Accuracy of the slave-boson method in calculations of the electronic structure of strongly correlated systems

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Specific representations of the effective Hamiltonian in the slave-boson method and of constraints on the fermion and boson variables are found. These representations are the best approximation of the exact solution in the multiband case.

A strong electron–electron interaction is a governing factor in the physical properties of several systems. Among these are heavy-fermion systems,[1] high-T_c superconductors,[2] and magnetic semiconductors based on chalcogenides of f-shell transition metals[3] (EuX, GdX, and DyX, where X=O, S, Se, or Te). The standard models for describing strongly correlated systems are the Hubbard model,[4] the Anderson model with an infinite repulsion,[5] and various modifications of the two. An effective method for analyzing this class of lattice models is the so-called slave-boson method, various versions of which were developed in Refs. 6–9. The most common version is that proposed by Kotliar and Ruckenstein[9] for the single-band Hubbard model.

The slave-boson method has been used in combination with the strong-coupling method to calculate the electron spectrum of strongly correlated systems in several papers (this approach has been used particularly frequently in the case of high-T_c superconductors). All such calculations have used the saddle-point approximation, in which the boson fields are replaced by mean fields. The parametrization for the boson fields introduced in Ref. 9 for the single-band scheme is applied directly to multiband models.

The problem is that the introduction of auxiliary bosons is not unambiguous at the operator level. All that is required is that the new effective Hamiltonian be exactly equivalent to the original one at the operator level. Since the introduction of bosons expands the space of states, constraints are imposed on the boson and fermion operators in order to maintain exact equivalence. The switch to the saddle-point approximation, on the other hand, reduces (roughly speaking) to the replacement of boson operators by their mean values. The exact equivalence is disrupted in an uncontrollable way in the process. There is no general rule for selecting a particular representation. The only selection condition is that the result agree best with the exact solution.

In the present letter we establish a parametrization of boson fields at a saddle point which leads to the best agreement in the multiband case through a comparison of results found by the slave-boson method and by the exact-diagonalization method.

Since the exact-diagonalization method makes it possible to work with small clusters, for definiteness (and also with an eye on further applications in realistic calculations

for the compounds EuX, GdX, and DyX, which crystallize in a NaCl lattice) we consider a plane square cluster of atoms of two species. We write the Hamiltonian in the form

$$H=\sum_{i=\sigma}\varepsilon_i f_{i\sigma}^{+} f_{i\sigma}+\sum_{NN\sigma} t_{ij} f_{i\sigma}^{+} f_{j\sigma}+\sum_{i} U_i f_{i_\uparrow}^{+} f_{i_\uparrow} f_{i_\downarrow}^{+} f_{i_\downarrow}, \tag{1}$$

where ε_i is the site energy ($i=1, 2$; t is the hopping integral between nearest neighbors). We assume that Coulomb repulsion is important only at sites of one species. For CuO_2, for example, we assume that this repulsion is important only at copper atoms, while for EuX we assume that it is important only for Eu atoms. The total number of electrons in the cluster is 6; this figure corresponds to the case of EuX (the chalcogen band is completely filled, while that of the transition metal in the f shells is half-filled). The spectrum of the Hamiltonian for this number of electrons is found by diagonalizing a 16×16 matrix.

We turn now to the slave-boson representation. Following Ref. 9, we define the effective Hamiltonian by

$$H_{\text{eff}}=\sum_{i\sigma}\varepsilon_i c_{i\sigma}^{+} c_{i\sigma}+\sum_{NN\sigma} t_{ij} z_{i\sigma}^{+} z_{j\sigma}\, c_{i\sigma}^{+} c_{j\sigma}+\sum_{i} U_i d_i^{+} d_i, \tag{2}$$

where $z_{i\sigma}=(d_i^{+}d_i+p_{i\sigma}^{+}p_{i\sigma})^{-1/2}(p_{i\sigma}^{+}e_i+d_i^{+}p_{i-\sigma})(e_i^{+}e_i+p_{i-\sigma}^{+}p_{i-\sigma})^{-1/2}$, $c_{i\sigma}^{+}$ and $c_{i\sigma}$ are fermion creation operators, and e_i^{+}, $p_{i\sigma}^{+}$, and d_i^{+} are creation operators for auxiliary bosons. Hamiltonian (2) acts in an expanded space of states which is the tensor product of the fermion and boson subspaces. In this expanded space we can single out a subspace defined by the constraints

$$e_i^{+}e_i+p_{i_\uparrow}^{+}p_{i_\uparrow}+p_{i_\downarrow}^{+}p_{i_\downarrow}+d_i^{+}d_i=1, \tag{3}$$

$$c_{i\sigma}^{+}c_{i\sigma}=p_{i\sigma}^{+}p_{i\sigma}+d_i^{+}d_i. \tag{4}$$

In this subspace H_{eff} is the same as H.

Representation (2) is not unique. We could obviously incorporate in $z_{i\sigma}$, as right and left factors, any operator expressions which satisfy the following conditions: 1) The factors are equal to one for all states for which the condition $(p_{i\sigma}^{+}e_i+d_i^{+}p_{i-\sigma})\neq0$ holds. 2) They have arbitrary values for states for which the condition $(p_{i\sigma}^{+}e_i+d_i^{+}p_{i-\sigma})=0$ holds. This arbitrariness was utilized in Ref. 9 to introduce some factors $(d_i^{+}d_i+p_{i\sigma}^{+}p_{i\sigma})^{-1/2}$ and $(e_i^{+}e_i+p_{i-\sigma}^{+}p_{i-\sigma})^{-1/2}$. The basic consideration was that the results found in the slave-boson method for the single-band Hubbard model agree with those found in the saddle-point approximation for an isolated center and with $U=0$.

In the multiband model, a corresponding ambiguity arises in the choice of the form of the very first term in (2). Along with those used above, the same matrix elements lead to the expressions

$$\sum_{i\sigma}\varepsilon_i z_{i\sigma}^{+} z_{i\sigma} c_{i\sigma}^{+} c_{i\sigma}\,, \tag{5}$$

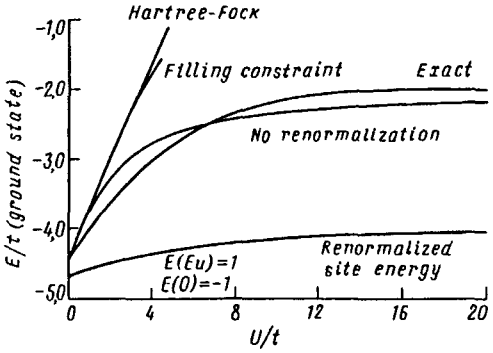

FIG. 1. Ground-state energy for the exact solution and for various types of constraints in the slave-boson method and the Hartree–Fock approximation.

$$\sum_{i\sigma} \varepsilon_i (p_{i\sigma}^+ p_{i\sigma} + d_i^+ d_i). \tag{6}$$

In the single-band scheme with site terms there is no ambiguity; all the ε_i are identical, and we can always choose $\varepsilon_i = 0$. This ambiguity also prevails for constraints (4), but not for (3). For example, we could replace constraints (4) by

$$c_{i\sigma}^+ c_{i\sigma} = (p_{i\sigma}^+ p_{i\sigma} + d_i^+ d_i)^{-1/2}, \tag{7}$$

which are satisfied in the same space of states as constraints (4).

These ambiguities are irrelevant in an exact solution of the problem; all representations must lead to the identical result. However, the slave-boson method has the practical value that one can use the saddle-point approximation in evaluating functional integrals over boson fields. In operator terms, this essentially means the replacement of the boson operators by c-number means and a search for a minimum of the energy under constraints (3) and (4). This solution method is approximate; the result depends on the particular choice of H_{eff}.

We have carried out calculations by the slave-boson method with various types of constraints. Constraint (3) was taken into account exactly for each individual site in these calculations (this is done conveniently by introducing some angular variables for the mean boson fields on a 4D sphere). For the intrasite terms we used representations (2), (5), and (6):

(1) Representation (6), along with constraints of the type $\langle c_{i\sigma}^+ c_{i\sigma} \rangle = p_{i\sigma}^* p_{i\sigma} + d_i^* d_i$ imposed at each site. In this case the mean values are determined self-consistently. This approximation is essentially the Hartree–Fock approximation.

(2) Representation (5) with renormalized site energies and also with unrenormalized ones, (2). In this case, only the total number of electrons in the system, $N = \Sigma_{i\sigma} n_{i\sigma}$, is fixed.

The best agreement with the exact solution is given by constraint (3), which fixes only the total number of electrons in the system, and by the expression with unrenormalized site energies. The results of calculations for these cases and for the exact solution are shown in Fig. 1. Even in this case, however, the mean numbers of electrons at a site calculated

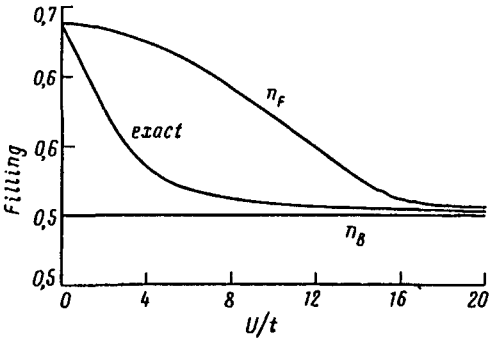

FIG. 2. Mean number of electrons at a site, $\langle c^+_{i\sigma}c_{i\sigma}\rangle$. The curve labeled "exact" corresponds to the exact solution, n_B corresponds to constraint (6), and n_F corresponds to the constraint which fixes the total number of electrons. The site energies are chosen in unrenormalized form, (2), for all curves.

in terms of the fermion means and the boson variables turn out to be different. An attempt to improve the agreement of the site means, i.e., a self-consistent incorporation of $\langle c^+_{i\sigma}c_{i\sigma}\rangle = p^*_{i\sigma}p_{i\sigma} + d^*_i d_i$, significantly degrades the agreement with the exact result. This circumstance means, at a qualitative level, that the fluctuations of the filling of the sites are not slight. Accordingly, if we drop this condition, and if we fix only the total number of electrons in the system, we weaken the constraints, and we find more accurate results. Figure 2 shows results calculated on the filling numbers by the slave-boson method, along with the results of an exact diagonalization of Hamiltonian (1) for a cluster. The best agreement with the exact result is thus found under the following conditions:

(1) Constraints (3) are taken into account exactly.
(2) The site terms are used in unrenormalized form, (2).
(3) The only quantity which is fixed is the total number of electrons in the system, not the number at each site individually, through the imposition of self-consistency with fermion means.

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