the slave-boson operators $\phi_{\Gamma,I}$ have been replaced by their mean-field expectation values, $\phi_{\Gamma,I} \mapsto \varphi_{\Gamma,I}$.

B. Local constraints

The variational parameters need to obey certain constraints which naturally arise in the evaluation in infinite dimensions. These are

$$\langle \hat{P}^\dagger \hat{P}\rangle_{\Psi_0} = 1, \tag{20}$$

$$\langle \hat{c}^\dagger_\sigma \hat{c}_{\sigma'} \hat{P}^\dagger \hat{P}\rangle_{\Psi_0} = \langle \hat{c}^\dagger_\sigma \hat{c}_{\sigma'}\rangle_{\Psi_0}. \tag{21}$$

Note that moving the operator $\hat{P}^\dagger\hat{P}$ relative to $\hat{c}^\dagger_\sigma$ or $\hat{c}_{\sigma'}$ in Eq. (21) would not alter the whole set of constraints. A set of constraints equivalent to Eq. (21) is obtained when we use the operators $\hat{h}^{(\dagger)}_\gamma$,

$$\langle \hat{h}^\dagger_\gamma \hat{h}_{\gamma'} \hat{P}^\dagger \hat{P}\rangle_{\Psi_0} = \langle \hat{h}^\dagger_\gamma \hat{h}_{\gamma'}\rangle_{\Psi_0}. \tag{22}$$

The constraint (20) can be written as

$$\sum_{\Gamma,\Gamma_1,\Gamma_2} \lambda^*_{\Gamma,\Gamma_1}\lambda_{\Gamma,\Gamma_2} m^0_{\Gamma_1,\Gamma_2} = 1, \tag{23}$$

which, by use of Eqs. (16) and (18), is found to be equivalent to

$$\sum_{\Gamma,I} \varphi^*_{\Gamma,I}\varphi_{\Gamma,I} = 1. \tag{24}$$

This is Eq. (28) in Ref. 19 at mean-field level. For the constraints (22) it follows that

$$\sum_{\Gamma,\Gamma_1,\Gamma_2} \sum_{H_1,H_2} \lambda^*_{\Gamma,\Gamma_1}\lambda_{\Gamma,\Gamma_2} T_{H_1,\Gamma_1} T^*_{H_2,\Gamma_2} \langle (\hat{h}^\dagger_\gamma \hat{h}_{\gamma'}|H_1\rangle\langle H_2|)\rangle_{\Psi_0}$$
$$= \langle \hat{h}^\dagger_\gamma \hat{h}_{\gamma'}\rangle_{\Psi_0}, \tag{25}$$

where, due to Eqs. (14) and (15), the expectation value on the left-hand side (LHS) can be written as

$$\langle (\hat{h}^\dagger_\gamma \hat{h}_{\gamma'}|H_1\rangle\langle H_2|)\rangle_{\Psi_0} = \langle H_2|\hat{h}^\dagger_\gamma \hat{h}_{\gamma'}|H_1\rangle \sqrt{m^0_{H_1} m^0_{H_2}}. \tag{26}$$

Then the identity

$$\langle H_2|\hat{h}^\dagger_\gamma \hat{h}_{\gamma'}|H_1\rangle = \sum_{I_1,I_2} \Omega_{H_2,I_2}\langle I_2|\hat{h}^\dagger_\gamma \hat{h}_{\gamma'}|I_1\rangle \Omega^*_{H_1,I_1} \tag{27}$$

transforms Eq. (25) into the form

$$\sum_\Gamma \sum_{I,I'} \varphi^*_{\Gamma,I}\varphi_{\Gamma,I'}\langle I'|\hat{h}^\dagger_\gamma \hat{h}_{\gamma'}|I\rangle = \langle \hat{h}^\dagger_\gamma \hat{h}_{\gamma'}\rangle_{\Psi_0}. \tag{28}$$

These equations can be transformed to the c-representation which leads to

$$\sum_\Gamma \sum_{I,I'} \varphi^*_{\Gamma,I'}\varphi_{\Gamma,I}\langle I|\hat{c}^\dagger_\sigma \hat{c}_{\sigma'}|I'\rangle = \langle \hat{c}^\dagger_\sigma \hat{c}_{\sigma'}\rangle_{\Psi_0}. \tag{29}$$

Equation (29) is equivalent to Eq. (29) in Ref. 19 at mean-field level.

C. Hopping renormalization

Finally, we investigate the expectation value of the electron transfer operators in the Hamiltonian (1). In infinite dimensions one finds that such an expectation value has the form $(i \neq j)$

$$\langle \hat{c}^\dagger_{i,\sigma_1}\hat{c}_{j,\sigma_2}\rangle_{\Psi_G} = \sum_{\sigma_1',\sigma_2'} r^{\sigma_1'}_{\sigma_1}(r^{\sigma_2'}_{\sigma_2})^*\langle \hat{c}^\dagger_{i,\sigma_1'}\hat{c}_{j,\sigma_2'}\rangle_{\Psi_0}, \tag{30}$$

or, alternatively, in the h representation

$$\langle \hat{h}^\dagger_{i,\gamma_1}\hat{h}_{j,\gamma_2}\rangle_{\Psi_G} = \sum_{\gamma_1',\gamma_2'} q^{\gamma_1'}_{\gamma_1}(q^{\gamma_2'}_{\gamma_2})^*\langle \hat{h}^\dagger_{i,\gamma_1'}\hat{h}_{j,\gamma_2'}\rangle_{\Psi_0}. \tag{31}$$

The local renormalization-matrix is most easily calculated in the h representation[4,7] where it has the rather simple form

$$q^{\gamma'}_\gamma = \frac{1}{n^0_{\gamma'}}\langle \hat{P}^\dagger \hat{h}^\dagger_\gamma \hat{P}\hat{h}_{\gamma'}\rangle_{\Psi_0}. \tag{32}$$

The matrix $r^{\sigma'}_\sigma$ in the c representation can then be derived from $q^{\gamma'}_\gamma$ by the transformation

$$r^{\sigma'}_\sigma = \sum_{\gamma,\gamma'} q^{\gamma'}_\gamma u_{\gamma,\sigma}u^*_{\gamma',\sigma'}. \tag{33}$$

With Eqs. (3) and (4), the matrix $q^{\gamma'}_\gamma$ reads explicitly

$$q^{\gamma'}_\gamma = \frac{1}{n^0_{\gamma'}}\sum_{\Gamma_1\ldots\Gamma_4} \lambda^*_{\Gamma_2,\Gamma_1}\lambda_{\Gamma_3,\Gamma_4}\langle\Gamma_2|\hat{h}^\dagger_\gamma|\Gamma_3\rangle\langle(|\Gamma_1\rangle\langle\Gamma_4|\hat{h}_{\gamma'})\rangle_{\Psi_0}, \tag{34}$$

where the expectation value in Eq. (34) can be written as

$$\langle(|\Gamma_1\rangle\langle\Gamma_4|\hat{h}_{\gamma'})\rangle_{\Psi_0} = \sum_{H_1,H_4} T_{H_1,\Gamma_1}T^*_{H_4,\Gamma_4}\langle H_4|\hat{h}_{\gamma'}|H_1\rangle \times \sqrt{m^0_{H_1}m^0_{H_4}}\sqrt{\frac{n^0_{\gamma'}}{1-n^0_{\gamma'}}}. \tag{35}$$

With Eqs. (17) and (18) we can rewrite Eq. (34) as

$$q^{\gamma'}_\gamma = \sqrt{\frac{1}{n^0_{\gamma'}(1-n^0_{\gamma'})}}\sum_{\Gamma,\Gamma'}\sum_{I,I'} \varphi^*_{\Gamma,I}\varphi_{\Gamma',I'}\langle\Gamma|\hat{h}^\dagger_\gamma|\Gamma'\rangle\langle I'|\hat{h}_{\gamma'}|I\rangle. \tag{36}$$

The transformation (33) from the h representation to the c representation is not as straightforward as the corresponding transformation from Eq. (28) to Eq. (29). Whereas the transformation with respect to the lower index γ is still simple

$$\langle\Gamma|\hat{c}^\dagger_\sigma|\Gamma'\rangle = \sum_\gamma \langle\Gamma|\hat{h}^\dagger_\gamma|\Gamma'\rangle u_{\gamma,\sigma}, \tag{37}$$

for the upper index γ' we need to take into account the factor $\sqrt{1/[n^0_{\gamma'}(1-n^0_{\gamma'})]}$ in Eq. (36) which also depends on γ'. For this purpose, we introduce the hole density-matrix $\tilde{D}$ with the elements

$$D^0_{\sigma,\sigma'} \equiv \langle \hat{c}_{\sigma'}\hat{c}^\dagger_\sigma\rangle_{\Psi_0}, \tag{38}$$

in addition to the density-matrix $\tilde{C}$ already defined in Eq. (5). Then the transformation (33) for the upper index γ' can be carried out along the lines

$$\sum_{\gamma'} u^*_{\gamma',\sigma'}\frac{\hat{h}_{\gamma'}}{\sqrt{n^0_{\gamma'}(1-n^0_{\gamma'})}} = \sum_{\gamma',\tilde{\sigma}}\frac{u^*_{\gamma',\sigma'}u_{\gamma',\tilde{\sigma}}}{\sqrt{n^0_{\gamma'}(1-n^0_{\gamma'})}}\hat{c}_{\tilde{\sigma}} \equiv \sum_{\tilde{\sigma}}[(\tilde{C}^0\tilde{D}^0)^{-1/2}]_{\tilde{\sigma},\sigma'}\hat{c}_{\tilde{\sigma}}. \tag{39}$$

Here, we used the notation

$$\sum_{\gamma'}\frac{u^*_{\gamma',\sigma'}u_{\gamma',\tilde{\sigma}}}{\sqrt{n^0_{\gamma'}(1-n^0_{\gamma'})}} = [(\tilde{C}^0\tilde{D}^0)^{-1/2}]_{\tilde{\sigma},\sigma'}. \tag{40}$$

With Eq. (40) and with $\langle I'|\hat{c}_{\tilde{\sigma}}|I\rangle = \langle I|\hat{c}^\dagger_{\tilde{\sigma}}|I'\rangle$ we can finally write the renormalization-matrix in the c representation as

$$r^{\sigma'}_\sigma = \sum_{\Gamma,\Gamma'}\sum_{I,I'}\varphi^*_{\Gamma,I}\varphi_{\Gamma',I'}\langle\Gamma|\hat{c}^\dagger_\sigma|\Gamma'\rangle \times \sum_{\tilde{\sigma}}[(\tilde{C}^0\tilde{D}^0)^{-1/2}]_{\tilde{\sigma},\sigma'}\langle I|\hat{c}^\dagger_{\tilde{\sigma}}|I'\rangle. \tag{41}$$

This expression matches Eq. (37) in Ref. 19 at mean field level, apart from the fact that there the constraints have been used to write the matrices $\tilde{C}^0\tilde{D}^0$ as a function of the fields $\varphi_{\Gamma,I}$; see Eqs. (35) and (36) in Ref. 19. However, as long as the constraints are fulfilled, this makes no difference because it does not change the variational energy functional.

IV. DISCUSSION

In this work, we showed that the multiband slave-boson mean-field theory of Lechermann *et al.* reproduces correctly the energy functional of the multi-band Gutzwiller theory developed earlier. As a by-product we were able to show how the different objects that appear in both approaches are related. This will turn out to be important for the comparison of future numerical results.

We believe that there are good reasons to prefer the derivation based on Gutzwiller wave functions over the slave-boson mean-field theory. First, these wave functions are well defined and they are evaluated exactly in the unambiguous limit of infinite spatial dimensions ($D \to \infty$). Therefore, e.g., the inclusion of superconducting pair correlations was straightforward.[4,6] In contrast, the slave-boson mean-field derivation is uncontrolled and quite adjustable in its outcome. Of all the different equations that one may derive within such an approach, the "right ones" are usually identified by some sophisticated guess. This guess, not surprisingly, always turns out to be equivalent to the Gutzwiller theory. This very equivalence is, by far, the most convincing argument for the credibility of the SBMFT results.

The Gutzwiller theory can also be used to calculate quasiparticle excitations within a Fermi-liquid approach[4,20] as well as spin-wave excitations.[21] The quasi-particle bands in the Gutzwiller theory coincide with those derived in the SBMFT. Therefore the zero-temperature spectral properties are equivalent in both approaches.

The ground-state energy functional also provides the Landau parameters for the description of thermodynamic properties.[11] Therefore, both approaches are equivalent in the Fermi-liquid regime when the temperature T is much smaller than the Fermi temperature T_F. Although the SBMFT equations can also be solved for $T \approx T_F$ or even for $T \gg T_F$, the approximation breaks down in this temperature regime.[22]

In principle, the SBMFT could be improved by computing fluctuations around the saddle point. To the best of our knowledge, however, this promise, although often made, has never materialized in any convincing improvement of the results, not even for the one-band Hubbard model.[23] In contrast, for Gutzwiller wave functions it is possible to calculate systematically $1/D$ corrections for all physical quantities.[14,20] Such calculations allow to estimate the accuracy of the results in infinite dimensions and to improve them, if necessary.

It should be kept in mind that the Gutzwiller theory is based on rather simple variational many-body wave functions which could be improved in many directions. Despite its limitations, however, the Gutzwiller theory appears to provide a suitable description of the quasiparticle bands in ferromagnetic nickel.[3,4]

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