Optimal auxiliary Hamiltonians for truncated boson-space calculations by means of a maximal-decoupling variational principle

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A new method based on a maximal-decoupling variational principle is proposed to treat the Pauli-principle constraints for calculations of nuclear collective motion in a truncated boson space. The viability of the method is demonstrated through an application to the multipole form of boson Hamiltonians for the single- j and nondegenerate multi- j pairing interactions. While these boson Hamiltonians are Hermitian and contain only one- and two-boson terms, they are also the worst case for truncated boson-space calculations because they are not amenable to any boson truncations at all. By using auxiliary Hamiltonians optimally determined by the maximal-decoupling variational principle, however, truncations in the boson space become feasible and even yield reasonably accurate results. The method proposed here may thus be useful for doing realistic calculations of nuclear collective motion as well as for obtaining a viable interacting-boson-model type of boson Hamiltonian from the shell model.

I. INTRODUCTION

Boson mapping methods [1–18] have played an important role in the study of nuclear collective motion as well as in the investigation of a possible microscopic foundation of the interacting-boson model (IBM) [19]. Through the use of boson mapping, one hopes that the shell-model fermion many-body problem can be made simpler and more transparent so that the complicated fermion structures related to nuclear collective motion can be described by means of relatively simple boson states or severely truncated boson space. This hope, however, has often been ruined by the fact that the simple boson states and/or truncated boson space one wishes to use often contain spurious components which do not have any counterparts in the original fermion space. In other words, they violate the Pauli-principle constraints of the original fermion problem. On the other hand, if one uses the so-called *physical states* and/or *physical subspace*, which do not contain any spurious components and thus strictly respect the Pauli-principle constraints, the boson calculations become at least as involved as the fermion calculations one intends to simplify. Consequently, one does not gain anything in using the boson mapping methods at all.

To make the boson description of nuclear collective motion really useful, therefore, it is essential to have a viable method to deal with the spurious-state problem [17] so that relatively simple boson states and/or severely truncated boson space can be used to give reasonably accurate results. The purpose of this paper is to propose and illustrate such a method which will allow one to effectively treat the Pauli-principle constraints for truncated boson-space calculations of nuclear collective motion.

This paper is organized as follows. In Sec. II, we first give a brief description of the maximal-decoupling principle, on which the present method of treating the Pauli-principle constraints for boson calculations is based. In

Sec. III, various boson mappings for the full nuclear shell-model algebra are briefly reviewed. There, in particular, we examine the multipole-form mapping procedure which yields Hermitian and finite boson Hamiltonians. The problems with this boson mapping procedure are solved with the present method in Sec. IV, where the viability of the method is demonstrated through applications to the monopole pairing models. In Sec. V we give a brief summary and discussion on the present work.

II. PRINCIPLE OF MAXIMAL DECOUPLING

In studying nuclear collective motion, it is essential that one have a viable method for determining the relevant collective degrees of freedom, such as the collective monopole and quadrupole degrees of freedom related to the SD -truncation (by retaining only the collective $J=0$ and 2 pairs) of the shell-model space. For example, if one insists that the collective states should have the lowest average energy, one can readily use the trace variational principle (TVP) of Klein and Vallières [20] to determine the relevant collective subspace. Alternatively, one can also use the recently developed maximal-decoupling principle (MDP) [21] to find the collective subspace. Like the TVP of Klein and Vallières, the MDP is also a trace variational principle. However, instead of minimizing the average energy of the states in the collective subspace, the MDP minimizes the coupling between the collective subspace and the rest of the space (hereafter termed the noncollective subspace). This feature of the MDP not only allows one to optimally pin down the collective degrees of freedom of the nuclear system under study, but also allows one to effectively treat the Pauli-principle constraints for the collective boson subspace chosen for calculations. To show that, we first give below a brief review on the essence of the MDP method.

Let $S = \{|i\rangle, i=1,2,\dots,\nu\}$ represent the collective subspace, such as the SD subspace, one chooses to work with for the nuclear system under study. Assuming $|i\rangle$

are orthonormal basis states, it is easy to see that the action of the Hamiltonian H on the basis states $|i\rangle$ can be written as

$$H|i\rangle = PH|i\rangle + QH|i\rangle \quad (1a)$$

with

$$P = \sum_{i=1}^v |i\rangle\langle i|, \quad Q = 1 - P. \quad (1b)$$

Here P and Q are, respectively, the projection operators for the collective and noncollective subspaces. If $QH|i\rangle$ vanish for all the basis states $|i\rangle$, one has a completely decoupled collective subspace which is an invariant space under the action of the Hamiltonian. In reality, however, this seldom happens. Thus, in order to have a reasonably decoupled collective subspace to work with, the norms of all $QH|i\rangle$ clearly should be made as small as possible. Since we usually have more than just one basis state, we democratically form the uniform sum

$$\sum_{i=1}^v \langle i|H^\dagger QH|i\rangle \equiv \text{Tr}(H^\dagger QH). \quad (2)$$

In (2), the trace is understood to be taken within the collective subspace S . This trace is clearly a non-negative quantity and represents an overall coupling between the collective and noncollective subspaces. By minimizing this coupling, one ends up with the following maximal-decoupling principle:

$$\delta \text{Tr}(H^\dagger QH) = 0, \quad (3)$$

where the variation is supposed to be performed with respect to parameters dictating the collective subspace, such as those representing the collective monopole and quadrupole degrees of freedom. In the limit that the collective subspace consists of only one state, say, $|\phi\rangle$, (3) simply reduces to the usual minimum variance principle [22,23]

$$\delta \left\{ \frac{\langle \phi|H^\dagger H|\phi\rangle}{\langle \phi|\phi\rangle} - \left| \frac{\langle \phi|H|\phi\rangle}{\langle \phi|\phi\rangle} \right|^2 \right\} = 0, \quad (4)$$

in which the variation is done with respect to the trial state $|\phi\rangle$. This is the single-state version of the MDP. Note that the quantity between the curly brackets in (4) is always non-negative and can be considered as a measure of deviation of the trial state from being an exact eigenstate of the Hamiltonian.

Being a trace variational principle, the maximal-decoupling principle given in (3) has the same advantage as the TVP of Klein and Vallières [20]. Namely, the relevant trace variations can be done before the actual diagonalization of the Hamiltonian within the chosen subspace is carried out because traces are invariant under the necessary transformations for diagonalizations. The TVP of Klein and Vallières, based on the idea that nuclear collective spectra usually lie lowest in energy, simply minimizes the average energy of the states in the chosen subspace. In contrast, by directly minimizing the coupling between the collective and noncollective subspaces, the MDP proposed here has several advantages: (1) Since the

trace defined in (2) is always non-negative and vanishes for complete decouplings, one always has a minimum variational principle. (2) In the cases where one has to work with non-Hermitian Hamiltonians, such as those resulting from using the Dyson boson mapping method [4,5,8,11–16], the present MDP can be readily applied, whereas the TVP of Klein and Vallières becomes nonapplicable unless complicated biorthogonal bases are used. (3) While the TVP of Klein and Vallières applies only to collective subspaces based on ground states, the present MDP can be applied to any subspaces chosen. In fact, (3) applies even to those subspaces consisting entirely of highly excited states as one may encounter in the study of various giant resonances. Moreover, the MDP proposed here has another unique applicability [24] which we shall illustrate and exploit below.

For example, in the Bardeen-Cooper-Schrieffer (BCS) type of calculations with quasiparticles, the number conservation is violated when quasiparticle states such as the BCS state $|\text{BCS}\rangle$ are used. The number conservation, of course, can be restored by invoking various number-projection techniques. However, if one sticks with the number-nonconserving quasiparticle states, one way to take care of the number conservation approximately is to work with the following Lipkin-Nogami type of auxiliary Hamiltonian [25]:

$$H' = H + \lambda_1 \hat{Z} + \lambda_2 \hat{Z}^2, \quad \hat{Z} \equiv N - \hat{N}, \quad (5)$$

instead of the original Hamiltonian H . Here, $\hat{N}$ is the number operator, N is the actual number of particles in the problem, and λ_1 and λ_2 are parameters to be determined. Note that, if one uses states with fixed particle number N , there is no difference between H and H' since $\hat{Z}$ gives null results when acting on such states. However, because one is working with quasiparticle states, depending on the actual values of the λ parameters, the auxiliary Hamiltonian H' can be very different from H . Thus, a crucial step in this type of quasiparticle calculations is to choose an appropriate H' .

For a given quasiparticle state, say, $|\phi\rangle = |\text{BCS}\rangle$, whether one can obtain sensible results depends very much on the actual values of the λ parameters in the auxiliary Hamiltonian H' . It seems reasonable to require that the λ parameters be chosen in such a way that $|\phi\rangle$ is as close as possible to an eigenstate of the auxiliary Hamiltonian H' . In accordance with the MDP given in (4), one thus ends up with the following novel variational principle:

$$\frac{\delta}{\delta \lambda_i} \left\{ \frac{\langle \phi|H'^\dagger H'|\phi\rangle}{\langle \phi|\phi\rangle} - \left| \frac{\langle \phi|H'|\phi\rangle}{\langle \phi|\phi\rangle} \right|^2 \right\} = 0, \quad i=1,2. \quad (6)$$

Equation (6) is exactly the same as the variational equation (4) except that one is now using an auxiliary Hamiltonian and that the variations are performed with respect to the parameters in the auxiliary Hamiltonian, instead of with respect to the parameters in the wave function. It is easy to see that the above novel variational principle yields

$$\langle \phi | \hat{Z} H' | \phi \rangle - \langle \phi | \hat{Z} | \phi \rangle \langle \phi | H' | \phi \rangle = 0, \quad (7a)$$

$$\langle \phi | \hat{Z}^2 H' | \phi \rangle - \langle \phi | \hat{Z}^2 | \phi \rangle \langle \phi | H' | \phi \rangle = 0. \quad (7b)$$

The relations in (7) imply another set of relations exactly in the same form as (7) but with the operator $\hat{Z}$ being replaced by the number operator $\hat{N}$. These latter relations are exactly what have been used previously [25] to determine the parameters λ_1 and λ_2 . Here, through the MDP, these relations clearly imply that we have an optimal auxiliary Hamiltonian for the Lipkin-Nogami type of BCS calculations. For standard BCS calculations, one sets $\lambda_2 = 0$. The present MDP, as given in (6) with $i = 1$, yields only the relation (7a) for the determination of the chemical potential λ_1 . In this case it can be easily proved that (7a) is consistent with the usual way of determining the chemical potential by the number condition $\langle \text{BCS} | \hat{N} | \text{BCS} \rangle = N$.

For multistate quasiparticle calculations, one can use the MDP as given in (3) with the trace variations being performed with respect to the λ parameters in the auxiliary Hamiltonian H' . Namely, one is trying to obtain an optimal auxiliary Hamiltonian so that there is a maximal decoupling for the given quasiparticle subspace.

We have seen from above that the variations for the MDP given in (3) or (4) can be performed not only with respect to the parameters in the wave functions but also with respect to the parameters in the auxiliary Hamiltonian. In the former case one endeavors to get a maximally decoupled subspace for a given Hamiltonian while in the latter case one endeavors to find an optimal auxiliary Hamiltonian for a given subspace or state. The reason why one should use an auxiliary Hamiltonian is because some symmetry property of the system, such as the number conservation, is violated by the states used in the calculations. In the following section, we will employ this MDP to determine an optimal auxiliary Hamiltonian for calculations with a severely truncated boson space so that there is no need to use the physical projection operator [4,14] directly to take care of the Pauli-principle constraints. Before we turn to this application, we shall first give a brief review and some new insight of the various boson mappings for the full shell-model algebra.

III. BOSON MAPPINGS FOR THE FULL SHELL-MODEL ALGEBRA

The idea of using boson mappings or expansions for the many-fermion problem was first introduced into nuclear physics by Belyaev and Zelevinsky [1]. It was then further developed by many others [2–6] through the years. For the *full* shell-model algebra there are basically two different boson mappings given for the bilinear forms of the shell-model single-particle creation (annihilation) operators $a_\alpha^\dagger$ (a_α), namely, the generalized Dyson mapping and the generalized Holstein-Primakoff mapping. Following Ref. [4], the generalized Dyson mapping is given by

$$a_\alpha^\dagger a_\beta^\dagger \rightarrow P_{\alpha\beta}^\dagger \equiv b_{\alpha\beta}^\dagger - \sum_{\gamma\delta} b_{\alpha\gamma}^\dagger b_{\beta\delta}^\dagger b_{\gamma\delta}, \quad (8a)$$

$$a_\beta a_\alpha \rightarrow b_{\alpha\beta}, \quad (8b)$$

$$a_\alpha^\dagger a_\beta \rightarrow \sum_\gamma b_{\alpha\gamma}^\dagger b_{\beta\gamma}, \quad (8c)$$

while the generalized Holstein-Primakoff mapping [1,2] is given by

$$a_\alpha^\dagger a_\beta^\dagger \rightarrow (b^\dagger \sqrt{1 - \hat{\rho}})_{\alpha\beta}, \quad (9a)$$

$$a_\beta a_\alpha \rightarrow (\sqrt{1 - \hat{\rho}} b)_{\alpha\beta}, \quad (9b)$$

$$a_\alpha^\dagger a_\beta \rightarrow \sum_\gamma b_{\alpha\gamma}^\dagger b_{\beta\gamma}, \quad (9c)$$

where $b^\dagger$, b , and $\hat{\rho}$ are matrices with $b_{\alpha\beta}^\dagger$, $b_{\alpha\beta}$, and $\hat{\rho}_{\alpha\beta} = \sum_\gamma b_{\beta\gamma}^\dagger b_{\alpha\gamma}$, respectively, as their elements. The antisymmetric bosons operators $b_{\alpha\beta}^\dagger = -b_{\beta\alpha}^\dagger$ in (8) and (9) satisfy the commutation relations

$$[b_{\alpha\beta}, b_{\alpha'\beta'}] = [b_{\alpha\beta}^\dagger, b_{\alpha'\beta'}^\dagger] = 0, \quad (10a)$$

$$[b_{\alpha\beta}, b_{\alpha'\beta'}^\dagger] = \delta_{\alpha\alpha'} \delta_{\beta\beta'} - \delta_{\alpha\beta'} \delta_{\beta\alpha'}. \quad (10b)$$

Furthermore, in both the Dyson and Holstein-Primakoff mappings, the fermion vacuum state $|0\rangle$ is mapped to the boson vacuum state $|0\rangle$, which is annihilated by the boson operators $b_{\alpha\beta}$.

Consider now the shell-model Hamiltonian

$$H = \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma, \quad (11)$$

where ϵ_α is the energy for the single-particle level $\alpha \equiv (n_\alpha, l_\alpha, j_\alpha, m_\alpha)$ and $V_{\alpha\beta\gamma\delta}$ are the two-body interaction matrix elements. One can utilize the boson mapping given either in (8) or in (9) to obtain the boson image of this shell-model Hamiltonian. In so doing, the boson images of the two-body interactions $a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$ are usually obtained by forming products of either (8a) and (8b) or (9a) and (9b), with appropriate single-particle indices. Namely,

$$(a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma)_B \rightarrow (a_\alpha^\dagger a_\beta^\dagger)_B (a_\delta a_\gamma)_B,$$

with the subscript B signifying a boson image in (8) or (9). These are the pairing-form or particle-particle boson images of the two-body interactions. For the shell-model Hamiltonian one can easily see that its pairing-form Dyson boson image is non-Hermitian but finite without infinite expansions while its pairing-form Holstein-Primakoff boson image is Hermitian but involves infinite expansions because of the square-root factors. Both the Dyson and the Holstein-Primakoff boson mappings done in the pairing form have been used extensively during the last 15 years or so for doing nuclear collective-motion calculations as well as for investigating the microscopic foundation of the IBM [19]. In recent years the nuclear community has seen a growing preference in using the Dyson mapping [8,11–16], largely owing to the finiteness of the mapping as well as our better ability to handle the resulting non-Hermitian quantum systems.

Kuchta [26], however, has recently emphasized the use of the Hermitian mapping of Holstein and Primakoff. He circumvented the problem of infinite expansions by first recoupling the two-body shell-model interactions

$a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}$ with

$$a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} = a_{\alpha}^{\dagger} a_{\gamma} a_{\beta}^{\dagger} a_{\delta} - \delta_{\beta\gamma} a_{\alpha}^{\dagger} a_{\delta} \quad (12)$$

and then exclusively using the boson mapping given in (9c) for the multipole operators $a_{\alpha}^{\dagger} a_{\beta}$ to the right-hand side of (12). The resulting boson images obtained this way are called the multipole-form or particle-hole boson images of the two-body interactions. In fact, once one uses the boson mapping to the two-body interactions in this fashion, there is actually no difference between the Dyson and Holstein-Primakoff mappings since (8c) and (9c) are exactly the same. The resultant boson Hamiltonian, which is Hermitian and involves only one- and two-body interactions, can be written as

$$H_B = \sum_{\alpha\beta} \epsilon_{\alpha} b_{\alpha\beta}^{\dagger} b_{\alpha\beta} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} b_{\alpha\beta}^{\dagger} b_{\gamma\delta}^{\dagger} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta\lambda\rho} V_{\alpha\beta\gamma\delta} b_{\alpha\lambda}^{\dagger} b_{\beta\rho}^{\dagger} b_{\gamma\lambda} b_{\delta\rho}, \quad (13)$$

where the notation that $\alpha \equiv (n_a, l_a, j_a, m_a)$ and $\beta \equiv (n_b, l_b, j_b, m_b)$, etc., has been used. This Hermitian boson Hamiltonian has been used extensively by Kuchta. In fact, people on and off have previously [27] come up

with this deceptively nice boson Hamiltonian for the original shell-model problem but have all given it up because this boson Hamiltonian is not amenable to any truncation at all. To see that, we take the following monopole pairing interaction as an example:

$$H = \sum_a \epsilon_a \hat{N}_a - G \sum_{ab} \sqrt{\Omega_a \Omega_b} A_{00}^{\dagger}(aa) A_{00}(bb), \quad (14)$$

where ϵ_a are shell-model single-particle energies, G the pairing strength, $\Omega_a = j_a + \frac{1}{2}$, and $\hat{N}_a = \sum_{m_a} a_{a\alpha}^{\dagger} a_{a\alpha}$ are, respectively, the pair degeneracy and number operator of the level $a \equiv (n_a, l_a, j_a)$. Furthermore, the spherical pair creation and annihilation operators are defined by

$$A_{JM}^{\dagger}(ab) = \frac{1}{\sqrt{2}} \sum_{m_a, m_b} (j_a m_a j_b m_b | JM) a_{a\alpha}^{\dagger} b_{\beta}^{\dagger} = [A_{JM}(ab)]^{\dagger}, \quad (15)$$

in which $(\cdots)$ is a Clebsch-Gordon coefficient for angular-momentum coupling. Using the recoupling scheme of (12) and the boson mapping (8c) or (9c) for the multipole operators, it is straightforward to obtain, for (14), the following boson Hamiltonian:

$$H_B = 2 \sum_{ab, JM} \epsilon_a B_{JM}^{\dagger}(ab) B_{JM}(ab) - G \sum_{ab} \sqrt{\Omega_a \Omega_b} B_{00}^{\dagger}(aa) B_{00}(bb) - G \sum_{abcd} \hat{J}_1 \hat{J}_2 \hat{J}_3 \hat{J}_4 \begin{Bmatrix} J_1 & J_2 & K \\ j_d & j_c & j_a \end{Bmatrix} \begin{Bmatrix} J_3 & J_4 & K \\ j_d & j_c & j_b \end{Bmatrix} [[B_{J_1}^{\dagger}(ca) B_{J_2}^{\dagger}(ad)]_K [\tilde{B}_{J_3}(cb) \tilde{B}_{J_4}(bd)]_K]_{00}, \quad (16)$$

where $\{\cdots\}$ is a 6- j symbol, $\hat{J}_1 = \sqrt{2J_1 + 1}$, etc., and $[\cdots]_{JM}$ denotes a standard angular momentum coupling. Also, $B_{JM}^{\dagger}(ab)$ and

$$\tilde{B}_{JM}(ab) \equiv (-1)^{J-M} B_{J, -M}(ab)$$

are spherical boson creation and annihilation operators with good angular momenta (JM) defined by

$$B_{JM}^{\dagger}(ab) = \frac{1}{\sqrt{2}} \sum_{m_a, m_b} (j_a m_a j_b m_b | JM) b_{a\alpha}^{\dagger} b_{\beta}^{\dagger} = [B_{JM}(ab)]^{\dagger}. \quad (17)$$

It is clear that the boson Hamiltonian in (16) not only is Hermitian but also contains only one- and two-boson interactions. This boson Hamiltonian looks deceptively nice because it contains bosons with all possible angular momenta. In practical calculations one is inevitably forced to make truncations by keeping only a few collective bosons with different angular momenta. In fact, the above multipole-form boson Hamiltonian usually yields very poor results under such truncations. To be specific, we take the single- j limit of (16) for $2n$ particles and keep only the $J=0$ boson. This truncation yields, for the “ap-

proximate” ground state $|s^n\rangle \equiv (B_{00}^{\dagger})^n |0\rangle / \sqrt{n!}$, the energy

$$\langle s^n | H_B | s^n \rangle = 2n\epsilon - nG \left[\Omega + \frac{n-1}{\Omega} \right], \quad (18)$$

which is not a good approximation to all the exact ground-state energy $E_0 = 2n\epsilon - nG(\Omega - n + 1)$. Note that the second term in the parentheses on the right-hand side of (18) not only has a wrong sign but also is of wrong order in the pair degeneracy Ω . Furthermore, the fact that $\langle s^n | H_B | s^n \rangle$ is smaller than E_0 implies there exist spurious states lying even lower in energy than the physical ground state $\hat{\mathcal{P}}|s^n\rangle$. Here $\hat{\mathcal{P}}$ is the so-called physical projection operator [4,14] whose effect is essentially to replace the various $b_{a\beta}^{\dagger}$ operators in the boson states by the corresponding $P_{a\beta}^{\dagger}$ operators defined in (8a). Therefore, the deceptively nice-looking boson Hamiltonian given in (16) not only is not amenable to truncations but also has a very serious spurious-state problem. In short, as it stands all by itself, this Hermitian boson Hamiltonian is not useful at all. In what follows, by means of the MDP, we shall show that one can easily find an appropriate auxiliary Hamiltonian to take the place of the original Hamiltonian H_B so that truncated boson-space calculations will be feasible.

IV. TRUNCATED BOSON-SPACE CALCULATIONS WITH OPTIMAL AUXILIARY HAMILTONIANS

A. Optimal auxiliary boson Hamiltonian for the monopole pairing model

Here we take the multipole-form boson Hamiltonian H_B for the pairing interaction given in (16) as an example. Instead of using H_B itself, we use the following auxiliary Hamiltonian:

$$H'_B = H_B + \sum_a \lambda_a \hat{Z}_a \quad (19)$$

$$\begin{aligned} \hat{Z}_a = & 4 \sum_{\substack{bcd \\ J_1 M_1 J_2 M_2}} B_{J_1 M_1}^\dagger(ac) B_{J_2 M_2}^\dagger(bd) B_{J_2 M_2}(bd) B_{J_1 M_1}(ac) \\ & + 4 \sum_{\substack{bcd \\ K J_1 J_2 J_3 J_4}} \hat{J}_1 \hat{J}_2 \hat{J}_3 \hat{J}_4 \begin{Bmatrix} j_a & j_c & J_1 \\ j_b & j_d & j_2 \\ J_4 & J_3 & K \end{Bmatrix} \left[[B_{J_1}^\dagger(ac) B_{J_2}^\dagger(bd)]_K [\tilde{B}_{J_3}(cd) \tilde{B}_{J_4}(ab)]_K \right]_{00}, \end{aligned} \quad (20b)$$

where $\{ \cdots \}$ is a 9- j symbol and for other quantities the same notations as those in (16) have been used.

The two terms on the right-hand side of (20a) are the boson images of the fermion operator $\hat{N}_a(\hat{N}-1) = \sum_{\beta, m_a} a_{\alpha}^\dagger a_{\beta}^\dagger a_{\beta} a_{\alpha}$ obtained, respectively, by forming appropriate products of (8c) or (9c) alone and by forming appropriate products of (8a) and (8b). Being the difference between these two boson images, which are equivalent within the physical boson subspace consisting of physical boson states such as $P_{\alpha_1, \beta_1}^\dagger P_{\alpha_2, \beta_2}^\dagger \cdots P_{\alpha_n, \beta_n}^\dagger |0\rangle$, $\hat{Z}_a$ yields null results when acting on these physical boson states. This special property of the two above-mentioned boson images have been exploited previously [14] by us to do approximate projections onto the physical subspace. Moreover, if one sums over all the levels $a \equiv (n_a, l_a, j_a)$ in (20), one will get exactly the so-called Park operator $\hat{Z} = \sum_a \hat{Z}_a$ [28]. Here, the $\sum_a \lambda_a \hat{Z}_a$ operator used in (19) for the auxiliary boson Hamiltonian H'_B can be considered as an extension of the Park operator. In principle, one could also include terms proportional to $\hat{Z}_a \hat{Z}_b$, etc., as well as terms of higher orders in the auxiliary Hamiltonian. However, in order to have an auxiliary boson Hamiltonian which is both Hermitian and contains only one- and two-boson terms, in what follows we will stick with the one given in (19). We emphasize that H_B and its auxiliary Hamiltonian H'_B have the same eigenvectors and eigenvalues within the physical boson subspace even though they give very different results outside this boson subspace. Adding a term like $\sum_a \lambda_a \hat{Z}_a$ to the boson Hamiltonian H_B , we are not changing any physics of the problem. In fact, we are taking advantage of this freedom to find an optimal auxiliary Hamiltonian to use so that calculations with truncated boson space will be feasible and the Pauli-principle constraints will also be taken care of, at least approximately. Whether this goal can be achieved depends on

with

$$\hat{Z}_a = \hat{N}_B(a)(\hat{N}_B - 1) - \sum_{m_a \beta} P_{\alpha \beta}^\dagger b_{\alpha \beta}. \quad (20a)$$

In (20a), $\hat{N}_B(a) = \sum_{m_a \beta} b_{\alpha \beta}^\dagger b_{\alpha \beta}$, $\hat{N}_B = \sum_a \hat{N}_B(a)$, and $P_{\alpha \beta}^\dagger b_{\alpha \beta}$, as have already been given in (8a) and (8b), are, respectively, the Dyson boson images of the fermion pair operators $a_{\alpha}^\dagger a_{\beta}^\dagger$, $a_{\beta} a_{\alpha}$. In terms of the spherical boson operators defined in (17), $\hat{Z}_a$ can be written as

how the λ_a parameters in the auxiliary Hamiltonian H'_B are chosen. Here, by means of the MDP, the λ_a parameters are to be determined in such a way that one has a maximal decoupling for the given truncated boson space or state. Namely,

$$\frac{\delta}{\delta \lambda_a} \text{Tr}(H_B^\dagger Q H'_B) = 0, \quad (21a)$$

or

$$\frac{\delta}{\delta \lambda_a} \left\{ \frac{(\phi | H_B^\dagger H'_B | \phi)}{(\phi | \phi)} - \left| \frac{(\phi | H'_B | \phi)}{(\phi | \phi)} \right|^2 \right\} = 0, \quad (21b)$$

depending on whether one is using a boson subspace or just a single-boson state. Equations (21a) and (21b) are the same as the two variational equations given in (3) and (4) except that the variations are now performed with respect to the parameters in the auxiliary Hamiltonian instead of those in the wave functions.

Note that auxiliary Hamiltonians similar to that in (19) have been used before [4, 26, 29]. In these previous works, the auxiliary Hamiltonian $H'(\mu) = H_D + \mu \hat{Z}$ was obtained by adding a term proportional to the Park operator $\hat{Z}$ to the original boson Hamiltonian H_D . In Refs. [4] and [29], the boson Hamiltonian was derived by using the Dyson boson mapping in the pairing form while in Ref. [26] it was derived by the same multipole-form mapping as has been used here in obtaining (19). The Park operator $\hat{Z}$ has the well-known property that $(\phi | \hat{Z} | \phi) \geq 0$ for any boson state $|\phi\rangle$, where the equality holds only when $|\phi\rangle$ is a physical boson state. Therefore, in Ref. [4], in order to minimize the spurious components in the state $|\phi\rangle$, the μ parameter was determined by the condition $(\partial/\partial \mu)(\phi | \hat{Z} | \phi) = 0$. This condition seems to have some problem with variational calculations and has never been used since. In Ref. [26], Kuchta used the condition

$\langle \phi | \hat{Z} | \phi \rangle = 0$ to determine the μ parameter in the auxiliary Hamiltonian. This condition, however, amounts to requiring that $|\phi\rangle$ be a physical boson state and thus is impossible to impose unless one uses a physical boson state [30]. In performing exact diagonalizations for a six-fermion problem in the boson space, a large enough value was used for the μ parameter in Ref. [29] to push the spurious states up in energy so that they stay outside the domain of the physical eigenstates of interest. When calculations are done in a truncated boson space, however, one cannot just use an arbitrary large enough value for the μ parameter. In fact, the quality of the results one will obtain in such calculations depends crucially on how the parameters in the auxiliary Hamiltonian are chosen. As will be seen shortly, the present MDP variational method as given in (21), which can also be termed as an optimal-auxiliary-Hamiltonian method, is indeed a viable

method for treating the spurious-state problem in truncated boson-space calculations. Moreover, by using $\sum_a \lambda_a \hat{Z}_a$ instead of the Park operator $\hat{Z}$, the auxiliary boson Hamiltonian H'_B given in (19) is more general than what has been used previously [4,26,29].

B. Single- j limit of the optimal auxiliary boson Hamiltonian

It is instructive to examine first the single- j limit of the auxiliary boson Hamiltonian H'_B given in (19) for the monopole pairing interaction defined in (14). If one uses the simple boson state $|s^n\rangle = (B_{00}^\dagger)^n |0\rangle / \sqrt{n!}$ for the ground-state calculation, it is straightforward to show that the MDP variational equation (21b) with $\lambda_a = \lambda$ implies that the optimal auxiliary boson Hamiltonian can be obtained with $\lambda = \frac{1}{4}G$. With this optimal value for λ , the auxiliary boson Hamiltonian becomes

$$\begin{aligned} H'_B &= H_B + \frac{1}{4}G\hat{Z} \\ &= 2n\epsilon - G(\hat{n} - \hat{n}_v)(\Omega - \hat{n} - \hat{n}_v + 1) + G\hat{n}_v(\hat{n}_v - 1) \\ &\quad + G \sum_{J's \neq 0}^K \hat{J}_1 \hat{J}_2 \hat{J}_3 \hat{J}_4 \left[\begin{Bmatrix} j & j & J_1 \\ j & j & j_2 \\ J_4 & J_3 & K \end{Bmatrix} - \begin{Bmatrix} J_1 & J_2 & K \\ j & j & j \end{Bmatrix} \begin{Bmatrix} J_3 & J_4 & K \\ j & j & j \end{Bmatrix} \right] [[B_{J_1}^\dagger B_{J_2}^\dagger]_K [\tilde{B}_{J_3} \tilde{B}_{J_4}]_K]_{00}, \end{aligned} \quad (22)$$

where

$$\begin{aligned} \hat{n} &= \hat{n}_s + \hat{n}_v, \\ \hat{n}_s &= B_{00}^\dagger B_{00}, \\ \hat{n}_v &= \sum_{J \neq 0, M} B_{JM}^\dagger B_{JM}. \end{aligned}$$

Use has been made of (16) and (20b) to obtain (22). The 9- j symbol and the product of the two 6- j symbols in the last term of (22) cancel exactly when any of the J_i ($i=1,2,3,4$) equals zero and thus in effect only the non- S (i.e., $J \neq 0$) boson operators are included in the summation. Consider first the states $|s^n\rangle$ and $B_{JM}^\dagger |s^{n-1}\rangle$, where $B_{JM}^\dagger$ ($\equiv B_{JM}^\dagger$ with $J \neq 0$) is a non- S boson creation operator. For these boson states, which contain at most one non- S boson (i.e., $n_v = 0$ or 1), the last two terms in (22) do not contribute. It is thus not difficult to see that they are exact eigenstates of the above auxiliary Hamiltonian with the correct eigenvalues

$$2n\epsilon - G(n - n_v)(\Omega - n - n_v + 1).$$

States with more than one non- S boson, such as $|n, n_v=2\rangle \sim B_{JM}^\dagger B_{J'M'}^\dagger |s^{n-2}\rangle$, are not eigenstates of H'_B . However, as long as the number of non- S bosons, i.e., n_v , is small compared to the number of S bosons n_s and to $\Omega - n$, the expectation value

$$\begin{aligned} \langle n, n_v | H'_B | n, n_v \rangle &\simeq 2n\epsilon - G(n - n_v)(\Omega - n - n_v + 1) \\ &\quad + Gn_v(n_v - 1) \end{aligned}$$

is still a reasonably good approximation to the exact en-

ergy eigenvalue. Note that here the contribution from the last term in (22), which has been ignored, is of order Gn_v^2/Ω .

We have seen in the last section that the multipole-form boson Hamiltonian for the single- j pairing interaction given in (16) is not amenable to truncations and thus is not useful at all for any practical calculation. Here, by using auxiliary boson Hamiltonians in the form of (19), the present maximal-decoupling variational principle enables one to choose an optimal one, as H'_B given in (22), so that calculations with severe boson truncations become feasible. In fact, in the present single- j limit, exact results have even been obtained with simple boson states such as $|s^n\rangle$ and $B_{JM}^\dagger |s^{n-1}\rangle$. This result is indeed encouraging.

C. Numerical application to the nondegenerate multi- j pairing model

To see whether we can still obtain reasonably accurate results in more general cases than the above single- j limit, we now apply the optimal-auxiliary-Hamiltonian method based on the MDP to the nondegenerate multi- j pairing interaction given in (14). This pairing interaction in the boson space is represented by the multipole-form boson Hamiltonian H_B in (16). In this case we still use an auxiliary boson Hamiltonian in the form of (19) but the λ_a parameters to be determined by the MDP variational equation (21b) are all taken as independent variational variables. For the ground-state calculation, the state $|\phi\rangle$ in (21b) is taken as the boson condensate

$$|s^n\rangle = \frac{1}{\sqrt{n!}} (s^\dagger)^n |0\rangle \quad (23a)$$

with

$$s^\dagger \equiv \sum_a c_a B_{00}^\dagger(aa), \quad \sum_a c_a^2 = 1. \quad (23b)$$

With this boson condensate, (21b) becomes

$$\frac{\delta}{\delta \lambda_a} \{ (s^n | H_B'^\dagger H_B' | s^n) - |(s^n | H_B' | s^n)|^2 \} = 0. \quad (24)$$

The c_a parameters defining the collective S boson in (23) above could have been determined by using the standard variational principle. Here, however, we use the MDP equation (4), which, in the present context, becomes

$$\frac{\delta}{\delta c_a} \{ (s^n | H_B'^\dagger H_B' | s^n) - |(s^n | H_B' | s^n)|^2 \} = 0, \quad (25)$$

subject to the constraint $\sum_a c_a^2 = 1$. Equations (24) and (25) mean that we are actually minimizing the non-negative quantity

$$(s^n | H_B'^\dagger H_B' | s^n) - |(s^n | H_B' | s^n)|^2$$

with respect to the parameters in the auxiliary Hamiltonian as well as those in the state. The end result is that we will have the best boson condensate state for the re-

sulting optimal auxiliary boson Hamiltonian.

The actual numerical applications of the MDP variational equations (24) and (25) are carried out for the tin isotopes. We take the single-particle energies $\epsilon_a = 0.0, 0.22, 1.90, 2.20$, and 2.80 MeV, respectively, for the valence j shells $a = 2d_{5/2}, 1g_{7/2}, 3s_{1/2}, 2d_{3/2}, 1h_{11/2}$. For the pairing strength, we use $G = 0.187$ MeV. The numerical results obtained for the nondegenerate multi- j pairing model using the auxiliary boson Hamiltonian H_B' in (19) are shown in Table I. There it can be seen that the energy eigenvalues for the ground states of the pairing interaction are quite accurately reproduced by the present method using $(s^n | H_B' | s^n)$, at least for all n up to near the middle of the major shell. For comparison we have also carried out the calculations using uniform λ parameters by setting $\lambda_a = \lambda$. This corresponds to using the Park operator $\hat{Z}$ multiplied by λ for the auxiliary Hamiltonian. As can be seen from the table, the ground-state energies are, in fact, not sensitive to whether one uses independent or uniform λ parameters in the MDP variational calculations.

To see whether we have obtained accurate wave functions, we also evaluated the occupation numbers for the various j shells. They are evaluated with the physical state projected from the boson condensate used in the calculation. Namely,

TABLE I. Ground-state energies and occupation numbers for even tin isotopes of N valence nucleons in the j shells $2d_{5/2}, 1g_{7/2}, 3s_{1/2}, 2d_{3/2}$, and $1h_{11/2}$ obtained by the present MDP method with independent and uniform λ_a parameters are compared with results of exact diagonalizations.

$n = N/2$	E_0	$v_{2d_{5/2}}^2$	$v_{1g_{7/2}}^2$	$v_{3s_{1/2}}^2$	$v_{2d_{3/2}}^2$	$v_{1h_{11/2}}^2$	Method
1	-1.534	0.1692	0.1022	0.0140	0.0113	0.0078	$\lambda_a = \lambda$
	-1.534	0.1692	0.1022	0.0140	0.0113	0.0078	Indep. λ_a
	-1.534	0.1692	0.1022	0.0140	0.0113	0.0078	Exact diag.
2	-2.619	0.3212	0.2113	0.0318	0.0258	0.0179	$\lambda_a = \lambda$
	-2.629	0.3260	0.2142	0.0284	0.0226	0.0152	Indep. λ_a
	-2.624	0.3252	0.2140	0.0287	0.0230	0.0156	Exact diag.
3	-3.254	0.4566	0.3248	0.0549	0.0447	0.0311	$\lambda_a = \lambda$
	-3.256	0.4693	0.3351	0.0447	0.0345	0.0230	Indep. λ_a
	-3.258	0.4676	0.3357	0.0442	0.0350	0.0234	Exact diag.
4	-3.445	0.5742	0.4406	0.0839	0.0691	0.0488	$\lambda_a = \lambda$
	-3.478	0.5961	0.4695	0.0611	0.0461	0.0301	Indep. λ_a
	-3.419	0.5971	0.4670	0.0607	0.0473	0.0309	Exact diag.
5	-3.185	0.6755	0.5522	0.1257	0.1022	0.0724	$\lambda_a = \lambda$
	-3.180	0.7090	0.6185	0.0768	0.0569	0.0347	Indep. λ_a
	-3.084	0.7153	0.6070	0.0784	0.0599	0.0379	Exact diag.
6	-2.476	0.7602	0.6551	0.1764	0.1466	0.1049	$\lambda_a = \lambda$
	-2.241	0.8236	0.7681	0.0946	0.0662	0.0383	Indep. λ_a
	-2.208	0.8245	0.7546	0.0978	0.0727	0.0441	Exact diag.
7	-1.318	0.8241	0.7425	0.2470	0.2060	0.1498	$\lambda_a = \lambda$
	-1.158	0.9189	0.8938	0.1413	0.0978	0.0552	Indep. λ_a
	-0.700	0.9277	0.9095	0.1200	0.0850	0.0481	Exact diag.

$$\begin{aligned}
v_a^2 &= \frac{1}{2\Omega_a} \frac{(\phi|\hat{N}_B(a)\hat{P}|\phi)}{(\phi|\hat{P}|\phi)} \\
&= \frac{1}{\Omega_a} \frac{(s^n|B_{00}^\dagger(aa)B_{00}(aa)\hat{P}|s^n)}{(s^n|\hat{P}|s^n)} \quad (26)
\end{aligned}$$

with $\hat{P}$ being the projection operator onto the physical boson subspace. Note that the effect of the physical projection operator $\hat{P}$ on a boson state is essentially to replace the $b_{\alpha\beta}^\dagger$ boson operators by the $P_{\alpha\beta}^\dagger$ operators defined in (8a) so that the resulting physical state will strictly obey the Pauli principle. Since physical boson states are usually very cumbersome to obtain in this fashion, the approximate projection method of Ref. [14] is useful when one is not too near the middle of the major shell. Here, in order to have an unambiguous assessment of the present MDP method, the occupation numbers given in the first two rows for each isotope in Table I are evaluated by using (26) with exact physical projections. One can easily see from the table that the calculation with independent λ_a yields much better occupation numbers compared to that with uniform λ_a . Thus, to obtain better wave functions, it is important to take all the λ_a as independent variational parameters so that one really has an optimal auxiliary Hamiltonian for the truncated boson space in the form of (19). Note also that, even when one gets bad ground-state energies with the simple boson state $|s^n\rangle$ near or over the middle of the major shell, the physical projected state $\hat{P}|s^n\rangle$ still yields reasonably accurate occupation numbers.

As to the actual values of the λ parameters in the auxiliary Hamiltonian, we obtained $\lambda_a = 0.0504, 0.0424, 0.1428, 0.1803$, and 0.2449 MeV, respectively, for the j shells $a = 2d_{5/2}, 1g_{7/2}, 3s_{1/2}, 2d_{3/2}$, and $1h_{11/2}$ when $n = 5$. For other isotopes, the values of the λ_a parameters change only slightly from the values given above. In the case when one uses uniform λ_a , their values are usually $\simeq 0.555$ MeV, slightly larger than the single- j value of $\frac{1}{4}G$.

It is worthwhile to emphasize one more time that the original multipole-form boson Hamiltonian H_B as given in (16) is not amenable to any truncation at all. By adding the term $\sum_a \lambda_a \hat{Z}_a$ to the Hamiltonian and working with the resultant auxiliary Hamiltonian in the form of (19) optimally determined by the MDP, reasonably accurate results have been obtained for the ground-state energies of the tin isotopes using just the simple boson state $|s^n\rangle$. In fact, our results for the energies here have about the same accuracy as that of the one-boson approximation of Ref. [31], in which a seniority-scheme boson mapping was used for the nondegenerate multi- j pairing interaction. This clearly shows that the present optimal-auxiliary-Hamiltonian method based on the MDP is indeed a viable method for treating the spurious-state problem in truncated boson-space calculations. Here we are concerned mainly with demonstrating how the MDP can be employed to find an optimal auxiliary Hamiltonian for truncated boson-space calculations. We therefore only mention in passing that more accurate results than those given in Table I for the ground-state energies of the

tin isotopes can be obtained if better trial states than the boson condensate $|s^n\rangle$ defined in (23) are used.

V. SUMMARY AND DISCUSSION

In this paper we have presented a maximal-decoupling principle and some of its novel applications. The MDP was originally developed as a viable alternative to the minimum-energy trace variational principle of Klein and Vallières [20] for effectively determining the collective degrees of freedom associated with nuclear collective motion. As it turns out, when the symmetry property of the system under study is broken by the states used in calculations, the MDP also allows one to minimize the errors due to this symmetry breaking by providing one with an optimal auxiliary Hamiltonian to replace the original Hamiltonian. This important feature of the MDP, which has been illustrated through an application to a Lipkin-Nogami type of BCS calculation, actually has applicability to a wide range of physical problems [24]. In the context of boson calculations using the multipole-form boson mapping, this MDP variational method enables one to treat the Pauli-principle constraints effectively (albeit indirectly) with an optimal auxiliary boson Hamiltonian so that severe truncations of the boson space become feasible.

As has been emphasized in Sec. II, with the MDP one minimizes the coupling between the collective and noncollective subspaces, instead of minimizing the average energy of the states in the collective subspace. In the context of boson calculations, this means that both the collective and noncollective degrees of freedom in the original fermion problem have to be mapped into bosons. Thus, boson mapping methods such as those given in Sec. III for the *full* shell-model algebra are best suited for applying the present MDP method, which is essentially an optimal-auxiliary-Hamiltonian method based on the maximal-decoupling variational principle.

According to conventional wisdom, the multipole-form boson mapping we have used in this work is more suitable for multipole interactions. The pairing interactions, on the other hand, are the worst case of this multipole-form boson mapping with respect to boson truncations. In the numerical applications to the single- j and nondegenerate multi- j pairing interactions above, however, by providing one with an optimal auxiliary boson Hamiltonian, the present MDP method has proved to be a viable method for treating the spurious-state problem in truncated boson-space calculations. We thus expect that the method should also work well for more general cases. To prove that, we are currently undertaking its application to more realistic shell-model interactions. The results of this application will be presented in a future publication. Finally, we stress that the optimal auxiliary Hamiltonian derived by the MDP method using the multipole-form boson mapping for any shell-model interaction is Hermitian and contains only one- and two-boson interactions. Therefore, the present MDP method should be useful for obtaining an IBM-like boson Hamiltonian from the shell model.

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