Exact criterion for choosing the hopping operator in the four-slave-boson approach

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We consider the N-component generalization of the four-slave-boson approach to the Hubbard model, where $1/N$ acts as the small parameter that controls the fluctuations about the saddle point, and address the problem of the appropriate choice of the bosonic hopping operator $z_{i\sigma}$. By suitably reorganizing the Fock space, we show that the square-root form for $z_{i,\sigma}$ (originally introduced by Kotliar and Ruckenstein) reproduces the exact independent-fermion ($U=0$) results not only at the mean-field ($N=\infty$) level but also to all orders in the $1/N$ expansion, provided one relaxes the usually adopted normal-ordered prescription for $z_{i,\sigma}$. This ensures that $z_{i,\sigma}$ need not be modified at successive orders in the fluctuation expansion, and implies that all correlation functions are correctly recovered in the $U=0$ limit, a nontrivial result for the slave-boson approach. In addition, it provides a stringent requirement on the form of $z_{i,\sigma}$, which might be also generalized to alternative slave-boson formalisms (like the spin-rotation-invariant formulation).

The four-slave-boson method has been widely used in the past few years to deal with the Hubbard model (with on-site repulsion U). This method is usually implemented via a mixed fermion-boson functional integral, which allows for a systematic expansion in terms of fluctuations about an appropriate mean field. The fluctuation expansion is, in turn, controlled by introducing an additional fermion degeneracy N and using $1/N$ as the expansion parameter.[1] Already at the mean-field level, the method provides a reasonable description of the phase diagram and of several static quantities for the Hubbard model, as shown by comparisons with quantum Monte Carlo calculations.[2] Since the slave-boson approach should be, by its conceiving, appropriate to the strong-coupling regime, it might not be expected to reproduce the noninteracting fermion limit at the same time. In this respect, Kotliar and Ruckenstein (KR) proposed choosing the hopping operator $z_{i,\sigma}$ (which, due to the redundancy of the slave-boson Fock space, it not uniquely defined) to obtain the correct result at the mean-field level in the $U\rightarrow 0$ limit.[3] It has, however, later been questioned whether the same form of $z_{i,\sigma}$ remains appropriate when corrections beyond mean field are introduced.[4] It turns out, in fact, that unphysical results occur when the KR form for $z_{i,\sigma}$ is used beyond mean field.[4,5]

It has been recently shown that the above anomalies stem from an inappropriate operator ordering of $z_{i,\sigma}$.[1] In fact, previous to the work of Ref. 1, all slave-boson calculations have been invariably carried out by assuming the normal-ordering prescription for $z_{i,\sigma}$, since normal ordering allows for a direct functional-integral representation of the Hamiltonian. If one adopts, instead, the KR form of $z_{i,\sigma}$ *without* modifying the original operator ordering, fluctuation corrections do not spoil the $U=0$ mean-field results (at least, for the free energy and related static quantities), in contrast to the normal-ordered version for $z_{i,\sigma}$. The question naturally arises whether the results of Ref. 1, which have been obtained up to leading order beyond mean field, also hold when higher-order corrections are considered, and not only for static but also for dynamic quantities.

In this paper, by exploiting some exact properties of the hopping operator and of the related constraints for arbitrary values of the degeneracy parameter N, we show that the $U=0$ independent-fermion result can be recovered (at zero temperature) to *all orders* in the $1/N$ expansion, *provided* the strict square-root form for $z_{i\sigma}$ is used instead of its normal-ordered version. This result holds not only for the ground-state energy, but also for the ground-state expectation values of operators written in terms of the *physical* fermion operators (obtained as the product of $z_{i\sigma}$ with a pseudofermion operator).

We consider the N-component generalization of the slave-boson single-band Hubbard Hamiltonian,[1,3] of the form

$$H=\sum_{i,i'}\sum_{\sigma=\pm 1}\sum_{S=1}^{N} t_{i,i'}f^{\dagger}_{i,S,\sigma}z^{\dagger}_{i,\sigma}z_{i',\sigma}f_{i',S,\sigma}+U\sum_{i}d^{\dagger}_{i}d_{i} \tag{1}$$

supplemented by the constraints

$$d^{\dagger}_{i}d_{i}+\sum_{\sigma=\pm 1}s^{\dagger}_{i,\sigma}s_{i,\sigma}+e^{\dagger}_{i}e_{i}=N\ , \tag{2a}$$

$$\sum_{S=1}^{N}f^{\dagger}_{i,S,\sigma}f_{i,S,\sigma}=s^{\dagger}_{i,\sigma}s_{i,\sigma}+d^{\dagger}_{i}d_{i}\ , \tag{2b}$$

which are straightforward generalizations of the $N=1$ case considered by KR. Although for $N>1$ constraints (2) no longer guarantee a one-to-one correspondence between the original fermion and the fermion-boson problems, we do not consider this an issue since $1/N$ has been introduced here merely as an expansion parameter, and the $N=1$ value will eventually be selected. In (1) and (2) e_i, $s_{i,\sigma}$, and d_i are slave-boson operators associated with empty, singly, and doubly occupied states, respectively;

$f_{i,S,\sigma}$ is a pseudofermion operator with spin σ and component S, and $i\,(i')$ extends over all lattice sites. For arbitrary N, the presence of the bosonic operator $z_{i,\sigma}$ in (1) is required to leave the subspace identified by the constraints (2) invariant; however, its choice is to some extent arbitrary due to the redundancy of the Fock space. Kotliar and Ruckenstein exploited this arbitrariness and suggested using the form[3]

$$z_{i,\sigma}=s_{i,-\sigma}^{\dagger}R_{i,\sigma}d_i+e_i^{\dagger}R_{i,\sigma}s_{i,\sigma}\ , \tag{3}$$

with

$$R_{i,\sigma}=R_{i,\sigma}^{KR}=:R_{i,\sigma}^{SQ}: \tag{4a}$$

and

$$R_{i,\sigma}^{SQ}=\frac{1}{\sqrt{N-d_i^{\dagger}d_i-s_{i,\sigma}^{\dagger}s_{i,\sigma}}}\times\frac{1}{\sqrt{N-e_i^{\dagger}e_i-s_{i,-\sigma}^{\dagger}s_{i,-\sigma}}} \tag{4b}$$

in order to reproduce the exact $U=0$ result at the mean-field level. The normal ordering $:R_{i,\sigma}^{SQ}:$ in (4a) stems from requiring a simple mapping of the Hamiltonian (1) into the corresponding action of the functional integral.

However, it has been shown in Ref. 1 that improved results are obtained beyond the mean field by relaxing the normal ordering in Eq. (4a) [whereby the normal-ordering requirements of the functional integral are met by suitably reordering the operators in (4b) within the $1/N$ expansion]. In the following, we shall not rely on the functional-integral formulation; rather, we will prove exact results *for arbitrary values of N* using the operator form (4b). Specifically, we will show that (i) the mixed fermion-boson Fock space restricted by (2) can be split into subspaces (labeled by a quantum number J_i) that remain invariant under the action of $z_{i,\sigma}$ when the form (4b) is adopted; and (ii) a particular subspace can be identified (with $J_i=0$ for all i), where a one-to-one correspondence between matrix elements of the original fermion and of the fermion-boson Hamiltonians can be established for all N. We will also argue that, when $U=0$, the ground state belongs to the subspace $\{J_i=0\}$.

We begin by analyzing the properties of operator (4b) in the bosonic Fock space at a given site i. We specify a generic basis state in this space via the bosonic occupation numbers n_e, $n_\uparrow$, $n_\downarrow$, and n_d associated with $e^{\dagger}e$, $s_\uparrow^{\dagger}s_\uparrow$, $s_\downarrow^{\dagger}s_\downarrow$, and $d^{\dagger}d$, in the order

$$|n_e,n_\uparrow,n_\downarrow,n_d\rangle\ . \tag{5}$$

Operator (4b) is diagonal in representation (5) [by contrast, its normal ordered version (4a) has nontrivial matrix elements in this representation]. This allows us to verify the following commutation relations for the operator $z_{i,\sigma}^{SQ}$ given by (3) with $R_{i,\sigma}=R_{i,\sigma}^{SQ}$, when acting on any state of the form (5) (below we will omit, for simplicity, the site index i and the label SQ):

$$[z_\uparrow,z_\downarrow]=0,\quad [z_\uparrow,z_\downarrow^{\dagger}]=0\ , \tag{6}$$

plus their Hermitian conjugates.

The physical (fermion-boson) subspace is identified by constraints (2). The set of bosonic states associated with a given fermionic configuration is thus determined via the pair of fermionic occupation numbers $N_{i,\sigma}=\sum_{S=1}^{N}f_{i,S,\sigma}^{\dagger}f_{i,S,\sigma}$ $(\sigma=\pm1)$ [a given pair $(N_\uparrow,\ N_\downarrow)$, may, on the other hand, be associated with more than one fermionic configuration]. Constraints (2) thus associate the pair $(N_\uparrow,N_\downarrow)$ with the bosonic subspace spanned by the basis states

$$|N_\uparrow,N_\downarrow;n_d\rangle_N=|N-N_\uparrow-N_\downarrow+n_d,N_\uparrow-n_d,N_\downarrow-n_d,n_d\rangle, \tag{7}$$

where n_d can take $1+\min(N_\uparrow,N_\downarrow,N-N_\uparrow,N-N_\downarrow)$ integer values ranging within $\max(0,-N+N_\uparrow+N_\downarrow)\le n_d\le\min(N_\uparrow,N_\downarrow)$. The subspaces $\{|N_\uparrow,N_\downarrow;n_d\rangle_N\}$ with different values of $(N_\uparrow,N_\downarrow)$ are connected by the operators z_σ and $z_\sigma^{\dagger}$. Consider, in particular, the application of the operators $z_\sigma^{\pm}$ (with $z_\sigma^{+}=z_\sigma^{\dagger}$ and $z_\sigma^{-}=z_\sigma$) on the state $|n,0;n_d=0\rangle_N$:

$$z_\uparrow^{\pm}|n,0;n_d=0\rangle_N=C_n^{\pm}|n\pm1,0;n_d=0\rangle_N\ , \tag{8}$$

where the normalization constants $C_n^{\pm}$ equal unity only for the *SQ* form (4b).[6] Therefore, the operators $z_\uparrow^{\pm}$ act as creation and destruction operators in the subspace spanned by $\{|n,0;n_d=0\rangle_N;n=0,\ldots,N\}$. The above conclusions hold, as well, if one exchanges up and down spins. Exploiting the commutation relations (6), one can then unambiguously define the subspace of the physical space spanned by the $(N+1)^2$ (normalized) states

$$|J=0;N_\uparrow,N_\downarrow\rangle_N\equiv(z_\uparrow^{\dagger})^{N_\uparrow}(z_\downarrow^{\dagger})^{N_\downarrow}|0,0;n_d=0\rangle_N\ , \tag{9}$$

with $0\le(N_\uparrow,N_\downarrow)\le N$. Here J is a *quantum number* which will be essential for the following arguments.

Consider, next, the subspace with $N_\uparrow=N_\downarrow=1$ spanned by the two states $|1,1;n_d=0\rangle_N$ and $|1,1;n_d=1\rangle_N$ [cf. Eq. (7)], since n_d takes the values 0 and 1 in this case. Recall that the state $|J=0;1,1\rangle_N=z_\uparrow^{\dagger}z_\downarrow^{\dagger}|0,0;n_d=0\rangle_N$ belongs to this subspace. The complement of this state in the subspace we are considering can then be found by Schwartz orthogonalization. Let us denote this state by $|J=1;1,1\rangle_N$. Similarly to what we have done in Eq. (9), from the state $|J=1;1,1\rangle_N$ one can construct a whole set of $(N-1)^2$ companion states as follows:

$$C_{(N_\uparrow,N_\downarrow)}^{(J=1)}|J=1;N_\uparrow,N_\downarrow\rangle_N=(z_\uparrow^{\dagger})^{N_\uparrow-1}(z_\downarrow^{\dagger})^{N_\downarrow-1}|J=1;1,1\rangle_N\ , \tag{10}$$

where $C_{(N_\uparrow,N_\downarrow)}^{(J=1)}$ is a normalization constant which is no longer unity as it was in Eq. (9). This difference between the values of the normalization constants for the cases $J=0$ and $J\ge1$ is due to the square-root choice (4b), and will be important in the following. It can further be shown that the states of the two sets $\{|J=0;N_\uparrow,N_\downarrow\rangle_N\}$ and $\{|J=1;N_\uparrow,N_\downarrow\rangle_N\}$ are mutually orthogonal.

One can then proceed by induction and identify $[N/2]+1$ orthogonal subspaces, labeled by the quantum number $J(=0,1,\ldots,[N/2])$ and spanned by the $(N-2J+1)^2$ states

$$C^{(J)}_{(N_\uparrow,N_\downarrow)}|J;N_\uparrow,N_\downarrow)_N=(z^\dagger_\uparrow)^{N_\uparrow-J}(z^\dagger_\downarrow)^{N_\downarrow-J}|J;J,J)_N \ , \quad (11)$$

with $J\le(N_\uparrow,N_\downarrow)\le N-J$. Note that successive applications of $z^\pm_\sigma$ do not change the value of J.

It remains to evaluate the constants $C^{(J)}_{(N_\uparrow,N_\downarrow)}(=C^{(J)}_{(N_\downarrow,N_\uparrow)}$, by symmetry), One can readily show that the quantity

$$\alpha^{(J)}_n\equiv\left|\frac{C^{(J)}_{(n+1,m)}}{C^{(J)}_{(n,m)}}\right|^2={}_N(J;n,m|z_\uparrow z^\dagger_\uparrow|J;n,m)_N \quad (12)$$

is the eigenvalue of the operator $z_\uparrow z^\dagger_\uparrow$ associated with the eigenstate $|J;n,m)_N$, and is independent of m. Consider then the trace of the operator $z_\uparrow z^\dagger_\uparrow$ in the subspace with given values of $N_\uparrow=n$ and $N_\downarrow=m$, where, for the sake of definiteness, we choose $m\le n\le N-m$. This subspace is spanned by $m+1$ states, which we can specify alternatively by $\{|J;n,m)_N$, with $0\le J\le m\}$ or by $\{|n,m;n_d\rangle_N$, with $0\le n_d\le m\}$. In the first (diagonal) basis the *restricted* trace takes the form

$$\mathrm{tr}(z_\uparrow z^\dagger_\uparrow)_{(n,m)}=\sum_{J=0}^{m}\alpha^{(J)}_n \ , \quad (13)$$

from which the eigenvalue $\alpha^{(m)}_n$ can be obtained as the difference

$$\alpha^{(m)}_n=\mathrm{tr}(z_\uparrow z^\dagger_\uparrow)_{(n,m)}-\mathrm{tr}(z_\uparrow z^\dagger_\uparrow)_{(n,m-1)} \ . \quad (14)$$

In the second (nondiagonal) basis, on the other hand, the restricted trace can be readily evaluated since the operator $z_\uparrow z^\dagger_\uparrow$ admits a simple representation. Comparing the two results, one obtains

$$\alpha^{(J)}_n=\frac{(n+1-J)(N-n-J)}{(N-n)(n+1)} \ . \quad (15)$$

Note that $\alpha^{(0)}_n=1$, as anticipated, and that $\alpha^{(J)}_n=0$ for the upper value $n=N-J$ (except for $J=0$; see Ref. 6). In addition, we have

$$0\le\alpha^{(J+1)}_n<\alpha^{(J)}_n<\alpha^{(J=0)}_{n'}=1 \quad (16)$$

for any pair (n,n') and $J\ge1$.

In conclusion, we have shown that (at any given lattice site) the constrained bosonic Fock space (for given N) can be split into the direct sum of subspaces spanned by the states $\{|J;N_\uparrow,N_\downarrow)_N$, with $J=0,\ldots,[N/2]\}$. Within each J subspace, the operators z_σ and $z^\dagger_\sigma$ act as "lowering" and "raising" operators with normalization constants given by (12) and (15) ($C^{(J)}_{(J,J)}=1$, by definition) and destroy the extremal states with $N_\sigma=J$ and $N_\sigma=N-J$, respectively. In this respect, the J subspaces bear some analogy with the sets of states obtained in elementary quantum mechanics by coupling two angular momenta.

We now return to the (physical) mixed fermion-boson Fock space. Constraints (2) associate every fermionic configuration with given values of $N_\uparrow$ and $N_\downarrow$, with the whole set of bosonic states $\{|J;N_\uparrow,N_\downarrow)_N$; $J=0,\ldots,\min(N_\uparrow,N_\downarrow,N-N_\uparrow,N-N_\downarrow)\}$ (and not just with a single bosonic state, like for $N=1$). This implies that a generic basis state of the mixed Fock space can be written (at any given lattice site) as the product of a fermionic and a bosonic state, as follows:

$$|\phi(N_\uparrow,N_\downarrow)\rangle|J;N_\uparrow,N_\downarrow)_N \ , \quad (17)$$

where $\phi(N_\uparrow,N_\downarrow)$ is a generic fermionic configuration consistent with the pair $(N_\uparrow,N_\downarrow)$. Note that the physical fermion operator $z_\sigma f_{S,\sigma}$ does not change the quantum number J when applied to (17).

Further concerning the Fock space for the whole lattice, this can also be split into distinct subspaces, each identified by a set of integers $\{J_i\}$ with i ranging over all lattice sites. Each subspace specified by the set $\{J_i\}$ is invariant under the slave-boson Hamiltonian with $U=0$, since $d^\dagger_i d_i$ is the *only* operator of the Hamiltonian (1) that modifies the quantum numbers J_i. In particular, within the subspace $\{J_i=0\}$ for *all i* the operators $z_{i,\sigma}$ and $z^\dagger_{i,\sigma}$ connect states of the type (17) with different $N_\uparrow$ and $N_\downarrow$, without changing their norm. In this subspace, the $U=0$ slave-boson Hamiltonian is thus *equivalent to its purely fermionic counterpart even when* $N>1$.[3] This finding is particularly relevant if the ground state of the Hamiltonian belongs to the subspace $\{J_i=0\}$. In this case, the ground-state expectation value of any operator in the purely fermionic representation equals the ground-state expectation value of the corresponding operator written in the slave-boson representation, *provided* the operator itself leaves the subspace $\{J_i=0\}$ invariant. This holds, e.g., for the correlation (Green's) functions, when the physical fermion operator $z_{i,\sigma}f_{i,S,\sigma}$ with $R_{i,\sigma}$ given by (4b) is used. Since all physical quantities in the purely fermionic representation scale simply with integer powers of N when $U=0$, the above conclusion implies that in the mixed fermion-boson representation all corrections (over and above the mean-field result) vanish identically *at any order in* $1/N$. This result confirms and extends on general grounds the numerical results obtained in Ref. 1 at the leading order in $1/N$.

There remains to prove that the ground state of (1) with $U=0$ belongs to the subspace $\{J_i=0\}$; that is,

$$E_0[\{J_i=0\}]<E_0[\{J'_i\}] \ \text{ with } \{J'_i\}\neq\{J_i=0\} \ , \quad (18)$$

where $E_0[\{J_i\}]$ stands for the lowest eigenvalue in the subspace specified by the set $\{J_i\}$. A property similar to (18) can be readily proved for a single-particle Hamiltonian with site-dependent hopping, of the form

$$H[\{Z_{i,\sigma}\}]=\sum_{i,i'}\sum_{\sigma=\pm1}\sum_{S=1}^{N}t_{i,i'}f^\dagger_{i,S,\sigma}Z_{i,\sigma}Z_{i',\sigma}f_{i',S,\sigma} \ , \quad (19)$$

where $t_{ii}=0$ (by assumption) and $Z_{i,\sigma}$ are real and positive numbers. Let $\tilde{E}_0[\{Z_{i\sigma}\}]$ be the ground-state energy associated with a given configuration $\{Z_{i,\sigma}\}$. Then

$$\tilde{E}_0[\{Z_{i,\sigma}\}]\le\tilde{E}_0[\{Z'_{i,\sigma}\}] \ , \quad (20)$$

whenever

$$Z_{i,\sigma}\ge Z'_{i,\sigma}\ge0 \quad (21)$$

for all i and σ, which can be shown by realizing that the ground-state expectation value

$$\left\langle\frac{\partial H[\{Z\}]}{\partial Z_{i,\sigma}}\right\rangle=\frac{\partial\tilde{E}_0[\{Z\}]}{\partial Z_{i,\sigma}} \quad (22)$$

is nonpositive for any chosen i and σ. At this point we note that the slave-boson Hamiltonian (1) with $U=0$ can be mapped, *within each subspace* $\{J_i\}$, onto the purely fermionic Hamiltonian (19) by replacing the c number $Z_{i,\sigma}$ with the Hermitian operator $(\alpha_{N_{i,\sigma}}^{(J_i)})^{1/2}$ [obtained by entering the fermionic operator $N_{i,\sigma}$ in the place of n in Eq. (15)].[7] Property (18) would thus follow from Eqs. (16), (20), and (21) if $\alpha_{N_{i,\sigma}}^{(J_i)}$ could be replaced by c numbers. In particular, this is approximately correct for large N where one can approximate

$$\alpha_{N_{i,\sigma}}^{(J_i)}=1-\frac{1}{\bar{n}_{i,\sigma}(1-\bar{n}_{i,\sigma})}\frac{J_i}{N}+\frac{J_i}{N^2}\frac{(1-\bar{n}_{i,\sigma}+J_i\bar{n}_{i,\sigma})}{(1-\bar{n}_{i,\sigma})\bar{n}_{i,\sigma}^2}+\frac{(1-2\bar{n}_{i,\sigma})}{\bar{n}_{i,\sigma}^2(1-\bar{n}_{i,\sigma})^2}\frac{J_i(N_{i,\sigma}-\langle N_{i,\sigma}\rangle)}{N^2}+O(N^{-3}) , \quad (23)$$

where $\langle N_{i,\sigma}\rangle=N\bar{n}_{i,\sigma}$ is the self-consistent ground-state value of $N_{i,\sigma}$ for given $\{J_i\}$. In this way Eq. (18) is validated for a sufficiently large (albeit finite) value of N. In this sense, we have proved order by order in $1/N$ that the slave-boson representation does not modify the exact ($U=0$) independent-fermion results.[8]

In conclusion, motivated by the encouraging numerical results obtained previously by implementing the $1/N$ expansion for the four-slave-boson method correctly,[1] in this paper we have analyzed in detail the structure of the enlarged slave-boson Fock space for $N>1$ and identified an intrinsic *dynamical symmetry* associated with a quantum number (J). We have thus been able to tune the four-slave-boson method at $U=0$ (where this dynamical symmetry holds exactly) by comparison with the independent-fermion results. Our finding considerably limits (and possibly eliminates) the arbitrariness of the choice of the hopping operator $z_{i,\sigma}$.

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[6]Problems occurring for the extremal states with $n=0$ and N can be suitably overcome by letting the pseudofermion operator act *before* $z_\sigma^{\pm}$ on any given state.

[7]By our convention, $\alpha_n^{(J)}=0$ for $n>N-J$ or $n<J-1$.

[8]An argument to exclude the possible occurrence of level crossing at finite N [whereby Eq. (18) would be invalidated] follows from the last inequality in Eq. (16).