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Nucleon-pair coupling scheme in Elliott's SU(3) model

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Elliott's SU(3) model is at the basis of the shell-model description of rotational motion in atomic nuclei. We demonstrate that SU(3) symmetry can be realized in a truncated shell-model space if constructed in terms of a sufficient number of collective S, D, G, \ldots pairs (i.e., with angular momentum zero, two, four, ...) and if the structure of the pairs is optimally determined either by a conjugate-gradient minimization method or from a Hartree-Fock intrinsic state. We illustrate the procedure for 6 protons and 6 neutrons in the pf (sdg) shell and exactly reproduce the level energies and electric quadrupole properties of the ground-state rotational band with SDG (SDGI) pairs. The SD-pair approximation without significant renormalization, on the other hand, cannot describe the full SU(3) collectivity. A mapping from Elliott's fermionic SU(3) model to systems with s, d, g, \ldots bosons provides insight into the existence of a decoupled collective subspace in terms of S, D, G, \ldots pairs.

Atomic nuclei exhibit a wide variety of behaviors, ranging from single-particle motion to superconducting-like pairing to vibrational and rotational modes. To a large extent the story of nuclear structure is the quest to encompass the widest range of behaviors within the fewest degrees of freedom. In the early stage of nuclear physics, the spherical nuclear shell model [1, 2] stressed the singleparticle nature of the nucleons in a nucleus, while the geometric collective model [3, 4] and the Nilsson meanfield model [5] pointed the way to describing rotational bands by emphasizing permanent quadrupole deformations [6] in "intrinsic" states. The reconciliation between these two pictures has been one of the most important advances in our understanding of the structure of nuclei. It was in large part due to Elliott who showed, on the basis of an underlying SU(3) symmetry, how to obtain deformed "intrinsic" states in a finite harmonicoscillator single-particle basis occupied by nucleons that interact through a quadrupole-quadrupole force [7]. This major step forward provided a microscopic interpretation of rotational motion in the context of the spherical shell model and, more recently, led to the symmetry-adapted no-core shell model [8].

Although the spherical shell model does provide a general framework to reproduce rotational bands [9] and shape coexistence [10] in light- and medium-mass nuclei, it is computationally still extremely challenging to describe deformation in heavier-mass regions [11]. Approximations must be sought. A tremendous simplification of the shell model occurs by considering only pairs of nucle-

ons with angular momentum 0 and 2, and treating them as (s and d) bosons. This approximation, known as the interacting boson model (IBM) [12, 13], is particularly attractive because of its symmetry treatment in terms of a U(6) Lie algebra, which allows a spherical U(5), a deformed SU(3), and an intermediate SO(6) limit. While the IBM has been connected to the shell model for spherical nuclei [14, 15], such relation has never been established for deformed nuclei, in which case the IBM has rather been derived from mean-field models [16, 17].

The nucleon-pair approximation (NPA) [18, 19] is one possible truncation scheme of the shell-model configuration space. The building blocks of the NPA are fermion pairs with certain angular momenta. Calculations are carried out in a fully fermionic framework, albeit in a severely reduced model space defined by the most important degrees of freedom in terms of pairs. The NPA therefore can be considered as intermediate between the full-configuration shell model and models that adopt the same degrees of freedom as the nucleon pairs but in terms of bosons. While the NPA has been successful for nearly spherical nuclei [20-27], previous studies for well-deformed nuclei are not satisfactory. For example, in the fermion dynamical symmetry model [28, 29] an SU(3) limit with Sp(6) symmetry can be constructed in terms of S and D pairs but their symmetry-determined structure is far removed from that of realistic pairs [30]. Also, the binding energy, moment of inertia, and electric quadrupole (E2) transitions calculated in an SD-pair approximation are much smaller than those obtained in Elliott's SU(3) limit for the pf and sdq shells [31].

In this Letter we successfully apply the NPA of the shell model to well-deformed nuclei. We show that the low-energy excitations of many-nucleon systems in Elliott's SU(3) limit can be exactly reproduced with a suitable choice of pairs in the NPA. We obtain an under-

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standing of this observation through a mapping to a corresponding boson model.

We consider an example system with even numbers of protons and neutrons in a degenerate pf or sdg shell, interacting through a quadrupole-quadrupole force of the form,

$$V_Q = -(Q_{\pi} + Q_{\nu}) \cdot (Q_{\pi} + Q_{\nu}), \tag{1}$$

where Q_{π} (Q_{ν}) is the quadrupole operator for protons (neutrons),

$$Q = -\sum_{\alpha\beta} \frac{\langle n_{\alpha} l_{\alpha} j_{\alpha} || r^2 Y_2 || n_{\beta} l_{\beta} j_{\beta} \rangle}{\sqrt{5} r_0^2} \left(a_{\alpha}^{\dagger} \times \tilde{a}_{\beta} \right)^{(2)}. \tag{2}$$

Greek letters α , β ,... denote harmonic-oscillator singleparticle orbits labeled by n, l, j, and j_z ; a_{α}^{\dagger} and \tilde{a}_{β} are the nucleon creation operator and its time-reversed form for the annihilation operator, respectively; and r_0 is the harmonic-oscillator length. As shown in Ref. [7], the interaction V_Q is a combination of the Casimir operators of SU(3) and SO(3), and its eigenstates are therefore classified by (irreducible) representations of these algebras with eigenenergies given by

$$-\frac{5}{2\pi} \left[\frac{1}{2} (\lambda^2 + \lambda \mu + \mu^2 + 3\lambda + 3\mu) - \frac{3}{8} L(L+1) \right], \quad (3)$$

in terms of the SU(3) labels (λ, μ) and the SO(3) label L, the total orbital angular momentum. Several useful SU(3) representations for low-lying states can be found in Ref. [31].

In the following we discuss in detail the case of 6 protons and 6 neutrons (6p-6n) in the NPA of the shell model and subsequently generalize to other numbers of nucleons. A nucleon-pair state of 6 protons is written as

$$|\varphi^{(I_{\pi})}\rangle = \left((A^{(J_{1})^{\dagger}} \times A^{(J_{2})^{\dagger}})^{(I_{2})} \times A^{(J_{3})^{\dagger}} \right)^{(I_{\pi})} |0\rangle, (4)$$

where I_2 is an intermediate angular momentum and $A^{(J)}^{\dagger}$ is the creation operator of a collective pair with angular momentum J:

$$A^{(J)\dagger} = \sum_{\alpha < \beta} y_J(\alpha\beta) \left(a_{\alpha}^{\dagger} \times a_{\beta}^{\dagger} \right)^{(J)}, \qquad (5)$$

where $y_J(\alpha\beta)$ is the pair-structure coefficient. For systems with protons and neutrons, we construct the basis by coupling the proton and neutron pair states to a state with total angular momentum I, i.e., $|\psi^{(I)}\rangle = (|\varphi^{(I_\pi)}\rangle \times |\varphi^{(I_\nu)}\rangle)^{(I)}$. Level energies and wave functions are obtained by diagonalization of the Hamiltonian matrix in the space spanned by $\{|\psi^{(I)}\rangle\}$, that is, from a configuration-interaction calculation. If a sufficient number of pair states are considered in Eq. (4), the NPA model space can be made exactly equivalent to the full

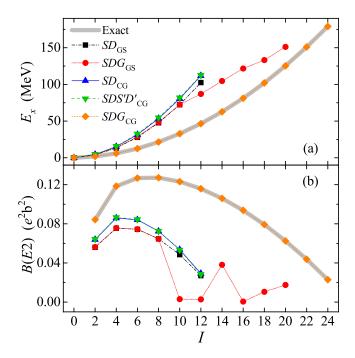


FIG. 1: (a) Excitation energy and (b) electric quadrupole reduced transition probability $B(E2;I\to I-2)$ for the ground rotational band of 6 protons and 6 neutrons in the pf shell in Elliott's SU(3) model. The subscript "GS" stands for generalized seniority and "CG" for conjugate gradient (see text).

shell-model space. The interest of the NPA, however, is to restrict to the relevant pairs and describe low-energy nuclear structure in a truncated shell-model space.

The selection of relevant pairs with the correct structure in Eq. (5) has been a long standing problem in NPA calculations. Recent applications choose pairs by the generalized seniority scheme (GS). Specifically, one optimizes the structure coefficients of the S pair by minimizing the expectation value of the Hamiltonian in the S-pair condensate and one obtains other pairs by diagonalizing the Hamiltonian matrix in the space spanned by GS-two (i.e., one-broken-pair) states [25, 32]. The collective pairs obtained with the GS approach provide a good description of nearly-spherical nuclei but, as recognized in Ref. [33] and as will also be shown below, they are inappropriate in deformed nuclei. Instead we use the conjugate gradient (CG) method [34, 35], where the structure coefficients of all pairs considered in the basis are simultaneously optimized by minimizing the groundstate energy in a series of iterative NPA calculations for a given Hamiltonian. The initial pairs in this iterative procedure are SU(3) tensors, obtained by diagonalizing V_Q in a two-particle basis and retaining the lowest-energy

Figure 1 shows, for a 6p-6n system in the pf shell, the results of various NPA calculations concerning excitation energies and E2 reduced transition probabilities (with the standard effective charges $e_{\pi}=1.5$ and $e_{\nu}=0.5$) for

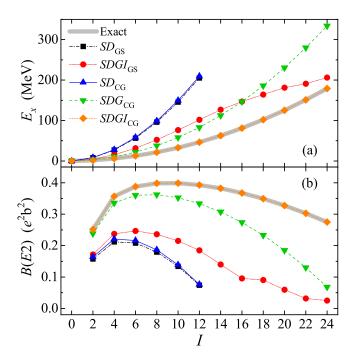


FIG. 2: Same as Fig. 1 for the sdg shell.

the lowest rotational band. These are compared to the exact results of Elliott's model, where the ground band belongs to the SU(3) representation $(\lambda, \mu) = (24, 0)$. Surprisingly, the SDG-pair approximation of the shell model in the CG approach (denoted as $SDG_{\rm CG}$) reproduces the exact binding energy, $810/\pi$ MeV according to Eq. (3), to a precision of eight digits, as well as the exact excitation energies for the entire ground band. One can understand the occurrence of the (24,0) representation from the coupling of (12.0) for the six protons and six neutrons separately and, in fact, all bands contained in the product $(12,0) \times (12,0)$, i.e. $(24,0), (22,1), \dots, (0,12)$, are exactly reproduced in the SDG_{CG} -pair truncated space. We also find that the results of the SDG-pair approximation are close to the exact results if the pairs are SU(3)tensors. For example, with such pairs the calculation reproduces 98% of the exact binding energy, 99% of the exact moment of inertia, and 97% of the exact B(E2)values.

On the other hand, the results of the SDG-pair approximation deteriorate if the pairs are obtained with the GS approach (denoted as $SDG_{\rm GS}$), which reproduces only 76% of the exact binding energy. Furthermore, $SDG_{\rm GS}$ fails to describe the quadrupole collectivity: The moment of inertia predicted by $SDG_{\rm GS}$ is only $\sim 43\%$ of the exact one, the predicted B(E2) values are too small, and the yrast states with angular momentum $I \geq 10$ do not follow the behavior of a quantum rotor. One concludes that the structure of the collective pairs, as determined by the GS approach, is not suitable for the description of well-deformed nuclei.

It is also of interest to investigate the standard SDpair approximation of the shell model and results of the SD_{GS} -, SD_{CG} -, and $SDS'D'_{CG}$ -pair approximations are shown in Fig. 1. Here S' and D' are collective pairs with angular momentum 0 and 2 but orthogonal to the S and D pairs, respectively. While the CG approach provides the numerically optimal solution in SD_{CG} - and $SDS'D'_{\text{CG}}$ -pair approximations, the results nonetheless are underwhelming. In the SD_{GS} , SD_{CG} , and $SDS'D'_{CG}$ spaces only 76%, 83%, and 84% of the exact binding energy are reproduced, respectively, and the predicted moments of inertia and B(E2) strengths are evidently smaller than the exact SU(3) results. We conclude that the collective SD pairs cannot fully explain the quadrupole collectivity of the SU(3) states. Interestingly, the excitation energies of the yrast states predicted by the SD-pair approximations follow an I(I+1) rule and the B(E2) strength exhibits a nearly-parabolic shape [see Fig. 1(b), two typical features of rotational motion. This raises the hope that an effective Hamiltonian and effective charges can be derived in the restricted SD_{CG} space, which takes into account the coupling with the excluded space. This conclusion is in line with a more phenomenological approach [17], in which an $L \cdot L$ term is added to the Hamiltonian, such that properties of low-lying states of well-deformed nuclei are reproduced in sd-IBM.

Figure 2 shows the corresponding results of for the 6p-6n system in the sdg shell. In this case the $SDGI_{CG}$ -pair approximation of the shell model reproduces exactly the SU(3) results and all states belonging to the coupled representation $(18,0) \times (18,0)$, i.e. $(36,0), (34,1), \dots, (0,18)$, are fully contained in the $SDGI_{CG}$ -pair truncated space. Again, if the pairs are SU(3) tensors, the SDGI-pair approximation is close to the exact result and reproduces 99% of the exact binding energy, 97% of the exact moment of inertia, and 99% of the exact B(E2) values. The SDG_{CG} -pair approximation yields 96% of the binding energy and 57% of the moment of inertia. The predicted B(E2) strength in the SDG_{CG} -pair approximation is close to the exact result for low angular momenta but deteriorates as angular momentum I increases. The necessity of renormalization is even larger in the $SD_{\rm CG}$ pair approximation.

Let us now try to understand the above results. Specifically, why is it that the SU(3) results in the pf shell are exactly reproduced with SDG but not with SD pairs? Similarly, why is it that SU(3) in the sdg shell cannot be represented with SD or SDG but requires SDGI pairs? To explain these findings, we invoke a mapping to a system with corresponding s, d, g, and i bosons (denoted as sd-, sdg-, or sdgi-IBM) and the bosonic realization of SU(3). The mapping is further specified by the fact that the quadrupole-quadrupole interaction V_Q is an SU(4) invariant and, consequently, one aims to realize the symmetries associated with Wigner's supermultiplet model [36] in terms of bosons. An SU(4)-invariant boson model,

known as IBM-4 [37], requires to assign to each boson a spin-isospin of (s,t) = (0,1) or (1,0), giving rise to a spin-isospin algebra $U_{st}(6)$.

The SU(3) limit can be realized in terms of bosons by first decoupling the orbital angular momentum from the spin-isospin of the bosons. For an n_b -boson state this leads to the classification

$$\begin{array}{cccc} \mathrm{U}(6\Lambda) \supset & \mathrm{U}(\Lambda) & \otimes & \mathrm{U}_{st}(6) \\ \downarrow & \downarrow & \downarrow & \downarrow \\ [n_b] & \left[\bar{h}\right] \equiv [h_1, ..., h_6] & \left[\bar{h}\right] \equiv [h_1, ..., h_6] \end{array}, (6)$$

with $\Lambda=6$, 15, and 28 for sd-, sdg-, and sdgi-IBM, respectively. The six labels $[\bar{h}]$ are a partition of n_b such that $h_1 \geq h_2 \geq \cdots \geq h_6$; they specify the representations of U(Λ) and U_{st}(6), which by virtue of the overall U(6Λ) symmetry of the bosons must be identical. For all above values of Λ (i.e., $\Lambda=6$, 15, and 28), Elliott's SU(3) appears as a subalgebra of U(Λ),

while Wigner's SU(4) occurs as a subalgebra of $U_{st}(6)$,

$$\begin{array}{cccc}
\mathbf{U}_{st}(6) \supset & \mathbf{SU}_{st}(4) \supset \mathbf{SU}_{s}(2) \otimes \mathbf{SU}_{t}(2) \\
\downarrow & \downarrow & \downarrow & \downarrow & \downarrow \\
[\bar{h}] & (\lambda', \mu', \nu') & S & T
\end{array} (8)$$

The quantum numbers (λ, μ) , K, and L in Eq. (7) and (λ', μ', ν') , S, and T in Eq. (8) have an interpretation identical to that in Elliott's fermionic SU(3) model [7, 38].

The SU(3) labels (λ, μ) in the different versions of the IBM can be worked out with the following procedure [39]. For a given number of bosons n_b , one enumerates all possible Young diagrams $[\bar{h}]$ of U(Λ) or U_{st}(6). For each $[\bar{h}]$ one obtains the SU_{st}(4) labels (λ', μ', ν') from the branching rule U(6) \supset SU(4), and retains only the ones that contain the favored supermultiplet. Finally, the SU(3) labels (λ, μ) for the above $[\bar{h}]$ are found from the U(Λ) \supset SU(3) branching rule.

Let us apply this procedure to the 6p-6n system in the pf shell. The lowest eigenstates of the quadrupole-quadrupole interaction belong to the favored SU(4) supermultiplet $(\lambda', \mu', \nu') = (0, 0, 0)$ and the leading (fermionic) SU(3) representation is $(\lambda, \mu) = (24, 0)$. For $n_b = 6$ bosons, the $U_{st}(6)$ or $U(\Lambda)$ representations containing this favored supermultiplet (0, 0, 0) are $[\bar{h}] = [6]$, [4, 2], $[2^3]$, and $[1^6]$, which have the SU(3) labels (λ, μ) as listed in Table I for the sd-, sdg-, and sdgi-IBM. The leading SU(3) representation (24, 0) is not contained in sd-IBM but is present in the [6] representation of U(15), and therefore it is contained in sdg-IBM. Similarly, 6p-6n in the sdg shell give rise to the leading SU(3) representation (36, 0), which is not contained in sd- nor sdg-IBM but present in sdgi-IBM.

TABLE I: Leading SU(3) representations for 6 bosons in sd-, sdg-, and sdgi-IBM occurring in the U(Λ) and U_{st}(6) representations [\bar{h}] containing the favored supermultiplet (0,0,0).

$(bosons)^{n_b}$	[h]	(λ,μ)
$(sd)^6$	[6]	$(12,0),(8,2),(4,4),(6,0),(0,6),\ldots$
		$(8,2), (6,3), (7,1), (4,4)^2, (5,2), \dots$
		$(6,0), (0,6), (3,3), (2,2)^2, (0,0)$
	$[1^6]$	(0,0)
$(sdg)^6$	[6]	$(24,0),(20,2),(18,3),(16,4)^2,(18,0),\dots$
	[4, 2]	$(20, 2), (18, 3), (19, 1), (16, 4)^3, (17, 2), \dots$
	$[2^{3}]$	$(18,0), (15,3), (12,6), (13,4), (14,2)^3, \dots$
	$[1^{6}]$	$(12,0),(8,5),(9,3),(3,9),(7,4),\ldots$
$(sdgi)^6$	[6]	$(36,0), (32,2), (30,3), (28,4)^2, (30,0), \dots$
	[4, 2]	$(32,2),(30,3),(31,1),(28,4)^3,(29,2)^2,\dots$
	$[2^3]$	$(30,0), (27,3), (24,6), (25,4), (26,2)^3, \dots$
	$[1^6]$	$(24,0), (20,5), (21,3), (18,6), (19,4), \dots$

TABLE II: Leading fermionic SU(3) representations (λ, μ) for n nucleons in the pf and sdg shells and the U(6), U(15), and U(28) representations of the $n_{\rm b}=n/2$ boson system that contain this (λ, μ) in sd-, sdg-, and sdgi-IBM.

$(shell)^n$	(λ, μ)	sd-IBM	$sdg ext{-}\mathrm{IBM}$	$sdgi ext{-}\mathrm{IBM}$
$(pf)^4$	(12,0)	_	_	[2]
	(16, 4)	_	_	$[4], [2^2]$
	(24, 0)	_	[6]	$[6], [4, 2], [2^3], [1^6]$
	(16, 0)	_	_	
$(sdg)^8$	(24, 4)	_	_	_
$(sdg)^{12}$	(36, 0)	_	_	[6]

The generalization to the 2p-2n (n = 4) and 4p-4n (n = 8) systems in the pf and sdg shells is summarized in Table II. The second column lists the leading fermionic SU(3) representations and the third, fourth, and fifth columns indicate whether this representation is contained in sd-, sdg-, and sdgi-IBM, respectively. A dash (—) indicates that it is not, in which case an NPA calculation adopting the corresponding SD, SDG, or SDGI pairs does not reproduce the full collectivity of the groundstate band in the fermionic SU(3) model. For n = 4and n = 8 nucleons in the sdq shell no exact mapping can be realized to sdgi-IBM and bosons with even higher angular momentum are needed. It should be noted, however, that this generally occurs for low nucleon number (e.g., for n = 12 nucleons in the sdg shell the problem does not occur), for which NPA calculations with high angular momentum pairs are still feasible.

While the best NPA solutions so far have been found by a numerically intensive optimization, it turns out they can also be obtained from a deformed "intrinsic" state. Again consider the 6p-6n system in the pf shell. An unconstrained Hartree-Fock (HF) calculation in this single-particle shell-model space [40] with a quadrupole-quadrupole interaction provides us with a HF state with an axially symmetric quadrupole deformed shape, a consequence of the spontaneous symmetry breaking [41] of

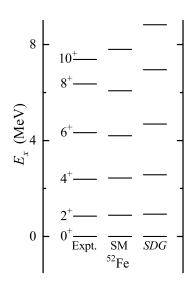


FIG. 3: The ground rotational band of 52 Fe. The experimental energies are taken from Ref. [44] and the shell-model results are obtained with the GXPF1 interaction.

rotational symmetry. One can project out a K=0 band with good angular momentum from this HF state [42], which exactly corresponds to the SU(3) representation (24,0) [7]. We use a and \bar{a} to denote the HF single-particle orbit and its time-reversal partner, respectively, and we write the creation operator of a nucleon as c_a^{\dagger} . A Slater determinant for an even number 2N of protons or neutrons can be written as a pair condensate:

$$\prod_{a=1}^{N} c_a^{\dagger} c_{\bar{a}}^{\dagger} |0\rangle = \mathcal{N} \left(\sum_{a} v_a \ c_a^{\dagger} c_{\bar{a}}^{\dagger} \right)^{N} |0\rangle. \tag{9}$$

The pair in the deformed HF state is a superposition of collective pairs of good angular momentum in the shell model [43]:

$$\sum_{a} v_a \ c_a^{\dagger} c_{\bar{a}}^{\dagger} = \sum_{IM} A_M^{(J)}^{\dagger}. \tag{10}$$

For the appropriate v_a one obtains SDG pairs, which are the same as the SDG pairs obtained by the CG-NPA calculations. Similarly, the SDGI pairs responsible for (36,0) for 6p-6n in the sdg shell can be also projected out from a deformed HF pair. The CG approach provides numerically optimal solutions in the NPA but is computationally heavy due to hundreds, even thousands of iterations. The HF approach derives pairs using an unconstrained HF calculation and the decomposition of pairs according to Eq. (10) has a very low computational cost.

Finally, we show that the NPA with CG-pairs provides a good description of low-lying states of rotational nuclei also if a realistic shell-model interaction is taken. We exemplify this with the nucleus 52 Fe, considered as a 6p-6n system in the pf shell with the GXPF1 effective interaction [45]. Figure 3 and Table III compare, for the ground

I^{π}	Expt.	SM	SDG
2^{+}	14.2(19)	19.2	17.0
4^+	26(6)	25.0	21.6
6^{+}	10(3)	17.4	20.0
8+	9(4)	11.5	15.5
10^{+}		12.7	10.5

TABLE III: $B(E2; I \rightarrow I-2)$ values (in W.u.) for the ground rotational band of 52 Fe. The experimental values are taken from Ref. [44] and the shell-model results are obtained with the GXPF1 interaction.

rotational band of 52 Fe, the experimental data [44], the full configuration shell model (SM), and the $SDG_{\rm CG}$ -pair approximation. Both the level energies and the B(E2) values obtained with $SDG_{\rm CG}$ are in good agreement with the data and with the shell model.

In summary, we construct in the NPA a collective subspace of the full shell-model space such that the former exactly reproduces, without any renormalization, the properties of the low-energy states of the latter. This construction is valid for an SU(3) quadrupole-quadrupole Hamiltonian and is achieved by determining the structure of the pairs with the conjugate-gradient minimization technique or on the basis of a deformed HF calculation. Exact correspondence is achieved only if a sufficient number of different pairs is considered. For example, a 6p-6n system in the pf (sdg) shell is reproduced exactly with SDG (SDGI) pairs; with just SD pairs, an important renormalization of all operators is required. We have analytic understanding of this result: The collective subspace of the NPA exactly captures the collectivity of the full space if and only if the mapping to a model constructed with bosons corresponding to the pairs gives rise to a leading bosonic SU(3) representation that is also leading in fermionic SU(3).

For many years a central problem in nuclear structure has been the construction of a collective subspace that decouples from the full shell-model space. With this work the conditions necessary for this decoupling to be exact are now understood for an SU(3) Hamiltonian. This understanding will pave the way for the construction of viable collective subspaces for more realistic shell-model interactions. It will also clarify the derivation of boson Hamiltonians appropriate for quadrupole deformed nuclei. Similar techniques conceivably might be applied elsewhere, such as to octupole-deformed nuclei with a $\mathrm{Sp}(\Omega)$ or $\mathrm{SO}(\Omega)$ symmetry [38].

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