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SYMPLECTIC NO-CORE CONFIGURATION INTERACTION FRAMEWORK FOR *AB INITIO* NUCLEAR STRUCTURE

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Abstract

We introduce a symplectic no-core configuration interaction (SpNCCI) framework for *ab initio* nuclear structure calculations, in a correlated many-body basis which encodes an approximate $\mathrm{Sp}(3,\mathbb{R})$ symmetry of the nucleus. Such a scheme potentially provides a means of restricting the many-body space to include only those highly-excited configurations which dominantly contribute to the nuclear wave function. We examine the symplectic symmetry structure arising in an illustrative *ab initio* SpNCCI calculation for ^{6}Li. We observe both the dominance of symplectic symmetry in individual wave functions and the emergence of families of states related by symplectic symmetry.

Keywords: *Ab initio* nuclear theory, symplectic group [$\mathrm{Sp}(3,\mathbb{R})$], no-core configuration interaction (NCCI).

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1 Introduction

A long-standing goal of nuclear physics is to quantitatively predict the structure of nuclei and understand their excitation modes *ab initio*, *i.e.*, directly from realistic internucleon interactions. However, in a traditional oscillator-basis no-core configuration interaction (NCCI) calculation [1,2], the dimension of the many-body basis explodes as the number of nucleons and included single-particle excitations is increased. The basis size which would be required in order to obtain quantitatively accurate predictions for nuclei with more than just a few nucleons becomes prohibitively large [3,4].

The symplectic no-core configuration interaction (SpNCCI) framework introduces a correlated many-body basis, one which encodes an approximate $\mathrm{Sp}(3,\mathbb{R})$ symmetry of the nucleus. Our aims in pursuing symplectic many-body symmetry are twofold: (1) to use symmetries to accelerate convergence of *ab initio* results and (2) to understand the symmetries underlying many-body correlations in nuclei, including emergent rotation [5].

The symplectic group in three dimensions $\mathrm{Sp}(3,\mathbb{R})$ [6] enters into the nuclear many-body problem both through its relation to kinematics (coordinates and momenta) and through its connection to the harmonic oscillator. It is generated by the bilinears in coordinates and momenta, *i.e.*, operators of the form $x_i x_j$, $x_i p_j$, $p_i x_j$, and $p_i p_j$ $(i,j = 1,2,3)$. It thus arises naturally in problems involving the coordinates and momenta. Symplectic symmetry has a close relation to collective deformation and rotational degrees of freedom [7], through its Elliott SU(3) [8,9] (and rotor model [10]) subgroup, which is generated by the orbital angular momentum and quadrupole operators. The group $\mathrm{Sp}(3,\mathbb{R})$ is also the dynamical group for the harmonic oscillator, which defines the underlying basis for nuclear configuration interaction (or interacting shell model) calculations.

These connections permit the construction of the symplectic shell model formalism, originally proposed by Rosensteel and Rowe [11]. While the goal of "diagonalising a realistic many-nucleon Hamiltonian in a $\mathrm{Sp}(3,\mathbb{R}) \supset \mathrm{SU}(3)$ shell model basis, to obtain a fully microscopic description of collective states from first principles" was envisioned early on [12], only recently has sufficient progress been made in the computational framework for *ab initio* calculations to allow this goal to be revisited [13–16].

From the viewpoint of accelerating convergence in NCCI calculations, it is perhaps most important to note that the need for including highly excited configurations in NCCI calculations exists, in large part, because the kinetic energy induces strong coupling across shells. The kinetic energy operator, as a generator of $\mathrm{Sp}(3,\mathbb{R})$, conserves $\mathrm{Sp}(3,\mathbb{R})$ symmetry. Thus, by reorganizing the many-body space according to irreducible representations (irreps) of $\mathrm{Sp}(3,\mathbb{R})$, it is broken into subspaces which cannot be connected by the kinetic part of the Hamiltonian, as portrayed in Fig. 1. Combining symplectic symmetry with the no-core configuration interaction frame-

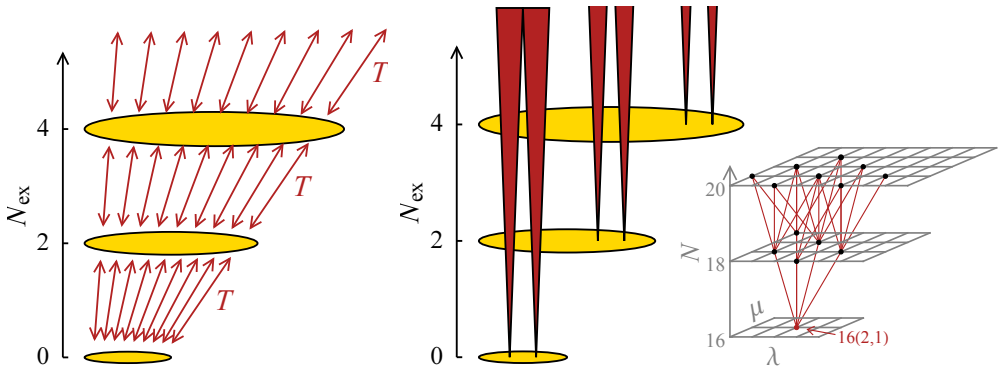

Figure 1: Reorganization of the NCCI many-body space into symplectic irreps: (left) the kinetic energy connects many-body states related by 0 or ± 2 oscillator quanta (as indicated by arrows), but (right) only connects states within a symplectic irrep (shaded cones). The detailed structure of an $\mathrm{Sp}(3,\mathbb{R})$ irrep in terms of U(3) irreps $N(\lambda,\mu)$ is illustrated in the inset (bottom right).

work potentially provides a means of identifying and restricting the basis to include only those highly excited configurations which dominantly contribute to the nuclear wavefunction, thereby (it is hoped) reducing the size of the basis necessary to obtain accurate results.

In this contribution, we briefly present a framework for *ab initio* calculations of nuclear structure in a SpNCCI scheme (Sec. 2). We then examine the symmetries arising in a SpNCCI calculation for ^{6}Li (Sec. 3). We observe both the dominance of symplectic symmetry in the individual wave functions and the emergence of families of states related by symplectic symmetry. These results are from work described in Ref. [17].

2 Symplectic NCCI framework

The SpNCCI basis for the nuclear many-body problem consists of states which reduce an $\mathrm{Sp}(3,\mathbb{R}) \supset \mathrm{U}(3) \supset \mathrm{SO}(3)$ subgroup chain, *i.e.*, which are arranged into nested irreps of all three of these groups. A symplectic irrep is built starting from some U(3) irrep with some lowest number of oscillator quanta, the *lowest grade irrep* (LGI). Laddering with the symplectic raising operator ($A \propto b^\dagger b^\dagger$), which creates pairs of oscillator quanta, generates the rest of the symplectic irrep, which is an infinite tower of U(3) irreps of increasing oscillator number. In practice, for SpNCCI calculations, this irrep must be truncated at some finite number of oscillator quanta.

To understand the quantum numbers for the SpNCCI basis, we first note that the group $\mathrm{U}(3) = \mathrm{U}(1) \times \mathrm{SU}(3)$ is the product of the U(1) generated by the harmonic oscillator number operator, with quantum number N, and the Elliott SU(3) group, which provides quantum numbers (λ,μ). Thus, a U(3) irrep is labeled by quantum

numbers $\omega \equiv N_\omega(\lambda_\omega, \mu_\omega)$. The structure of a symplectic irrep is uniquely defined by the U(3) quantum numbers $\sigma \equiv N_\sigma(\lambda_\sigma, \mu_\sigma)$ of its LGI, which thus serve as the $\mathrm{Sp}(3,\mathbb{R})$ quantum numbers of the symplectic irrep. The detailed structure of an $\mathrm{Sp}(3,\mathbb{R})$ irrep in terms of U(3) irreps is illustrated in the inset of Fig. 1, specifically for the $16(2,1)$ irrep of ^{8}Be.[1]

At the bottom of the group chain, SO(3) is the orbital angular momentum group, which provides the quantum number L. While the $\mathrm{Sp}(3,\mathbb{R})$ subgroup chain describes orbital (spatial) structure, there is also the complementary SU(2) spin group, with quantum number S. Orbital and spin angular momenta couple to give total angular momentum J. The SpNCCI basis is therefore classified according to symmetry labels for the subgroup chain

$$\underset{N_\sigma(\lambda_\sigma,\mu_\sigma)}{[\mathrm{Sp}(3,\mathbb{R})} \supset \underset{N_\omega(\lambda_\omega,\mu_\omega)}{\mathrm{U}(3)} \supset \underset{L}{\mathrm{SO}(3)}] \times \underset{S}{\mathrm{SU}_S(2)} \supset \underset{J}{\mathrm{SU}_J(2)}. \tag{2.1}$$

Recall that here $N_\omega(\lambda_\omega, \mu_\omega)$ are the U(3) quantum number of the basis state itself — so, if we are only interested in U(3) symmetry, we can simply designate these $N(\lambda, \mu)$. Then, $N_\sigma(\lambda_\sigma, \mu_\sigma)$ are the U(3) quantum numbers of the LGI from which the entire symplectic irrep is built.

When defining an NCCI basis, it is more transparent and convenient to work with the number of oscillator *excitations* N_{ex} relative to the lowest Pauli-allowed oscillator configuration for the nucleus. Configurations with $N_{\mathrm{ex}} = 0$ are traditionally known as "$0\hbar\omega$" configurations, those with $N_{\mathrm{ex}} = 2$ as "$2\hbar\omega$" configurations, *etc.* Similarly, for a SpNCCI basis, we shall refer to the number $N_{\omega,\mathrm{ex}}$ (or simply N_{ex}) of excitation quanta for U(3) irreps and $N_{\sigma,\mathrm{ex}}$ for the LGIs of $\mathrm{Sp}(3,\mathbb{R})$ irreps. Thus, in the symplectic decomposition of the many-body space shown schematically Fig. 1 (right), each disk (light shading) respresents states with a given $N_{\mathrm{ex}} = 0$, 2, or 4, while each cone (dark shading) represents a symplectic irrep with LGI at $N_{\sigma,\mathrm{ex}} = 0$, 2, or 4.

In our SpNCCI framework, matrix elements of the Hamiltonian (or other operators) in the symplectic many-body basis are determined from certain "seed" matrix elements by use of symplectic laddering operations. The approach is based on ideas initially proposed by Suzuki and Hecht [18, 19], but these have now been extended to accommodate general, realistic internucleon interactions.

In order to evaluate the matrix elements of an operator in the SpNCCI basis, we first decompose the operator in terms of SU(3)-coupled components, or *unit tensors*. We then apply commutation relations of these unit tensors with the symplectic laddering operators to recursively express all matrix elements in terms of matrix elements among certain lowest states, specifically, the LGIs. We explicitly expand

[1] The U(1) label N appearing in the U(3) labels $N(\lambda, \mu)$ is actually not the number of oscillator quanta, *per se*, but rather the dimensionless oscillator Hamiltonian, which also includes a zero-point contribution of 3/2 for each nucleon [12]. Thus, in the lowest Pauli-allowed oscillator configuration of ^{8}Be, the four s-shell nucleons contribute 3/2 each, and the four p-shell nucleons contribute 5/2 each, giving $N = 16$, as in the $16(2,1)$ irrep shown.

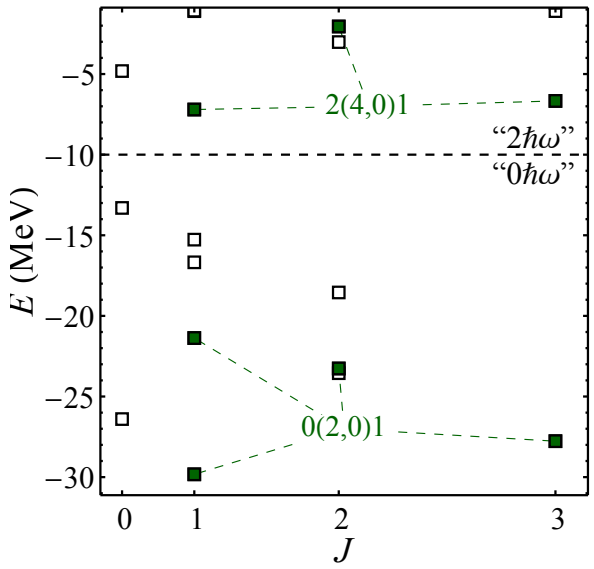

Figure 2: Energy eigenvalues from an SpNCCI calculation for ^{6}Li. Energies are plotted *vs.* $J(J+1)$, as conventional for rotational analysis [5]. States below the dashed line are predominantly $0\hbar\omega$, while those above the line have predominantly $2\hbar\omega$ (or higher) contributions. States having dominant U(3) $\times$ SU(2) contributions with $N_{\rm ex}(\lambda,\mu)S$ quantum numbers $0(2,0)1$ and $2(4,0)1$ are highlighted (solid symbols, as labeled).

these LGIs in terms of the SU(3) no-core shell model [SU(3)-NCSM] basis and use the SU(3)-NCSM code `LSU3shell` [20] to evaluate the seed matrix elements. The recurrence then involves coefficients obtained through vector coherent state (VCS) methods [21–23].

3 Illustration: Symplectic symmetry in ^{6}Li

Since SpNCCI calculations are carried out in an $\mathrm{Sp}(3,\mathbb{R}) \supset \mathrm{U}(3)$ basis, we can immediately extract the decomposition of each eigenfunction into contributions with different symmetry characters, for all the groups in the chain (2.1). That is, we can decompose the wave function according to any combination of the quantum numbers $\sigma = N_\sigma(\lambda_\sigma,\mu_\sigma)$ for $\mathrm{Sp}(3,\mathbb{R})$ and $\omega = N_\omega(\lambda_\omega,\mu_\omega)$ for U(3), as well as the more familiar orbital angular momentum L and spin S.

By examining such decompositions, we can start to answer some of the questions we laid out above: Do the highly-excited oscillator-basis contributions to the nuclear wave functions primarily come from low-lying symplectic irreps, suggesting that symplectic truncation may be feasible? And can an $\mathrm{Sp}(3,\mathbb{R}) \supset \mathrm{U}(3)$ irrep structure provide a useful classification scheme for understanding the nuclear eigenspectrum?

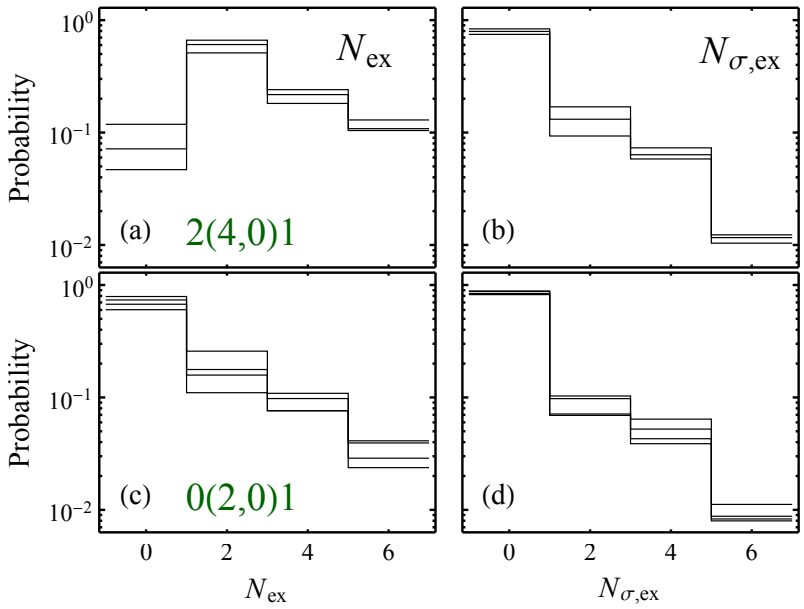

Figure 3: Decompositions of calculated eigenstates by oscillator excitation quanta $N_{\rm ex}$ (left) and by the $N_{\sigma,\rm ex}$ of the contributing symplectic irrep (right). Decompositions are shown for the highlighted states from Fig. 2, with dominant contributions from U(3) $\times$ SU(2) symmetry $0(2,0)1$ (bottom) or $2(4,0)1$ (top). Only oscillator configurations with even values of $N_{\rm ex}$ contribute to natural parity states.

Here we consider a SpNCCI calculation of ^{6}Li, for which the low-lying energy spectrum is shown in Fig. 2. This calculation is based on the JISP16 internucleon interaction [24], with no Coulomb interaction (*i.e.*, pure isoscalar). For initial examination and benchmarking purposes, we simply choose a space which is truncated at 6 oscillator quanta, with oscillator basis parameter $\hbar\omega = 20\,\mathrm{MeV}$. That is, we take all symplectic irreps with LGIs having up to $N_{\sigma,\rm max} = 6$ excitation quanta, then truncate each symplectic irrep to basis states with up to $N_{\rm max} = 6$ excitation quanta.[2]

Each of the states in Fig. 2 is found to have at most one or two dominant U(3) $\times$ SU(2) contributions, that is, well-defined ω and spin quantum numbers.

[2]The resulting spectrum is identical to that for a traditional $N_{\rm max} = 6$ M-scheme NCCI calculation, since both spaces include all intrinsic excitations of up to 6 quanta (this equivalence permits rigorous numerical validatation against traditional NCCI codes such as MFDn [25, 26]). While the traditional M-scheme NCCI basis consists of laboratory-frame Slater determinants (which include center-of-mass excitations and which, while having definite M, are in general admixtures of all $J \geq |M|$), the SpNCCI basis is defined in the intrinsic frame (consisting of states which are free of center-of-mass excitations and which are also naturally J-coupled). Compare the resulting dimension of 197 822 for the laboratory-frame $M = 0$ space [3] with 3484 for the intrinsic-frame $J = 0$ space [27], for ^{6}Li at $N_{\rm max} = 6$.

However, we focus on two specific U(3)×SU(2) "families" of states in this discussion, identified by the filled symbols in Fig. 2. We shall see that these together form part of a larger family of states with the same dominant symplectic symmetry.

Let us start by classifying the states in the spectrum of Fig. 2 according to contributions from configurations with different numbers of oscillator quanta. The calculated states below an excitation energy of $\sim 20\,\mathrm{MeV}$, as demarcated by the horizontal dashed line in Fig. 2, are dominated by $N_{\mathrm{ex}} = 0$ contributions. That is, in traditional shell model parlance, they have predominantly $0\hbar\omega$ character. Above this point in the spectrum, eigenstates dominated by $N_{\mathrm{ex}} = 2$ contributions, or $2\hbar\omega$ states, begin to appear.

To provide a more quantitative picture of this situation, decompositions by N_{ex} are shown in Fig. 3 (left): specifically, decompositions for the $0\hbar\omega$ states highlighted at the bottom of Fig. 2 are overlaid in the lower panel [Fig. 3(b)], and decompositions for the $2\hbar\omega$ states highlighted at the top of Fig. 2 are overlaid in the upper panel [Fig. 3(a)].[3] Clearly the "$0\hbar\omega$" states are not described entirely in the valence shell, but rather are heavily "dressed" with excited oscillator configurations, nor are the "$2\hbar\omega$" states entirely orthogonal to the valence space. However, the $0\hbar\omega$ states are dominated by $N_{\mathrm{ex}} = 0$ contributions at the 60%–80% level, while, for the $2\hbar\omega$ states, the $N_{\mathrm{ex}} = 0$ contributions fall below the 15% level.

We now look at the full decomposition with respect to U(3) × SU(2) character, labeled by the U(3) × SU(2) quantum numbers $N_{\mathrm{ex}}(\lambda,\mu)S$, in Fig. 4. The states in the $0\hbar\omega$ family highlighted at the bottom of Fig. 2 all have dominant U(3) × SU(2) contribution $0(2,0)1$. [For the ground state of ^{6}Li, the U(3) structure — and $0(2,0)1$ dominance — was explored by Dytrych *et al.* [28], on the basis of *ab initio* SU(3)-NCSM calculations.] Contributions from the other $0\hbar\omega$ U(3) × SU(2) irreps appear at the few percent level. This pattern of U(3)×SU(2) contributions is shown for the 1^+_1 ground state and 3^+_1 first excited state in Fig. 4(c,d). The states in the $2\hbar\omega$ family highlighted at the top of Fig. 2 instead have dominant U(3) × SU(2) contribution $2(4,0)1$, as shown for the 1^+ and 3^+ states of that family in Fig. 4(a,b).

While the U(3) × SU(2) decomposition begins to tell us about the symmetry properties of these states, it provides only partial information on the symplectic structure. Any SpNCCI basis state with N_{ex} excitation quanta comes from a symplectic irrep with $N_{\sigma,\mathrm{ex}} \leq N_{\mathrm{ex}}$. That is, the basis state may itself be part of an LGI ($N_{\sigma,\mathrm{ex}} = N_{\mathrm{ex}}$), or it may be obtained by the action of the symplectic raising operator from a lower LGI ($N_{\sigma,\mathrm{ex}} < N_{\mathrm{ex}}$).

Each bar in the U(3) × SU(2) decomposition histograms in Fig. 4 represents the total probability contribution of many basis states from several U(3) × SU(2)

[3] When interpreting these, and subsequent, decompositions in an oscillator basis, it is important to keep in mind that they reflect a particular choice of oscillator length (here, corresponding to $\hbar\omega = 20\,\mathrm{MeV}$) and are subject to change as the oscillator basis is dilated to other values of $\hbar\omega$. Therefore, one should be cautious in attaching undue physical significance, *e.g.*, interpreting them to mean that any given state has fundamentally a "$0\hbar\omega$" or "$2\hbar\omega$" nature with respect to some true mean-field vacuum.

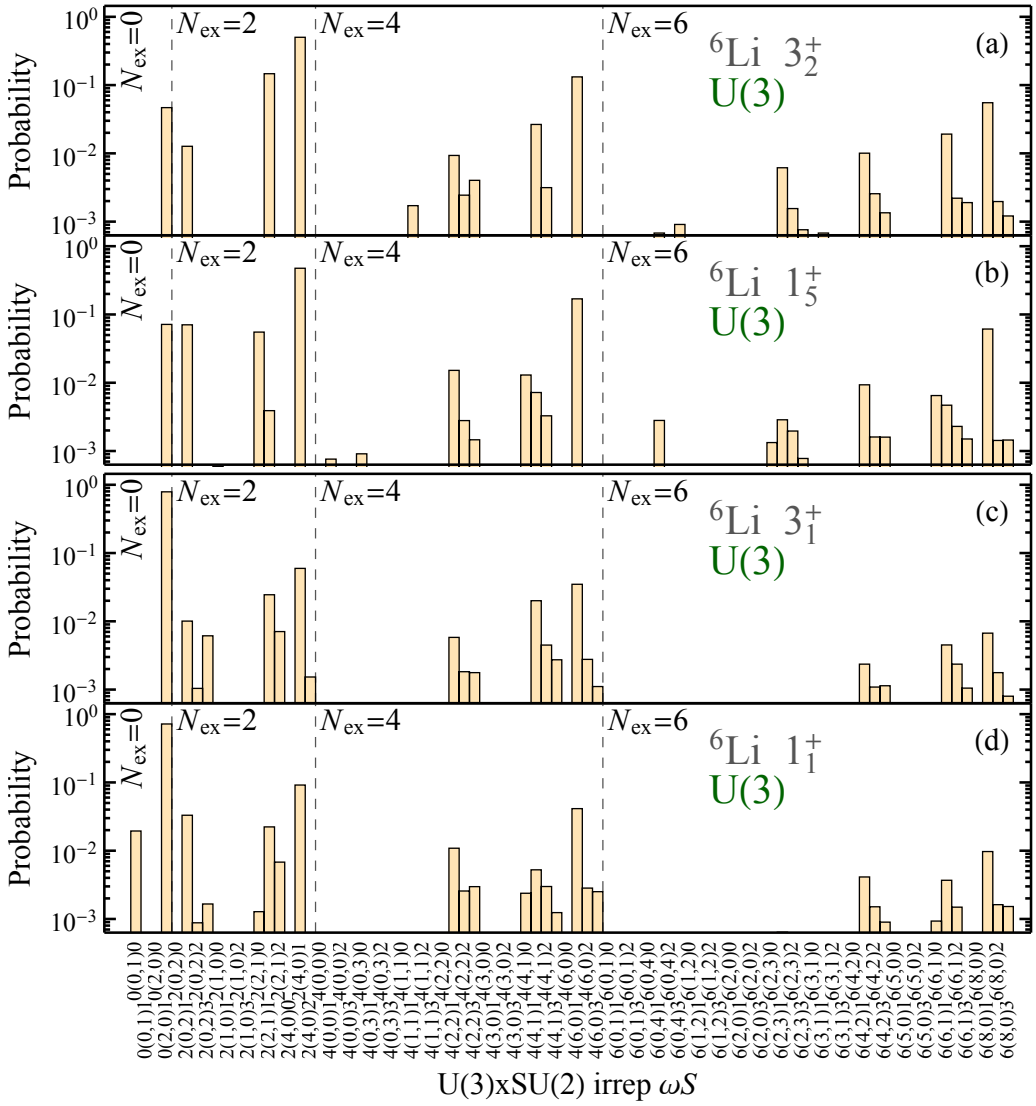

Figure 4: Decompositions of calculated eigenstates by U(3) × SU(2) contributions $N_{\rm ex}(\lambda,\mu)S$: for the lowest 1^+ and 3^+ states (c–d) and for excited 1^+ and 3^+ states of predominantly $2\hbar\omega$ character (a–b). The contributions are ordered, from left to right in the figure, first by $N_{\rm ex}$, and then by SU(3) and spin quantum numbers.

irreps sharing the same quantum numbers. For instance, there are in fact 8 different U(3) × SU(2) irreps with quantum numbers $2(4,0)1$, for ^{6}Li. One of these comes from the $N_{\sigma,\rm ex} = 0$ symplectic irrep $0(2,0)1$, while the rest are themselves LGIs of $N_{\sigma,\rm ex} = 2$ symplectic irreps.

Before breaking each wave function down into contributions from specific $\mathrm{Sp}(3,\mathbb{R})$ quantum numbers, it is informative to simply look at the decomposition of each wave

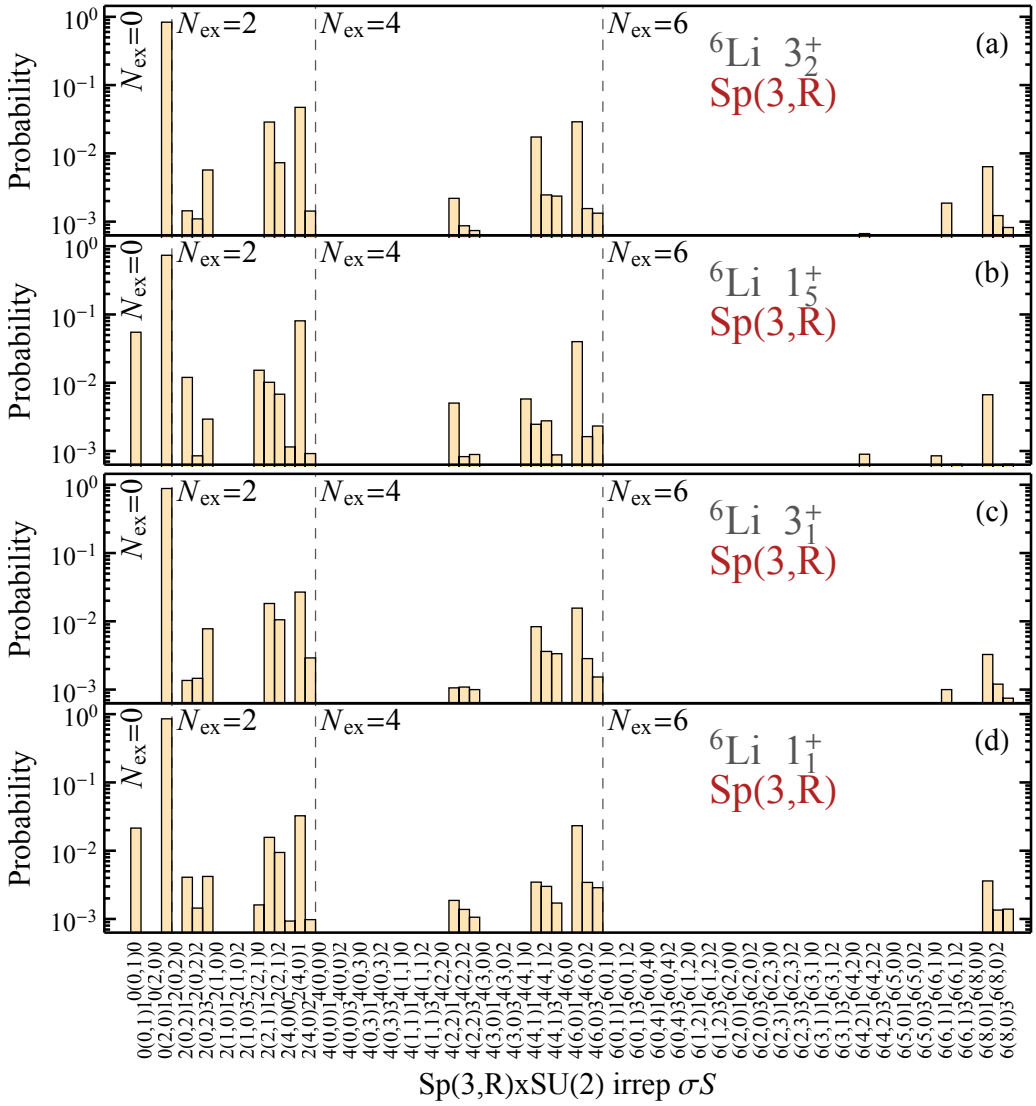

Figure 5: Decompositions of calculated eigenstates by $\mathrm{Sp}(3,\mathbb{R})\times\mathrm{SU}(2)$ contributions $N_{\sigma,\mathrm{ex}}(\lambda_\sigma,\mu_\sigma)S$: for the lowest 1^+ and 3^+ states (c–d) and for excited 1^+ and 3^+ states of predominantly $2\hbar\omega$ character (a–b).

function with respect to how "excited" the contributing symplectic irreps are. Decompositions by $N_{\sigma,\mathrm{ex}}$ are shown in Fig. 3 (right).

Since the $N_{\sigma,\mathrm{ex}} = 0$ contribution must be at least as large as the $N_{\mathrm{ex}} = 0$ contribution, clearly the $0\hbar\omega$ states will have a significant $N_{\sigma,\mathrm{ex}} = 0$ contribution. In particular, for the highlighted family of states with $\mathrm{U}(3) \times \mathrm{SU}(2)$ character $0(2,0)1$ [Fig. 3(d)], the $N_{\sigma,\mathrm{ex}} = 0$ contributions are in the 70%–90% range. Thus, a substantial portion of the excited oscillator contributions [Fig. 3(c)] actually comes

from $N_{\sigma,\mathrm{ex}} = 0$ sympletic irreps. This is encouraging for the viability of symplectic truncation schemes.

But what about the $2\hbar\omega$ states? For the highlighted family of states with $\mathrm{U}(3) \times \mathrm{SU}(2)$ character $2(4,0)1$ [Fig. 3(b)], recall that this $2(4,0)1$ contribution could come either from the $N_{\sigma,\mathrm{ex}} = 0$ symplectic irrep $0(2,0)1$ or from the $2(4,0)1$ LGIs of $N_{\sigma,\mathrm{ex}} = 2$ symplectic irreps. So, are these $2\hbar\omega$ states dominated by contributions from $N_{\sigma,\mathrm{ex}} = 0$ symplectic irreps or from $N_{\sigma,\mathrm{ex}} = 2$ symplectic LGIs? From the $N_{\sigma,\mathrm{ex}}$ decompositions [Fig. 3(b)], it is immediately apparent that they are dominated by contributions from $N_{\sigma,\mathrm{ex}} = 0$, at the $> 70\%$ level.

The full decompositions with respect to $\mathrm{Sp}(3,\mathbb{R}) \times \mathrm{SU}(2)$ character, labeled by the $\mathrm{Sp}(3,\mathbb{R}) \times \mathrm{SU}(2)$ quantum numbers $N_{\sigma,\mathrm{ex}}(\lambda_\sigma,\mu_\sigma)S$, are shown in Fig. 5. The most notable feature apparent in Fig. 5 is the dominance of the contribution from the $0(2,0)1$ symplectic irrep, for all these states. In fact, all the highlighted states in Fig. 2 — both the low-lying $0\hbar\omega$ states with $0(2,0)1$ $\mathrm{U}(3) \times \mathrm{SU}(2)$ character and the high-lying $2\hbar\omega$ states with $2(4,0)1$ $\mathrm{U}(3) \times \mathrm{SU}(2)$ character — receive their dominant contribution from this single $N_{\sigma,\mathrm{ex}} = 0$ symplectic irrep, the $0(2,0)1$ symplectic irrep.

Thus, states with very different oscillator excitation content [Fig. 3 (left)], and consequently very different U(3) content (Fig. 4), nonetheless form a larger family of states sharing the same symplectic symmetry. This is fundamentally the idea of the classification scheme for the SpNCCI *basis* states in an $\mathrm{Sp}(3,\mathbb{R}) \supset \mathrm{U}(3)$ scheme (2.1): many U(3) irreps form a single $\mathrm{Sp}(3,\mathbb{R})$ irrep, as illustrated in Fig. 1 (inset). However, here we find the same $\mathrm{Sp}(3,\mathbb{R}) \supset \mathrm{U}(3)$ organizational scheme holding for the physical spectrum of energy *eigen*states obtained from an *ab initio* calculation.

4 Conclusions

In conclusion, a framework for *ab initio* no-core configuration interaction calculations in an $\mathrm{Sp}(3,\mathbb{R}) \supset \mathrm{U}(3)$ symplectic basis is now in place. This scheme builds on an existing SU(3)-coupled framework for the nuclear problem and combines it with the group-theoretical machinery for $\mathrm{Sp}(3,\mathbb{R})$.

In initial calculations, illustrated here with ^{6}Li, we confirm $\mathrm{Sp}(3,\mathbb{R})$ as an approximate symmetry of states throughout the low-energy spectrum. These states are characterized by mixing of a few dominant symplectic irreps. Then, families of states arise with similar symplectic structure, despite their differing U(3) content.

To take full advantage of approximate symplectic symmetry in nuclei, as a means of accelerating convergence of NCCI calculations, it will be necessary to go beyond the simple benchmark $N_{\max}$ truncation scheme for the SpNCCI space illustrated here. While some gains can likely be made by truncating the space to dominant $N_\sigma(\lambda_\sigma,\mu_\sigma)S$ symplectic subspaces, these subspaces are highly degenerate, especially as we go to higher $N_{\sigma,\mathrm{ex}}$.

The most effective truncation will therefore likely come by identifying the few dominant symplectic irreps from within these subspaces (*e.g.*, by some variant of importance truncation [29]). Once these "Hamiltonian preferred" symplectic irreps are identified, a more stringent truncation can be carried out to a relatively small number of symplectic irreps within each subspace.

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