A slave-boson mean-field theory for general multi-band Hubbard models

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We introduce a new slave-boson mean-field theory which allows the investigation of general multi-band Hubbard models. Unlike earlier attempts of such a generalisation, in our approach the quantum-mechanical problem is exactly reformulated in an extended Hilbert space of Fermions and Bosons before a mean-field approximation is applied. Systems with superconducting order parameters are naturally included in our formalism. Our ground-state energy functional agrees with the corresponding quantity derived within the Gutzwiller theory.

1 Introduction For the investigation of correlated electron systems in two or three dimensions only few theoretical approaches exist which lead to sensible results for small, medium, as well as strong Coulomb interaction parameters. A widely used approach which fulfils this criterion is the slave-boson mean-field theory. It has been introduced by Kotliar and Ruckenstein for an investigation of the single band Hubbard model [1]. The approach is based on two main ideas:

i) The original quantum-mechanical problem, described by a fermionic Hamiltonian $\hat{H}$, is reformulated by introducing bosonic degrees of freedom at each lattice site $i$ of the system. As long as certain constraints are exactly fulfilled, the resulting new Hamiltonian $\hat{H}$ in the enlarged bosonic-fermionic Hilbert space is mathematically equivalent to $\hat{H}$.

ii) The Hamiltonian $\hat{H}$ is investigated by means of a mean field theory or, in the language of functional integrals, by a saddle-point approximation.

Unfortunately, there is an infinite number of Hamiltonians $\hat{H}$, equivalent to $\hat{H}$, which may all lead to different results on mean-field level. Therefore, the approach requires a sophisticated guess in order to find the ‘right’ Hamiltonian which yields sensible mean-field results. The choice, made by Kotliar and Ruckenstein, leads to the same ground-state energy functional as it is found by an exact evaluation of Gutzwiller wave-functions in the limit of infinite spatial dimensions [2,3].

For the investigation of real materials one usually has to take into account the multi-orbital electronic structure of such systems. This requires the study of multi-band Hubbard models. While the generalisation of the Gutzwiller theory for multi-band models is rather straightforward even for systems with superconducting ground states [4,5,6], the very same generalisation of the slave-boson theory turned out to be difficult. Only recently such a generalised slave-boson scheme has been introduced for the treatment of general multi-band models [7]. The ground-state energy functional, derived in that work, has been shown to agree with the Gutzwiller functional [8]. In a more recent work [9], the scheme introduced in [7] was generalised in order to study superconducting systems. For such systems, however, the ground-state energy functional derived in [9] seems not to agree with the corresponding Gutzwiller functional [5].

In the derivations of Refs. [7,9] there is a fundamental shortcoming. While in the single-band case the derivation of the slave-boson theory is exact up to the point where the mean-field approximation is applied, the multi-band derivation of Ref. [7] requires additional approximations already on the level of the operator equations. It is the main purpose of this work to introduce an alternative slave-boson scheme for multi-band models which avoids these additional approximations and is exact apart from the final mean-field treatment. In addition, our new approach automatically covers systems with superconducting order parameters.
The presentation is organised as follows: In section 2 we introduce the general multi-band models that are investigated in this work. We briefly summarise the results of the Gutzwiller theory for multi-band Hubbard models in section 3. A reminder of the Kotliar-Ruckenstein theory for the one-band Hubbard model is given in section 4. Previous attempts to generalise this approach are discussed in section 5. In section 6 we derive our new slave-boson theory for the investigation of general multi-band models. A summary closes our presentation in section 6.

2 Model Hamiltonians

We study the general class of multi-band Hubbard models

\[ \hat{H} = \sum_{\sigma, \sigma'} \varepsilon_{\sigma, \sigma'} \hat{c}_{i, \sigma}^{\dagger} \hat{c}_{i, \sigma'} \quad \text{where} \quad \varepsilon_{\sigma, \sigma'} = \varepsilon_{\sigma} - U_{\sigma, \sigma'} \]

for each lattice site $i$. The Hamiltonian (2) is determined by the orbital-dependent on-site energies $\varepsilon_{\sigma, \sigma'}$ and by the two-particle Coulomb interaction $U_{\sigma, \sigma'}$. It contains $2N$ local spin-orbit states $\sigma$, which we assume to be ordered in some arbitrary way, $\sigma = 1, \ldots, 2N$. Here, $N$ is the number of orbitals per lattice site. In order to set up a proper basis of the local Hilbert space, we introduce the following notations for the $2^{2N}$ possible configurations:

i) An atomic configuration $I$ is characterised by the electron occupation of the orbitals,

\[ I \in \{ \emptyset; (1); (1,2); (1,2,3); \ldots (2N-1,2N); (1,2,\ldots,2N) \} \]

where the elements in each set $I = (\sigma_1, \ldots)$ are ordered, i.e., it is $\sigma_1 < \sigma_2 < \ldots$. The symbol $\emptyset$ in (3) means that the site is empty. In general, we interpret the indices $I$ as sets in the usual mathematical sense. For example, in the atomic configuration $I$ only those orbitals in $I$ that are not in $I'$ are occupied. The complement of $I$ is $\bar{I} \equiv (1,2,\ldots,2N) \setminus I$, i.e., in the atomic configuration $\bar{I}$ all orbitals but those in $I$ are occupied.

ii) The absolute value $|I|$ of a configuration is the number of elements of $I$, i.e.,

\[ |I| = \sum_{\sigma} n_{\sigma} \quad \text{where} \quad n_{\sigma} = \begin{cases} 1 & \text{if } \sigma \in I \\ 0 & \text{if } \sigma \in \bar{I} \end{cases} \]

\[ |I| = \sum_{\sigma} n_{\sigma} = \text{total number of orbitals} \]

iii) A state with a specific configuration $I$ is given as

\[ |I\rangle = \hat{C}_I^\dagger |0\rangle \equiv \prod_{\sigma \in I} \hat{c}_{i, \sigma}^{\dagger} |0\rangle = \hat{c}_{i, \sigma_1}^{\dagger} \cdots \hat{c}_{i, \sigma_{|I|}}^{\dagger} |0\rangle \]

where the operators $\hat{c}_{i, \sigma}^{\dagger}$ are in ascending order, i.e., it is $\sigma_1 < \sigma_2 < \ldots < \sigma_{|I|}$. Products of annihilation operators, such as

\[ \hat{C}_I \equiv \prod_{\sigma \in I} \hat{c}_{i, \sigma} = \hat{c}_{i, \sigma_1} \cdots \hat{c}_{i, \sigma_{|I|}} \]

will always be placed in descending order, i.e., with $\sigma_1 > \sigma_2 \cdots > \sigma_{|I|}$. Note that we have introduced the operators $\hat{C}_I^\dagger$ and $\hat{C}_I$ just as convenient abbreviations. They must not be misinterpreted as fermionic creation or annihilation operators.

iv) The operator $\hat{m}_{I, I'} \equiv |I\rangle \langle I'|$ describes the transfer between configurations $I'$ and $I$. It can be written as

\[ \hat{m}_{I, I'} = \hat{C}_I^\dagger \hat{C}_{I'} \prod_{\sigma'} (1 - \hat{n}_{\sigma'}) \]

where $J \equiv I \cup I'$. A special case, which derives from (7), is the occupation operator

\[ \hat{n}_{I} \equiv |I\rangle \langle I| = \prod_{\sigma \in I} \hat{n}_{\sigma} \prod_{\sigma' \in I} (1 - \hat{n}_{\sigma'}) \]

The states $|I\rangle$ form a basis of the atomic Hilbert space. Therefore, any other basis $|I'\rangle$ of the atomic Hilbert space can be written as

\[ |I'\rangle = \sum_{I} T_{I, I'} |I\rangle \]

with coefficients $T_{I, I'}$. With such a general basis, the atomic Hamiltonian has the form

\[ \hat{H}_{I, \text{loc}} = \sum_{I, I'} E_{I, I'} \hat{m}_{I, I'} \]

\[ \hat{m}_{I, I'} \equiv |I\rangle \langle I'| \]

In case that we deal with only one orbital per lattice site, the Hamiltonian (14) reads

\[ \hat{H}_{1\text{B}} = \sum_{i, j} \sum_{\sigma=1}^2 t_{i, j} \hat{c}_{i, \sigma}^\dagger \hat{c}_{j, \sigma} + \sum_{i} U_i \hat{m}_{i, 12} \]

Here, the indices $\sigma = 1, 2$ represent the two possible spin directions and $\hat{m}_{i, 12} = \hat{n}_{i, \sigma} \hat{n}_{i, \sigma'}$ with $\hat{n}_{i, \sigma} \equiv \hat{c}_{i, \sigma}^\dagger \hat{c}_{i, \sigma}$ is the “double-occupancy operator” on lattice site $i$.

3 The Gutzwiller Energy Functional for Multi-Band Systems

For later comparison with the slave-boson mean-field theories, we briefly summarise the results of the Gutzwiller theory for multi-band Hubbard models. For all technical details, we refer the reader to Refs. 4-5.

Multi-band Gutzwiller wave-function have the form

\[ |\Psi_G\rangle = \hat{P}_G |\Psi_0\rangle = \prod_i \hat{P}_i |\Psi_0\rangle \]
where $|\Psi_0\rangle$ is a normalized single-particle product state and the local Gutzwiller correlator is defined as

$$\hat{P}_{l} = \sum_{I'} \lambda_{l}^{(I)} |I'_I| |I'_I\rangle .$$

Note that, instead of Eq. (13), one can also work with a non-diagonal variational parameter matrix $\lambda_{l}^{(I',I)}$.

$$\hat{P}_{l} = \sum_{I,I'} \lambda_{l}^{(I,I')} |I'_I| |I'_I\rangle .$$

Since we work with an arbitrary atomic basis $|I\rangle$, however, both correlation operators (13) and (14) define the same variational space. In the following, we summarise the main results for a correlation operator of the form (13).

In general, the local uncorrelated density matrix

$$C_{i,\sigma} = \langle \hat{\epsilon}_{i,\sigma}^{\dagger} \hat{\epsilon}_{i,\sigma}^{\dagger} \rangle |\Psi_0\rangle$$

is non-diagonal with respect to $\sigma, \sigma'$. In superconducting systems, it additionally exhibits anomalous elements such as $\langle \hat{\epsilon}_{i,\sigma}^{\dagger} \hat{\epsilon}_{i,\sigma'} \rangle |\Psi_0\rangle$. By means of a unitary transformation (i.e., a Bogoliubov transformation for superconductors) one always finds a local basis with a diagonal density matrix and vanishing anomalous elements. In the following, we only work with such a local basis, since it simplifies the results for the variational energy. Nonetheless, we use the notations which we introduced in the previous section. For superconducting systems, this means that the single-particle Hamiltonian in [11] has the more complicated form

$$\hat{H}_{0} = \sum_{i\neq j} \sum_{\sigma,\sigma'} \left[ t_{i,j}^{\sigma,\sigma'} \hat{\epsilon}_{i,\sigma}^{\dagger} \hat{\epsilon}_{j,\sigma'} + t_{i,j}^{\sigma',\sigma} \hat{\epsilon}_{i,\sigma'}^{\dagger} \hat{\epsilon}_{j,\sigma} \right] .$$

Note that for our ‘orbital’ basis $|\sigma\rangle$ the expectation value of the operator (17) with respect to $|\Psi_0\rangle$ is given as

$$\langle \hat{\epsilon}_{i,\sigma}^{\dagger} \hat{\epsilon}_{i,\sigma}^{\dagger} \rangle |\Psi_0\rangle = \delta_{I,I'} \eta_{i,\sigma}^{0} .$$

where

$$\eta_{i,\sigma}^{0} \equiv \langle \hat{\epsilon}_{i,\sigma}^{\dagger} \hat{\epsilon}_{i,\sigma} \rangle |\Psi_0\rangle .$$

The variational parameters $\lambda_{l}^{(I)}$ need to obey certain constraints, which naturally arise in the evaluation in infinite dimensions [3,5]. These are

$$1 = \sum_{I'} \lambda_{l}^{*} \lambda_{l} \langle \hat{m}_{i,I'} \rangle |\Psi_0\rangle ,$$

$$\langle \hat{\epsilon}_{i,\sigma}^{\dagger} \hat{\epsilon}_{i,\sigma'} \rangle |\Psi_0\rangle = \lambda_{l}^{*} \lambda_{l} \langle \hat{m}_{i,I'} \rangle |\Psi_0\rangle .$$

With the expectation value

$$m_{i,I'} = \langle \hat{m}_{i,I'} \rangle |\Psi_0\rangle = \langle \hat{m}_{i,I'} \rangle |\Psi_0\rangle ,$$

one can readily calculate the local energy $\langle \hat{H}_{i,\text{loc}} \rangle |\Psi_0\rangle$. For the calculation of the single-particle energy, we have to determine the expectation values of normal and anomalous hopping operators,

$$\langle \hat{\epsilon}_{i,\sigma}^{(1)} \hat{\epsilon}_{j,\sigma'}^{(1)} \rangle |\Psi_0\rangle = \sum_{\sigma_1,\sigma_2} \langle \hat{\epsilon}_{i,\sigma_1}^{\dagger} \hat{\epsilon}_{j,\sigma_2} \rangle \langle \hat{\epsilon}_{i,\sigma_1}^{\dagger} \hat{\epsilon}_{j,\sigma_2} \rangle |\Psi_0\rangle ,$$

where, to simplify the notation, we dropped the lattice site index of the ‘renormalisation matrix’ $q_{\sigma}$. This renormalisation matrix is given as

$$q_{\sigma} = \sum_{I,I'} \lambda_{l}^{*} \lambda_{l} \langle \hat{m}_{i,I'} \rangle |\Psi_0\rangle .$$

where we introduced the operator

$$\hat{m}_{i,I'}^{\sigma} = \langle 1 - f_{\sigma'} |I'I'\rangle |\Psi_0\rangle ,$$

Here, we use the abbreviation $f_{\sigma} = \langle I'I'\rangle |\Psi_0\rangle$ and the operator

$$\hat{m}_{i,I'}^{\sigma} = \hat{C}_{i}^{\dagger} \hat{C}_{i} \prod_{\sigma' \in J} (1 - n_{\sigma'}) .$$

which is defined for $\sigma \in J \equiv \bar{I} \cup T$. Note that the expectation value of Eq. (23) in Eq. (22) can be readily evaluated with equations (17).

4 The Kotliar-Ruckenstein Theory

In the first part of this section, we introduce the auxiliary particle method, which was proposed by Kotliar and Ruckenstein for an investigation of the single-band Hubbard model. In the second part, previous attempts to generalise this approach for multi-band Hubbard models are discussed.

4.1 The One-Band Model

We start from the Hamiltonian [11] with its four-dimensional local Hilbert space $\mathcal{H}_{i}$ for each lattice site $i$, represented by the four states $|I\rangle = |0\rangle, |\sigma\rangle, |12\rangle$ (with $\sigma = 1, 2$ for the two spin directions). The Hilbert space of the whole lattice system is given by the tensor product

$$\mathcal{H} = \bigotimes_{i} \mathcal{H}_{i} .$$

Kotliar and Ruckenstein introduced auxiliary bosonic operators $\hat{\tilde{\epsilon}}_{i}\hat{\tilde{\epsilon}}_{i}^{\dagger}$, which lead to an enlarged local Hilbert space $\mathcal{H}_{i,\text{FB}}$ defined by the basis states

$$|I',I\rangle_{i,\text{FB}} = |I\rangle_{i} \bigotimes |I'\rangle_{i} .$$
Here, \(|I⟩\) is the fermionic configuration state defined in equation (5), and \(|I⟩_{i:B}\) is the bosonic state
\[
|I⟩_{i:B} ≡ |φ^+_i,1⟩|0⟩_{i:B} .
\] (26b)
with the bosonic vacuum state \(|0⟩_{i:B}\). The original quantum mechanical problem can be recovered in the following way:

i) One has to find a subspace \(\mathcal{H}^I\) of \(\mathcal{H}^FB\) which is isomorphic to the physical Hilbert space \(\mathcal{H}\) for each lattice site \(i\). Kotliar and Ruckenstein defined this subspace by means of the constraints
\[
\hat{F}_{i,0} ≡ 1 − \sum_j \hat{b}^+_{i,j} = 0 ,
\] (27a)
\[
\hat{F}_{i,σ} ≡ \hat{c}^+_{i,σ} \hat{c}_{i,σ} − \hat{n}^B_{i,σ} = 0 ,
\] (27b)
with the bosonic occupation operators
\[
\hat{n}^B_{i,σ} ≡ \hat{φ}^+_{i,1} \hat{φ}_{i,1} .
\] (28)
The constraints (27) define the subspace \(\mathcal{H}^I\) via the conditions
\[
\hat{F}_{i,σ} |Ψ⟩ = 0
\] (29)
for each \(|Ψ⟩ \in \mathcal{H}^I\) and \(σ \in \{0, 1, 2\}\). Alternatively, we can define \(\mathcal{H}^I\) directly by specifying its basis
\[
|I⟩_i ≡ |I⟩_{i:FB} |I⟩_{i:B} .
\] (30)
The corresponding Hilbert space for the lattice system is given by
\[
\mathcal{H} ≡ ⊗_i \mathcal{H}_i .
\] (31)
Note that, by construction, there is now a one-to-one correspondence of all physical states \(|Ψ⟩ \in \mathcal{H}\) and their counterparts \(|Ψ⟩ \in \mathcal{H}^I\).

ii) With the auxiliary Hilbert spaces \(\mathcal{H}_i\) and \(\mathcal{H}^I\) properly defined, one can find operators \(\hat{O}_i\) in \(\mathcal{H}_i\) that are similar to the physical operators \(\hat{O}_i\) in \(\mathcal{H}_i\). Here, ‘similarity’ means that
\[
⟨I| \hat{O}_i |I⟩ = ⟨I| \hat{O}^I_i |I⟩ \quad \text{for all configurations} \quad |I⟩, |I⟩ .
\] (32)
With similar local operators \(\hat{O}_i\), one can set up an ‘effective’ Hamiltonian \(\hat{H}^{1B}\) which is similar to the physical Hamiltonian \(\hat{H}\) in \(\mathcal{H}\), i.e., it obeys
\[
⟨Ψ| \hat{H}^{1B} |Ψ⟩ = ⟨Ψ| \hat{H}^I |Ψ⟩
\] (33)
for all physical states \(|Ψ⟩ , |Ψ⟩ \in \mathcal{H}\) and their counterparts \(|Ψ⟩ , |Ψ⟩ \in \mathcal{H}^I\). In this way, we have introduced an exact mapping of the original physical problem, described by the Hamiltonian \(\hat{H}\) in its Hilbert space \(\mathcal{H}\) and the effective Hamiltonian \(\hat{H}^{1B}\) in \(\mathcal{H}^I\).

To set up \(\hat{H}^{1B}\), we start with an identification of operators that are similar to the fermionic operators \(\hat{c}^{(1)}_{i,σ}\) in \(\mathcal{H}_i\). Their counterparts \(\hat{c}^{(1)}_{i,σ}\) in \(\mathcal{H}^I\) can be chosen as
\[
\hat{c}^+_i ;c_{i,σ} = \hat{r}^+_i ;c_{i,σ} , \quad \hat{c}^-_i ;c_{i,σ} = \hat{v}^+_i ;c_{i,σ} ,
\] (34a)
where the bosonic operators
\[
\hat{r}^+_i ;c_{i,σ} ≡ \hat{c}^{1^+_i}_i ;c_{i,σ} + \hat{c}^{1^-}_i ;c_{i,σ} , \quad \hat{r}^-_i ;c_{i,σ} = \hat{c}^{1^-}_i ;c_{i,σ} + \hat{c}^{1^+_i}_i ;c_{i,σ} ,
\] (34b)
have been introduced. As required, the operators \(\hat{c}^{(1)}_i ;c_{i,σ}\) obey equation (32). To set up the Hamiltonian \(\hat{H}^{1B}\) in \(\mathcal{H}^I\), we further need to find an operator \(\hat{m}_{i:12}\) that is similar to \(\hat{m}_{i:12} = \hat{n}_{i:1} \hat{n}_{i:2}\). The most obvious choice is
\[
\hat{m}_{i:12} = \hat{n}^B_{i:12} .
\] (35)
Note, however, that there is a large amount of arbitrariness. For example, the operators
\[
\hat{m}_{i:12} = \hat{n}^B_{i:1} \hat{n}_{i:2} \quad \text{or} \quad \hat{m}_{i:12} = \hat{n}_{i:1} \hat{n}^B_{i:2}
\] (36)
are also similar to \(\hat{m}_{i:12}\) since both obey equation (32). The same ambiguity arises for the operators (34a). For example, they may equally well be chosen as
\[
\hat{L}^+_i ;c_{i,σ} = \hat{q}^+_i ;c_{i,σ} \hat{c}^+_i , \quad \hat{L}^-_i ;c_{i,σ} = \hat{q}^-_i ;c_{i,σ} \hat{c}^-_i ,
\] (37a)
with
\[
\hat{q}^+_i ;c_{i,σ} ≡ (\hat{Δ}^+_i ;c_{i,σ})^{-1/2} \hat{r}^+_i ;c_{i,σ} (1 − \hat{Δ}^+_i ;c_{i,σ})^{-1/2} , \quad \hat{q}^-_i ;c_{i,σ} = (1 − \hat{Δ}^+_i ;c_{i,σ})^{-1/2} \hat{r}^+_i ;c_{i,σ} (\hat{Δ}^+_i ;c_{i,σ})^{-1/2} ,
\] (37b)
and
\[
\hat{Δ}^+_i ;c_{i,σ} ≡ \hat{n}^B_{i:12} + \hat{r}^-_i ;c_{i,σ} .
\] (37c)
In fact, this choice is better than (34a) and was used by Kotliar and Ruckenstein since it yields the correct ground-state energy in the uncorrelated limit \(U = 0\) if the resulting effective Hamiltonian
\[
\hat{H}^{1B} = \sum_{i,j,s} t_{i,j} \hat{q}_{i,σ}^* \hat{q}_{j,σ} \hat{c}^+_i \hat{c}^-_j + U \sum_i \hat{n}^B_{i:12}
\] (38)
is investigated on a mean-field level, see below.

Kotliar and Ruckenstein used a functional integral approach to calculate the free energy of the Hamiltonian (38). For ground-state properties, i.e., at zero temperature, their saddle-point approach is equivalent to a replacement of the bosonic operators \(\hat{φ}_{i,1}\) by the amplitudes \(\varphi_{i,1}\). They govern the bosonic occupations
\[
⟨\hat{N}^B_{i,σ}⟩ = |\varphi_{i,σ}|^2 .
\] (39)
and have to be determined by a minimisation of the ground-state energy functional
\[
⟨\hat{H}^{1B}⟩_{\varphi_{i,σ}} = \sum_{i,j,s} t_{i,j} \hat{q}_{i,σ}^* \hat{q}_{j,σ} \langle \hat{c}^+_i \hat{c}^-_j⟩ \varphi_0 + U \sum_i \hat{n}^B_{i:12} .
\] (40)
Here, the factors \(\hat{q}^+_i ;c_{i,σ}\) and \(\hat{q}^-_i ;c_{i,σ}\) are defined in (37) with the operators \(\hat{c}^{(1)}_i ;c_{i,σ}\) replaced by \(\varphi_{i,σ}^*\). Note that all quantities in this section are real and the asterisks, e.g., in equation (40),
are only used in anticipation of the corresponding multi-band results in section 5.

Instead of dealing with the exact constraints, they are also satisfied only on a ‘mean-field level’ by Kotliar and Ruckenstein, i.e., for the expectation values

\[ 1 = \sum_I n^I_{i,\sigma}, \quad n^0_{i,\sigma} = n^I_{i,1,2} + n^I_{i,\sigma}. \]  

(41a)  

(41b)

The constraints (41) and the energy functional (40) are the same as those derived for the Gutzwiller wave function in the limit of infinite spatial dimensions or evaluated by means of the Gutzwiller approximation.

4.2 Multi-Band Hubbard Models

A generalisation of the slave-boson theory is straightforward for multi-band Hubbard models with a local Coulomb interaction of the form

\[ \hat{H}_I = \sum_{\sigma,\sigma'} U_{\sigma,\sigma'} \hat{n}_\sigma \hat{n}_{\sigma'} = \sum_I U_I \hat{n}_I, \]  

(42)

where

\[ U_I = \sum_{\sigma,\sigma'} U_{\sigma,\sigma'} \]  

(43)

It yields the same energy functional as derived within the Gutzwiller theory. For the treatment of general multi-band Hubbard models a generalised slave-boson theory has been derived by Dai et al. and, more successfully, by Lechermann et al.

As demonstrated in the previous sections, the slave-boson approach contains a number of adjustable objects. These rather flexible elements of the theory are the definition of the extended Hilbert space \( \mathcal{H}_s^{\text{FB}} \), the definition of its physical subspace \( \mathcal{H}_s \), the form of the constraint equations \( \hat{F}_I = 0 \), and finally, the particular definition of similar operators \( \hat{O}_i \). Despite this huge flexibility, in both works and the authors fail to derive an exact mapping of Hilbert spaces and Hamiltonians which, on a mean-field level, leads to satisfactory results. We will briefly summarise the previous attempts to formulate a generalised slave-boson scheme for multi-band Hubbard models in this section. Our own derivation for such an approach is discussed in section 5.

Dai et al. use constraint equations which do not define the correct physical Hilbert space. This problem has been pointed out and solved by Lechermann et al. In their work, however, they fail to derive proper fermionic operators \( \hat{c}^{(1)}_{i,\sigma} \). Instead, symmetry arguments are used in order to guess the form of certain operators \( \hat{c}^{(1)}_{i,\sigma} \), which lead to a reasonable energy functional on mean-field level. These operators, however, are not similar to the physical operators \( \hat{c}^{(1)}_{i,\sigma} \), see below. Therefore, the whole derivation seems even less controlled than for the single-band model. In this section, we briefly summarise the main ideas of the slave-boson mean-field theory introduced by Lechermann et al.

As in case of the single-band model one has to set up a local Hamiltonian \( \mathcal{H}_I \) which is isomorphic to the physical fermionic Hamiltonian \( \mathcal{H}_I \) with its basis \( |I\rangle \). Lechermann et al. discuss various possibilities to define such local Hilbert spaces consisting of bosons and fermions. At first sight, it seems that \( \mathcal{H}_I \) is most naturally defined as a generalisation of (30) through a basis

\[ |I\rangle_i = |I\rangle_i \otimes |I\rangle_i ; B \]  

(44)

with bosonic operators \( \hat{c}^{(1)}_{i,\sigma} \) and the corresponding states \( |I\rangle_i ; B \equiv |I\rangle_i \otimes |0\rangle_i B \). However, the Hilbert-space \( \mathcal{H}_I \) defined by this basis is discarded by Lechermann et al. on the grounds that there is no way to find a reasonable set of constraint equations as an alternative definition of \( \mathcal{H}_I \). In section 5 we show that the basis (44) can, in fact, be used for a slave-boson theory, which, however, has to be different from the original scheme introduced by Kotliar and Ruckenstein.

Instead of (44), Lechermann et al. introduce the basis

\[ |I\rangle_i = \frac{1}{\sqrt{|I|}} \sum_{I(I| = |I')} \phi_{i,I,I'} |0\rangle_i B \otimes |I\rangle_i \]  

(45)

as a definition of their Hilbert space \( \mathcal{H}_I \). Note that in their derivation they draw a distinction between physical particles and quasi-particles, described by operators \( \hat{c}^{(1)}_{i,\sigma} \) and \( \hat{j}^{(1)}_{i,\sigma} \), respectively. Our derivation in this section indicates that this distinction is unnecessary.

The Ansatz (45) employs bosonic operators \( \hat{O}_{i,I} \) for each pair of multiplet states \( |I\rangle \) and configurations states \( |I\rangle \) with the same particle number \( |I| = |I| \). The number of these operators is much larger than the dimension of the local Hilbert space, which is different from the original single-band scheme introduced by Kotliar and Ruckenstein. Despite this large number of operators, the space \( \mathcal{H}_I \) is isomorphic to the physical Hilbert space \( \mathcal{H}_I \) with its basis \( |I\rangle_i \). Therefore, it is possible to find operators \( \hat{O}_{i,I} \) in \( \mathcal{H}_s \) that are similar to the physical operators \( \hat{O}_i \) in \( \mathcal{H}_s \), see below.

For the mean-field treatment, one has to find constraints which define the Hilbert space \( \mathcal{H}_I \) in a unique way. As shown in [7], this is achieved by means of the operator identities

\[ \hat{F}_{1,0} = 1 - \sum_{I,J} \hat{c}^{(1)}_{i,I,I} \hat{O}_{i,I,I} = 0, \]  

(46a)

\[ \hat{F}_{i,\sigma,\sigma'} = \hat{c}^{(1)}_{i,\sigma} \hat{c}^{(1)}_{i,\sigma'} - \sum_{I,I',J} \hat{O}_{i,I,I'} |I\rangle_i \hat{c}^{(1)}_{i,\sigma} \hat{c}^{(1)}_{i,\sigma'} |I\rangle_i = 0. \]  

(46b)
The representation \( \hat{w}_{i,\Gamma}',\Gamma' \) of local operators in \( \mathcal{H}_i \) is readily given by
\[
\hat{w}_{i,\Gamma}',\Gamma' = \sum_I \hat{\phi}_{i,\Gamma,\Gamma}',I \hat{\phi}_{i,\Gamma,\Gamma}',I^\dagger .
\]
(47)
This result leads to the representation
\[
\hat{H}_{i,\text{loc}} = \sum_{\Gamma,\Gamma'} E_{i,\Gamma,\Gamma'}^\text{loc} \sum_I \hat{\phi}_{i,\Gamma,\Gamma}',I \hat{\phi}_{i,\Gamma,\Gamma}',I^\dagger
\]
(48)
of the local Hamiltonian \( \mathcal{H} \).

In order to set up the effective Hamiltonian \( \hat{\mathcal{H}} \), one needs representations \( \hat{c}_{i,\sigma}' \) of fermionic creation operators. As shown in (49), a conceivable choice for \( \hat{c}_{i,\sigma}' \) would be
\[
\hat{c}_{i,\sigma}' = \sum_{\sigma'} \hat{q}_{i,\sigma,\sigma'} \hat{c}_{i,\sigma'}\dagger ,
\]
(49a)
where
\[
\hat{q}_{i,\sigma,\sigma'} = \sum_{\Gamma,\Gamma''} \sum_{I,I'} \frac{\langle I'|\hat{c}_{i,\sigma}'|\Gamma''\rangle \langle I'|\hat{c}_{i,\sigma}|\Gamma\rangle}{\sqrt{|\langle I'|\rangle (N - |\Gamma\rangle^2)}} \hat{\phi}_{i,\Gamma,\Gamma',I'} \hat{\phi}_{i,\Gamma',I} .
\]
(49b)
is a bosonic operator and \( N \) is the number of spin-orbital states \( |\sigma\rangle \) per site. Evaluated on mean-field level, however, expression (49) does not lead to a reasonable energy functional since it does not yield the correct results in the uncorrelated limit. Note that the situation here is different from the single-band model since, there, it was possible to find improved expressions for the operator \( \hat{c}_{i,\sigma}' \), which are still similar to the physical operators \( \hat{c}_{i,\sigma} \). In case of the operators (49), it seems to be unfeasible to improve them accordingly. Instead, Lechermann et al. introduce the following ‘improved’ expression for \( \hat{c}_{i,\sigma}' \), which, though leading to reasonable results on the mean-field level, is mathematically not similar to \( \hat{c}_{i,\sigma} \),
\[
\hat{q}_{i,\sigma,\sigma'} = \sum_{\Gamma,\Gamma''} \sum_{I,I'} \hat{\phi}_{i,\Gamma,\Gamma',I} \hat{\phi}_{i,\Gamma',I} \hat{c}_{i,\sigma}'\dagger \hat{c}_{i,\sigma'}\dagger ,
\]
(50)
where
\[
\hat{M}_{i,\sigma,\sigma'} \equiv \left( \frac{1}{2} \hat{\Delta}_{i,\sigma}'\dagger \hat{\Delta}_{i,\sigma}' + \hat{\Delta}_{i,\sigma}'\dagger \hat{\Delta}_{i,\sigma}' - 1/2 \right)_{\sigma,\sigma'} ,
\]
(52)
and
\[
\hat{\Delta}_{i,\sigma,\sigma'}^{(p)} = \sum_{\Gamma,\Gamma'} \hat{\phi}_{i,\Gamma,\Gamma',I} \hat{\phi}_{i,\Gamma',I} \hat{c}_{i,\sigma}'\dagger \hat{c}_{i,\sigma'}\dagger ,
\]
(53a)
\[
\hat{\Delta}_{i,\sigma,\sigma'}^{(h)} = \sum_{\Gamma,\Gamma'} \hat{\phi}_{i,\Gamma,\Gamma',I} \hat{\phi}_{i,\Gamma',I} \hat{c}_{i,\sigma}'\dagger \hat{c}_{i,\sigma'}\dagger .
\]
(53b)
Note that \( \hat{\Delta}_{i,\sigma,\sigma'}^{(h,p)} \) and \( \hat{M}_{i,\sigma,\sigma'} \) are considered as matrices with respect to the indices \( \sigma, \sigma' \) whose elements are bosonic operators. The inversion \([\ldots]^{-1/2}\) and the square root in (52) are defined with respect to this matrix structure.

The operators (48) and (50) define an effective Hamiltonian
\[
\hat{H} = \sum_{i,j} \hat{\epsilon}^{\sigma,\sigma'}_{i,j} \sum_{\sigma,\sigma';\gamma,\gamma'} \hat{q}_{i,\sigma} \hat{q}_{j,\sigma'}^\dagger \hat{c}_{i,\gamma}^\dagger \hat{c}_{j,\gamma'} + \sum_i \hat{H}_{i,\text{loc}}
\]
(54)
which can now be evaluated on mean-field level, i.e., by replacing the operators \( \hat{q}_{i,\Gamma} \) by their corresponding amplitudes \( \varphi_{i,\Gamma,\Gamma,\Gamma'}^{(\tau)} \). These amplitudes then serve as variational parameters.

In Ref. [8], it was shown that the energy functional that results from the mean-field treatment of the constraints (46) and of the Hamiltonian (54) agrees with the Gutzwiller variational results introduced in Refs. [45].

5 A New Slave-Boson Theory for Multi-Band Hubbard Models As discussed in the previous section, a generalisation of the Kotliar-Ruckenstein scheme for the investigation of multi-band models faces significant problems, which, up to now, have not been solved satisfactorily. Here, we show that, due to the enormous flexibility of the 

slave-boson approach, it is, in fact, relatively easy to reproduce the Gutzwiller energy functional for multi-band Hubbard models. To this end, however, one has to approach the problem in a different way than Kotliar and Ruckenstein. In the first part of this section, we introduce our new slave-boson scheme by reconsidering the single-band model. In the second part, we show that our new approach can be easily applied to multi-band models including those with superconducting ground states.

5.1 The Single-Band Model For our alternative formulation of the slave-boson theory, we introduce the operators
\[
\hat{m}_{i,I}^B = \hat{\xi}_{i,I}^B\hat{\theta}_{i,I}
\]
(55a)
where
\[
\hat{\theta}_{i,I}^B \equiv \hat{\theta}_{i,I}^B \prod_{I'} \hat{\epsilon}_{i,I'}
\]
(55b)
and
\[
\hat{\epsilon}_{i,I} \equiv \prod_{n=1}^{\infty} \left( 1 - \frac{\hat{\phi}_{i,\Gamma,\Gamma'}^\dagger \hat{\phi}_{i,\Gamma}^\dagger \hat{\phi}_{i,\Gamma} \hat{\phi}_{i,\Gamma'} \hat{\phi}_{i,\Gamma'}\dagger \hat{\phi}_{i,\Gamma}\dagger \hat{\phi}_{i,\Gamma}\dagger \hat{\phi}_{i,\Gamma'}\dagger \hat{\phi}_{i,\Gamma'}\dagger }{n} \right)
\]
(55c)
is the projection operator onto the vacuum state of the boson created by \( \hat{\phi}_{i,\Gamma} \). The operator (55a) therefore projects onto the sub-space with exactly one boson in the state \( |i; I\rangle \) occupied.

As pointed out before, there is a large amount of arbitrariness in the choice, e.g., of the constraints (27). Instead of those equations, we can also work with
\[
\hat{F}_{i,0} = 1 - \sum_I \tilde{m}_{i,I}^B m_{i,I}^B = 0 ,
\]
(56a)
\[
\hat{F}_{i,\sigma} = \hat{n}_{i,\sigma} - \hat{n}_{i,\sigma} \sum_I \tilde{m}_{i,I}^B m_{i,I}^B = 0 ,
\]
(56b)
where \( \hat{n}_{i,\sigma} \) has been defined in Eq. (8). Note that the Hilbert space \( \hat{H} \), given by the basis (31), is already uniquely defined by the first constraint, equation (56a). In \( \hat{H} \), however, the second equation is equally valid, i.e., we have \( \hat{F}_{i,\sigma} \langle \hat{I} \rangle = 0 \) for all states (56d).

In the Kotliar-Ruckenstein scheme, the operators \( \hat{\varphi}_{i,\sigma} \) are chosen as \( \hat{n}_{i,\sigma}^\dagger \), c.f. equation (28). In our approach, we work with

\[
\hat{\varphi}_{i,\sigma} \equiv \hat{m}_{i,1} m_{i,1}^B \; .
\]

(57)

Since we are only interested in the derivation of an approximate ground-state-energy functional, we avoid functional integral techniques here and employ the variational wave function

\[
|\psi_0^F\rangle \equiv |\psi_0^B\rangle \otimes |\psi_0\rangle
\]

(58a)

where \( |\psi_0\rangle \) is a fermionic single-particle product state and

\[
|\psi_0^B\rangle \equiv \prod_i \hat{D}_i |0\rangle
\]

(58b)

a coherent bosonic state with

\[
D_i \equiv \prod_j \exp \left( \varphi_{i,T}^\dagger \hat{\varphi}_{i,\sigma} - \varphi_{i,T}^\dagger \hat{\varphi}_{i,\sigma}^\dagger \right) .
\]

(58c)

By construction, (58b) is a normalised eigenstate of \( \hat{\varphi}_{i,\sigma} \) with eigenvalues \( \varphi_{i,\sigma} \); see, e.g., Ref. [19]. In addition, we have

\[
\langle \hat{\varphi}_{i,T} \rangle |\psi_0^B\rangle = \exp ( - |\varphi_{i,\sigma}|^2 ) ,
\]

(59a)

\[
\langle \hat{\varphi}_{i,T}^\dagger \hat{\varphi}_{i,T} \rangle |\psi_0^B\rangle = |\varphi_{i,\sigma}|^2 \prod_i \exp ( - |\varphi_{i,\sigma}|^2 )
\]

(59b)

which leads to the expectation value

\[
\langle \hat{m}_{i,1} \rangle |\psi_0^B\rangle = \langle \hat{m}_{i,1} \rangle |\psi_0\rangle |\psi_{i,\sigma}|^2
\]

(60)

where we introduced

\[
\varphi_{i,\sigma} \equiv \varphi_{i,\sigma} \prod_i \exp ( - |\varphi_{i,\sigma}|^2 / 2 ) .
\]

(61)

A comparison with the corresponding result in the Gutzwiller theory [20] shows that the Gutzwiller variational parameters \( \lambda_i \) correspond to the 'renormalised' bosonic amplitudes

\[
\varphi_{i,\sigma} \equiv \lambda_i .
\]

(62)

The constraints (56d), evaluated on mean-field level (i.e., using the wave-functions (58b)), have the form

\[
1 = \sum_i |\varphi_{i,\sigma}|^2 \langle \hat{m}_{i,1} \rangle |\psi_0\rangle ,
\]

(63a)

\[
\hat{n}_{i,\sigma}^0 = |\varphi_{i,\sigma}|^2 (\hat{m}_{i,1})^\dagger |\psi_0\rangle + |\varphi_{i,\sigma}|^2 (\hat{m}_{i,1})^\dagger |\psi_0\rangle
\]

(63b)

which is in agreement with equations (41) if we equate \( \hat{n}_{i,\sigma}^B \) (in the Kotliar-Ruckenstein scheme) with \( |\varphi_{i,\sigma}|^2 \langle \hat{m}_{i,1} \rangle |\psi_0\rangle \) (in our new slave-boson scheme).

Finally, we choose the operators \( \hat{\varphi}_{i,\sigma}^\dagger \) in \( \hat{H} \) as

\[
\hat{\varphi}_{i,\sigma}^\dagger = \hat{\varphi}_{i,\sigma}^\dagger \hat{\varphi}_{i,\sigma}^\dagger \; ,
\]

(64a)

\[
\hat{\varphi}_{i,\sigma} = \hat{\varphi}_{i,\sigma}^\dagger \hat{\varphi}_{i,\sigma}^\dagger
\]

(64b)

where

\[
\varphi_{i,\sigma} \equiv \theta_{i,12} \varphi_{i,\sigma}^\dagger \varphi_{i,\sigma} + \theta_{i,\sigma}^\dagger \varphi_{i,\sigma}^\dagger (1 - \varphi_{i,\sigma}^\dagger ) .
\]

(64b)

Note that here, unlike in the Kotliar-Ruckenstein scheme, the operators \( \varphi_{i,\sigma}^\dagger \) contain both fermionic and bosonic degrees of freedom. Evaluated with the wave function (58), one finds

\[
\varphi_{i,\sigma} = \langle \varphi_{i,\sigma}^\dagger \varphi_{i,\sigma} \rangle = \theta_{i,12} \varphi_{i,\sigma}^\dagger \varphi_{i,\sigma} + \theta_{i,\sigma}^\dagger \varphi_{i,\sigma}^\dagger (1 - \varphi_{i,\sigma}^\dagger ) ,
\]

(65)

which agrees with equations (37) on mean-field level. However, the expectation value of a hopping operator is the same as in the Gutzwiller theory,

\[
\langle \hat{\varphi}_{i,\sigma}^\dagger \hat{\varphi}_{i,\sigma} \rangle \varphi_{i,\sigma}^\dagger \varphi_{i,\sigma} = \varphi_{i,\sigma}^\dagger \varphi_{i,\sigma}^\dagger \varphi_{i,\sigma}^\dagger \varphi_{i,\sigma} = 0 .
\]

(66)

These terms emerge when the fermionic expectation value \( \langle \hat{n}_{i,\sigma} \hat{\varphi}_{i,\sigma}^\dagger \hat{\varphi}_{i,\sigma} \rangle \varphi_{i,\sigma}^\dagger \varphi_{i,\sigma} = \varphi_{i,\sigma}^\dagger \varphi_{i,\sigma}^\dagger \varphi_{i,\sigma}^\dagger \varphi_{i,\sigma} \)

(68)

Since the three-line terms vanish in the limit of infinite spatial dimensions, our slave-boson approach yields the same variational ground-state energy as the Gutzwiller theory.

5.2 General Multi-Band Models

A generalisation of our new slave-boson scheme for multi-band Hubbard models is straightforward. We work with an arbitrary set of local multiplet states \( |\Gamma\rangle \), which define the basis (51) of a Hilbert space \( \hat{H} \). For these states, we introduce bosonic operators \( \hat{m}_{i,\Gamma}^B \) and \( \hat{\theta}_{i,\Gamma}^\dagger \), i.e., only with \( I \) replaced by \( \Gamma \).

As a generalisation of (56), we work with the constraints

\[
\hat{F}_{i,0} \equiv 1 = \sum_{\Gamma} \hat{m}_{i,\Gamma}^B \hat{m}_{i,\Gamma}^B = 0 ,
\]

(69a)

\[
\hat{F}_{i,\sigma,\sigma'} \equiv \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma'}^\dagger - \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma'} + \sum_{\Gamma} \hat{m}_{i,\Gamma}^B \hat{m}_{i,\Gamma}^B = 0 ,
\]

(69b)

which yield an alternative way to define the Hilbert space \( \hat{H} \).

The operators \( \hat{m}_{i,\Gamma,\Gamma'} \) are properly represented in \( \hat{H} \) by

\[
\hat{m}_{i,\Gamma,\Gamma'} \equiv \sum_{\sigma} \hat{m}_{i,\Gamma}^B \hat{m}_{i,\Gamma}^B \hat{\theta}_{i,\Gamma}^\dagger \hat{\theta}_{i,\Gamma'}^\dagger
\]

(70)

An evaluation of these operators on mean-field level, i.e., by means of a wave function (58), with

\[
\hat{D}_i \equiv \prod_i \exp \left( \varphi_{i,\sigma} \hat{\varphi}_{i,\Gamma}^\dagger - \varphi_{i,\sigma}^\dagger \hat{\varphi}_{i,\Gamma} \right) ,
\]

(71)
leads to
\[ m_{i,G,G'} = \langle \hat{m}_{i,G,G'} \rangle_0 = \langle \hat{m}_{i,G,G'} \rangle_0 \theta_{i,G} \theta_{i,G'} \quad (72) \]
with
\[ \theta_{i,G} \equiv \varphi_{i,G} \prod_{G'} \exp \left( -|\varphi_{i,G'}|^2/2 \right). \quad (73) \]
A comparison with Eq. (19) reveals the correspondence of the variational parameters \( \lambda_{i,G} \) in the Gutzwiller theory and the amplitudes \( \theta_{i,G} \) in our new slave-boson mean-field approach.

An evaluation of the constraints (69) on mean-field level leads to
\[ 1 = \sum_{G,G'} \theta_{i,G}^* \theta_{i,G'} \langle \hat{m}_{i,G,G'} \rangle_0 , \quad (74a) \]
\[ \langle \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma'} \rangle_0 = \sum_{G,G'} \theta_{i,G}^* \theta_{i,G'} \langle \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma'} \hat{m}_{i,G,G'} \rangle_0 , \quad (74b) \]
which matches the Gutzwiller constraints, equations (18).

Finally, we define the operator
\[ \hat{\xi}_{i,\sigma} \equiv \sum_{\sigma'} \tilde{q}_{i,\sigma} \hat{c}_{i,\sigma'} \quad (75a) \]
with
\[ \tilde{q}_{i,\sigma} = \sum_{G,G'} \hat{\theta}_{i,G} \hat{\theta}_{i,G'} \langle \hat{G} | \hat{G}' \rangle \sum_{I,I'} T_{I,I'} T_{G,G'}^{*} \hat{H}_{I,I'}^{*} . \quad (75b) \]
Here, we dropped the lattice-site index \( i \) and use the operator \( \hat{H}_{I,I'} \) defined in Eq. (23). The operator \( \hat{\xi}_{i,\sigma} \) in \( \hat{H}_i \) is similar to the physical creation operator \( \hat{c}_{i,\sigma} \) because the sums over \( \sigma' \) and \( I, I' \) in equations (75) are just a complicated expression for
\[ |I\rangle \langle I'| = \sum_{\sigma,\sigma'} T_{I,I'} T_{I',I}^{*} \hat{H}_{I,I'}^{*} \hat{c}_{I',\sigma} \hat{c}_{I,\sigma'} . \quad (76) \]
A mean-field evaluation of (75b) leads to the renormalisation matrix
\[ q_{i,\sigma} = \sum_{G,G'} \hat{\theta}_{i,G} \hat{\theta}_{i,G'} \langle \hat{G} | \hat{G}' \rangle \sum_{I,I'} T_{I,I'} T_{G,G'}^{*} \hat{H}_{I,I'}^{*} \hat{c}_{I',\sigma} \hat{c}_{I,\sigma'} , \quad (77) \]
which matches equation (22) in the Gutzwiller theory. As in the single-band model, the expectation values of normal and anomalous hopping operators agree with those in the Gutzwiller theory
\[ \langle \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma'} \rangle_0 = \sum_{\sigma_1,\sigma_2} \tilde{q}_{i,\sigma_1} \tilde{q}_{j,\sigma_2} \langle \hat{c}_{i,\sigma_1}^\dagger \hat{c}_{j,\sigma_2} \rangle_0 , \quad (78) \]
only if we neglect the contributions with more than one line connecting the sites \( i \) and \( j \). This is ensured in the limit of infinite spatial dimensions, where both approaches then yield the same ground-state energy functional.

6 Conclusions

In summary, we have developed a new slave-boson scheme for general multi-band Hubbard models which, in the limit of infinite dimensions, reproduces the results of the Gutzwiller theory. The main advantage of our new approach is its exactness up to the point where a mean-field approximation is applied. In addition, it automatically covers the cases of systems with superconducting order parameters.

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