Applicability of the slave-boson method for calculating the electronic structure of multiband systems with strong Coulomb correlations

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(Submitted 27 April 1995)
Pis'ma Zh. Éksp. Teor. Fiz. **61**, No. 11, 941–946 (10 June 1995)

Calculations of the electronic structure of strongly correlated systems carried out by the slave-boson method are compared with exact numerical solutions for finite clusters. The "slave-boson" method is found to be a very good approximation for studying not only the single-band Hubbard model but also multiband Hubbard models. It yields the characteristics of the ground state within an error $\sim 1\%$. The reasons for the large discrepancy observed previously [S. N. Molotkov *et al.*, JETP Lett. **59**, 847 (1994)] between the slave-boson results and the exact solution are identified. © *1995 American Institute of Physics.*

Strongly correlated compounds, including, in particular, high-T_c superconductors, heavy-fermion systems, and magnetic semiconductors, have attracted considerable research interest in recent years. Because of the exceptional complexity of a theoretical description of the electronic structure of these compounds (even on the basis of simplified model Hamiltonians), the usual approach in the literature has been to adopt various approximations. Exact solutions can be derived only numerically, and then only for small clusters.[1,2]

One of the most powerful of these approximate methods is the "slave-boson" method, which was proposed in Ref. 3 for the one-band Hubbard model. This method is essentially a mean-field theory which is capable of incorporating strong correlation effects which usually arise from a Coulomb repulsion of electrons. This method is widely used to study magnetically ordered phases, metal–insulator transitions, the Kondo effect, and other topics.

The one-band Hubbard model is not adequate, however, for describing certain classes of compounds. It has thus become necessary to generalize the slave-boson method to multiband model Hamiltonians of various types. This approach was taken in Ref. 4, for example, for the 2D Emery model (a multiband Hubbard model), which was developed for the purpose of calculating electronic characteristics of the copper–oxygen planes in high-T_c superconductors.[5]

The slave-boson method was recently used[6] to determine the ground-state energy

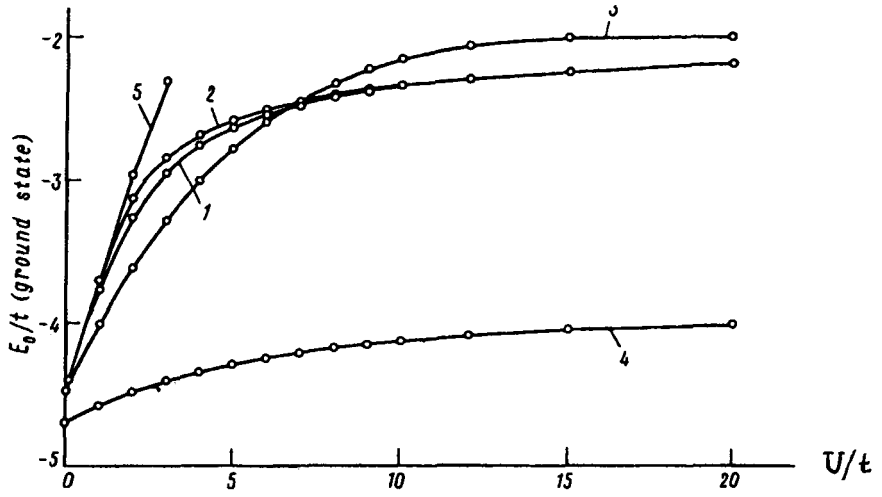

FIG. 1. Energy of the ground state, E_0, of a 2D Eu_2X_2 cluster versus the Coulomb repulsion energy U at Eu sites. *1*—Exact numerical solution; *2*—solution derived in the present study by the slave-boson method; *3–5*—results of Ref. 6 for various types of bonds in the slave-boson method.

E_0 and the average number of electrons per site, $n_{i\sigma}$, in a version of the multiband Hubbard model which describes magnetic semiconductors on the basis of chalcogenides of transition metals with f-shells (e.g., EuX, where X=O, S, Te, or Se). Comparing results calculated with an exact solution calculated numerically for a four-site cluster, Molotkov *et al.*[6] summarized their results as follows: "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."

We need to stress that the correspondence with the exact solution is the only criterion for testing the reliability of an approximate method, since the "physical plausibility" of the results is often deceptive. Accordingly, the approach taken in Ref. 6 appears to us to be completely justified. However, the discrepancy between the "best approximation" of Ref. 6 and the exact solution is so large (see Figs. 1 and 2 of Ref. 6) that one is led to doubt the very validity of the slave-boson method for multiband models. This question requires clarification, since the use of the slave-boson method to study multiband systems has now become so popular (see, for example, Ref. 7 and the papers cited there) that a large discrepancy with the exact solution (if such were to be found in even one specific case) would force us to reexamine the many results which have been derived by the slave-boson method.

The slave-boson method is used in this study, as in Ref. 6, to calculate E_0 and $n_{i\sigma}$ in a magnetic semiconductor of the EuX type. The same characteristics are calculated for the copper–oxygen plane which is a basic structural element of the high-T_c superconductors. Comparing the results of these calculations with exact numerical solutions found for finite numbers of clusters, we show that the slave-boson method is a very good

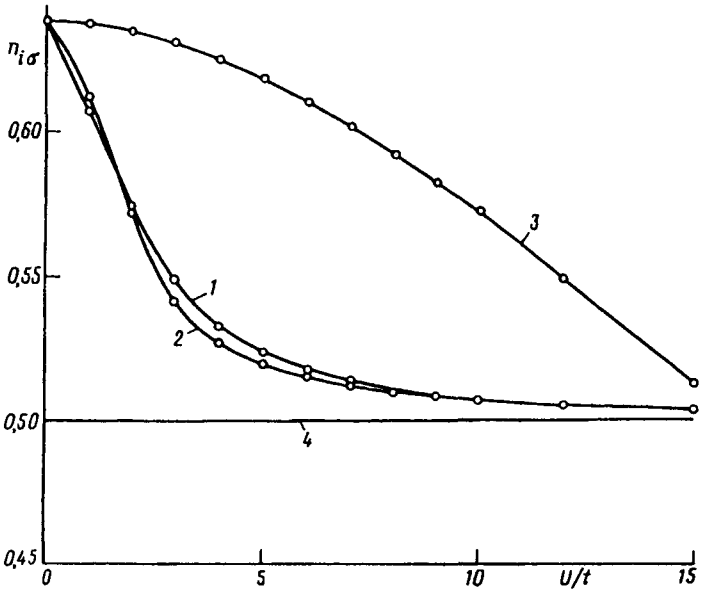

FIG. 2. Expectation value of the number of electrons (with a fixed spin projection) at Eu sites, $n_{i\sigma}=\langle f_{i\sigma}^{+}f_{i\sigma}\rangle$, versus the Coulomb repulsion energy U at Eu sites in a 2D Eu_2X_2 cluster. *1*—Exact numerical solution; *2*—solution found in the present study by the salve-boson method; *3, 4*—calculated in Ref. 6 in terms of fermion expectation values *(3)* and boson variables *(4)*.

approximation for studying not only the one-band Hubbard model, but also multiband Hubbard models. This method can reveal the ground-state characteristics within an error $\sim 1\%$.

To describe the electronic structure of EuX we use a 2D multiband model as in Ref. 6, with the Hamiltonian

$$H=\epsilon_f\sum_{i,\sigma} f_{i\sigma}^{+}f_{i\sigma}+\epsilon_c\sum_{j,\sigma} c_{j,\sigma}^{+}c_{j\sigma}+t\sum_{\langle ij\rangle,\sigma}(f_{i\sigma}^{+}c_{j\sigma}+\text{H.a.})+U\sum_{i} f_{i\uparrow}^{+}f_{i\uparrow}f_{i\downarrow}^{+}f_{i\downarrow}, \qquad (1)$$

where the operators $f_{i\sigma}^{+}$ ($f_{i\sigma}$) and $c_{j\sigma}^{+}$ ($c_{j\sigma}$) create (annihilate) an electron with a spin projection σ at the Eu and X atoms, respectively (the index i refers to Eu sites, and j to X cites), t is the hopping integral for the hopping of electrons between nearest Eu and X sites, ϵ_f and ϵ_c are the site energies, and U is the energy of the Coulomb repulsion of electrons at Eu atoms.

Let us go over to the slave-boson representation. We introduce some auxiliary bosons which correspond to different degrees of filling of the Eu levels with electrons (an empty site; one electron, with spin $\uparrow$ or $\downarrow$; or two electrons). We denote by e_i^{+}, $s_{i\uparrow}^{+}$, $s_{i\downarrow}^{+}$, and d_i^{+} operators which create the corresponding bosons. We define the constraints

$$e_i^{+}e_i+s_{i\uparrow}^{+}s_{i\uparrow}+s_{i\downarrow}^{+}s_{i\downarrow}+d_i^{+}d_i=1, \qquad (2)$$

$$f_{i\sigma}^{+}f_{i\sigma}=s_{i\sigma}^{+}s_{i\sigma}+d_i^{+}d_i\,, \tag{3}$$

which are the completeness condition and the condition of charge conservation.[3] These constraints identify a subspace in which the following Hamiltonian acts:

$$H_{\rm sb}=\sum_{i,\sigma}(\epsilon_f+\lambda_{i\sigma})f_{i\sigma}^{+}f_{i\sigma}+\epsilon_c\sum_{j,\sigma}c_{j\sigma}^{+}c_{j\sigma}+U\sum_i d_i^{+}d_i+t\sum_{\langle ij\rangle,\sigma}(z_{i\sigma}^{+}f_{i\sigma}^{+}c_{j\sigma}+\text{H.a.})$$

$$-\sum_i\lambda_{i\sigma}(s_{i\sigma}^{+}s_{i\sigma}+d_{i\sigma}^{+}d_{i\sigma})+\sum_i\lambda_i^{0}(e_i^{+}e_i+s_{i\uparrow}^{+}s_{i\uparrow}+s_{i\downarrow}^{+}s_{i\downarrow}+d_i^{+}d_i-1), \tag{4}$$

where $\lambda_{i\sigma}$ and λ_i^0 are Lagrange multipliers. These multipliers are introduced in order to satisfy constraints (2) and (3). The operator $z_{i\sigma}$ is given by

$$z_{i\sigma}=(1-d_i^{+}d_i-s_{i\sigma}^{+}s_{i\sigma})^{-1/2}(e_i^{+}s_{i\sigma}^{+}+s_{i-\sigma}^{+}d_i)(1-e_i^{+}e_i-s_{i-\sigma}^{+}s_{i-\sigma})^{-1/2}, \tag{5}$$

where the operator factors on the left and right are chosen in such a way that the operator matrix elements H and $H_{\rm sb}$ agree in the case $U=0$. We wish to stress that this form of the operator factors, which was proposed in Ref. 3 for a half-filled Hubbard band, is also valid for a multiband model with an arbitrary degree of filling of the band, with Coulomb correlations (in the compounds under consideration here, a band of the transition metal Eu with f-shells). This point can be verified quite easily by considering the limiting case $U=0$.

To calculate E_0 and $n_{i\sigma}=\langle f_{i\sigma}^{+}f_{i\sigma}\rangle$, we use the saddle-point approximation,[3] in which all boson fields are replaced by their expectation values, found from the condition that the quantity $E_0=\langle H_{\rm sb}\rangle$ have an absolute minimum as a function of the variables $\lambda_{i\uparrow}$, $\lambda_{i\downarrow}$, and d_i^2. Since we do not know at the outset whether the ground state is paramagnetic or antiferromagnetic, we break up the 2D lattice into two sublattices (A and B). In the paramagnetic phase we would have $\lambda_{i\sigma}^{A}=\lambda_{i\sigma}^{B}=\lambda$, and in the antiferromagnetic phase we would have $\lambda_{i\sigma}^{A}=\lambda_{i-\sigma}^{B}=\lambda_\sigma$ (regardless of the value of i, by virtue of translational invariance). Since d_i^2 is also independent of i, the problem reduces to one of minimizing the functional $E_0(\lambda_\uparrow,\lambda_\downarrow,d^2)$. Of the two possible types of states (paramagnetic or antiferromagnetic), the ground state is of course that for which the energy E_0 is smallest. The quantity $n_{i\sigma}$ is found in a self-consistent way through the use of condition (3).

As in Ref. 6, we tested the accuracy of the slave-boson method by carrying out calculations for a four-site Eu_2X_2 cluster with six electrons and comparing the results with the solution found through a numerical diagonalization of the original Hamiltonian, (1). The relative error of the numerical calculations is less than 10^{-8}; i.e., the numerical solution is essentially exact. Figure 1 shows a plot of E_0 versus U according to our calculations for the case $\epsilon_f/t=1$, $\epsilon_c/t=-1$. Also shown in this figure are three curves of $E_0(U)$ calculated by the algorithms described in Ref. 6 (these curves coincide with those given in Ref. 6; we would simply note that curves *1* and *3* are mixed up in Ref. 6).

It follows from Fig. 1 that the error of the slave-boson method does not exceed 3%. It is well below 1% in the case of most physical interest, that of values $U/t>10$, in which the repulsion energy is larger than the band width. This assertion stands in sharp contrast

with curves *3–5* in Ref. 6. Our curve *2* lies above exact solution *1* for all values of U (this is a natural result, since any variational method will overestimate E_0), while curve *3* (the "best approximation" in Ref. 6 crosses curve *1* at $U/t \approx 7$.

The primary reason for the large discrepancy between the data of Ref. 6 and the exact solution is that we have ignored the possibility that an antiferromagnetic state will prevail. Our calculations show that the ground state is paramagnetic only for values $U/t \lesssim 1.5$. The question of the nature of the ground state is an important one, since the answer to this question determines what we can conclude about the presence or absence of various effects in the system. For example, while a Brinkman–Rice transition occurs in the paramagnetic state of the cluster under consideration (in this case, E_0 and $n_{i\sigma}$ become independent of U beginning at a certain value of U), this transition does not occur in the antiferromagnetic state (which is the ground state!). Furthermore, since no variation with respect to the parameters $\lambda_{i\sigma}$ was carried out in Ref. 6, an incorrect result was derived even in paramagnetic region.

Figure 2 shows $n_{i\sigma}$ versus U. The correspondence between the slave-boson method (curve *2*) and the exact solution (curve *1*) is again very good. This cannot be said of curves *3* and *4* from Ref. 6, which we calculated by the algorithm described in Ref. 6 (these two curves coincide with the corresponding curves in Ref. 6). We wish to stress that the curves of $n_{i\sigma}=\langle f_{i\sigma}^{+} f_{i\sigma}\rangle$ and $n_{i\sigma}=\langle s_{i\sigma}^{+} s_{i\sigma}+d_i^{+} d_i\rangle$ versus U found in terms of fermion expectation values and boson variables, respectively, agree with each other (curve *2*). This is a predictable consequence of the self-consistent procedure which we used to minimize the functional $E_0(\lambda_{\uparrow},\lambda_{\downarrow},d^2)$ (see also Ref. 4). Since the quantities $\langle f_{i\sigma}^{+} f_{i\sigma}\rangle$ and $\langle s_{i\sigma}^{+} s_{i\sigma}+d_i^{+} d_i\rangle$ were different in Ref. 6 (curves *3* and *4* in Fig. 2), the calculation method is not self-consistent.

Finally, we present some results which we found for the 2D Emery model.[5] This model describes the CuO_2 planes in high-T_c superconductors. The corresponding Hamiltonian is (we are ignoring the Coulomb repulsion at oxygen sites and also the repulsion between copper and oxygen sites)

$$H=\epsilon\sum_{j,\sigma} p_{j\sigma}^{+} p_{j\sigma}+t\sum_{\langle ij\rangle,\sigma}(p_{j\sigma}^{+} d_{i\sigma}+\text{H.a.})+U_d\sum_i d_{i\uparrow}^{+} d_{i\uparrow} d_{i\downarrow}^{+} d_{i\downarrow}\,. \tag{6}$$

Here the operators $d_{i\sigma}^{+}$ ($d_{i\sigma}$) and $p_{j\sigma}^{+}$ ($p_{j\sigma}$) create (annihilate) a hole at copper and oxygen atoms, respectively; t is the hopping integral for hops between nearest copper and oxygen sites; ϵ is the difference between the energies of a hole at oxygen and copper sites, and U is the energy of the Coulomb repulsion of holes and copper atoms.

Figures 3 and 4 show $n_{i\sigma}=\langle d_{i\sigma}^{+} d_{i\sigma}\rangle$ and E_0 versus ϵ found by exact calculations (based on the Lanczos numerical algorithm[2]) and by the slave-boson method[4] for a Cu_4O_8 cluster with $U_d/t=8$. (We are assuming that the total number of holes in a cluster is equal to the number of oxygen sites, i.e., four; this assumption corresponds to an undoped, insulating state of the CuO_2 plane in the high-T_c superconductor.) We see that the error of the slave-boson method does not exceed 1% at either $\epsilon/t<1$ (this is a "charge-transfer" insulating state) or $\epsilon/t\gg 1$ (a Mott–Hubbard antiferromagnetic state). We wish to stress that the excellent agreement between the results found by slave-boson

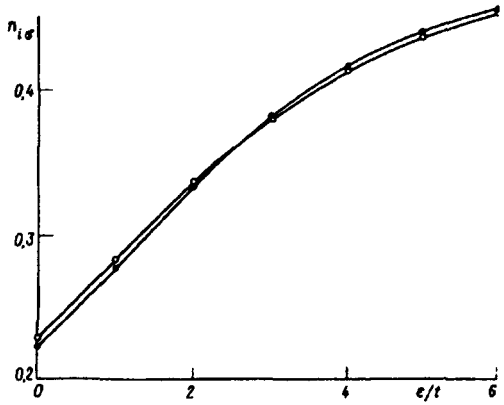

FIG. 3. Expectation value of the number of holes (with a fixed spin projection) at a copper site, $n_{i\sigma}=\langle d_{i\sigma}^{+}d_{i\sigma}\rangle$, versus the difference between the site energies of oxygen and copper, ϵ, in a Cu_4O_8 cluster with four holes. ○—Exact numerical solution; ●—slave-boson solution.

method and the exact solutions is also seen for other numbers of holes in a cluster and in calculations of various correlation functions, e.g., $\langle n_{i\sigma}n_{j\sigma'}\rangle$.

Our basic conclusion, therefore, is that the slave-boson method is a very good approximation for studying not only the one-band Hubbard model, but also multiband versions of this model, making it possible to determine characteristics of the ground state within an error $\sim 1\%$. Necessary conditions for the correct use of this method are as follows: 1) The possible realization of both paramagnetic and antiferromagnetic states in the system must be taken into account. 2) Variational parameters $\lambda_{i\sigma}$ must be incorpo-

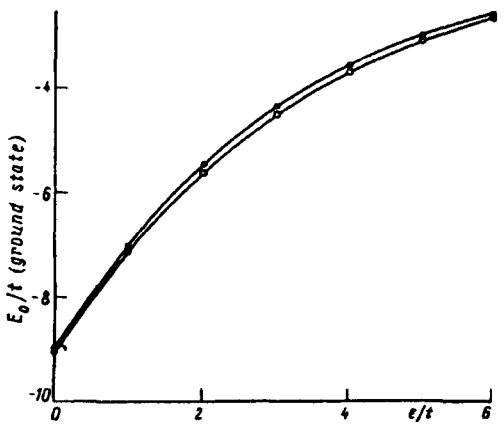

FIG. 4. Ground-state energy E_0 of a 2D Cu_4O_8 cluster with eight holes versus the difference between the site energies of oxygen and copper, ϵ. ○—Exact numerical solution; ●—slave-boson solution.

rated in the Hamiltonian. 3) A self-consistent procedure must be used in minimizing the energy functional.

This study was supported by the Scientific Council on the Problem of High-Temperature Superconductivity. It was carried out within the framework of Project 94031 of the State Program on High-Temperature Superconductivity. This study was also supported by Grants 94-02-05755 and 94-02-04-843 of the Russian Fund for Fundamental Research and Grant M67300 of the International Science Foundation and the Russian Government.

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Translated by D. Parsons