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SU(3) versus deformed Hartree-Fock

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Deformation is fundamental to understanding nuclear structure. We compare two ways to efficiently realize deformation for many-fermion wavefunctions, the leading SU(3) irrep and the angular-momentum projected Hartree-Fock state. In the absence of single-particle spin-orbit splitting the two are nearly identical. With realistic forces, however, the difference between the two is non-trivial, with the angular-momentum projected Hartree-Fock state better approximating an “exact” wavefunction calculated in the fully interacting shell model. The difference is driven almost entirely by the single-particle spin-orbit splitting.

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I. INTRODUCTION

Deformation is one of the most salient features of atomic nuclei. The Bohr-Mottelson model, a quantum realization of the ellipsoidal surface of a liquid drop, was a major triumph in understanding nuclear structure [1]. The other major fundamental nuclear structure theory is, of course, the independent-particle or shell model, which is usually realized in a spherical basis. Elliott combined these two paradigms in the SU(3) model [2]: the antisymmetric (fermionic) irreducible representations (irreps) of SU(3) in a spherical shell-model basis give rise to band structures associated with quadrupole deformed shapes.

The nuclear Hamiltonian is not invariant under SU(3), however. Important parts of the nuclear Hamiltonian mix SU(3) irreps, like pairing and the single-particle spin-orbit splitting. To include symmetry breaking realistic interactions requires a more sophisticated version of the SU(3) model [3, 4, 5]. The Nilsson model [1, 6] of deformation describes single-particle levels by including quadrupole deformation and spin-orbit splitting, but one can think of Nilsson levels as a simplified version of deformed mean-field, or Hartree-Fock, levels.

It is commonly accepted that the simplest SU(3) theory, one that takes only the leading SU(3) irrep into account, is a reasonable approximation to the exact ground state wavefunction of light *sd*-shell nuclei and not an unreasonable first approximation as one moves to mid and upper *sd*-shell nuclei and on into the lower *fp*-shell. This understanding provided motivation for a recent proposal for a “mixed-mode” approach to the selection of shell-model basis states, combining a few irreps of SU(3) to account for deformation with spherical configurations favored by pairing-like modes and single-particle degrees of freedom, keeping the combined total number of basis states well-below that of the full space [7].

While the mixed-mode approach has tremendous

promise, SU(3) irreps are not the only means of realizing deformation. Projected Hartree-Fock states would be an obvious alternative. In fact, both SU(3) and projected Hartree-Fock have been made the basis of shell-model calculations [8, 9, 10]. However, a systematic comparison of SU(3) and Hartree-Fock as starting points for shell-model calculations has not been made. This paper addresses that issue. Specifically, setting aside questions related to the advantages or disadvantages of algebraic versus numeric methods, we compare the leading SU(3) irrep and the angular-momentum-projected, deformed Hartree-Fock state as approximations to “exact” shell-model ground state wavefunctions for *sd*- and lower *fp*-shell nuclei for “realistic” interactions.

We find that projected Hartree-Fock is a better first approximation to the exact solution than the single leading SU(3) irrep. Upon further investigation, however, we find that by removing the spin-orbit splitting of single-particle energies, the differences become almost negligible, similar to the results found in [5]. So although SU(3) has many advantages, being an algebraic theory, the results of in this paper serve as a useful caveat. We also discuss some technical details of SU(3) versus projected Hartree-Fock, especially with regards to computational burden, in the concluding section.

II. METHOD OF CALCULATION

We start with a shell-model Hamiltonian which for the purposes of this paper we consider to be the true interaction. We compare the full numerical solution from shell-model diagonalization, $|SM\rangle$, against two approximate wavefunctions: a state from the leading SU(3) irrep, $|SU(3)\rangle$, and the projected Hartree-Fock state $|PHF\rangle$. We consider only even-even nuclei.

A. The model spaces

We work in complete $0\hbar\omega$ model spaces, either the $1s_{1/2}-0d_{3/2}-0d_{5/2}$ (or *sd*) shell or the $1p_{1/2}-1p_{3/2}-0f_{5/2}-0f_{7/2}$ (*pf*) shell. This means there is an inert core, ^{16}O

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for the *sd*-shell and ^{40}Ca for the *pf* shell. Valence particles are restricted to the single-particle states of a single major harmonic oscillator shell.

B. The interactions

We use general one+two-body interactions which conserve angular momentum and isospin. For the “true” interaction we use semi-empirical interactions such as the Brown-Wildenthal USD interaction for the *sd* shell [11] and the modified Kuo-Brown (KB3) interaction for the *pf* shell [12]. These interactions were derived by taking a realistic G-matrix interaction computed from NN phase shifts, and then adjusting matrix elements to fit to a large number of levels over a wide range of A ; for the USD interaction, this includes a phenomenological scaling of the two-body matrix elements by $A^{-0.3}$ (if one does not scale, the results below are qualitatively similar but quantitatively slightly weaker). What is important for our purposes is that these interactions describe very well the binding energies for a large number of nuclei and aside from the restriction to two-body, rotationally and isospin invariant interactions, were not restricted, that is, not assumed to have some schematic form such as quadrupole + pairing. Although less directly relevant to this paper, these interactions describe well excitation spectra and transition matrix elements. (Despite their general success, these general interactions are not perfect. For example, they have great difficulty in satisfactorily reproducing K-band splitting, something that is easily accomplished in an SU(3) basis by using a special scalar interaction that is of third+fourth order in the generators of SU(3) [13].)

In the *pf* shell we also investigated the Brown-Richter interaction [14]. The results were qualitatively the same, although the effect of spin-orbit splitting was smaller. For this paper we present only the KB3 results for the *pf* shell.

Gueorguiev et al [5] projected exact shell-model wavefunctions in the *pf*-shell onto SU(3) irreps and found that single-particle spin-orbit splitting made a significant contribution to mixing of SU(3) irreps in exact shell-model wavefunctions. Therefore for this study, analogous to [5], we removed the spin-orbit splitting of the single-particle energies for both the USD and KB3 interactions.

Pairing also contributes to mixing of SU(3) irreps [3]. Unlike single-particle spin-orbit splitting, however, pairing and $Q \cdot Q$ interactions share matrix elements in common, so it is not trivial to disentangle pairing from $Q \cdot Q$ in realistic interactions such as USD and KB3. Therefore in this paper we focus only on the simpler case of spin-orbit splitting.

C. “Exact” solutions

The many-body Hamiltonians were constructed from the one+two-body interactions and diagonalized using a descendent of the Glasgow shell-model code [15].

In principle we allow all possible many-body configurations within that space; but because the Hamiltonian is rotationally invariant, we can without loss of generality restrict ourselves to those many-body states with $M = 0$, the so-called M-scheme basis.

D. SU(3) solutions

To construct the leading irreps of SU(3), we diagonalized the SU(3) two-body Casimir $C_2 = Q \cdot Q + 3L^2$ (subtracting a small amount of L^2 in order to split states with the same (λ, μ) but different L). Because this is a two-body, real Hermitian operator, it can be treated as a Hamiltonian and therefore diagonalized by the same code that handles the realistic Hamiltonian. Unfortunately, because the shell-model code we used cannot handle three-body operators, we could not use the third-order SU(3) Casimir to split states with different (λ, μ) but with degenerate values of C_2 . Fortunately, for the leading irrep this was not a problem.

E. Hartree-Fock solutions

To construct the Hartree-Fock solutions, we took a Slater determinant wavefunction, and minimized the expectation value of a given Hamiltonian using gradient descent. We then projected the Hartree-Fock Slater determinant onto the $M = 0$ shell-model basis states used in computing the ‘exact’ and SU(3) solutions. This state did not have good angular momentum, but we projected out the $J = 0$ part of the wavefunction. (We projected onto states of good angular momentum by a Lanczos moment method similar to that used in [5] to project onto SU(3) states and in [16] to generate Gamow-Teller strength distributions. The unprojected state is used as the starting Lanczos vector, or “pivot,” and then one performs a few Lanczos iterations using J^2 as the Hamiltonian, splitting the pivot into components with good J . Although Ref. [5] used this technique to decompose shell-model wavefunctions among SU(3) irreps, for this paper we computed the wavefunction for the leading SU(3) irrep in the same shell model basis, as described in the previous subsection, and computed the overlap as a simple dot product, the wavefunctions being vectors in the M-scheme basis.)

Our results for the ground state were insensitive to the orientation of the HF state. Results for excited states for triaxial nuclei were, however, sensitive to the orientation of the HF state. In general, results for excited states were qualitatively similar to the ground state, although quantitatively less pronounced, so we do not present results for excited states here.

TABLE I: Energies of approximate wavefunctions, relative to the exact (shell-model) ground state, where HF = unprojected Hartree-Fock, PHF = projected Hartree-Fock, and SU(3) = leading irrep. All energies are in MeV. The label “nls” means single-particle spin-orbit splitting has been removed.

Nucleus	H	ΔE HF	ΔE PHF	ΔE SU(3)
^{20}Ne	USD	4.25	0.95	2.78
	USD-nls	4.55	1.02	1.01
^{24}Mg	USD	6.47	1.75	7.97
	USD-nls	6.59	1.45	2.42
^{32}S	USD	7.16	3.26	10.07
	USD-nls	6.12	1.50	2.36
^{36}Ar	USD	3.95	1.58	5.29
	USD-nls	3.70	0.80	0.84
^{44}Ti	KB3	3.72	1.18	6.46
	KB3-nls	3.80	1.11	2.54

III. RESULTS

A. Energies

In Table I we compare the ground state energies, relative to the exact (diagonalization of all valence configurations) ground state energy. That is, we compute

$$\Delta E = \langle \Psi | \hat{H} | \Psi \rangle - \langle SM | \hat{H} | SM \rangle,$$

where $|SM\rangle$ is the exact shell model wavefunction, and $|\Psi\rangle =$ projected Hartree-Fock (PHF) or leading SU(3) irrep. We also show the energy of the unprojected Hartree-Fock (HF) for comparison.

The expectation value of the exact Hamiltonian, with spin-orbit splitting, is considerably lower for the PHF state than for the SU(3) state, in one case by nearly 7 MeV. When spin-orbit splitting is removed, the difference becomes much smaller, nearly vanishing for nuclei with axial symmetry.

B. Wavefunctions

In addition to computing the energies, we calculated the overlap of wavefunctions, shown in Table II. The trends from the energies continue. For realistic interactions, the leading SU(3) has a smaller overlap with the exact shell model wavefunction than the projected Hartree-Fock state. When single-particle splitting is removed, the SU(3) state and the projected Hartree-Fock state come much closer to one another. The remaining difference may be due to pairing or other pieces of the realistic interaction.

Note: the small overlap between the ^{32}S PHF state and the leading SU(3) irrep is due to the large fragmentation of the exact-shell model wavefunction over SU(3),

TABLE II: Overlaps of wavefunctions. SM= exact shell model ground state wavefunction, PHF = projected Hartree-Fock, and SU(3) = leading irrep. The symbol “nls” means single-particle spin-orbit splitting has been removed.

Nucl	H	$\langle SM PHF \rangle$	$\langle SM SU(3) \rangle$	$\langle SU(3) PHF \rangle$
^{20}Ne	USD	0.957	0.881	0.948
	USD-nls	0.948	0.952	0.999
^{24}Mg	USD	0.926	0.667	0.494
	USD-nls	0.936	0.892	0.942
^{32}S	USD	0.847	0.358	0.171
	USD-nls	0.925	0.865	0.944
^{36}Ar	USD	0.923	0.636	0.586
	USD-nls	0.948	0.960	0.973
^{44}Ti	KB3	0.933	0.462	0.473
	KB3-nls	0.909	0.727	0.883

confirmed by spectral decomposition as in [5]. This fragmentation is very sensitive to the single-particle spin-orbit splitting: a reduction of the spin-orbit splitting by merely 15% will nearly triple $\langle SU(3) | PHF \rangle$.

C. Ground state geometry

In addition to computing the overlap probabilities of wavefunction, it is useful to analyze the wavefunctions in terms of quadrupole deformation, i.e., the classic deformation parameters β and γ .

We computed the deformation parameters β, γ for the unprojected Hartree-Fock state by diagonalizing the mass quadrupole tensor of the valence particles, as described by Ormand et al [17]. For the interactions we chose the exact Hamiltonians (USD and KB3), the exact Hamiltonians with the single-particle spin-orbit splitting removed (USD-nls and KB3-nls), and the SU(3) second-order Casimir. (Note: although in principle one can compute deformation of SU(3) wavefunctions directly from (λ, μ) [3, 4], for consistency we also applied Hartree-Fock to the SU(3) Hamiltonian.)

Table III shows that all three interactions yield similar results, but in particular the removal of spin-orbit splitting makes the deformation geometry nearly identical to that of SU(3). This supports the overlap results from section III B. We also see that inclusion of the spin-orbit force “softens” the deformation of the Hartree-Fock state, presumably through mixing of SU(3) irreps and similar to that seen in [4].

IV. DISCUSSION AND CONCLUSIONS

In phenomenological but high-quality shell-model interactions, meaning that the one- and two-body matrix elements are fit to a large number of levels over a substan-

TABLE III: Deformation geometry of unprojected Hartree-Fock states for different Hamiltonians. (For SU(3) we used the second-order Casimir C_2 as the Hamiltonian.)

Nucleus	H	β	γ
^{20}Ne	USD	0.458	0°
	USD-nls	0.476	0°
	SU(3)	0.476	0°
^{24}Mg	USD	0.284	13.7°
	USD-nls	0.312	18.6°
	SU(3)	0.315	19.1°
^{32}S	USD	0.112	24.6°
	USD-nls	0.155	40.4°
	SU(3)	0.157	40.9°
^{36}Ar	USD	0.081	60°
	USD-nls	0.094	60°
	SU(3)	0.095	60°
^{44}Ti	KB3	0.440	0°
	KB3-nls	0.527	0°
	SU(3)	0.556	0°

tial range of A , a J -projected Hartree-Fock state does a nontrivially better job of approximating the “exact” ground state wavefunctions and binding energies derived from diagonalization in a full $0\hbar\omega$ shell-model space, than does the leading SU(3) irrep. The difference is driven almost entirely by the single-particle spin-orbit splitting, similar to that seen in previous work [4, 5].

Does this mean that Hartree-Fock is necessarily superior to SU(3)? The short answer is no; for a longer answer we compare HF and SU(3) along two axes: analytic insight and computational burden.

SU(3) allows a tremendous degree of analytic insight into the structure of nuclear wavefunctions: for rotational nuclei both the ground state and excited states are often dominated by just a few SU(3) irreps, which can then illuminate the structure of band spectra including E2 transition strengths. SU(3) is especially useful for systems such as the rare earths [18], where a full spherical shell-model calculation would be prohibitive.

The computational burden can best be expressed by the number of basis Slater determinants needed to project out a good quantum number (such as J , M , λ or μ), because modern shell-model codes use occupation-representation Slater determinants. In other words, one defines a single-particle basis and represents a many-body basis state as a binary word (1=occupied single particle state and 0=unoccupied). Much of the physics is contained by the choice of the single-particle basis.

In a j - j coupled codes, such as Glasgow [15], OXBASH [19], ANTOINE [20], or REDSTICK/ELDORADO [21], the single-particle states couple l and s up to good j and m . An important advantage of j - j coupling is that spin-orbit splitting is trivial. The many-body basis states such single-particle states individually have good total M , and

hence are called an M-scheme basis, but generally do not have good J . However one generally only needs a few hundred M -scheme Slater determinants to project out good J , as J^2 is block-diagonal in j - j basis. Deformation is harder, however: to project out good λ or μ usually requires the entire many-body basis, which can be of order $10^4 - 10^5$ in the sd -shell and larger in the pf -shell.

SU(3) shell model codes [22] use L - S coupling built upon a cylindrical single-particle basis. In this basis spin-orbit splitting is hard (=requires many irreps) but deformation is simple. For the leading irrep, to construct states of good λ, μ one needs exactly one determinant, for the next-to-leading irrep the number is typically two or four depending upon whether the irrep occurs once or twice, and so on. Thus, because higher-weight irreps dominate the low-lying spectra, deformation is very simple. In fact most of the computational burden lies again in projecting out states of good J , and is roughly similar to that for the spherical (j - j coupled) shell model.

Finally we consider the Hartree-Fock state, which in principle incorporates both deformation and spin-orbit splitting. The HF state is not an exact eigenstate of SU(3) Casimirs, but that is not troubling as SU(3) is not an exact symmetry. Instead, as with other bases, the computational burden arises from projection of angular momentum. Formally one projects out states of good J by integrating over wavefunctions rotated by the Euler angles weighted by Wigner D-functions. If, however, the HF state has axial symmetry (that is, good M) then one can project out a state of good J with just $J_{max} + 1$ Slater determinants, where J_{max} is the largest total angular momentum possible. For the sd -shell this is 14; for the pf -shell, this is 30. That is, one could get deformation, spin-orbit splitting, and rotational invariance with just a handful of Slater determinants. One could also imagine using particle-hole excitations on top of the Slater determinants and projecting onto good angular momentum, and indeed this approach has been used [9, 10].

Unfortunately, for triaxial HF states one must in addition project out states of good M ; the number of states required goes from 10-30 to a few thousand. Furthermore, HF states present additional difficulties when one considers multi- $\hbar\omega$ shells, where center-of-mass motion comes into play. Projection of a Hartree-Fock state onto a nonspurious state is difficult because the generators of center-of-mass motion are complicated and incomplete in a Hartree-Fock single-particle basis. The generalization of SU(3) to multi- $\hbar\omega$ shells, the symplectic model [23], automatically separates out spurious from nonspurious states. Therefore, while projected Hartree-Fock has some computational advantages, for multi-shell calculations the symplectic extension of SU(3) may still be the method of choice.

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- [1] A. Bohr and B. R. Mottelson, *Nuclear Structure*, Vol II (W. A. Benjamin, Inc., Boston, 1975).
- [2] J. P. Elliott, Proc. Roy. Soc. (London) **A245**, 128 and 562 (1958); M. Harvey, Adv. Nucl. Phys. **1**, 67 (1968).
- [3] C. Bahri, J. Escher, and J. P. Draayer, Nucl. Phys. **A 592**, 171 (1995).
- [4] J. Escher, C. Bahri, D. Troltenier, and J. P. Draayer, Nucl. Phys. **A 633**, 662 (1998).
- [5] V. Gueorguiev, J. P. Draayer, and C. W. Johnson, Phys. Rev. **C 63**, 014318 (2000).
- [6] S. G. Nilsson, K. Dan. Vidensk. Selks. Mat.-fys. Medd., **29**, No. 16 (1955).
- [7] V. Gueorguiev, W. E. Ormand, C. W. Johnson, and J. P. Draayer, Phys. Rev. **C 65** 024314 (2002) .
- [8] J. P. Draayer and K. J. Weeks, Ann. of Phys. **156**, 41 (1984); O. Castaños, J. P. Draayer and Y. Lebscher, Ann. of Phys. **180**, 290 (1987).
- [9] T. Hjelt, K. W. Schmid, and A. Faessler, Nucl. Phys. **A 697**, 164 (2002); E. Bender, K. W. Schmid and A. Faessler, Prog. Part. Nucl. Phys. **38**, 159 (1997).
- [10] V. Velásquez, J. G. Hirsch and Y. Sun, Nucl. Phys. **A 643**, 39 (1998).
- [11] B.H. Wildenthal, Prog. Part. Nucl. Phys. **11**, 5 (1984).
- [12] T.T.S. Kuo and G.E. Brown, Nucl. Phys. **A114**, 235 (1968); A. Poves and A.P. Zuker, Phys. Rep. **70**, 235 (1981).
- [13] J. P. Draayer and G. Rosensteel, Nucl. Phys. **A439**, 61 (1985).
- [14] W. A. Richter, M. G. van der Merwe, R. E. Julies, and B. A. Brown, Nucl Phys. **A523**, 325 (1991).
- [15] R. R. Whitehead, *et al*, Adv. Nucl. Phys. **9**, 123 (1977).
- [16] E. Caurier, A. Poves, and A. P. Zuker, Phys. Lett. **B 252**, 13 (1990); Phys. Rev. Lett. **74**, 1517 (1995).
- [17] W. E. Ormand, D. J. Dean, C. W. Johnson, G. H. Lang, and S. E. Koonin, Phys. Rev. **C 49**, 024314 (1994).
- [18] G. Popa, J. G. Hirsch and J. P. Draayer, Phys. Rev. **C 62**, 064313 (2000); C. E. Vargas, J. G. Hirsch and J. P. Draayer, Nucl. Phys. **A 673**, 219 (2000);
- [19] A. Etchegoyen, et al, MSU-NSCL Report 524 (1985).
- [20] E. Caurier, computer code ANTOINE, CRN, Strasbourg, 1989 (unpublished); E. Caurier, A. P. Zuker, and A. Poves, in *Nuclear Structure of Light Nuclei Far from Stability*, Proceedings of the Obernai Workshop, 1989, edited by G. Klotz (CRN, Strasbourg, 1989).
- [21] W. E. Ormand, private communication.
- [22] Y. Akiyama and J. P. Draayer, Comp. Phys. Comm. **5** , 405 (1973); C. Bahri and J. P. Draayer, Comp. Phys. Comm. **83** , 59 (1994).
- [23] G. Rosensteel and D. J. Rowe, Ann. Phys. (N.Y.) **126**, 343 (1980); J. Escher and J. P. Draayer, J. Math. Phys. **39**, 5123 (1998); J. Escher and J. P. Draayer, Phys. Rev. Lett. **82**, 5221 (1999).