Supplemental material for "A nucleus-dependent valence-space approach to nuclear structure"

DETAILS OF THE CALCULATION

Unless otherwise noted, all calculations are carried out using the same interaction as in Ref. [1]: a chiral NN interaction at N^{3}LO [2] with a 3N interaction at N^{2}LO [3], consistently free-space SRG evolved to $\lambda_{\rm SRG} = 1.88\,{\rm fm}^{-1}$ in a harmonic oscillator basis with a frequency of 24 MeV [4]. We employ a model space truncation defined by all single-particle states with $2n + \ell \leq e_{\rm max} = 12$, except for the case of the calcium isotopes in Fig. 2, where we use e_{max}=14 to compare with previous calculations. The interaction is then transformed to the Hartree-Fock basis of the fractionally-filled ENO reference. It is perhaps worth remarking that in order to ensure that the one-body density matrix remains diagonal, the Hartree-Fock calculation should be carried out on the entire ensemble, maintaining a consistent single-particle basis. At this point the normal-ordered residual 3N part is discarded.

The IM-SRG decoupling is performed using the Magnus formulation presented in Ref. [5] with the arctangent variant of the White generator [6, 7]

$$\eta = \frac{1}{2}\arctan\frac{2H_{\rm od}}{\Delta}, \tag{1}$$

where $H_{\rm od}$ and Δ are the suitably-defined [8] off-diagonal part of the Hamiltonian and the energy denominator, respectively. Briefly, in the Magnus formulation, the transformed Hamiltonian is written as

$$\begin{aligned} H_s &= e^{\Omega_s} H_0 e^{-\Omega_s} \\ &= H_0 + [H_0, \Omega_s] + \frac{1}{2}[\Omega_s, [\Omega_s, H_0]] + \ldots \end{aligned} \tag{2}$$

where Ω_s is the anti-hermitian generator of the full unitary transformation. The generator Ω_s is updated at each step in the flow using the Baker-Campbell-Hausdorff formula

$$\begin{aligned} e^{\Omega_{s+ds}} &= e^{\eta_s ds} e^{\Omega_s} \\ \Omega_{s+ds} &= \eta_s ds + \Omega_s + \frac{1}{2} ds\,[\eta_s, \Omega_s] + \ldots \end{aligned} \tag{3}$$

Both equations (2) and (3) are carried out until convergence is achieved.

The procedure used for this work may be summarized as the following:

1. Set the starting Hamiltonian H_0 as relative kinetic energy plus NN+3N interaction
2. Perform a Hartree-Fock calculation using the occupation numbers of the ensemble reference ρ
3. Transform H_0 to the resulting Hartree-Fock basis
4. Normal order H_0 w.r.t. ρ and discard the residual 3N part
5. Use IM-SRG to decouple the core orbits from all other orbits
6. Use IM-SRG to decouple the valence space from all other orbits
7. Normal order w.r.t. the core of the valence space
8. Diagonalize the transformed valence-space Hamiltonian with a standard shell-model code

In all cases the valence space is defined by one major harmonic-oscillator shell for protons and neutrons (e.g., for ^{16}N, protons in the $0p$ shell and neutrons in the $1s0d$ shell). For details on the IM-SRG decoupling, see Refs. [8, 9]. The code used for this work is written in `C++` and is freely available online [10]. The valence-space diagonalizations are performed with NuShellX@MSU [11].

For some light nuclei, we compare with results of the importance-truncated no-core shell model (IT-NCSM). Since the IT-NCSM and IM-SRG employ different model space truncations (many-body states and single-particle states, respectively), only converged results can be meaningfully compared. Consequently the oscillator frequencies need not be the same, as the converged result should be independent of this parameter.

ENSEMBLE REFERENCE STATE

As stated in the text, the details of the ensemble reference state do not enter into the calculation. We simply use the corresponding fractional occupation numbers during the normal ordering and IM-SRG decoupling. However we give here a qualitative description of the reference, and we will present a more detailed formal discussion elsewhere. The reference should be constructed so that all irreducible density matrices encountered in the generalized Wick theorem of Ref. [12] vanish aside from the diagonal one-body density matrix corresponding to the occupation fraction n. For a j shell with $N_j = 2j+1$ m-states, the elimination of the N_j-body density matrices necessitates the inclusion of an N_j-particle (totally filled) Slater determinant in the ensemble. Eliminating the $N_j - 1$-body density matrices requires the additional inclusion of all determinants with $N_j - 1$ particles, etc. In the end, one finds that the ensemble will include all determinants with particle number ν ranging from 0 to N_j, and all possible m-state configurations, with weights given by $c_\alpha(\nu) = n^\nu (1-n)^{N_j - \nu}$.

PERFORMANCE

A necessary consequence of the present approach is that a distinct valence-space Hamiltonian is produced for each nucleus, in contrast to the standard shell model approach where one Hamiltonian is used for an entire region of nuclei. An impressive part of the IM-SRG is the low computational cost associated with decoupling a valence-space Hamiltonian in this manner, comparable with the cost of a (closed shell) single-reference IM-SRG or coupled cluster with singles and doubles (CCSD) calculation. The $e_{\max} = 14$ results require less than one day on a single node with 24 CPUs. Therefore converged results for the entire *sd* shell, for instance, may be obtained with only tens of thousands of CPU-hours.

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