Importance Truncated No-Core Shell Model *

R. Roth

Institut für Kernphysik, TU Darmstadt, Schlossgartenstr. 9, 64289 Darmstadt, Germany

One of the most universal tools for the *ab initio* solution of the nuclear many-body problem is the No-Core Shell Model (NCSM). It is widely used for the description of ground states and low-lying excited states of nuclei throughout the p-shell [1]. Apart from energies, detailed spectroscopic information and form-factors can be extracted from the resulting many-body eigenstates. The limitation of converged NCSM calculations to the p-shell results solely from the dimension of the $N_{\max}\hbar\omega$ model space, which grows factorially with the number of particles and the truncation parameter $N_{\max}$. However, for the description of an individual eigenstate, e.g. the ground state, many of the basis states are irrelevant, i.e., their amplitude in the expansion of the eigenstates is extremely small or zero. If these irrelevant states were known beforehand one could restrict the model space to the important basis states and thus reduce the dimension significantly.

Such an *a priori* measure for the importance of individual basis states for the description of a selected target state can be derived within many-body perturbation theory [2]. Starting from an initial approximation of the target state $|\Psi_{\text{ref}}\rangle$, the importance of a basis state $|\Phi_\nu\rangle$ can be estimated through its amplitude in the first-order perturbative expansion of the target state,

$$\kappa_\nu = -\frac{\langle\Phi_\nu|\,\mathrm{H}\,|\Psi_{\text{ref}}\rangle}{\epsilon_\nu - \epsilon_{\text{ref}}} \;.$$

In the framework of multiconfigurational perturbation theory the reference state can already be a superposition of many basis states. Note, however, that the perturbative importance measure entails a npnh-hierarchy: assuming a two-body Hamiltonian, only those states that differ form the reference state by a 2p2h excitation at most can have non-zero κ_ν. We therefore use an iterative scheme for the construction of the importance truncated $N_{\max}\hbar\omega$ model space: We start from a simple shell-model Slater determinant as initial reference state and, in the first iteration, construct all 1p1h and 2p2h configurations, keeping only those with $|\kappa_\nu| > \kappa_{\min}$. After solving the eigenvalue problem in this basis, the eigenstate is used as new reference state for the second iteration, which extends the importance truncated model space up to the 4p4h level.

Typically we use as sequence of values for $\kappa_{\min}$ starting from $\kappa_{\min} = 3\times10^{-5}$ and extrapolate the energies to $\kappa_{\min} \to 0$, thus recovering the full space. That this scheme is very reliable is demonstrated in Fig. 1, where the importance truncated NCSM results after one and two iteration are compared to the full NCSM (using ANTOINE [4]) for ^{4}He with the V_{UCOM} interaction [3]. Although the dimension of the model space is reduced by up to two orders of magnitude through the importance truncation, the full NCSM result is reproduced after two iterations to an accuracy of 10 keV for all $N_{\max}$ and $\hbar\omega$. The reduction of the model space dimension becomes more significant for heavier nuclei. For ^{16}O as depicted in Fig. 1, this allows us to go to large $N_{\max}$ whereas the full NCSM is restricted to $N_{\max} \leq 8$. The importance truncated NCSM after two iterations already shows good agreement with the full NCSM results. The effect of configurations up to the 6p6h level can be included either via a third iteration or perturbatively and turns out to be small (cf. Fig. 1).

The importance truncated NCSM combines the intrinsic advantages of the NCSM (translational invariance, variation upper bound) with a computationally efficient and physically motivated truncation scheme that extends its range to medium-heavy nuclei.

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References

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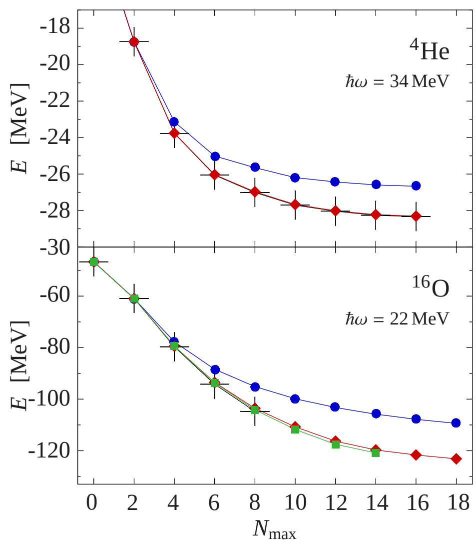

Figure 1: Convergence of the ground state energy of ^{4}He and ^{16}O as function of $N_{\max}$ using the V_{UCOM} interaction. The crosses indicate full NCSM results. The disks and diamonds depict results of the importance truncated NCSM after one and two iterations, i.e. up to 2p2h and 4p4h configurations, respectively. The squares include a perturbative correction for up to 6p6h configurations.