Analysis of the truncation schemes for the physical boson states with Dyson's description

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We analyze various truncation schemes for the physical boson basis states which are required for the calculations in the boson space, in the Dyson boson mapping formalism. The available approximate schemes violate the Pauli principle and are found to be inadequate. The necessity to evolve yet a reliable and useful truncation scheme is stressed.

In recent years much effort has gone into the formulation of a microscopic theory with the sole aim to relate the phenomenological neutron-proton interacting boson model (IBM2) (Ref. 1) to the nuclear shell model. These microscopic theories, also referred to as boson expansion theories, start with the expansion of bifermion operators in terms of bosons through a suitable mapping procedure. The mapping is determined through the requirement that the respective commutation algebras be fully preserved. Both unitary and nonunitary mappings have been used. The nonunitary mapping of bifermion operators is achieved through the generalized Dyson boson mapping (DBM) and is represented for the uncoupled case as

$$(C_\alpha^\dagger C_\beta^\dagger)\rightarrow \bar{b}_{\alpha\beta}^\dagger \equiv b_{\alpha\beta}^\dagger - \sum_{\gamma\delta} b_{\alpha\gamma}^\dagger b_{\beta\delta}^\dagger b_{\gamma\delta} \ , \tag{1a}$$

$$(C_\beta C_\alpha)\rightarrow \bar{b}_{\alpha\beta} \equiv b_{\alpha\beta} \ , \tag{1b}$$

$$(C_\alpha^\dagger C_\beta)\rightarrow \sum_\gamma b_{\alpha\gamma}^\dagger b_{\beta\gamma} \ . \tag{1c}$$

$C_\alpha^\dagger$ (C_α) are the fermion single-particle (s.p.) creation (annihilation) operators for the state $|\alpha\equiv nljm\rangle$ and obey anticommutation relations; the fermion vacuum $|0\rangle$ is defined through $C_\alpha|0\rangle=0$. The $b_{\alpha\beta}^\dagger$ ($b_{\alpha\beta}$) are the boson creation (annihilation) operators, and satisfy

$$[b_{\alpha\beta}, b_{\gamma\delta}^\dagger] = \delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma} \ , \tag{2a}$$

$$[b_{\alpha\beta}, b_{\gamma\delta}] = [b_{\alpha\beta}^\dagger, b_{\gamma\delta}^\dagger] = 0 \ . \tag{2b}$$

The boson vacuum $|0\rangle$ is likewise defined through $b_{\alpha\beta}|0\rangle=0$. Equations (1a)–(1c) ensure that any fermion operator in DBM will have a finite number of terms in the boson space. The DBM mapping [Eqs. (1a)–(1c)] can be generalized[2] for the case of coupled and/or collective bifermion operators in a straightforward manner. The collective bifermion operators can be introduced either before[2] or after[3] the mapping, i.e., either in the fermion space itself or in the boson space.

We begin by introducing collective fermion pair excitation operators $Q^\dagger$ defined as

$$Q_\mu^\dagger = \sum_{a\le b} \tilde{\chi}_{J_\mu}^\mu(ab) \frac{A_{J_\mu}^\dagger(ab)}{\sqrt{1+\delta_{ab}}} \ , \tag{3a}$$

with

$$A_{J_\mu}^\dagger(ab) = [C_a^\dagger C_b^\dagger]_{J_\mu} \ . \tag{3b}$$

The label a represents all but the magnetic quantum number m_a of the sp state $|\alpha\rangle$. The amplitudes $\tilde{\chi}$ appearing in Eq. (3a) should be calculated taking into account all the valence fermions using shell-model techniques. We use here the broken-pair approximation (BPA) (Ref. 4) which has been found to be suitable[5] in such microscopic theories. The BPA assumes the ground state $|\Phi_0\rangle$ for p pairs of identical valence nucleons to be of the form

$$|\Phi_0\rangle \rightarrow S_+^p |0\rangle \ , \tag{4}$$

where the pair distributed operator S_+ is analogous to the $Q_\mu^\dagger$ operator with $J_\mu=0$. The distribution coefficients $\tilde{\chi}_{J_\mu=0}$ appearing in the definition of S_+ operators can be calculated by minimizing the Hamiltonian with respect to the ground state $|\Phi_0\rangle$. This is termed as zero-BPA (BPA0).[4] Next, the BPA basis states $|\Phi_{JM}(ab)\rangle$ are obtained through the replacement of one of the S_+ operators appearing in Eq. (4) by an operator $A_{JM}^\dagger(ab)$. For the case of $J=0$ these basis states are not orthonormal and therefore an orthonormal set is constructed from these BPA basis states. The Hamiltonian is then diagonalized in this space. This is termed as one-BPA or simply referred to as BPA. The eigenstates $|\Psi_\mu\rangle$ so obtained can be rewritten as

$$\Psi_\mu = \sum_{a\le b} \alpha_{J_\mu}^\mu(ab) |\Phi_{J_\mu M_\mu}(ab)\rangle \rightarrow N_{J_\mu}^\mu Q_\mu^\dagger (S^\dagger)^{p-1}|0\rangle \ . \tag{5}$$

The amplitudes $\tilde{\chi}$ are explicitly related to $\alpha_{J_\mu}^\mu$ and the normalization $N_{J_\mu}^\mu$ and hence may in general depend on the Hamiltonian H and p—the number of pairs of valence nucleons. It should be pointed out that an accurate set of $\chi_{J_\mu=0}(aa)$ for the lowest $\Psi_{\mu(J_\mu=0)}$ can be obtained through the following iterative procedure, starting from any arbitrary set of $\tilde{\chi}_{J_\mu=0}$; the BPA wave function Eq. (5) for the ground state is rewritten as

$$\sum_a \mathscr{C}_{J_\mu=0}^{(aa)} A_{00}^\dagger(aa)(S^\dagger)^{p-1}|0\rangle \ . \tag{6}$$

The new set of $\tilde{\chi}_{J_\mu=0}(aa)$ are determined from the calculated $\mathscr{C}_{J_\mu=0}(aa)$ by requiring that Eq. (6) has the same form as Eq. (4). The BPA calculations are again performed and the new set of $\tilde{\chi}_{J_\mu=0}(aa)$ determined. This procedure is repeated until the convergence is obtained. This iterative procedure avoids minimization (BPA0) and is fast converging, in fact, in practice two or three iterations are sufficient to yield an accurate set of $\tilde{\chi}_{J_\mu=0}(aa)$.

For the purpose of analyzing the original fermion prob-

TABLE I. Calculated ground state energies E_0 and occupation probabilities for the tin isotopes. The strength G of the Hamiltonian and s.p. energies ϵ_a used are $G=0.187$ MeV and $\epsilon_a=0.22$, 1.90, 2.20, and 2.80 MeV for $1d_{5/2}$, $1g_{7/2}$, $3s_{1/2}$, $2d_{3/2}$, and $1h_{11/2}$, respectively.

p	E_0	$\vartheta^2_{2d_{5/2}}$	$\vartheta^2_{1g_{7/2}}$	$\vartheta^2_{3s_{1/2}}$	$\vartheta^2_{2d_{3/2}}$	$\vartheta^2_{2d_{3/2}}$	$\vartheta^2_{1h_{11/2}}$
2	−2.269	0.315	0.221	0.029	0.023	0.016	BCS
	−2.621	0.306	0.226	0.032	0.025	0.016	NOA
	−2.623	0.325	0.214	0.029	0.023	0.016	Li
	−2.623	0.325	0.214	0.029	0.023	0.016	BPA0
	−2.624	0.325	0.214	0.029	0.023	0.016	Exact
5	−2.450	0.706	0.610	0.085	0.063	0.038	BCS
	−3.150	0.765	0.565	0.081	0.062	0.040	NOA
	−3.085	0.712	0.609	0.079	0.060	0.038	Li
	−3.074	0.713	0.609	0.078	0.060	0.038	BPA0
	−3.084	0.715	0.607	0.078	0.060	0.038	Exact
7	−0.150	0.902	0.869	0.189	0.126	0.063	BCS
	−1.200	1.070	0.791	0.113	0.087	0.056	NOA
	−0.741	0.913	0.912	0.127	0.090	0.051	Li
	−0.634	0.930	0.913	0.118	0.082	0.046	BPA0
	−0.700	0.936	0.909	0.120	0.085	0.048	Exact
8	2.925	0.931	0.914	0.368	0.247	0.114	BCS
	3.200	1.223	0.933	0.130	0.100	0.064	NOA
	1.506	1.030	1.010	0.208	0.135	0.067	Li
	2.200	0.936	0.922	0.388	0.234	0.107	BPA0
	2.150	0.931	0.914	0.370	0.249	0.115	Exact

TABLE II. Calculated ground state energies E_0 and occupation probabilities for the tin isotopes, with the energy shift $\Delta E=1.0$ MeV relative to the $2d_{5/2}$ level. The parameters G and ϵ_a are the same as those of Table I.

p	E_0	$\vartheta^2_{2d_{5/2}}$	$\vartheta^2_{1g_{7/2}}$	$\vartheta^2_{3s_{1/2}}$	$\vartheta^2_{2d_{3/2}}$	$\vartheta^2_{1h_{11/2}}$	
3	−1.277	0.861	0.081	0.015	0.013	0.009	Li
	−1.256	0.865	0.079	0.015	0.012	0.009	BPA0
4	−0.318	1.078	0.161	0.021	0.017	0.113	Li
	0.040	0.885	0.289	0.033	0.026	0.017	BPA0
5	1.606	1.050	0.406	0.041	0.031	0.020	Li
	1.943	0.914	0.496	0.049	0.038	0.025	BPA0

TABLE III. Calculated ground state energies E_0 and occupation probabilities for the nickle isotopes. The parameters used for the pairing Hamiltonian are the following: $G=0.331$ MeV, and $\epsilon_a=0$, 0.78, 1.56, and 4.52 MeV for $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$, and $1g_{9/2}$, respectively.

p	E_0	$\vartheta^2_{2p_{3/2}}$	$\vartheta^2_{1f_{5/2}}$	$\vartheta^2_{2p_{1/2}}$	$\vartheta^2_{1g_{9/2}}$	
2	−1.670	0.565	0.236	0.096	0.013	BCS
	−2.090	0.624	0.201	0.081	0.013	Li
	−2.090	0.624	0.201	0.082	0.013	BPA0
	−2.100	0.629	0.198	0.081	0.013	Exact
3	−0.160	0.732	0.420	0.177	0.020	BCS
	−1.770	0.801	0.383	0.148	0.020	Li
	−1.740	0.759	0.407	0.155	0.021	BPA0
	−1.750	0.764	0.404	0.153	0.021	Exact
5	2.500	0.928	0.827	0.532	0.026	BCS
	1.720	0.925	0.866	0.395	0.031	Li
	1.730	0.932	0.855	0.416	0.031	BPA0
	1.700	0.934	0.856	0.408	0.031	Exact

TABLE IV. Calculated ground state energies E_0 and occupation probabilities for the nickel isotopes with the energy shift $\Delta E = 0.5$ MeV relative to the $2p_{3/2}$ level.

p	E_0	$\vartheta^2_{2p_{3/2}}$	$\vartheta^2_{1f_{5/2}}$	$\vartheta^2_{2p_{1/2}}$	$\vartheta^2_{1g_{9/2}}$	
2	−1.529	0.802	0.102	0.046	0.009	Li
	−1.529	0.802	0.102	0.046	0.009	BPA0
3	−0.618	1.056	0.024	0.091	0.013	Li
	−0.369	0.858	0.357	0.126	0.017	BPA0

lem in the boson space, all the relevant fermion operators are first expressed in terms of bosons with the help of Dyson boson mapping [Eqs. (1a)—(1c)]. For carrying out the explicit calculations in the boson space, one needs to construct a suitable set of basis states. This is a nontrivial problem, the prime reason being that the ordinary boson basis (BB) states are overcomplete and do violate the Pauli principle; as a result these basis states contain spurious components. An obvious way to rectify these drawbacks is to start with an orthonormal set of fermion states involving $Q^\dagger$ operators, which with the help of mapping [Eqs. (1a)—(1c)] yields the corresponding basis states in terms of boson operators. The states so obtained are referred to as the physical boson basis (PBB) states. Due to the nonunitary nature of the Dyson mapping, this procedure yields biorthonormal set of PBB states. The PBB bra states are trivially obtained just by replacing Q_μ fermion operators by the corresponding coupled collective boson operators b_μ. On the other hand, an explicit expression for a general PBB ket state is quite involved. However, for the case of a single $b^\dagger_\mu$ for each spin and parity (J^π_μ), the lowest PBB ket state corresponding to each J^π_μ can be expressed in a closed form.[6]

The calculations in the boson space with the full PBB states is equivalent to carrying out the exact shell-model calculations in the fermion space. Therefore, various schemes for truncating the PBB states are being envisaged, the idea being to consider only a limited number of terms appearing in the expression of PBB states. This would therefore violate the Pauli principle. This is still an open problem and awaits a satisfactory solution. As an example, we consider the lowest $J=0$ PBB state, the only case studied extensively. The explicit expression for this state is

$$(S^\dagger)^p|0\rangle \rightarrow \left[\frac{(s^\dagger)^p}{\sqrt{p!}} + \sum_\nu \Gamma^{(0\nu)0}(b^\dagger_\nu)_{J_{\nu=0}}(s^\dagger)^{p-1} + \sum_{\mu\nu}\Gamma^{(\mu\nu)0}(b^\dagger_\mu b^\dagger_\nu)_{J=0}(s^\dagger)^{p-2} + \sum_{\mu\nu\rho}\Gamma^{(\mu\nu)\rho}[(b^\dagger_\mu b^\dagger_\nu)_{J_\rho} b^\dagger_\rho]_{J=0}(s^\dagger)^{p-3}\right]|0\rangle + \cdots . \tag{7}$$

Here we have used $s^\dagger$ to represent the lowest $J=0$ boson analogous to the $S^\dagger$ operator employed in the fermion case. The coefficients $\Gamma^{(0\nu)0}$, $\Gamma^{(\mu\nu)0}$, $\Gamma^{(\mu\nu)\rho}$, etc., are functions of the amplitudes $\tilde{\chi}_\mu$ and the coupling coefficients. Their explicit expressions are lengthy and therefore will not be presented here. In the lowest order one considers just the first term of the PBB state [Eq. (7)]. This corresponds to the complete neglect of the Pauli principle and

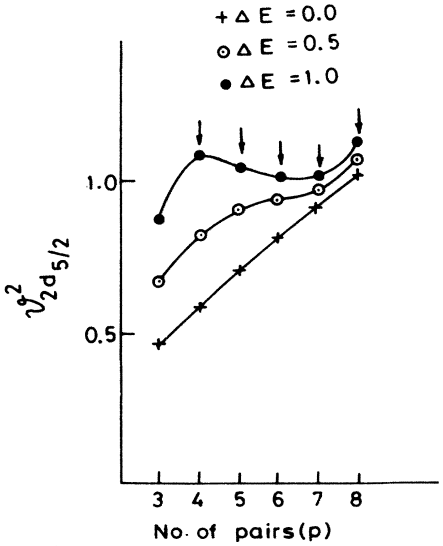

FIG. 1. The calculated occupation probabilities $\vartheta^2_{2d_{5/2}}$ with Li's prescription using the shift $\Delta E = 0.0$, 0.5, and 1.0 MeV are plotted versus the number of neutron pairs p for even Sn isotopes. The arrows indicate the values exceeding unity.

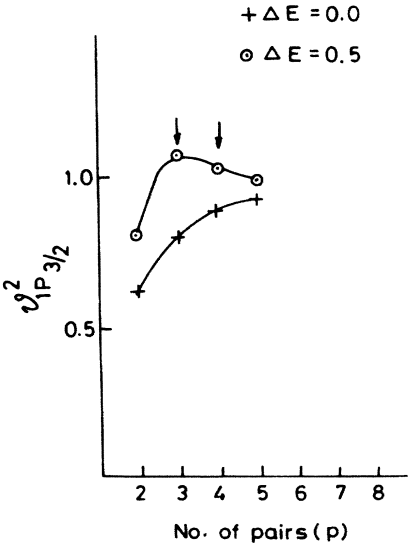

FIG. 2. The calculated occupation probabilities $\vartheta^2_{1p_{3/2}}$ with Li's prescription using the shift $\Delta E = 0.0$ and 0.5 MeV are plotted versus the number of neutrons pairs p for even Ni isotopes. The arrows indicate the values exceeding unity.

is referred to as the one-boson approximation[3] In the next order one retains all the terms involving a maximum of two $b^\dagger$ operators or up to the terms containing a minimum of $(p-2)$ $s^\dagger$ operators. This truncation scheme is exact for two pairs ($p=2$) of particles. Recently, Li[7] proposed an iterative procedure and in practice advocates retaining only the terms with a maximum of two $b^\dagger_\mu$ operators. The author introduces the collective operators in the boson space—and determines the corresponding coefficients $\tilde{\chi}_\mu(ab)$ through the minimization of the expectation value of the transformed Hamiltonian between the truncated lowest $J=0$ PBB state. As stated before, all the relevant expression for $p=2$ pairs are exact; however, the differences do creep in for higher p values. It is to be noted that the inclusion of all the terms in Eq. (7) corresponds to the exact shell model/BPA0 state depending upon the use of the corresponding $\tilde{\chi}$ coefficients. The BPA0 has been shown to be a good approximation to the shell model ground state which is also revealed through the results presented later.

In order to ascertain quantitatively the extent of violation of the Pauli principle in the various truncation schemes for the PBB states, explicit numerical calculations for even Ni and Sn isotopes have been performed. This will also demonstrate the limitations, if any, of these approximate schemes. For Sn isotopes the neutrons outside the $Z=50$, $N=50$ inert core are restricted to occupy five ($2d_{5/2}$, $1g_{7/2}$, $3s_{1/2}$, $2d_{3/2}$, and $1h_{11/2}$) valence levels having 0.0, 0.22, 1.90, 2.20, and 2.80 MeV unperturbed sp energies, respectively. The pairing Hamiltonian with strength $G=0.187$ MeV has been used as the model interaction. In the case of Ni isotopes the neutrons outside the ^{56}Ni inert core ($Z=28$, $N=28$) are restricted to occupy four ($2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$, and $1g_{9/2}$) valence levels having 0.0, 0.78, 1.56, and 4.52 MeV s.p. energies, respectively, and $G=0.331$ MeV has been used. This input information is identical to that used by Li in his investigations. The results of the calculations obtained with Li's approximation scheme labeled "Li" are presented in Tables I and III for selected Sn and Ni isotopes. The tables also include the corresponding results obtained with the BCS, the BPA0, and the exact shell model and are labeled BCS, BPA0, and Exact, respectively. The results obtained with number operator approximations (NOA's) are also included in Table I. The method seems to work up to $p=7$ (the shell closure of $2d_{5/2}$ and $1g_{7/2}$, which are nearly degenerate; energy difference 0.22 MeV). It is found that for $p=8$ (16 particles) in the case of Sn, the occupation probability of the $2d_{5/2}$ level with Li's procedure exceeds unity. The maximum error in energy is found to be exactly at this value of p and is equal to ~ 0.5 MeV (see Table I for $p=8$). The differences in the calculated occupation probabilities are also substantial for this value of p ($p=8$). In general, Li overestimates the occupation probabilities (ϑ^2) for the lowest level(s).

The extent of overestimation of ϑ^2, i.e., the violation of the Pauli principle for the set "Li," sensitively depends upon the single particle energies for a given Hamiltonian. To dramatize this, we introduced a shift ΔE in the s.p. energies relative to the lowest s.p. valence state. The results are displayed for three sets of $\Delta E=0.0$, 0.5, and 1.0 MeV for Sn isotopes in Fig. 1 and for two sets of $\Delta E=0.0$ and 0.5 MeV for Ni isotopes in Fig. 2. The similar results with $\Delta E=1.0$ for Sn isotopes are presented in Table II, while those with $\Delta E=0.5$ MeV for Ni isotopes are presented in Table IV. It is observed that even at $p=4$ the $\vartheta^2_{2d_{5/2}}$ in the case of Sn and at $p=3$ the $\vartheta^2_{1p_{3/2}}$ in the case of Ni exceed unity. The maximum error in the energy is found to occur exactly at these values of p for which the occupation probability exceeds unity. The difference in the calculationed ϑ^2 are also substantial for these values of p. Thus the iterative scheme proposed by Li is found to work for the case of (near) degenerate s.p. levels. The extent of the Pauli violations depends sensitively upon the explicit values of the s.p. energies for a given interaction. Therefore, this iterative scheme may or may not work in the realistic cases depending upon the explicit values of the s.p. energies. It further implies that the model studies with a single level or degenerate levels may not reveal important effects like the Pauli principle, etc. Therefore, the model case studies may not necessarily be sufficient to demonstrate the general applicability of a particular formalism.

In conclusion, we note that the available truncation schemes for the PBB states may not be adequate in realistic cases. Therefore, the need to evolve yet a reliable and useful truncation scheme for working in the boson space is stressed.

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