Comment on "*Ab initio* Study of ^{40}Ca with an Importance-Truncated No-Core Shell Model"

In a recent Letter [1], Roth and Navrátil present an importance-truncation scheme for the no-core shell model. The authors claim that their truncation scheme leads to converged results for the ground state of ^{40}Ca. We believe that this conclusion cannot be drawn from the results presented in the Letter [1]. Furthermore, the claimed convergence is at variance with general expectations of many-body theory. In particular, coupled-cluster calculations indicate that a significant fraction of the correlation energy is missing.

The truncation proposed in the Letter [1] is based on an importance sampling that selects the most important particle-hole (ph) excitations. It produces unlinked diagrams and lacks size extensivity [2]. This implies that the quality of the truncation in large systems (such as ^{40}Ca) cannot be judged from its behavior in small systems (such as ^{4}He or ^{16}O). In the absence of exact results for ^{40}Ca, one needs to show that the truncation converges (i) with respect to (w.r.t.) the number of states retained in the importance sampling, (ii) w.r.t. the size of the model space (i.e., the maximal number of excited oscillator quanta approaches $N_{\max} \to \infty$), and (iii) w.r.t. the number of ph excitations. For ^{40}Ca, the Letter [1] fails to provide convincing evidence for the full convergence, in particular, with respect to (iii).

Figure 4 of the Letter [1] shows the convergence for ^{40}Ca and the V_{UCOM} potential. The convergence w.r.t. step (ii) is not yet established due to the considerable slopes at $N_{\max} = 16$. We consider the convergence w.r.t. (iii) and note that a model space of size $N_{\max}$ can accommodate up to $N_{\max}$ ph excitations. Thus, no judgment about $4p4h$ excitations is possible when $N_{\max}$ does not exceed the value 4 by a considerable amount. The agreement between the $4p4h$ results and the exact results up to $N_{\max} = 4$ merely demonstrates the convergence of step (i) in small model spaces. Beyond $N_{\max} = 4$, no exact results are provided to judge the quality of the $4p4h$ truncation. Beyond $N_{\max} = 8$, the description is limited to $3p3h$ excitations. Clearly, the explicit demonstration of the convergence w.r.t. (iii) is missing.

A second calculation for ^{40}Ca and the $V_{\mathrm{low}k}$ potential is shown in Fig. 5b of the Letter [1]. This figure demonstrates that step (i) converges for the small model space with $N_{\max} = 4$. It also shows that the results are converged w.r.t. (ii) *for fixed* $3p3h$ excitations. Again, the convergence w.r.t. (iii) is missing.

How accurate are the $3p3h$ results presented in Fig. 5b of the Letter [1]? To answer this question, we performed coupled-cluster calculations [3] for the same nucleus and interaction. This method is size extensive, includes a significant fraction of the $4p4h$ excitations, and is very accurate [2]. The Hamiltonian is translationally invariant, and the operator of the kinetic energy is exactly as in the Letter [1] and as in our 2007 papers. The CCSD expectation value of the center-of-mass Hamiltonian is below 200 keV and similar in size to the result cited in the Letter [1]. The CCSD(T) results [3] indicate that the ground-state energy for ^{40}Ca and $V_{\mathrm{low}k}$ is about 40 MeV lower than obtained in the Letter [1]. The authors of the Letter [1] seem to have missed this result from our work [3], and in their comparison for ^{16}O, they referred to our CCSD result but not to the more accurate CCSD(T) result.

The shortcomings of a $3p3h$ truncation are well known. First, $N = Z$ nuclei have strong α-particle correlations which are of $4p4h$ character. Second, the calculation of the ground state of the $N = Z$ nucleus ^{56}Ni (See Table 1 of Ref. [4]) shows that the $3p3h$ truncation (CISDT) is of rather poor quality compared to $4p4h$ (CISDTQ) and inferior to coupled-cluster theory. Third, calculations for small molecules (see, e.g., Fig. 3 of Ref. [2]) show that the $3p3h$ truncation is much less accurate than coupled-cluster theory.

In summary, the claim of a converged $3p3h$ truncation for ^{40}Ca has not been substantiated in the Letter [1]. This claim disagrees with expectations from many-body theory [2,4], and the reported result deviates considerably from coupled-cluster calculations [3].

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