Nilsson-based truncation of the nuclear shell model

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A method for truncating the nuclear shell model in terms of Nilsson orbits is developed and tested in the context of a simple model that admits coexistence between deformed and spherical configurations. The method reproduces the exact-diagonalization spectra of both the spherical and deformed configurations if angular momentum projection is carried out prior to diagonalization. Implementation of this method in m-scheme shell-model codes is discussed.

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The nuclear shell model has evolved to the stage where it can be used for systematic studies of nuclear properties [1]. Its practical application is limited, however, to regions of nuclei in which the shell-model dimensions are small enough to be manageable. Typically, this means light nuclei or nuclei relatively near closed shells. In other regions, including those in which collectivity arises in its many manifestations, shell-model techniques are not directly applicable without the introduction of severe truncations. In spherical nuclei, truncations can be implemented via weak-coupling considerations. In deformed nuclei, truncations based on weak coupling are in general not appropriate. To produce a deformed correlation structure from a spherical shell-model basis, one must mix a large number of neutron and proton configurations.

In recent years, several methods for truncating the shell model in deformed (and other collective) nuclei have been developed. One example is the interacting boson model (IBM) [2], in which the shell-model Hamiltonian is approximately diagonalized in a truncated weak-coupling basis of selected neutron and proton configurations via a bosonization assumption. Despite the enormous phenomenological success of the IBM, a detailed microscopic derivation for deformed nuclei has not yet been obtained. Two other methods that have received much attention in recent years are the fermion dynamical symmetry model (FDSM) [3] and the pseudo-SU(3) scheme [4]. Both are purely fermionic approaches that make use of symmetry considerations to define a collective truncated basis. Since the single-particle splittings between active orbitals do not respect the symmetries used in defining either the FDSM basis or the pseudo-SU(3) basis, their detailed application may require considerable mixing of the fundamental configurations.

In this Brief Report, we consider an alternative fermionic method that truncates the shell model in well-deformed nuclei through the use of the Nilsson scheme [5]. Since Nilsson-model wave functions explicitly include the splittings between active single-particle orbitals, such a method may permit the description of deformed nuclear states with relatively little configuration mixing.

Nilsson wave functions are characterized by good K values (but not good J) and thus are most naturally treated in the m scheme. In earlier efforts [6] to describe deformed light nuclei in terms of Nilsson orbits, the analysis was carried out by first coupling to states of good angular momentum and isospin and then using JT-scheme methods. Because of recent advances in shell-model technology, this is no longer necessary. Several shell-model codes now exist [7] that work directly in the m scheme, and they can be readily adapted to our purposes. As a reminder, the m scheme is particularly well suited for programming purposes since the presence or absence of a particle in a given single-particle state may be described by a 1 or a 0 and represented directly in binary language.

The Nilsson model gives single-nucleon wave functions in an axially symmetric deformed potential. The starting point of our proposed method is to generate an optimum set of Nilsson levels. The deformation parameter β may be chosen either from a Hartree-Fock or a Hartree-Fock-Bogolyubov calculation [5] for the nucleus (or band) of interest. If we denote the creation operators for the deformed single-particle orbitals by $b^\dagger$ and those for the spherical orbitals by $a^\dagger$, there exists a unitary transformation connecting these two single-particle bases:

$$b_K^\dagger = \sum_j c_{jK} a_{j,m=K}^\dagger . \tag{1}$$

The basic idea is to work in a basis in which the valence particles are distributed over the deformed orbitals,

$$b_{K_1}^\dagger b_{K_2}^\dagger \cdots b_{K_n}^\dagger |0\rangle . \tag{2}$$

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By inserting (1) into (2), the deformed basis states can be transformed into a sum over spherical states. Care must be taken to end up with patterns in standard order, but this amounts to an overall sign depending on the number of permutations required.

We gain nothing, however, by simply transforming from one single-particle basis to another. If all deformed orbits are included, the deformed-space diagonalization will yield identical results to those obtained in the spherical basis. The essence of our method is to impose truncations based on Nilsson energetics. It is our hope that this will permit us to incorporate the strong configuration mixing induced by the neutron-proton interaction in a small (and tractable) model space.

Once we carry out a truncation in terms of deformed single-particle states, it is imperative that we incorporate angular momentum projection. The Hamiltonian acting in a *truncated* deformed basis will in general not separate states of different J values. States of good angular momentum can be retrieved by introducing the standard projection operator [5]

$$P^J = \prod_{J' \neq J} [\hat{J}^2 - J'(J'+1)]/[J(J+1) - J'(J'+1)] , \qquad (3)$$

which is already incorporated in the m-scheme shell-model code OXBASH [7]. In principle, angular momentum projection can be implemented either before or after diagonalization of the truncated Hamiltonian matrix. As we will see in the calculations to follow, it is usually necessary to carry out the projection prior to diagonalization, particularly if pairing is important. Isospin projection, if necessary, can be implemented in a similar way.

To test the utility of our proposed method, we have applied it to a simple shell-model problem involving four identical nucleons occupying $p_{3/2}$, $d_{5/2}$, and $s_{1/2}$ orbits and interacting via a sum of a pairing and a quadrupole force. We have in mind a scenario common to many nuclei near closed shells in which quadrupole correlations pull down deformed core-excited states into the energy region of the dominant spherical closed-shell states. With this in mind, we assume that the $p_{3/2}$ level is 10 MeV below the other two (which are assumed to be degenerate). We furthermore assume a pairing force strength of $G=1$ MeV and quadrupole strength of $\kappa=1$ MeV.

Exact solutions for this model can be readily obtained by direct diagonalization of the Hamiltonian matrix. The resulting spectrum is shown in Fig. 1 (labeled EXACT). Indeed the calculation produces a typical coexistence pattern. The 0_1^+ ground state is primarily a filled $p_{3/2}$ orbit. The 0_2^+, 2_1^+, and 4_1^+ states to a good approximation form a rotational band:

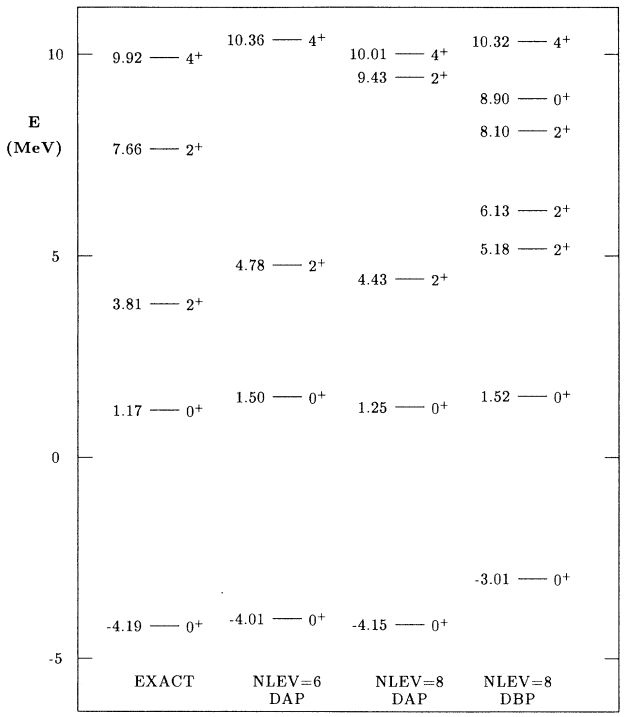
$$[E(4_1^+) - E(0_2^+)]/[E(2_1^+) - E(0_2^+)] = 3.32$$

This rotational band arises by exciting two particles from the $p_{3/2}$ orbit into the $d_{5/2}$ and $s_{1/2}$ orbits, where they are correlated strongly by the quadrupole force. The occupation numbers for the lowest states are illustrated in Table I. Note that pairing induces some mixing between the spherical and deformed 0^+ states, as reflected in the 2p-2h (two-particle–two-hole) admixture in the ground state and the 0p-0h admixture in the 0_2^+ state.

TABLE I. Orbit occupation numbers for the exact eigenstates of the shell-model Hamiltonian described in the text.

State	Occupation numbers $p_{3/2}$	$d_{5/2}$	$s_{1/2}$
0_1^+	3.189	0.556	0.255
0_2^+	2.755	0.812	0.433
2_1^+	1.995	1.280	0.725
2_2^+	1.989	1.441	0.570
4_1^+	1.989	1.785	0.226

Next we turn to a discussion of how we implement Nilsson-based truncations in obtaining approximate solutions for this model. A deformed basis corresponding to the active levels of this model involves 12 single-particle states, for which the deformed creation operators are



11

FIG. 1. Calculated spectra for the shell-model calculations described in the text. The spectrum labeled EXACT refers to an exact diagonalization of the shell-model Hamiltonian. Subsequent spectra give the results associated with Nilsson-based truncations; they are labeled according to the number of deformed orbits included (NLEV) and whether diagonalization was carried out after angular momentum projection (DAP) or before angular momentum projection (DBP).

$$
\begin{aligned}
b^{\dagger}_{1,K=(1/2)^-} &= a^{\dagger}_{p_{3/2,1/2}} , \\
b^{\dagger}_{2,K=-(1/2)^-} &= a^{\dagger}_{p_{3/2,-1/2}} , \\
b^{\dagger}_{3,K=(3/2)^-} &= a^{\dagger}_{p_{3/2,3/2}} , \\
b^{\dagger}_{4,K=-(3/2)^-} &= a^{\dagger}_{p_{3/2,-3/2}} , \\
b^{\dagger}_{5,K=(1/2)^+} &= \alpha\, a^{\dagger}_{d_{5/2,1/2}} + \sqrt{1-\alpha^2}\, a^{\dagger}_{s_{1/2,1/2}} , \\
b^{\dagger}_{6,K=-(1/2)^+} &= \alpha\, a^{\dagger}_{d_{5/2,-1/2}} + \sqrt{1-\alpha^2}\, a^{\dagger}_{s_{1/2,-1/2}} , \\
b^{\dagger}_{7,K=(3/2)^+} &= a^{\dagger}_{d_{5/2,3/2}} , \\
b^{\dagger}_{8,K=-(3/2)^+} &= a^{\dagger}_{d_{5/2,-3/2}} , \\
b^{\dagger}_{9,K=(1/2)^+} &= \sqrt{1-\alpha^2}\, a^{\dagger}_{d_{5/2,1/2}} - \alpha\, a^{\dagger}_{s_{1/2,1/2}} , \\
b^{\dagger}_{10,K=-(1/2)^+} &= \sqrt{1-\alpha^2}\, a^{\dagger}_{d_{5/2,-1/2}} - \alpha\, a^{\dagger}_{s_{1/2,-1/2}} , \\
b^{\dagger}_{11,K=(5/2)^+} &= a^{\dagger}_{d_{3/2,5/2}} , \\
b^{\dagger}_{12,K=-(5/2)^+} &= a^{\dagger}_{d_{5/2,-5/2}} .
\end{aligned}
\tag{4}
$$

Because of the simplicity of the model, the only mixing that arises in a deformed basis is between the two $K=\frac{1}{2}^+$ states (denoted by subscripts 5 and 9) and the two related $K=-\frac{1}{2}^+$ states (6 and 10). This mixing is represented by a single parameter α.

To determine the *optimum* Nilsson basis, we carry out a variational calculation appropriate to the 2p-2h deformed band. Namely we consider as a trial state

$$
|\Phi\rangle = b^{\dagger}_1 b^{\dagger}_2 b^{\dagger}_5 b^{\dagger}_6 |0\rangle \tag{5}
$$

and determine α so as to minimize the expectation value of the Hamiltonian. This is equivalent to a (prolate) deformed Hartree-Fock treatment of the 2p-2h configuration. The minimum energy occurs for $\alpha=0.84$.

We then carried out several sets of calculations truncated according to this deformed basis. The simplest reasonable truncation would be to include only the four levels of the $p_{3/2}$ orbit (levels 1–4) and the lowest $K=\pm\frac{1}{2}^+$ levels (5 and 6). Including just these six levels and *implementing angular momentum projection prior to diagonalization* in the truncated basis yields the spectrum labeled NLEV=6 DAP in the figure. Already we see a reasonable reproduction of the lowest states of the system. The deformed band, which at the level of single-particle energies lies 20 MeV above the ground band, is brought down dramatically by the deformed correlations; its band head lies 5.51 MeV above the ground state, in fairly good agreement with the exact-diagonalization excitation energy of 5.36 MeV. Furthermore, this extremely simple calculation gives a qualitative reproduction of the spectrum of states in the deformed band. It should be noted that in this calculation, the 0^+, 2^+, and 4^+ dimensions are 3, 2, and 2, respectively, significantly smaller than the corresponding dimensions (7, 12, and 8) of the full calculation.

Adding one more (time-reversed) pair of Nilsson levels (7 and 8) leads to the results labeled NLEV=8 DAP in the figure. Now the agreement is in fact quantitative, with the exception of the second 2^+ state. Clearly, truncation of the full space in terms of a fairly small number of deformed Nilsson orbits (appropriately chosen) is able to describe the complicated coexistence dynamics of this system quite accurately.

Finally, in the last spectrum shown in the figure (labeled NLEV=8 DBP), we present results obtained with the same eight Nilsson levels (1–8) but with angular momentum projection carried out after a diagonalization in the intrinsic basis. These results are in rather poor agreement with the exact results; in particular, the two bands lie much too close in energy. And the reason for this is quite easy to understand. The spherical $p^4_{3/2}(0)$ configuration can only have a pairing interaction with the 0^+ member of the deformed 2p-2h band. But the *intrinsic* 2p-2h $K=0^+$ state contains *all* allowed even angular momenta. Thus, treating pairing in the intrinsic frame prior to diagonalization leads to a strongly reduced pairing effect on the ground state. And this is why the ground-state energy is so poorly reproduced. The message is clear; angular momentum projection must be carried out prior to diagonalization when pairing is important.

In Table II, we show the overlaps between states obtained at the various levels of approximation and those of the exact calculation. The same conclusions that emerged from the comparison of spectra show up here as well. In particular, the NLEV=8 calculation with projection before diagonalization gives excellent quantitative reproduction of the exact results.

At first glance, these results seem very promising. They suggest that it is possible to quantitatively reproduce the dynamics of strong deformation in the shell model in a relatively small basis built up in terms of appropriate deformed Nilsson (HF) single-particle states. Such a treatment not only reduces the size of the basis but also gives a clear picture of the dominant physics underlying the low-lying states. However, there are two caveats that should be noted: (i) Even though the deformed basis is amenable to drastic truncation, it is still necessary to calculate all of the Hamiltonian matrix elements in the large spherical basis. Thus, an important issue still to be addressed before applying these methods to more realistic situations is how large a valence space can be handled with this method before the problem becomes CPU-time prohibitive. (ii) While the method we have discussed is able to describe a single deformed configuration and also its interplay with a spherical configuration corresponding to closed shells, it cannot be used with similar confidence in a scenario involving two collective

TABLE II. Overlap of approximate eigenstates obtained in truncated calculations with those resulting from exact diagonalization of the shell-model Hamiltonian described in the text.

	Overlaps				
Calculation	0^+_1	0^+_2	2^+_1	2^+_2	4^+_1
NLEV=6 (1–6)	0.996	0.991	0.894	· · ·	0.970
NLEV=8 (1–8)	0.999	0.998	0.944	0.821	0.997

configurations with very different deformations (e.g., one prolate and one oblate). There, one would most likely need to include two sets of Nilsson levels, and appropriately orthogonalize the resulting states.

There is one final point to note. The test model that we have used builds collective rotations from a quadrupole interaction between like nucleons. In real nuclei, deformation arises predominantly through the quadrupole component of the neutron-proton interaction [8]. The same methods that we have discussed here should also be applicable in such cases.

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