Roth and Navrátil Reply: In the preceding Comment [1] Dean *et al.* criticize our calculations for the ground-state energy of 40 Ca within the importance-truncated no-core shell model (NCSM) [2]. In particular, they address the role of configurations beyond the $3\,p3h$ level, which have not been included in our 40 Ca calculations for large model spaces.

Before responding to this point, the following general statements are in order. For the atomic nucleus as a self-bound system, translational invariance is an important symmetry. The only possibility to preserve translational invariance when working with a Slater determinant basis is to (i) use the harmonic oscillator (HO) single-particle states and (ii) truncate the model space according to the total HO excitation energy $N_{\rm max}\hbar\Omega$, as done in the *ab initio* NCSM. This is important not only for obtaining proper binding or excitation energies, but also for a correct extraction of physical wave functions.

The minimal violation of the translational invariance was one of the main motivations for developing the importance-truncation scheme introduced in [2]. In this scheme, we start with the complete $N_{\rm max}\hbar\Omega$ HO model space and select important configurations via perturbation theory. All symmetries are under control and our importance-truncated NCSM calculations are completely variational, i.e., they provide an upper bound for the ground-state energy of the system.

The restriction to the 3p3h level, made for computational reasons in the $N_{\rm max}>8$ calculations for $^{40}{\rm Ca}$, is not inherent to the importance-truncation scheme. The explicit inclusion of 4p4h configurations—though computationally more demanding—is straightforward, even for the largest $N_{\rm max}\hbar\Omega$ model spaces discussed. To demonstrate this we have performed full 4p4h calculations for $^{40}{\rm Ca}$ in a $14\hbar\Omega$ no-core model space at $\hbar\Omega=24$ MeV using the $V_{\rm low}k$ interaction employed in [2]. The resulting groundstate energy of $E_{4p4h}=-471.0$ MeV can be compared with $E_{3p3h}=-461.2$ MeV for the 3p3h calculation reported in Fig. 5(b) with an uncertainty of typically 1 MeV due to the extrapolation $\kappa_{\rm min}\to 0$. Thus the 4p4h configurations change the resulting ground-state energy of $^{40}{\rm Ca}$ by approximately 2%.

In addition to the explicit inclusion of 4p4h or higher-order configurations one can use perturbative corrections based on the eigenstates obtained in the importance truncated space, to account for excluded higher-order configurations. Alternatively, Davidson-type corrections, which are employed successfully in quantum chemistry [3], can be employed. These techniques even restore size extensivity in an approximate way.

The coupled-cluster method (CCM) used by the authors of [1] lacks the above discussed features important for the nuclear many-body problem, in particular, it violates translational invariance from the very beginning and it does not fulfill the variational principle. The problem of a spurious center-of-mass contamination of the many-body states in

CCM is not resolved and often not even mentioned (see, e.g., Ref. [4]). In [1] it is stated that the CCM Hamiltonian is translationally invariant. By inspecting Eqs. (4) and (6) in [5], one can see that it is not the case as the parameter β_{CoM} is fine-tuned and thus nonzero in general. Moreover, noniterative triples corrections like CCSD(T), as referred to in [1], tend to overestimate the correlation energy or even collapse. It is claimed that the CCM is very accurate. A closer inspection of recently published nuclear manybody results does not support this statement. In Ref. [6], the ⁴He binding energy with the chiral nucleon-nucleon (NN) potential was determined with an uncertainty of several MeV. The same is obtained in the ab initio NCSM with accuracy of 10 keV [7]. The CCM binding energy results for ¹⁶O with the identical chiral N³LO NN potential obtained in Refs. [5,8] differ by more than 5 MeV.

The CCSD(T) ground-state energy for 40 Ca with V_{lowk} reported in Ref. [4] is about 30 MeV lower than our 4p4h result (CCSD is about 20 MeV lower). Taking into account the small 2% difference of our 3p3h and 4p4h results and the violation of the variational principle and the translational invariance in the CCM method, we believe that the CCM result overestimates the exact ground-state energy in this case.

In conclusion, the importance truncation provides an efficient way to extend the domain of NCSM calculations to medium-heavy nuclei while preserving translational invariance and the variational principle and allowing for systematic and controlled improvements.

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- [1] D. J. Dean *et al.*, preceding Comment, Phys. Rev. Lett. **101**, 119201 (2008).
- [2] R. Roth and P. Navrátil, Phys. Rev. Lett. 99, 092501 (2007).
- [3] W. Duch and G. H. F. Diercksen, J. Chem. Phys. **101**, 3018 (1994) and references therein.
- [4] G. Hagen et al., Phys. Rev. C 76, 044305 (2007).
- [5] J. R. Gour et al., Phys. Rev. C 74, 024310 (2006).
- [6] D. J. Dean and M. Hjorth-Jensen, Phys. Rev. C **69**, 054320 (2004).
- [7] S. Quaglioni and P. Navrátil, Phys. Lett. B 652, 370 (2007).
- [8] M. Wloch et al., Phys. Rev. Lett. 94, 212501 (2005).