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Numerical optimization algorithm for rotationally invariant multi-orbital slave-boson method

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ABSTRACT

We develop a generalized numerical optimization algorithm for the rotationally invariant multi-orbital slave boson approach, which is applicable for arbitrary boundary constraints of high-dimensional objective function by combining several classical optimization techniques. After constructing the calculation architecture of rotationally invariant multi-orbital slave boson model, we apply this optimization algorithm to find the stable ground state and magnetic configuration of two-orbital Hubbard models. The numerical results are consistent with available solutions, confirming the correctness and accuracy of our present algorithm. Furthermore, we utilize it to explore the effects of the transverse Hund's coupling terms on metal–insulator transition, orbital selective Mott phase and magnetism. These results show the quick convergency and robust stable character of our algorithm in searching the optimized solution of strongly correlated electron systems.

1. Introduction

Introducing auxiliary bosons to strongly correlated fermionic systems is an important method for many-body physics, such as the slave boson, the slave spin and slave rotor techniques [1–3]. Amongst these approaches, the Kotliar–Ruckenstein slave boson approach [1] is a very useful tool in dealing with correlated electron system. In this approach, the Hilbert space is enlarged to include fermionic and auxiliary slave bosonic degrees of freedom. The fermionic degree of freedom describes Landau quasiparticles, and the bosonic degrees describe the local states [4]. By setting a series of constraints, which select the physical states out of enlarged Hilbert space, the local physical configurations can be coherently described by the fermionic and bosonic degrees of freedom.

Slave-boson mean-field theory is mainly developed to calculate the quasiparticle (QP) weight of correlated electron systems, and a part of spin and orbital fluctuations is taken into account. The Fermi surfaces of the correlated systems are determined by the QP weight and Lagrange multipliers, which globally ensure the physical constraints. The slave-boson mean-field theory is able to eliminate local repulsive interaction through introducing local constraints, and projects a highly correlated system into an uncorrelated state [1]. Thus it is convenient to deal with complicated spin and orbital-ordered states [5–7], superconductive state [4] and spin liquid state [8]. The high-energy fluctuation processes could also be described by the auxiliary boson fields [9].

The single-orbital slave-boson functional-integral method introduced by Kotliar and Ruckenstein [1] was extended to two-orbital degenerate Hubbard model by Hasegawa et al. [5,10,11], hence could be used to investigate multi-orbital metal–insulator transitions. However, the multi-orbital Kotliar–Ruckenstein slave boson (KRSB) method is only suitable to handle with the model Hamiltonian with density–density interactions [1,12]. The rotationally invariant slave boson (RISB) method was proposed by Wölfle et al. [13,14] and generalized to multi-orbital case by Lechermann et al. [12,15–17]. In the complicated magnetic configurations or multiorbital systems, the number of slave bosons increases exponentially with the increase of the number of freedom degrees, the slave-boson mean-field approximation still costs much computation resource when searching for the ground state of multi-orbital correlated systems, even in the KRSB framework [18,19]. Meanwhile, when we further consider the contributions of the spin flip and pair hopping terms to reveal the roles of spin and orbital fluctuations, the RISB method should be applied, and we need to optimize a total-energy problem with many slave boson variables. In this case, the classical single optimization technique hardly finishes such a task. So it is desirable to develop a

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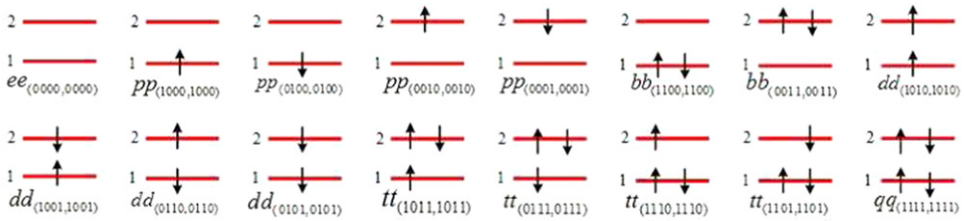

Fig. 1. The atomic spin and orbital configurations of two-orbital system and the corresponding slave bosons. Here e, p, b, d, t, q denote states from empty to four occupations in the corresponding graphs. The first group numbers in the indexes of slave bosons, for example $ee_{(0000,0000)}$, etc., describe the occupations on electron species in the sequence of (spin up of orbital 1, spin down of orbital 1, spin up of orbital 2 and spin down of orbital 2) in the physical Fock state, the second group numbers in the indexes have the similar meaning in the QP Fock state, where 0 denotes empty and 1 is occupied.

more efficient and stable numerical algorithm for both the KRSB and RISB methods.

In this paper, we develop a numerical optimization algorithm by synthesizing the pattern search method [20], the gradient method [21] and the Rosenbrock technique [22]. This algorithm is applicable for arbitrary boundary constraint of the objective function. Then we employ it to search for the ground state of the two-orbital Hubbard model in the RISB framework, and discuss the effects of spin–flip and pair-hopping Hund's rule coupling terms on Mott metal–insulator transition and magnetic moments. The comparisons between our solutions and available results confirm that the present algorithm is accurate, efficient and stable for numerically optimizing the total energy of multi-orbital slave boson approach. The rest of this paper is organized as follows: we firstly describe the model Hamiltonian and theoretical approach in Section 2; then the numerical optimization algorithm and numerical method for two-orbital slave-boson approach are described in Section 3; in Section 4, the numerical accuracy and stability of our algorithm applied for two-orbital RISB model are analyzed; finally the concluding remarks are given in Section 5.

2. Rotationally invariant slave boson formulas of two-orbital Hubbard model

To describe the low-energy physical processes in strongly correlated electron systems, we usually adopt the multi-orbital Hubbard model Hamiltonian, which can be written in the following form:

$$H = H_0 + H_I \tag{1}$$

with

$$H_0 = -\sum_{\langle ij\rangle,\alpha,\beta,\sigma}\left(t_{ij}^{\alpha,\beta}d_{i\alpha\sigma}^{\dagger}d_{j\beta,\sigma} + h.c.\right) + \sum_{i,\alpha,\sigma}(\varepsilon_\alpha - \mu)\, n_{i\alpha\sigma} \tag{2}$$

and

$$\begin{aligned} H_I =\ & U\sum_{i,\alpha} n_{i\alpha\uparrow}n_{i\alpha\downarrow} + \sum_{i,\sigma,\sigma',\alpha>\beta}\left(U' - J_Z\delta_{\sigma\sigma'}\right) n_{i\alpha\sigma}n_{i\beta\sigma'} \\ & - J_X\sum_{i,\alpha\neq\beta}\left(d_{i\alpha\uparrow}^{\dagger}d_{i\alpha\downarrow}d_{i\beta\downarrow}^{\dagger}d_{i\beta\uparrow}\right) + J_P\sum_{i,\alpha\neq\beta}\left(d_{i\alpha\uparrow}^{\dagger}d_{i\alpha\downarrow}^{\dagger}d_{i\beta\downarrow}d_{i\beta\uparrow}\right) \end{aligned} \tag{3}$$

where $d_{i\alpha\sigma}^{\dagger}$ creates an electron with the orbital index α and spin σ at the lattice site i, $n_{i\alpha\sigma}$ denotes the corresponding occupation number operator, ε_α is the energy level of the α orbital, μ is the chemical potential. The hopping integral between two orbitals α and β is denoted by $t_{ij}^{\alpha\beta}$, and the intra-orbital (inter-orbital) Coulomb repulsion is U (U'). The density–density interaction term, spin–flip term and pair-hopping term of the Hund's rule coupling are denoted by J_Z, J_X and J_P, respectively. Throughout this paper we set $U' = U - 2J_Z$ and $J_Z = 0.25U$, and the two orbitals are degenerate, *i.e.* $\varepsilon_1 = \varepsilon_2$.

Next, we project the original Hamiltonian (1) into the RISB representation. In the RISB framework (see the Appendix), sixteen Fock states in two-orbital case are shown in Fig. 1, which have been used for the two-orbital KRSB model [23], the corresponding slave bosons are plotted. It is obviously that the electron occupations associated with physical space are identical to those associated with QP space in KRSB method. We chose these Fock states as the bases of the physical and QP spaces. The matrix that is made up of 256 slave bosons is shown in Fig. 2. The local atomic Fock bases in physical and QP spaces are also plotted at the heads of each row and line. The same sequences of the Fock bases in the physical and QP spaces are adopted, thus the KRSB fields only appear in the diagonal. The off-diagonal slave bosons are classified into six groups, according to their described physics as shown Fig. 2. For example, the off-diagonal slave bosons in the SR region describe the physics with regard to the spin-rotation symmetry. The off-diagonal slave bosons between different lattices are neglected since the interaction between different lattices is not considered in the present two-orbital Hubbard model. As shown in the Appendix, in the rotational-invariant saddle-point approximation, the complicated model Hamiltonian given by Eqs. (1) and (2) reduces to a optimization problem of total energy functional, see Eqs. (A.12) and (A.13).

In the saddle-point approximation, the total energy of two-orbital Hubbard model is given by:

$$E_{gs} = E_{kin} + E_{loc} \tag{4}$$

with

$$\begin{aligned} E_{kin} =\ & \begin{pmatrix}\mathbf{R}_{\mathbb{A}}^{\dagger} & 0\\ 0 & \mathbf{R}_{\mathbb{B}}^{\dagger}\end{pmatrix}\boldsymbol{\varepsilon}(\mathbf{k})\begin{pmatrix}\mathbf{R}_{\mathbb{A}} & 0\\ 0 & \mathbf{R}_{\mathbb{B}}\end{pmatrix} + \begin{pmatrix}\boldsymbol{\Lambda}_{\mathbb{A}} & 0\\ 0 & \boldsymbol{\Lambda}_{\mathbb{B}}\end{pmatrix} \\ & + \begin{pmatrix}\mathbf{E}_{0\mathbb{A}} - \mu & 0\\ 0 & \mathbf{E}_{0\mathbb{B}} - \mu\end{pmatrix} \end{aligned} \tag{5}$$

and

$$\begin{aligned} E_{loc} =\ & tr\left[\begin{pmatrix}\boldsymbol{\Phi}_{\mathbb{A}} & 0\\ 0 & \boldsymbol{\Phi}_{\mathbb{B}}\end{pmatrix}\begin{pmatrix}\mathbf{E}_{\mathbb{A}}^{(b)} & 0\\ 0 & \mathbf{E}_{\mathbb{B}}^{(b)}\end{pmatrix}\begin{pmatrix}\boldsymbol{\Phi}_{\mathbb{A}} & 0\\ 0 & \boldsymbol{\Phi}_{\mathbb{B}}\end{pmatrix}\right] \\ & + U\lambda\left[\sum_{aAm}|\phi_{aAm}|^2 - 2\right] \\ & - \sum_{mn}\left[\begin{pmatrix}\boldsymbol{\Lambda}_{\mathbb{A}} & 0\\ 0 & \boldsymbol{\Lambda}_{\mathbb{B}}\end{pmatrix}\circ\begin{pmatrix}\mathbf{n}_{\mathbb{A}} & 0\\ 0 & \mathbf{n}_{\mathbb{B}}\end{pmatrix}\right]_{mn}. \end{aligned} \tag{6}$$

Here $\boldsymbol{\varepsilon}(\mathbf{k})$ is the energy dispersion matrix of the system. $\mathbf{R}_{\mathbb{A}}$ and $\mathbf{R}_{\mathbb{B}}$ in Eq. (5) are the renormalization factor matrices of lattices A and B defined by Eq. (A.5), which is written in a more compact matrix form as follows:

$$\mathbf{R}_a = \mathbf{C}_a\mathbf{M}_a^T \tag{7}$$

with

$$C_{a\alpha\gamma} = \sum_{ij}[\mathbf{D}_a \circ (\boldsymbol{\Phi}_a\mathbf{F}_a\boldsymbol{\Phi}_a)]_{ij}, \tag{8}$$

where $\boldsymbol{\Phi}_a$ is the slave boson matrix, and the symbol '$\circ$' denotes Hadamard product. The index a denotes sublattice A or sublattice B.