PHYSICAL REVIEW C VOLUME 50, NUMBER 4 OCTOBER 1994

Comparison between two variational approaches for non-Hermitian boson Hamiltonians

M. C. Cambiaggio
Departamento de Física, Comisión Nacional de Energía Atómica, Avenida del Libertador 8250, 1429 Buenos Aires, Argentina

J. Dukelsky
Grupo de Física Nuclear, Facultad de Ciencias, Universidad de Salamanca, 37008 Salamanca, Spain
(Received 20 October 1993; revised manuscript received 22 June 1994)

The non-Hermitian Hartree approximation and the variational principle with quasi-Hermitian operators are compared in two different boson models. In a very simple schematic model the two methods provide comparable results. For the non-Hermitian boson Hamiltonian obtained applying the Dyson boson expansion to a two-level pairing model the results obtained are different. The first approach, although it does not provide an upper bound for the ground state energy, is not limited by the appearance of spurious states that break the quasi-Hermiticity of the Hamiltonian.

PACS number(s): 21.60.Jz, 21.90.+f

Boson expansion theories are often used as a convenient means for describing collective nuclear properties. In the particular case of the nonunitary Dyson boson mapping a non-Hermitian boson Hamiltonian is obtained. A complete diagonalization of this Hamiltonian is not always possible in realistic calculations and consequently adequate approximations must be performed. In a previous paper [1] we have proposed to use a Hartree approach that takes into account the non-Hermitian nature of the mapped Hamiltonian and have shown that it gives good ground-state results when applied to a simplified shell model defined by a monopole pairing Hamiltonian. However, these results are not upper bounds for the exact ground-state energies.

On the other hand, the approximate results are worse when the spurious components are important. The presence of spurious states, an always present problem when working with boson expansions, is due to the fact that the boson Hilbert space is larger than the original fermion Hilbert space and consequently part of the former, called the unphysical subspace, does not take into account Pauli effects.

In a recent paper [2] Scholtz *et al.* address the problem of how to perform a mean-field calculation when the Hamiltonian, and possibly other physical observables, are quasi-Hermitian rather than Hermitian. This happens not only when one studies the boson image of a Hermitian fermion Hamiltonian but also in some other cases as for example in the theory of effective interactions [3]. They formulate a variational principle which conforms to all the criteria of a proper variational principle; i.e., it is real, bounded from below by the exact ground-state energy, and, upon variation over the whole space, it yields the eigenvalue equations. They illustrate the procedure in a simple schematic model.

It is interesting to compare the two approaches and study their differences. With this aim we apply them to the schematic boson model of Ref. [2] and to the boson Hamiltonian obtained applying the Dyson mapping to the two-level pairing model.

In the model introduced in Ref. [2] one has two types of boson creation (annihilation) operators $a_i^\dagger$ $(a_i); i = 1, 2$. The Hamiltonian is

$$H = \hat{n}_2 + \frac{(\beta+\gamma)}{N} a_1^\dagger a_1^\dagger a_2 a_2 + \frac{(\beta-\gamma)}{N} a_2^\dagger a_2^\dagger a_1 a_1, \quad (1)$$

where $\hat{n}_2 = a_2^\dagger a_2$ is the number operator for boson 2 and N is the total number of bosons. It is to be noted that γ must be different from zero for the Hamiltonian being non-Hermitian. The exact results are obtained diagonalizing this Hamiltonian using as basis states the ones labelled by the total number operator and $\hat{n}_2$.

According to Scholtz *et al.* [2] a set of operators A_i in a finite-dimensional space is called quasi-Hermitian if there exists a linear operator T (a metric) that is Hermitian and positive definite and satisfies

$$TA_i = A_i^\dagger T. \quad (2)$$

In this case a new scalar product may be defined with respect to which the operators A_i are Hermitian. Consequently, all the usual theorems applicable to Hermitian operators hold if this new scalar product is employed.

A proper variational principle is easily formulated for the Hamiltonian H when this is one of the quasi-Hermitian operators. According to Eq. (2)

$$TH = H^\dagger T. \quad (3)$$

The energy functional E is defined as

$$E(\varphi) = \frac{\langle\varphi|TH|\varphi\rangle}{\langle\varphi|T|\varphi\rangle} \quad (4)$$

and shown to be greater than or equal to the lowest eigenvalue of H. Moreover, variation of E over the whole space yields the eigenvalue equations [2].

Within the schematic model described previously we take the Hamiltonian, the total number of particles, and the number of particles in state two as the set of observables A_i. They change neither the number of particles n_2 by an odd number nor the total number of particles. To avoid the problems associated with reducibility and the nonuniqueness of the metric [2], we restrict ourselves to the irreducible invariant subspace corresponding to even values of n_2. Studying the conditions under which the metric T exists, different regions of the $\beta - \gamma$ plane are identified (see Fig. 1 of Ref. [2]). For $|\gamma| > |\beta|$ there are two regions, one in which the Hamiltonian has complex eigenvalues and consequently, the set of operators is not quasi-Hermitian and another in which, although all the eigenvalues are real, T still does not exist. Only for $|\gamma| < |\beta|$ the model is well defined and a T exists, namely,

$$T = \left(\frac{\beta+\gamma}{\beta-\gamma}\right)^{\frac{\hat{n}_2}{2}} . \tag{5}$$

In this region the model exhibits a phase transition that occurs on the curves $\beta^2 - \gamma^2 = \frac{1}{4}$.

The trial wave function in the variational calculation performed in Ref. [2] is

$$|\varphi\rangle = \sum_{n_2=0}^{N} \frac{(\cos\theta)^{N-n_2}(\sin\theta)^{n_2}}{n_2!(N-n_2)!}(a_1^\dagger)^{N-n_2}(a_2^\dagger)^{n_2}|0\rangle. \tag{6}$$

The sum runs over even integers n_2 only. It is to be noted that Eq. (6.10) in Ref. [2] has two misprints [4]: the sum runs up to N and not $\frac{N}{2}$ and the factorials are missing. The ground-state energy obtained minimizing the energy functional E given in Eq. (4) with respect to θ agrees well with the exact result. As an example we show in Table I the variational results obtained for $N = 50$, $\gamma = -0.8\beta$ and different values of β from -2 to 0. The exact results are also given for comparison. The approximation is very good before the phase transition that occurs at $|\beta|_{\rm crit} = 0.8333$ for these values of the parameters, gets worse around the critical value of β and improves with increasing $|\beta|$.

As the usual trial wave function when working in boson systems is a boson condensate we have also considered

$$|\varphi\rangle = (a_1^\dagger + \mu a_2^\dagger)^N|0\rangle \tag{7}$$

and minimized the energy functional E given in Eq. (4) with respect to μ. This provides an analytic result for the ground-state energy which is zero up to the phase transition and

$$E_{gs} = \frac{[2(N-1)(\beta+\gamma)+N\rho]^2}{8(N-1)(\beta+\gamma)\rho} \tag{8}$$

after it. Here $\rho = \sqrt{\frac{\beta+\gamma}{\beta-\gamma}}$. The phase transition occurs at

$$\frac{2(N-1)|\beta+\gamma|}{N} = \rho. \tag{9}$$

For the above-mentioned values of the parameters one gets $|\beta_{\rm crit}| = 0.85$ and the energies listed in the last column of Table I. These results are worse than the previous ones before and on the vicinity of the phase transition and coincide with them for larger values of $|\beta|$.

For implementing the Hartree approach in a boson system one introduces collective boson operators $\Gamma_n^\dagger$ by means of a canonical transformation, assumes that the ground-state wave function is that of a condensate of only one kind of collective bosons, and minimizes the expectation value of the Hamiltonian with respect to the transformation coefficients [5]. For a non-Hermitian Hamiltonian one has to consider [1] a trial bra $\langle\bar{\varphi}|$ that is not equal to the Hermitian conjugate of the trial ket $|\varphi\rangle$.

Within the schematic boson model described above one defines

$$\Gamma^\dagger = \frac{1}{\sqrt{\mathcal{N}}}(\eta_1 a_1^\dagger + \eta_2 a_2^\dagger) \tag{10}$$

$$\bar{\Gamma} = \frac{1}{\sqrt{\mathcal{N}}}(\bar{\eta}_1 a_1 + \bar{\eta}_2 a_2), \tag{11}$$

where $\mathcal{N} = \eta_1\bar{\eta}_1 + \eta_2\bar{\eta}_2$, such that the operators $\bar{\Gamma}$ and $\Gamma^\dagger$ satisfy boson commutation relations. The trial bra and ket are

$$\langle\bar{\varphi}| = \langle 0|\frac{1}{\sqrt{N!}}\bar{\Gamma}^N \tag{12}$$

$$|\varphi\rangle = \frac{1}{\sqrt{N!}}(\Gamma^\dagger)^N|0\rangle. \tag{13}$$

Then one has to minimize the expectation value of the Hamiltonian with respect to η_i and $\bar{\eta}_i$. The normalization condition $\mathcal{N} = 1$ is not enough to normalize the bra and the ket separately because if we multiply the η_i by a constant k and divide the $\bar{\eta}_i$ by the same constant k the equations remain the same [1,6]. This is not a problem if we only want to calculate the ground-state energy but allows us to add another condition which we have chosen to be $\eta_1 = \bar{\eta}_1$. The minimization provides an analytic result for the ground-state energy which coincides with the one obtained applying the variational principle with quasi-Hermitian operators and a trial wave function that is a boson condensate [Eq. (8)]. As in the latter case, one also obtains that the energy before the phase transition is zero and that the critical values of the parameters are determined by condition (9).

With the aim of performing a more complete compar-

TABLE I. Ground-state energies in the schematic model for $N = 50$, $\gamma = -0.8\beta$, and different values of β.

β	Exact	Variational	Hartree	Boson condensate
-0.2	-0.0143	-0.0142	-0.0141	0
-0.4	-0.0595	-0.0573	-0.0568	0
-0.6	-0.145	-0.132	-0.130	0
-0.8	-0.301	-0.243	-0.236	0
-1.0	-0.666	-0.404	-0.333	-0.329
-1.2	-1.698	-1.498	-1.498	-1.498
-1.4	-3.342	-3.172	-3.172	-3.172
-1.6	-5.324	-5.163	-5.163	-5.163
-1.8	-7.524	-7.365	-7.365	-7.365
-2.0	-9.875	-9.715	-9.715	-9.715

ison we have also used as trial bra and ket the ones obtained from Eqs. (12) and (13) restricting the sums that appear in the expansions of Γ^N and $(\Gamma^\dagger)^N$ to even values of n_2. The results obtained from the minimization of the expectation value of the Hamiltonian in this case are to be compared with the ones obtained when using the trial wave function (6) in the variational principle with quasi-Hermitian operators. For $N = 50$ and $\gamma = -0.8\beta$ these Hartree energies are given in Table I. They are very similar to the variational results except near the phase transition where the latter are better.

The second model used in this comparison is the two-level pairing model. The fermion pairing Hamiltonian for two levels of the same degeneracy $\Omega = j + \frac{1}{2}$ and single-particle energies $\frac{\varepsilon}{2}$ and $-\frac{\varepsilon}{2}$ is

$$H_F = \sum_{\sigma m} \sigma \frac{\varepsilon}{2} b^\dagger_{\sigma m} b_{\sigma m} - \frac{G}{4} \sum_{\sigma\sigma'} P^\dagger_\sigma P_{\sigma'} \tag{14}$$

with $\sigma = \pm 1$ and

$$P^\dagger_\sigma = \sum_m (-)^{j-m} b^\dagger_{\sigma m} b^\dagger_{\sigma -m}. \tag{15}$$

G is the strength of the pairing interaction.

The exact solution may be obtained by diagonalizing this Hamiltonian on the basis provided by the number of pairs in level one and the total number of pairs.

The two-level pairing model exhibits a phase transition as a function of the dimensionless parameter $x = \frac{2\Omega G}{\varepsilon}$. For $x < 1$ the single-particle splitting between the two levels dominates and particles in different levels are not pair correlated. For $x > 1$ the pairing interaction dominates over the single-particle term producing a superfluid solution.

The Dyson boson expansion maps bifermion operators in terms of ideal boson creation and annihilation operators through a nonunitary and finite transformation [1,7]. Truncating the expansion by considering only zero angular momentum bosons one gets the following boson images:

$$(P^\dagger_\sigma)_B = 2\sqrt{\Omega} S^\dagger_\sigma - \frac{2}{\sqrt{\Omega}} S^\dagger_\sigma S^\dagger_\sigma S_\sigma \tag{16}$$

$$(P_\sigma)_B = 2\sqrt{\Omega} S_\sigma \tag{17}$$

$$(K)_B = \sum_\sigma \sigma \varepsilon S^\dagger_\sigma S_\sigma, \tag{18}$$

where K is the one-body term in Eq. (14) and $S^\dagger_\sigma$ (S_σ) is the creation (annihilation) operator of a collective boson in the level σ. Therefore, the mapped Hamiltonian turns out to be a non-Hermitian boson Hamiltonian

$$H_B = \varepsilon \sum_\sigma \sigma S^\dagger_\sigma S_\sigma - G\Omega \sum_{\sigma\sigma'} S^\dagger_\sigma S_{\sigma'} + G \sum_{\sigma\sigma'} S^\dagger_\sigma S^\dagger_\sigma S_\sigma S_{\sigma'}. \tag{19}$$

For applying the variational principle with quasi-Hermitian operators we take the Hamiltonian (19), the total number of bosons $\hat{N}$, and the number of bosons in level one $\hat{n}_1$ for the set of operators A_i. This set is irreducible on the boson space considered that corresponds to a fixed value of N, $0 \leq N \leq 2\Omega$, and $0 \leq n_1 \leq N$. We look for the metric T. Applying condition (2) to $\hat{N}$ and $\hat{n}_1$ and taking into account that we can label all the states by the eigenvalues of these two operators, we conclude that T must be a function of them, $T = T(\hat{N}, \hat{n}_1)$. On the other hand, applying (2) to the Hamiltonian we get a relation between the matrix elements of the operator T

$$t(N, n_1 + 1) = t(N, n_1) \frac{(\Omega - N + n_1 + 1)}{(\Omega - n_1)}. \tag{20}$$

Consequently, a positive definite metric only exists for $N \leq \Omega$. If $N > \Omega$ the operators are not quasi-Hermitian which is consistent with the fact that in this case the Hamiltonian has complex eigenvalues due to the appearance of spurious states related to violations of the Pauli principle. Note that the recursive relation (20) will diverge and then change sign for values of n_1 greater than Ω. Solving this recursion relation and choosing $t(N, 0) = 1$ we have

$$T(\hat{N}, \hat{n}_1) = \frac{(\Omega - \hat{N} + \hat{n}_1)!(\Omega - \hat{n}_1)!}{\Omega!(\Omega - \hat{N})!}. \tag{21}$$

For applying the variational principle to the energy functional given in (4) we use a boson condensate as the trial wave function

$$|\varphi\rangle = (S^\dagger_{-1} + \delta S^\dagger_1)^N |0\rangle = \sum_{l=0}^{N} \binom{N}{l} (S^\dagger_{-1})^{N-l} \delta^l (S^\dagger_1)^l |0\rangle. \tag{22}$$

The ground-state energies obtained from the minimization procedure for $\varepsilon = 2, \Omega = N = 10$ are shown in Table II. The exact results are also given for comparison. We have added εN to the energies. The superconducting phase transition occurs at $G_{\text{crit}} = 0.1$. The approximate results agree quite well with the exact ones before the phase transition but get worse with increasing coupling constants.

Trying to improve the variational results in the superconductive region we have used different trial wave functions which look like the one in Eq. (22) but with the combinatorial number to different powers: 0, 2, and 3. The best results are the ones obtained using the square of the combinatorial number and are also shown in Table II. These results are not so good as the previous ones before the phase transition but instead they are much better for larger values of G.

For applying the non-Hermitian Hartree approximation to the boson Hamiltonian given in (19) we use the procedure described before when considering the schematic boson model. In definitions (10) and (11) we replace the boson operators $a^\dagger_i$ and a_i by $S^\dagger_\sigma$ and S_σ, calculate the expectation value of the Hamiltonian with

TABLE II. Ground-state energies ($+\varepsilon N$) in the two-level pairing model for $\varepsilon = 2$ and $\Omega = N = 10$.

G	Exact	Variational	(comb. number)^2	Hartree
0.025	-0.268	-0.268	-0.250	-0.268
0.050	-0.582	-0.582	-0.578	-0.582
0.075	-0.972	-0.971	-0.944	-0.974
0.100	-1.503	-1.488	-1.467	-1.523
0.125	-2.322	-2.200	-2.240	-2.416
0.150	-3.605	-3.115	-3.542	-3.777
0.175	-5.311	-4.194	-5.259	-5.506
0.200	-7.291	-5.401	-7.240	-7.482
0.500	-37.11	-24.66	-37.08	-37.20
1.000	-91.05	-62.44	-91.04	-91.10
2.000	-200.5	-141.2	-200.5	-200.6

respect to the trial bra and ket (12) and (13), and minimize it. As before, we use the normalization condition and $\eta_1 = \bar{\eta}_1$. The Hartree energies obtained for $\varepsilon = 2$ and $\Omega = N = 10$ are shown in Table II. They agree well with the exact results but are not upper bounds to the exact ground-state energies.

In summary, we have compared two different mean-field approximations appropriate for non-Hermitian Hamiltonians. In a schematic boson model the two approaches give comparable results, what has been checked for different sets of parameter values, but it is a very simple model.

In the two-level pairing model some differences appear. The non-Hermitian Hartree approximation applied to the Dyson boson image of the Hamiltonian gives good ground-state energies but this approach has a drawback: it does not provide upper bounds for those energies. However, the method has an important advantage: it is not limited by the appearance of spurious states although the approximate results are worse when the spurious components are more important. This has been already seen in Ref. [1]. On the other hand, it is possible within this approach to study excited states.

With respect to the variational principle with quasi-Hermitian operators, it also gives reasonable results when applied to the above-mentioned Dyson boson Hamiltonian. In this case, for getting the best results one has to use different trial wave functions before and after the phase transition. For $G < G_{\text{crit}}$ one gets excellent results using a boson condensate as the trial wave function, which is the usual choice, but then the results are very poor after the phase transition. It is possible to improve the ground-state energies in the latter region using a different wave function but in this case one gets not so good results for small coupling constants. Consequently, the phase transition present in the model is pointed out by a change in the most appropriate wave function whereas with the previous method it is well represented by a boson condensate.

Once again, these conclusions have been checked for different values of the model parameters.

The drawback of the method based on quasi-Hermitian operators is that, in its present form, it cannot deal with spurious states originated in Pauli violations. These spurious states may be related to complex eigenvalues of the Hamiltonian, breaking the condition of quasi-Hermiticity. In our calculation of the two-level pairing model this problem can be overcome by performing a truncation to the physical space, disregarding states with $n_i > \Omega$, or equivalently by changing from particles to holes for $N > \Omega$. This limitation could be very serious in more realistic situations. In particular, in the five-level pairing model with parameters appropriate for the tin isotopes studied in Ref. [1] one of the levels has degeneracy one which implies that spurious states are always present. Practical techniques for performing a truncation to physical states should be combined with this variational approach in order to be able to treat more realistic problems.

On the other hand, the non-Hermitian Hartree approximation, even if it is not limited by the appearance of spurious states, provides worse results when spurious components are more important. These conclusions emphasize the relevance of the still unsolved problem of identifying and projecting out spurious states, particularly on applying boson mapping methods in cases where the collective bosons are not completely decoupled from those bosons which have to be included to obtain an exact realization of the operators involved [8].

Therefore, it would be very interesting to study the possibility of using the metric T for detecting the spurious states and extending the region of validity of the variational principle with quasi-Hermitian operators without loosing the property of being a proper variational calculation which provides upper bounds to the energies. However, the construction of the metric is not an easy task in not so simple models.

This work has been supported in part by the Carrera del Investigador Científico y Técnico of the CONICET, Argentina.

[1] M. C. Cambiaggio and J. Dukelsky, Phys. Lett. B **197**, 479 (1987).
[2] F. G. Scholtz, H. B. Geyer, and F. J. W. Hahne, Ann. Phys. **213**, 74 (1992).
[3] T. H. Schucan and H. A. Weidenmüller, Ann. Phys. **73**, 108 (1973); **76**, 483 (1973).
[4] H. B. Geyer (private communication).
[5] J. Dukelsky, G. G. Dussel, R. P. J. Perazzo, S. L. Reich, and H. M. Sofia, Nucl. Phys. **A425**, 93 (1984).
[6] Y. K. Gambhir, J. A. Sheikh, P. Ring, and P. Schuck, Phys. Rev. C **31**, 1519 (1985).
[7] E. R. Marshalek, Nucl. Phys. **A347**, 253 (1980).
[8] J. Dobaczewski, H. B. Geyer, and F. J. W. Hahne, Phys. Rev. C **44**, 1030 (1991).