Iterative boson expansion procedure for fermion systems

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A new approach to many-body dynamics that combines successive boson expansion and mean-field techniques, and which was recently developed for boson systems, is extended to fermion systems. The procedure is developed for both the ground state and for low-lying excited states and is tested in the context of the two-level pairing model. Special attention is focused on the problem of unphysical states.

I. INTRODUCTION

In a recent note,[1] an iterative boson expansion procedure (IBEP) was proposed as a practical and systematic means of approximating the ground state of a system of interacting bosons. Basic to this procedure were three important observations: (1) that boson expansion techniques (BET),[2] traditionally used in the context of fermion systems, can be extended to boson systems, (2) that problems related to unphysical states, which are common to any BET, are less severe for boson systems than for fermion systems, particularly when treating the ground state, and (3) that the BET can be iteratively combined with mean-field techniques (MFT) to systematically build in additional many-body correlation effects. In the present work, we extend the IBEP to systems of interacting fermions and apply it to the two-level pairing model. We also extend the procedure to the description of low-lying excited states and discuss a partial approach to the problem of unphysical states.

II. THE FORMALISM

A. Review of boson expansions

We begin with a brief review of boson expansions. Consider a system of particles, either fermions or bosons, distinguished by a signature label

$$\sigma=\begin{cases}1 & \text{for fermions}\\ 0 & \text{for bosons}\ .\end{cases} \tag{1}$$

We denote the creation and annihilation operators of the system as $a_i^\dagger$ and a_i, respectively. These operators satisfy the generalized (anti)commutation relation

$$a_i a_j^\dagger-(-1)^\sigma a_j^\dagger a_i=\delta_{ij}\ . \tag{2}$$

In a BET, the Hilbert space associated with these particles is *mapped* onto an ideal boson space defined by the pair-boson creation and annihilation operators $B_{ij}^\dagger$ and B_{ij}, respectively. These pair bosons *take the place of* pairs of the original particles and thus satisfy the requirement of being either antisymmetric ($\sigma=1$) or symmetric ($\sigma=0$) under the interchange of indices,

$$B_{ij}^\dagger=(-1)^\sigma B_{ji}^\dagger\ . \tag{3}$$

Furthermore, they satisfy ideal boson commutation relations

$$\begin{aligned}&[B_{ij},B_{kl}^\dagger]=\delta_{ik}\delta_{jl}+(-1)^\sigma\delta_{il}\delta_{jk}\ ,\\ &[B_{ij},B_{kl}]=[B_{ij}^\dagger,B_{kl}^\dagger]=0\ .\end{aligned} \tag{4}$$

To completely define the ideal boson space, it is necessary to include a vacuum state $|0\rangle_B$, defined by

$$B_{ij}|0\rangle_B=0 \quad \text{for } all\ i,j\ . \tag{5}$$

There are several ways to define the mapping so as to preserve the dynamics of the original problem. In the Belyaev-Zelevinski-Marshalek (BZM) approach, this is accomplished by requiring that the mapping preserve the commutation algebra of the original system. We will, in this work, use the Dyson non-Hermitian version of the BZM mapping. Violation of Hermiticity permits the commutation algebra to be preserved with a finite mapping. The relevant Dyson images of the fundamental biparticle operators, either for fermions or for bosons, are

$$\begin{aligned}&(a_i^\dagger a_j^\dagger)_B=B_{ij}^\dagger+(-1)^\sigma\sum_{kl}B_{ik}^\dagger B_{jl}^\dagger B_{kl}\ ,\\ &(a_i a_j)_B=B_{ji}\ ,\\ &(a_i^\dagger a_j)_B=\sum_k B_{ik}^\dagger B_{jk}\ .\end{aligned} \tag{6}$$

Note that the signature enters both in the intrinsic character of the bosons [(3) and (4)] and in the mapping (6). It is through the signature that the permutation symmetry character of the original problem is transmitted.

In applying the IBEP to boson systems,[1] it was possible to use the particle-hole mapping equations, at least for the description of the ground state of the system. In treating fermion systems, it is more appropriate to map the Hamiltonian in particle-particle form, even for the ground state; it is in this way that the physics of the Pauli principle is most naturally transmitted. As we see from (6), use of the particle-particle mapping leads to a non-Hermitian Hamiltonian in the ideal boson space.

B. Mean-field techniques for non-Hermitian systems

As in the earlier development of the IBEP to boson systems, we use the BET in conjunction with MFT. For the ground state, we treat the non-Hermitian Hamiltonian system using the Hartree-Bose (HB) approximation and for low-lying excited states we use the Tamm-Dancoff (TD) approximation. We also consider the use of the broken pair (BP) approximation for such systems.

The Hartree and Tamm-Dancoff approximations, as appropriate to non-Hermitian Hamiltonian systems, were discussed by Cambiaggio and Dukelsky.[3] The starting point is the introduction of a canonical transformation from the noncollective bosons $B_{ij}^\dagger$ and B_{ij} to collective bosons

$$\Gamma_p^\dagger = \tfrac{1}{2}\sum_{ij} z_{ij}^p B_{ij}^\dagger \tag{7a}$$

and

$$\gamma_p = \tfrac{1}{2}\sum_{ij} y_{ij}^p B_{ij} \ . \tag{7b}$$

Note that for a non-Hermitian system, the bra and ket transformations are in principle different; however, to ensure that the transformation is canonical, it is necessary that the x and y transformation matrices be the inverses of one another.

In Hartree approximation, one searches for the optimum description of the system as a boson condensate. Namely, one assumes trial bra and ket vectors

$$|\text{Hartree}\rangle = \frac{1}{\sqrt{N!}}(\Gamma_0^\dagger)^N|0\rangle_B \tag{8a}$$

and

$$\langle\text{Hartree}| = \frac{1}{\sqrt{N!}}\,{}_B\langle 0|(\gamma_0)^N \tag{8b}$$

and determines the structure coefficients of the *dominant* collective bosons $\Gamma_0^\dagger$ and γ_0 by minimizing the expectation value of the non-Hermitian boson Hamiltonian, subject to the constraint that the transformation to collective bosons be canonical.

The Hartree variational calculations also provide a set of collective bosons, $\Gamma_p^\dagger$ and γ_p ($p\neq 0$), that are orthogonal to those of the ground condensate. In Tamm-Dancoff approximation, one assumes that the lowest excited states can be described in terms of one-boson excitations of the Hartree ground state. Once again, separate bra and ket excitations are required. The relevant basis states can be written as ($p\neq 0$)

$$|p\rangle = \frac{1}{\sqrt{(N-1)!}}\Gamma_p^\dagger(\Gamma_0^\dagger)^{N-1}|0\rangle_B \tag{9a}$$

and

$$\langle p| = \frac{1}{\sqrt{(N-1)!}}\,{}_B\langle 0|(\gamma_0)^{N-1}\gamma_p \ . \tag{9b}$$

Diagonalization of the non-Hermitian boson Hamiltonian must also be carried out subject to the constraint that the right and left eigenvector matrices are inverses of one another, as well as to a further normalization constraint, which is described in Ref. 3.

The formalism necessary for a BP treatment of a non-Hermitian boson system has to our knowledge not yet been presented. Here, the assumption is that the ground state can be represented as a pair condensate of the form

$$|BP\rangle = (\Delta^\dagger)^{N/2}|0\rangle_B \tag{10a}$$

and

$$\langle BP| = {}_B\langle 0|(\delta)^{N/2} \ , \tag{10b}$$

with

$$\Delta^\dagger = \sum_{ijkl}\alpha_{ijkl}B_{ij}^\dagger B_{kl}^\dagger \tag{10c}$$

and

$$\delta = \sum_{ijkl}\beta_{ijkl}B_{ij}B_{kl} \ . \tag{10d}$$

The optimum pair condensate can then be obtained using an iterative diagonalization procedure, similar to the one used by Scholten[4] in generalized-seniority shell-model calculations. More precisely, we iteratively diagonalize the Hamiltonian in the basis

$$|ijkl\rangle = B_{ij}^\dagger B_{kl}^\dagger(\Delta^\dagger)^{(N-1)/2}|0\rangle_B \ , \tag{11a}$$

$$\langle ijkl| = {}_B\langle 0|(\delta)^{(N-1)/2}B_{ij}B_{kl} \ , \tag{11b}$$

until the lowest bra and ket eigenvectors agree with the input α and β structure coefficients of the $\Delta^\dagger$ and δ correlated boson pairs. Again, the right and left eigenvector matrices are constrained to be inverses of one another. At each step of the iterative procedure, it is convenient to first diagonalize the non-Hermitian norm matrix, and then to diagonalize the Hamiltonian in the resulting biorthogonal basis.

At the point of convergence, the energetically lowest eigenvector represents the (self-consistent) ground state of the system. Furthermore, the eigenvectors that are higher in energy represent (low-lying) excited states.

C. Unphysical states and the Park operator

A general feature of boson mappings is the occurrence of unphysical states that do not preserve the symmetry character of the system. The origin of these unphysical states can be seen by considering states involving two bosons

$$|ij,kl\rangle = B_{ij}^\dagger B_{kl}^\dagger|0\rangle_B \ . \tag{12}$$

Such a state preserves the symmetry character of the original system under the interchange of the labels i and j and under the interchange of the labels k and l, but not under the interchange of one of the labels of the first boson with one of the labels of the second. To construct a state with the proper symmetry character, it is necessary to take the linear combination

$$|ijkl\rangle=[B_{ij}^{\dagger}B_{kl}^{\dagger}+(-1)^{\sigma}B_{ik}^{\dagger}B_{jl}^{\dagger}+(-1)^{\sigma}B_{kj}^{\dagger}B_{il}^{\dagger}]|0\rangle_B \ . \tag{13}$$

Such a state has a direct counterpart in the system prior to the mapping and is referred to as a physical state. The two linear combinations orthogonal to it have no such counterparts and are referred to as unphysical states.

In an exact diagonalization of the Hamiltonian that results from a boson mapping, the unphysical states completely decouple from the physical states. This is no longer true, however, when the system is treated approximately. Variational calculations mix physical and unphysical states, with the degree of mixing dictated by their proximity in energy.

As noted earlier, unphysical states that arise in the mapping of fermion systems onto boson systems are of particular concern since they often emerge from variational calculations as the lowest states of the system. Those arising in boson→boson mappings are of less concern when focusing on the ground state of the system; however, they too become a problem when treating excited states. The lack of a procedure for effectively treating unphysical states is the principal problem that has precluded the practical application of boson expansion techniques.

Recently, Park[5] introduced an operator that can be used to assess the symmetry character of a state resulting from a boson mapping, whether physical, unphysical, or of mixed character. This operator was first introduced in the context of fermion systems, but it can be readily generalized to any system. By definition, it is given by

$$P=(N_{ph}^2)_{\rm Dyson}-(N_{pp}^2)_{\rm Dyson} \ , \tag{14a}$$

where

$$N_{ph}^2=\sum_{ij} a_i^{\dagger}a_i a_j^{\dagger}a_j \ , \tag{14b}$$

is the square of the number operator expressed in particle-hole form and

$$N_{pp}^2=\sum_{i} a_i^{\dagger}a_i+\sum_{ij} a_i^{\dagger}a_j^{\dagger}a_j a_i \tag{14c}$$

is the corresponding expression in particle-particle form. Using the generalized mapping equations (6), we obtain an explicit form for the Park operator

$$P=\sum_{ijkl} B_{ik}^{\dagger}B_{jl}^{\dagger}[B_{ik}B_{jl}-(-1)^{\sigma}B_{kl}B_{ij}] \ . \tag{15}$$

It is straightforward to confirm that all physical states $|P_i\rangle$ are eigenstates of this operator with eigenvalue zero

$$P|P_i\rangle=0 \ . \tag{16}$$

This statement follows trivially from the fact that the difference between N_{ph}^2 and N_{pp}^2 prior to the mapping was identically zero. Equally true, although a bit less obvious, is that for any unphysical state $|U_i\rangle$

$$\langle U_i|P|U_i\rangle>0 \ . \tag{17}$$

Thus, by evaluating the expectation value of the Park operator we get a measure of the mixing of unphysical states in the low-lying wave functions of interest.

Another possible use of the Park operator is as a pseudo-Majorana interaction. The idea is to replace the boson Hamiltonian H_B that results from the mapping by a modified Hamiltonian $H_B(\lambda)$, defined by

$$H_B(\lambda)=H_B+\lambda P \ . \tag{18}$$

If $\lambda>0$, the only effect of the additional term on the exact spectrum is to lift up all unphysical states relative to all physical states, precisely as desired. Indeed, an analogous approach is commonly used in the shell model to remove states with spurious center-of-mass motion.

But, as noted earlier, variational approximations, such as Hartree, do not fully decouple physical and unphysical states. What will be the effect of adding a pseudo-Majorana interaction in such calculations? To answer this question, it is useful to first address a related question: Under what condition does Hartree approximation produce a purely physical state? Taking the expectation value of the Park operator (15) between the Hartree self-consistent states [(7) and (8)] and equating the result to zero yields the following condition that must be satisfied by the x^0 and y^0 structure coefficients:

$$N(N-1)\sum_{ijkl} y_{ik}^0 y_{jl}^0[x_{ik}^0 x_{jl}^0-(-1)^{\sigma}x_{ij}^0 x_{kl}^0]=0 \ . \tag{19}$$

This equation has no solution for fermion systems ($\sigma=1$). As a consequence, the Hartree wave functions that emerge after a fermion→boson mapping have large admixtures of physical and unphysical components. Clearly, a pseudo-Majorana interaction will not be useful in such cases. This was first pointed out by Hahne and collaborators[6] in the context of a pure pairing model, although in the recent work of Kuchta[7] there are implied claims to the contrary. While our work tends to support the claim of Ref. 6, further clarification is called for.

For boson systems ($\sigma=0$), Eq. (19) has solutions. In particular, it is satisfied whenever the x_{ij}^0 coefficients are separable, i.e., whenever

$$x_{ij}^0=\eta_i\eta_j \ . \tag{20}$$

In the extreme limit in which there are no new (pairing) correlations produced by the mapping, the x_{ij}^0 will indeed be separable, with the η_i coefficients being those arising in a Hartree treatment of the system prior to the mapping.

It is for this reason that a pseudo-Majorana approach applied after a boson→boson mapping may have a greater chance of success. The Hartree wave functions that emerge after such a mapping can be approximately physical. When this is indeed the case, the inclusion of a pseudo-Majorana interaction will still have the effect of lifting up the predominantly unphysical states relative to the predominantly physical states.

However, there is also a cautionary message that follows from the above analysis. Inclusion of the Park operator as a pseudo-Majorana interaction has the further effect of suppressing the pair correlations that are incorporated by the mapping. Thus, there is a subtle interplay between two effects; the desirable effect of lifting up unphysical components and the undesirable effect of removing the new pair correlations. Clearly, if the Park operator is to be a useful means of suppressing the influence of unphysical states, it is essential that it lifts them in energy more rapidly than it causes pair correlations to be lost. We will return to this point in the applications to follow.

III. APPLICATION OF THE IBEP TO THE TWO-LEVEL PAIRING MODEL

A. The model

As a first application of the IBEP to a fermion system, we have studied the two-level pairing model.[8] In this model, N identical fermions, limited to two active levels with the same pair degeneracy $\Omega=j+\frac{1}{2}$, interact via the Hamiltonian

$$H_F=\sum_{\alpha}\alpha\frac{\epsilon}{2}T_\alpha-\frac{G}{4}\sum_{\alpha\alpha'}P_\alpha^\dagger P_{\alpha'} \ , \tag{21a}$$

where

$$T_\alpha=\sum_m a_{\alpha m}^\dagger a_{\alpha m} \ , \tag{21b}$$

$$P_\alpha^\dagger=\sum_m(-1)^{j-m}a_{\alpha m}^\dagger a_{\alpha -m}^\dagger \ , \tag{21c}$$

and $\alpha=\pm 1$, corresponding to the two active levels. The full shell-model space appropriate to this model contains a collective subspace, involving $L=0$ pairs in each of the two active orbits, that completely decouples from the noncollective subspace involving other pairs. In what follows, we will focus solely on the description of the physics of the collective subspace.

The two-level pairing model exhibits a phase transition as a function of the dimensionless parameter $x=2\Omega G/\epsilon$. For $x\ll 1$, the single-particle splitting between the two levels dominates and particles in one level are not pair correlated with those in the other level. We refer to this as the normal solution. For $x\gg 1$, the pairing interaction dominates over the single-particle splitting and thus can effectively scatter particles from one level to the other, producing a superfluid solution. At a critical intermediate value of $x\sim 1$, a phase transition from the normal to the superfluid domain occurs.

B. The first Dyson mapping

For this system, the first Dyson mapping (of the collective subspace) is already well known. The pair and particle-hole operators that enter the Hamiltonian (21) map according to

$$(P_\alpha^\dagger)_{B1}=2\sqrt{\Omega}s_\alpha^\dagger-\frac{2}{\sqrt{\Omega}}s_\alpha^\dagger s_\alpha^\dagger s_\alpha \ , \tag{22a}$$

$$(P_\alpha)_{B1}=2\sqrt{\Omega}s_\alpha \ , \tag{22b}$$

and

$$(T_\alpha)_{B1}=2s_\alpha^\dagger s_\alpha \ , \tag{22c}$$

where s_α is the pair boson that *replaces* the $L=0$ collective pair in level α. The subscript $B1$ is included to indicate that this is the *first boson* mapping.

Using the mapping Eqs. (22), we obtain for the Dyson image of H_F the non-Hermitian pair-boson Hamiltonian

$$\begin{aligned}H_{B1}=&\epsilon(s_1^\dagger s_1-s_{-1}^\dagger s_{-1})\\&-G\Omega(s_1^\dagger s_1+s_1^\dagger s_{-1}+s_{-1}^\dagger s_1+s_{-1}^\dagger s_{-1})\\&+G(s_1^\dagger s_1^\dagger s_1 s_1+s_1^\dagger s_1^\dagger s_1 s_{-1}\\&\quad+s_{-1}^\dagger s_{-1}^\dagger s_{-1}s_1+s_{-1}^\dagger s_{-1}^\dagger s_{-1}s_{-1}) \ .\end{aligned}\tag{23}$$

C. The second Dyson mapping

The second Dyson mapping takes the collective pair-boson space into a quartet-boson space, defined by two-index bosons $\Lambda_{\alpha_1\alpha_2}^\dagger$, which likewise have angular momentum $L=0$. The relevant mapping equations are

$$\begin{aligned}(s_{\alpha_1}^\dagger s_{\alpha_2}^\dagger)_{B2}&=\Lambda_{\alpha_1\alpha_2}^\dagger+\sum_{\alpha_2\alpha_4}\Lambda_{\alpha_1\alpha_3}^\dagger\Lambda_{\alpha_2\alpha_4}^\dagger\Lambda_{\alpha_3\alpha_4} \ ,\\(s_{\alpha_1}s_{\alpha_2})_{B2}&=\Lambda_{\alpha_1\alpha_2} \ ,\\(s_{\alpha_1}^\dagger s_{\alpha_2})_{B2}&=\sum_{\alpha_3}\Lambda_{\alpha_1\alpha_3}^\dagger\Lambda_{\alpha_2\alpha_3} \ .\end{aligned}\tag{24}$$

We can simplify the treatment of the quartet-boson space by exploiting the symmetry property (3). The four possible Λ bosons are then replaced by three independent bosons $p_1^\dagger$, $p_0^\dagger$, and $p_{-1}^\dagger$, via the defining relations

$$\Lambda_{11}^\dagger=\sqrt{2}p_1^\dagger, \quad \Lambda_{-1-1}^\dagger=\sqrt{2}p_{-1}^\dagger, \quad \Lambda_{1-1}^\dagger=\Lambda_{-11}^\dagger=p_0^\dagger \ . \tag{25}$$

These operators satisfy the usual boson commutation relation

$$[p_i,p_j^\dagger]=\delta_{ij} \ . \tag{26}$$

Finally, the boson Hamiltonian H_{B2} resulting from the second mapping can be expressed in terms of the three $p_i^\dagger$ quartet bosons,

$$\begin{aligned}H_{B2}=&2\epsilon(p_1^\dagger p_1-p_{-1}^\dagger p_{-1})-G\Omega[2p_1^\dagger p_1+2p_0^\dagger p_0+2p_{-1}^\dagger p_{-1}+\sqrt{2}p_1^\dagger p_0+\sqrt{2}p_{-1}^\dagger p_0+\sqrt{2}p_0^\dagger p_1+\sqrt{2}p_0^\dagger p_{-1}]\\&+G(2p_1^\dagger p_1+2p_{-1}^\dagger p_{-1}+\sqrt{2}p_1^\dagger p_0+\sqrt{2}p_{-1}^\dagger p_0)\\&+2G\Big[2p_1^\dagger p_1^\dagger p_1 p_1+2p_{-1}^\dagger p_{-1}^\dagger p_{-1}p_{-1}+2p_1^\dagger p_0 p_1+2p_{-1}^\dagger p_0^\dagger p_0 p_{-1}+2p_0^\dagger p_0^\dagger p_1 p_{-1}+\sqrt{2}p_1^\dagger p_1^\dagger p_1 p_0\\&\quad+\sqrt{2}p_{-1}^\dagger p_{-1}^\dagger p_{-1}p_0+\sqrt{2}p_1^\dagger p_0^\dagger p_0 p_0+\sqrt{2}p_{-1}^\dagger p_0^\dagger p_0 p_0+\frac{1}{\sqrt{2}}p_0^\dagger p_0^\dagger p_0 p_{-1}+\frac{1}{\sqrt{2}}p_0^\dagger p_0^\dagger p_0 p_{-1}\Big] \ .\end{aligned}\tag{27}$$

D. Mapping of the number operator

The two mappings can of course be applied to all operators of interest. As a particular example, consider the fermion number operator, $N_F=\sum_{\alpha m} a^\dagger_{\alpha m} a_{\alpha m}$. The first mapping transforms it according to

$$N_F \rightarrow 2\sum_\alpha s^\dagger_\alpha s_\alpha = 2N_{B1} ,$$

and the second mapping according to

$$2N_{B1} \rightarrow 4(p^\dagger_1 p_1 + p^\dagger_0 p_0 + p^\dagger_{-1} p_{-1}) = 4N_{B2} , \qquad (28)$$

confirming that the number of bosons is indeed reduced in half at each step of the iterative procedure.

E. Unphysical states in the two-level pairing model

As noted earlier, a general feature of boson mappings is that they produce unphysical states that do not preserve the symmetry character of the system. In the two-level pairing model, however, there are no unphysical states produced in the first mapping, as long as (a) we restrict the mapping to the collective subspace only, and (b) the number of fermion pairs does not exceed the pair degeneracy Ω of each level. The second mapping, however, does produce unphysical states. To illustrate this point, consider a system with $N_p = \frac{1}{2}N_F = 10$ active fermion pairs and a pair degeneracy of $\Omega = 10$. The number of states in both the collective fermion space and the first ideal boson space is 11, confirming that no unphysical states arise in the first mapping. However, the dimension of the second ideal space is 21, indicating that the second mapping produces ten states that do not preserve the symmetry character of the first ideal boson space.

Since the second mapping produces unphysical states, it is useful to introduce its associated Park operator P_{B2}. The explicit form for this operator is

$$P_{B2} = 2U^\dagger_{B2} U_{B2} , \qquad (29a)$$

where

$$U_{B2} = 2p_1 p_{-1} - p_0 p_0 . \qquad (29b)$$

To better appreciate the physical content of the Park operator (29), it is useful to rewrite U_{B2} in terms of the two-index Λ bosons,

$$2p_1 p_{-1} - p_0 p_0 = \Lambda_{11}\Lambda_{-1-1} - \Lambda_{1-1}\Lambda_{-11} . \qquad (30)$$

From this, we can readily confirm that the two-boson state $U^\dagger_{B2}|0\rangle_{B2}$ is indeed orthogonal to the *physical* two-boson state given in (13). Thus, requiring that the Park operator has zero expectation value is equivalent to imposing the additional symmetry that is missing in the mapping.

F. Calculations and results

The specific calculations that we report here are for a system in which $N_p = \Omega = 10$ and $\epsilon = 2$. In Table I, we present results for the ground-state energy of the system (as a function of the pairing strength G). The column denoted Exact refers to an exact diagonalization of the fermion Hamiltonian in the collective pair subspace. The results denoted $IT=1$ and $IT=2$ refer to Hartree calculations carried out after the first mapping ($B1$) and after the second mapping ($B2$), respectively. The column denoted BP1 refers to broken pair calculations carried out after the first mapping. For this system, the phase transition from normal to superfluid occurs for a critical value of $G \sim 0.1$.

TABLE I. Ground-state energy (in MeV) for the two-level pairing model. Calculations were carried out for $\epsilon = 2$ MeV, $\Omega = 10$, and $N_p = 10$. The column denoted Exact gives results of exact diagonalization, the other three give results obtained at various levels of approximation, which are described in the text.

G	Exact	$IT=1$	BP1	$IT=2$
0	−20	−20	−20	−20
0.025	−20.268	−20.268	−20.268	−20.268
0.050	−20.582	−20.582	−20.582	−20.582
0.075	−20.972	−20.974	−20.972	−20.972
0.100	−21.503	−21.523	−21.502	−21.505
0.125	−22.322	−22.416	−22.314	−22.333
0.150	−23.605	−23.777	−23.609	−23.600
0.175	−25.311	−25.506	−25.323	−25.249
0.200	−27.291	−27.482	−27.302	−27.167
0.500	−57.107	−57.199	−57.108	−56.797
1	−111.053	−111.100	−111.053	−110.832
2	−220.526	−220.603	−220.526	−220.404

The $IT=1$ calculations reproduce the ground-state energy when the system is in the normal phase. But they cease to be able to reproduce the exact results at and after the phase transition. In contrast, the BP1 calculations provide excellent reproduction of the exact results both in the normal and superfluid phases. The improvement of BP1 over $IT=1$ reflects the importance of correlations between the pair bosons in the superfluid phase. Note that both of these calculations were based on the same Hamiltonian and furthermore were carried out in a system ($B1$) with physical states only.

As a first guess, we might expect the $IT=2$ results to be similar in quality to the BP1 results, since both incorporate up to four-fermion correlations. Up to a coupling strength of $G \sim 0.2$, the two calculations indeed give roughly comparable results. However, for $G > 0.2$, the BP1 results are significantly better than the $IT=2$ results. The reason for this is that in the $IT=2$ calculations, there is some mixing with unphysical states. As we will see shortly, unphysical states move down in energy as we increase the pairing strength G, and this has the effect of increasing their admixtures in the variational ground state.

Similar conclusions follow from a consideration of the lowest excited state, for which we present the analogous results in Table II. But here the effect is even more dramatic. Now the $IT=2$ calculations begin to show significant discrepancies for a pairing strength of only $G \sim 0.15$, somewhat closer to the phase transition. Once again this is a direct reflection of increased mixing with unphysical states with increasing G.

To confirm that unphysical states of the second mapping come down in energy as the pairing strength in-

TABLE II. Energy of the lowest excited state (in MeV) for the two-level pairing model. Calculations were carried out for $\epsilon=2$ MeV, $\Omega=10$, and $N_p=10$. The various columns have the same significance as in Table I. The energies given in the column denoted $IT=2$ are for the lowest predominantly physical excited states.

G	Exact	$IT=1$	BP1	$IT=2$
0	4.00	4.00	4.00	4.00
0.025	3.53	3.53	3.53	3.53
0.050	3.02	3.00	3.02	3.02
0.075	2.48	2.40	2.48	2.47
0.100	1.97	1.82	1.98	1.95
0.125	1.71	1.68	1.57	1.81
0.150	1.97	2.98	1.99	2.19
0.175	2.58	2.63	2.65	2.71
0.200	3.24	3.20	3.28	3.17
0.500	9.75	9.65	9.73	10.40
1	19.88	19.83	19.87	20.27
2	39.94	39.91	39.93	40.15

creases, we carried out a diagonalization of the non-Hermitian Hamiltonian H_{B2}. As noted earlier, an exact diagonalization completely decouples unphysical states from physical states. Thus, by comparing the $IT=2$ results with the exact results obtained by diagonalizing the original fermion Hamiltonian, we can distinguish physical from unphysical states. In Fig. 1, we show results for the lowest three physical states (solid lines) and the lowest three unphysical states (dashed lines) as a function of G. The lowest unphysical states all move down in energy as the pairing strength increases. Furthermore, for $G>0.15$ the lowest unphysical state and the lowest excited state are very close in energy, so that the mixing induced in TD approximation should be very large.

The variational mean-field calculations mix physical and unphysical states. To assess the degree of mixing, we present in Table III the mean value of P for the ground state and the lowest few excited states obtained in the Hartree and TD approximations, respectively. As suggested above, the ground state and the lowest excited state are almost purely physical up to the critical value, after which the degree of unphysical state mixing gradually increases. These results confirm our earlier remark that the origin of the discrepancies that occur in the $IT=2$ calculations beyond the phase transition are a reflection of mixing with unphysical states. This mixing becomes particularly large in the low-lying excited states. Clearly, if we wish to be able to use the second Dyson expansion as a reliable means of approximating this many-body system, we must first develop a procedure to effectively remove the influence of these unphysical states, particularly from the low-lying TD excitations.

Following the discussion of Sec. II C, we consider the use of the Park operator of the second mapping, P_{B2}, as a pseudo-Majorana interaction. The fact that the degree of mixing of unphysical states is relatively weak suggests that such an approach may be useful. But, as noted in the earlier discussion, such a procedure will only be of practical use if it pushes up unphysical states in energy

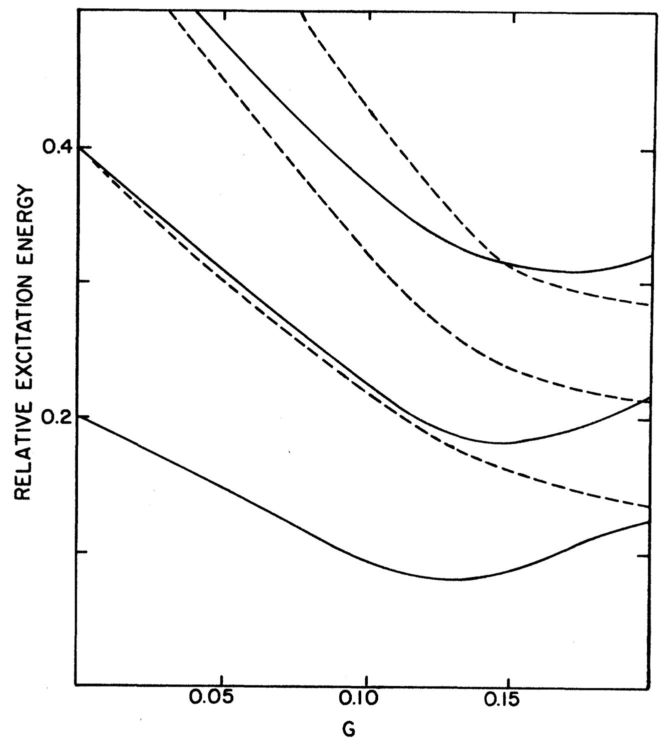

FIG. 1. Relative energies of low-lying excited states of the two-level pairing model following a second Dyson mapping. The results were obtained by diagonalization of the non-Hermitian boson Hamiltonian H_{B2} given in Eq. (27), for the parameter values $\epsilon=2$, $N_{B2}=5$, $\Omega=10$. Physical states are denoted by solid lines and unphysical states by dashed lines.

more rapidly than it destroys the new pair correlations.

To assess the usefulness of introducing a pseudo-Majorana Park operator in the two-level pairing model, we have carried out a series of Hartree and TD calculations using the modified Hamiltonian

$$H_{B2}(\lambda)=H_{B2}+\lambda P_{B2} , \qquad (31)$$

TABLE III. Mean value of the Park operator P for the ground state (GS) and lowest few excited states (TDA1 and TDA2) obtained in the $IT=2$ calculations described in the text.

G	GS	TDA1	TDA2
0	0.0	0.0	32.00
0.025	0.0	−0.034	32.03
0.050	−0.001	−0.195	32.19
0.075	−0.018	−0.610	32.61
0.100	−0.109	−1.344	33.30
0.125	−0.559	−1.806	33.58
0.150	−1.328	−0.882	32.35
0.175	−2.008	2.215	28.98
0.200	−2.508	8.501	22.50
0.500	−2.893	31.65	−0.808
1	−1.283	32.03	−0.540
2	−0.380	32.01	−0.167

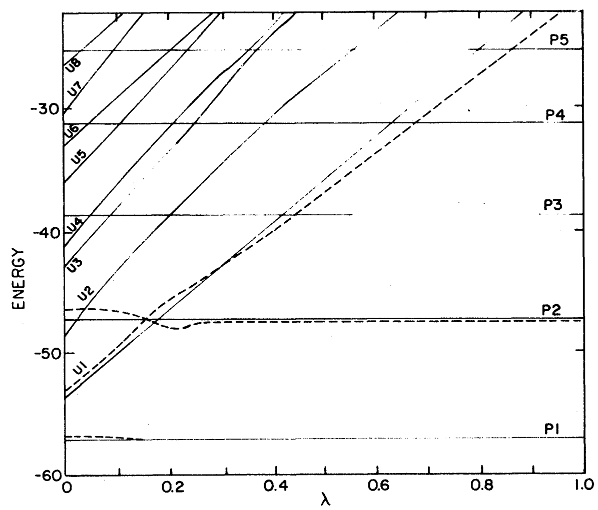

FIG. 2. Energies of low-lying excited states of the two-level pairing model following a second Dyson mapping and including a pseudo-Majorana interaction. The results are based on the Hamiltonian given in Eq. (30) with the same parameter values $\epsilon=2$, $N_{B2}=5$, $\Omega=10$ as in Fig. 1 and with $G=0.5$. The solid curves are the result of *exact* diagonalization; the dashed curves result from mean-field Hartree and Tamm-Dancoff calculations. The notation P_n (U_n) refers to the nth physical (unphysical) excited state, as discussed in the text.

with a pairing strength of $G=0.5$. For this value of G, the original $\lambda=0$ calculations produce two unphysical states between the ground state and the first excited state. In Fig. 2, we display the results as a function of the pseudo-Majorana strength λ. The notation P_n (U_n) denotes the nth physical (unphysical) state. Solid lines correspond to the exact results and dashed lines to the Hartree and TD results.

The first point to note is that, as expected, the exact physical states are completely unaffected by the addition of the pseudo-Majorana term. In contrast, the exact unphysical states are pushed up in energy very rapidly as λ is increased. Note further that, for $\lambda<0.15$, the lowest excited state is unphysical. At $\lambda \sim 0.15$, however, it crosses the lowest physical excited state, after which both the ground state and the first excited state are physical.

Since the mean-field calculations do not completely decouple physical and unphysical states, they produce significant mixing in the vicinity of the crossing. However, for $\lambda>0.3$, they provide an excellent reproduction of the exact spectrum. On the basis of these calculations, we conclude that for this model the Park operator is useful as a means of suppressing the effects of unphysical states that arise in the second boson$\rightarrow$boson mapping. The $IT=2$ calculations including a pseudo-Majorana interaction produce results that are comparable to the essentially exact BP1 calculations, *but more simply*. It is our hope that these remarks may apply more generally to the unphysical states that arise in any boson$\rightarrow$boson mapping, but further testing is clearly needed.

IV. SUMMARY

In summary, we have discussed in this paper the application of an IBEP to approximately describe the collective dynamics of many-body fermion systems. We have developed the formalism necessary to implement this procedure, following on recent developments in the application of boson expansion techniques to boson systems. Each stage of the IBEP in principle introduces unphysical states. Furthermore, in variational calculations, these unphysical states mix into the lowest states of the system, which are the states that are of particular interest. By focusing on the two-level pairing model, we have shown that the inclusion of a pseudo-Majorana interaction may be effective as a means of suppressing the influence of unphysical states that arise in boson$\rightarrow$boson mappings. In the two-level pairing model, no unphysical states arise in the first fermion$\rightarrow$boson mapping (if the number of active fermion pairs does not exceed the pair degeneracy of each active level). In more general problems, however, they will arise, and it will be necessary to find a practical procedure for removing their influence. We are currently investigating several possible approaches for accomplishing this. In our view, this remains the one outstanding problem that must be satisfactorily addressed before the IBEP can be viewed as a practical microscopic approach to the collective dynamics of many-fermion quantum systems.

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