Convergence in the Symplectic No-Core Configuration Interaction Framework

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Abstract

The symplectic no-core configuration interaction (SpNCCI) framework for *ab initio* nuclear structure predictions carries out calculations in a correlated many-body basis which encodes an approximate $\mathrm{Sp}(3,\mathbb{R})$ symplectic symmetry of the nucleus. This framework opens up the possibility of identifying and restricting the many-body space to include only the basis states which dominantly contribute to the nuclear wavefunctions of interest. We examine the convergence of ^{3}He binding energy and matter radius in a basis truncated according to a simple scheme based on the symplectic symmetry.

Keywords: *Symplectic no-core configuration interaction (SpNCCI); symmetry adapted basis; ab initio nuclear physics*

1 Introduction

In no-core configuration interaction (NCCI) approaches to solving the nuclear many-body problem, one of the biggest challenges is tied to the necessity of describing both short and long range correlations within the chosen basis. In the harmonic oscillator basis, this translates to the need to include oscillator configurations (distributions of particles over harmonic oscillator shells) with many oscillator quanta. However, the basis grows rapidly as the number of oscillator quanta increases, and the size of the resulting basis quickly exceeds current computational limits. So, we must look to methods which allow us to reduce the necessary size of the basis while still capturing the relevant physics. In the symplectic no-core configuration interaction (SpNCCI) framework, the many-body problem is solved in a basis consisting of highly correlated states which have definite $\mathrm{Sp}(3,\mathbb{R})$ symmetry. The goal is then to use the approximate symplectic symmetry of the nucleus [1–6] to significantly reduce the basis size.

Truncation of the many-body basis by symplectic symmetry is well-suited for long range observables that are sensitive to the tail of the wavefunction, e. g., nuclear radii and $E2$ transition strengths. The need to include highly excited configurations in the

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http://www.ntse.khb.ru/files/uploads/2018/proceedings/McCoy.pdf.

nuclear wavefunction is largely due to the kinetic energy term of nuclear Hamiltonian. The nuclear interaction dominates the Hamiltonian at for low number of oscillator quanta, whereas the kinetic energy dominates for highly excited states. Since the symplectic symmetry is conserved by the kinetic energy [7,8], the SpNCCI basis is broken into subspaces, or irreducible representations (irreps), which are not connected by the kinetic energy. Moreover, while the nuclear interaction does mix states within different symplectic irreps, it has been observed [1–6] that the interaction only strongly mixes states belonging to a relatively small number of symplectic irreps. Thus, identifying the relatively small number of symplectic irreps containing the dominantly contributing low-lying states also provides a selection criteria for the "important" high-lying states. The overall effect is that more of the the highly excited basis states necessary for describing the tail of the wavefunction are included in the basis than would have been possible with the traditional $N_{\max}$ truncated many-body basis [9].

In this paper, we briefly present the SpNCCI basis (Section 2) and computational framework (Section 3). In Section 4, we then discuss convergence behaviour in a symplectic truncated basis using the ^{3}He binding energy and matter radius to illustrate.

2 The symplectic basis

The SpNCCI many-body basis is composed of states with definite $\mathrm{Sp}(3,\mathbb{R})$ symmetry. These states can be thought of as linear combinations of the harmonic oscillator configurations (or Slater determinants) that form the traditional NCCI [or no-core shell model (NCSM)] basis [9]. In this sense, the SpNCCI basis states build in single-particle correlations. However, in actual calculations, the SpNCCI basis states are never explicitly expressed in terms of Slater determinants, as discussed in Section 3.

In the symplectic basis, the states are first organized into irreducible representations (irreps) of $\mathrm{Sp}(3,\mathbb{R})$ [7, 8]. Within each symplectic irrep, the basis states are then organized into irreps of U(3). That is, the basis reduces the subgroup chain $\mathrm{Sp}(3,\mathbb{R}) \supset \mathrm{U}(3)$. The U(3) group factorizes into $\mathrm{U}(3) \sim \mathrm{U}(1) \times \mathrm{SU}(3)$, where U(1) is the group of the harmonic oscillator Hamiltonian, for which the quantum number is the total number N of oscillator quanta, and SU(3) is Elliott's SU(3) group, generated by orbital angular momentum and quadrupole operators [10, 11]. Thus, basis states within the U(3) irrep are characterized by definite U(3) symmetry $\omega = N_\omega(\lambda_\omega, \mu_\omega)$. In other words, the basis states have definite total number of oscillator quanta N_ω, as in traditional NCCI calculations, as well as definite Elliott SU(3) symmetry $(\lambda_\omega, \mu_\omega)$.

Each symplectic irrep is then labeled according to the single U(3) irrep with the fewest number of oscillator quanta in the symplectic irrep. This irrep is referred to as the *lowest grade irrep* (LGI). An LGI can be identified as the states which are annihilated by the symplectic lowering operator $B^{(0,2)}$. The remaining states in the symplectic irrep are obtained by repeatedly acting on the LGI with the symplectic raising operator $A^{(2,0)}$. Each raising operation adds two oscillator quanta. Thus, a single symplectic irrep contains states with oscillator quanta $N_\omega = N_\sigma,\ N_\sigma + 2,\ \ldots$ The laddering operator can be applied infinitely many times, so the symplectic irrep is, in principle, unbound. However, the SpNCCI framework requires a finite basis, so each irrep must be truncated, e. g., to some finite number of oscillator quanta.

3 Calculations in symplectic basis

In the SpNCCI framework, the matrix elements of the nuclear Hamiltonian (and other observables) are obtained directly in the symplectic basis via recurrence. Such an approach was first proposed for a symplectic shell model by Reske, Suzuki and Hecht [12–14]. These methods are extended in the SpNCCI framework to accommodate general spin and isospin-dependent nonlocal nuclear interactions for *ab initio* calculations [5].

In this recurrence, the matrix elements between high-lying SpNCCI basis states (with many oscillator quanta) are expressed in terms of states with fewer number of oscillator quanta. This expression is obtained by making use of commutation relation of the Hamiltonian operator with the symplectic ladder operator, which relate states with different number of oscillator quanta [5]. The recurrence starts with the matrix elements between the lowest lying states in each symplectic irrep (between LGIs). The matrix elements between LGIs are obtained by expanding the LGIs in terms of SU(3) coupled configurations and then using the existing symmetry adapted no-core shell model (SA-NCSM) code `LSU3Shell` [15] to compute the matrix elements.

The expansion of the LGIs in terms of SU(3) coupled configurations is obtained by solving for the simultaneous null space of the $\mathrm{Sp}(3,\mathbb{R})$ lowering operator $B^{(0,2)}$ and the center-of-mass oscillator number operator $N_{\mathrm{cm}}^{(0,0)}$, in the SA-NCSM basis. The resulting states are fully antisymmetric by construction with zero center-of-mass excitations [center-of-mass free (CMF)]. The intrinsic symplectic raising operator preserves both the antisymmeterization and CMF nature of the states. Consequently, the basis state obtained by acting on the LGI with the raising operator are likewise both antisymmeterized and CMF.

4 Convergence

The efficacy of the SpNCCI framework depends on how well we can obtain converged values for nuclear observables in a symplectic truncated basis. Before we can develop effective truncation schemes, we need first to understand the convergence behaviour of these observables. As a simple example, we consider the convergence behaviour of the ^{3}He binding energy (Fig. 1) and matter radius (Fig. 2) obtained using the code `spncci` [17].

For this illustration, we simply restrict the basis to symplectic irreps generated from LGIs with oscillator quanta less than or equal to some fixed number. We quote this number in terms of excitation quanta N_{ex}, i. e., number of oscillator quanta above the lowest Pauli allowed number of quanta N_0 for the given nucleus. Thus the restriction on the LGI is given by $N_{\sigma,\mathrm{ex}} \leq N_{\sigma,\mathrm{max}}$ where $N_{\sigma,\mathrm{ex}} = N_\sigma - N_0$. Each of the panels in Fig. 1 and Fig. 2 correspond to a different value of $N_{\sigma,\mathrm{max}}$. For example, the calculations in Fig. 1(a) are carried out in a symplectic basis which includes only the symplectic irreps with $N_{\sigma,\mathrm{ex}} \leq 2$, i. e., in an $N_{\sigma,\mathrm{max}} = 2$ truncated basis.

Within each $N_{\sigma,\mathrm{max}}$ truncated space, each of the symplectic irreps in the basis must be truncated to some finite number of states. Here we include only the states in each irrep with number of excitation quanta ($N_{\mathrm{ex}} = N_\omega - N_0$) less than some maximum value N_{max}, i. e., $N_{\mathrm{ex}} \leq N_{\mathrm{max}}$. Each of the curves shown in the panel corresponds to successively higher maximum allowed excitation quanta ($N_{\mathrm{max}} = 2, 4, \ldots, 16$). A

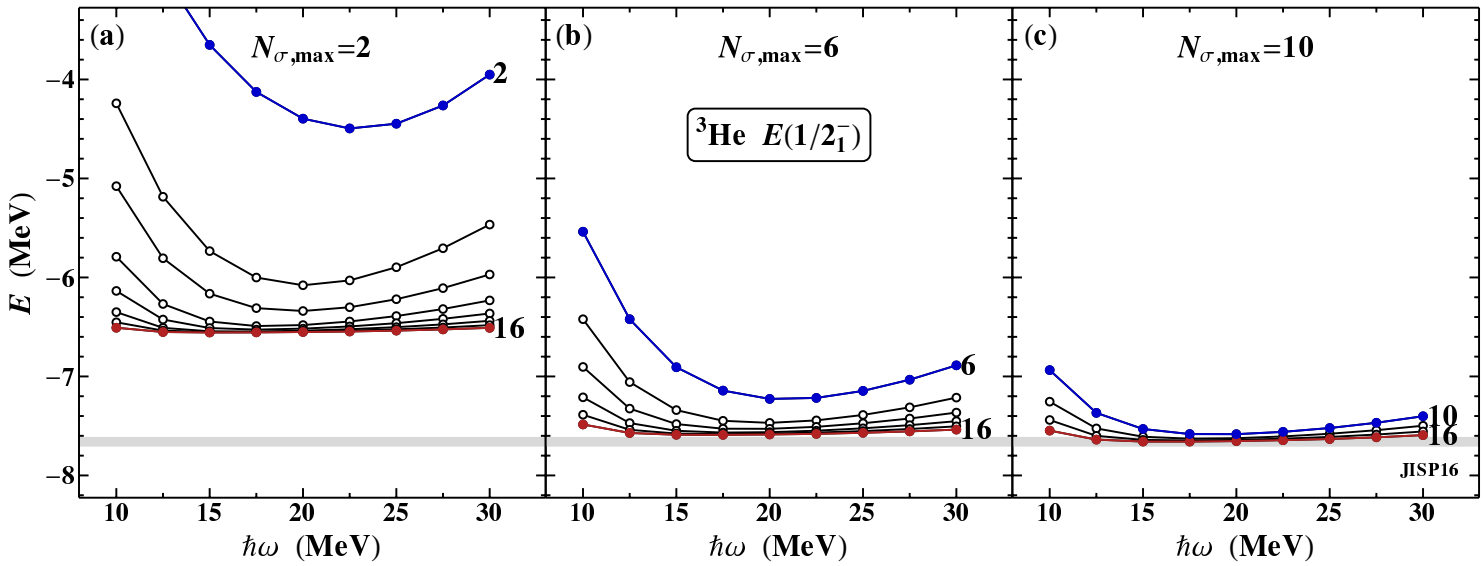

Figure 1: Convergence of the binding energy of ^{3}He in the SpNCCI framework. The set of symplectic irreps included in the calculation is given by (a) $N_{\sigma,\max} = 2$, (b) $N_{\sigma,\max} = 6$, or (c) $N_{\sigma,\max} = 10$. Each curve is labeled by the $N_{\max} = N_{\sigma,\max}, N_{\sigma,\max} + 2, \ldots, 16$ truncation used within these irreps. The gray band indicates the approximate full-space value. These calculations are based on the JISP16 internucleon interaction [16].

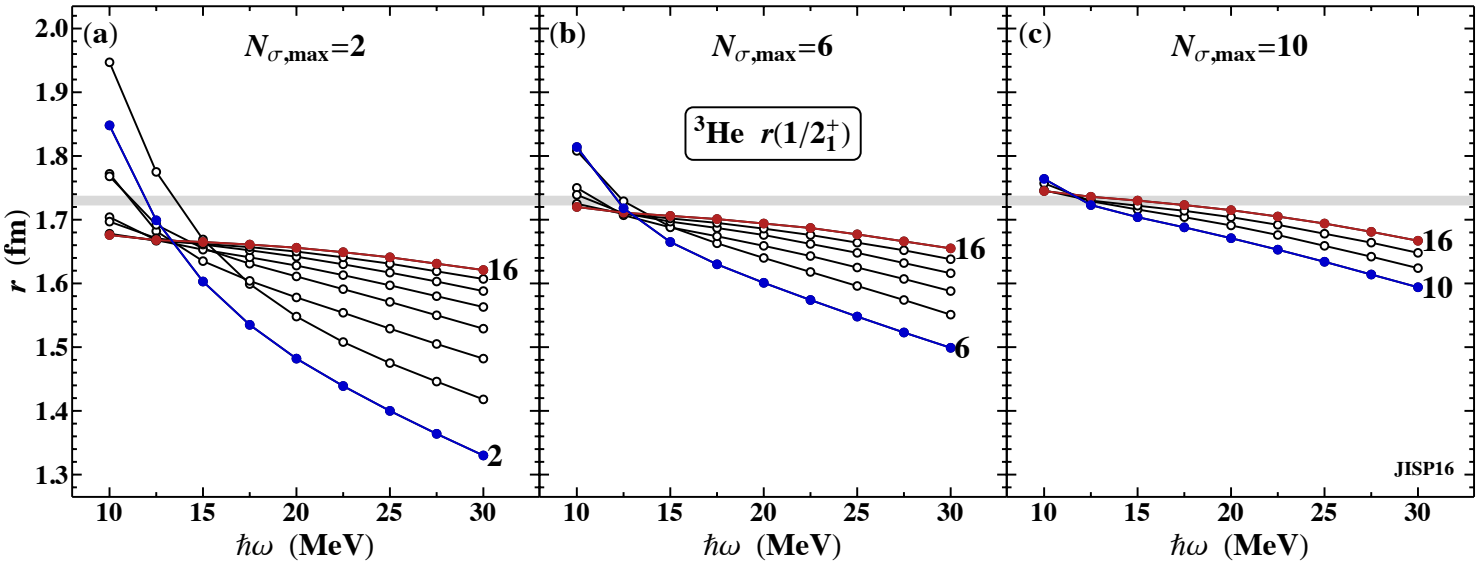

Figure 2: Convergence of the ^{3}He r.m.s. matter radius in the SpNCCI framework. The set of symplectic irreps included in the calculation is given by (a) $N_{\sigma,\max} = 2$, (b) $N_{\sigma,\max} = 6$, or (c) $N_{\sigma,\max} = 10$. Each curve is labeled by the $N_{\max} = N_{\sigma,\max}, N_{\sigma,\max} + 2, \ldots, 16$ truncation used within these irreps. The gray band indicates the approximate full-space value. These calculations are based on the JISP16 internucleon interaction [16].

truncated basis in which $N_{\sigma,\max} = N_{\max}$ (blue curve) will yield identical results to those obtained in the traditional NCCI framework in an $N_{\max}$ truncated basis.

Let us first consider the binding energy of ^{3}He shown in Fig. 1. When convergence is achieved, the results obtained no longer depend on the choice of many-body basis. In the SpNCCI framework, this means that convergence is signalled when results no longer depend on the length scale of the oscillator basis (results are independent of $\hbar\omega$) and when they no longer change as additional basis states are included in the basis (as $N_{\max}$ and $N_{\sigma,\max}$ increase). In Fig. 1(a), the results for $N_{\max} = N_{\sigma,\max} = 2$ (blue curve) vary significantly for different values of $\hbar\omega$. However, with each successive $N_{\max}$, the curves begin to flatten, signalling the results are approaching convergence with respect to $\hbar\omega$. Similarly, with increasing $N_{\max}$, the curves fall closer together, indicating that the values are approaching convergence with respect to $N_{\max}$. By $N_{\max} = 16$ (red curve) the results are comparatively independent of $\hbar\omega$ and $N_{\max}$.

However, the convergence within an $N_{\sigma,\max}$ space is not the same as convergence within the full space (all symplectic irreps included). Note that the converged value obtained in the $N_{\sigma,\max} = 2$ space [Fig. 1(a)] is not the same as value obtained in the full many-body basis[1] (gray line). Thus, the results are not yet converged with respect to the number of symplectic irreps included, i. e., with respect to $N_{\sigma,\max}$. In Fig. 1(b), the energies obtained in the space including the $N_{\sigma,\max} = 6$ irreps are, again, converging with respect to $\hbar\omega$ and $N_{\max}$. However, now they are converging to a different value. Similarly, in Fig. 1(c), the energies converge within the $N_{\sigma,\max} = 10$ space with increasing $N_{\max}$, but, again, to a different value. However, the difference between the $N_{\max} = 16$ curve for $N_{\sigma,\max} = 6$ and $N_{\max} = 10$ is significantly smaller than the difference between the $N_{\sigma,\max} = 2$ and $N_{\sigma,\max} = 6$ curves. This relatively small shift of the energy curves at fixed $N_{\max}$ between $N_{\sigma,\max} = 6$ and $N_{\sigma,\max} = 10$ indicates that the results are nearing convergence with respect to $N_{\sigma,\max}$.

Let us now take a look at the r.m.s radius of ^{3}He. In traditional NCCI calculations, which corresponds here to the $N_{\sigma,\max} = N_{\max}$ calculations, we see a strong dependence on the length scale $\hbar\omega$ [20, 21]. However, within an $N_{\sigma,\max}$ truncated space, as more and more excited configurations are included in the basis (increasing $N_{\max}$), the values for the radius converge with respect to both $N_{\max}$ and $\hbar\omega$, just as they did for the energy. The effect of including additional $\mathrm{Sp}(3,\mathbb{R})$ irreps (increasing $N_{\sigma,\max}$) is then to simply shift the value of the radius obtained at large $N_{\max}$.

This behaviour suggests that a reasonable approximate value may be obtained within a comparatively small subspace composed of a relatively small number of symplectic irreps. In this example, the inclusion of just the higher N_{ex} states belonging to the $N_{\sigma,\max} = 2$ irreps is sufficient to obtain a value for the radius which is converged with respect to $\hbar\omega$ and $N_{\max}$ and which is within 0.1 fm of the full space value. For $N_{\max} = 16$, the largest calculation shown for $N_{\sigma,\max} = 2$ in Fig. 2(a), the dimension of the space for $J = 1/2$ is 217 where as the full M-scheme space (basis for traditional NCCI calculations) at $N_{\max} = 16$ with angular momentum projection $M = 1/2$ has dimension 392 039, which is more than three orders of magnitude larger than that of the corresponding symplectic basis.

[1] The approximate full space values are obtained using the NCCI code `MFDn` [18, 19].

5 Conclusion

Carrying out calculations in a symplectic basis opens up the possibility obtaining accurate predictions in a much smaller basis than possible in the traditional NCCI framework, particularly for long range observables. The simple $N_{\sigma,\max}$ truncation scheme used in the results shown in Fig. 1 and Fig. 2 barely begins to touch on the potential uses of the symplectic symmetry as a means of defining efficient truncation schemes. The challenge is to identify the relevant symplectic irreps by, e. g., a perturbative approach similar to the method employed in the importance truncated no-core-shell model (IT-NCSM) [22].

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