Truncation and Extrapolation of Ab initio Calculations in a Finite Model Space

Sidney A. Coon

Department of Physics, University of Arizona, Tucson, Arizona 85721, USA

Estimating the errors due to the truncation to a model space is crucial for successful *ab initio* calculations which must always employ an extrapolation scheme to obtain a result, be it an energy spectrum or another property of the calculated nucleus. A popular model space is formed by the construction of a variational trial wavefunction which uses a complete set of many-body basis states based upon a summation over products of three-dimensional harmonic oscillator (HO) functions [1]. These model spaces are defined by a truncation of the expansion characterized by a counting number (\mathcal{N}) and by the intrinsic scale ($\hbar\omega$) of the basis HO functions chosen; in short by the ordered pair $(\mathcal{N}, \langle \omega \rangle)$. In calculations such as no-core shell model or the no-core full configuration method [2] traditional extrapolations are made with the truncation parameter N_{max} related to the maximum number of oscillator quanta, above the minimum configuration, kept in the model space. In the spirit of effective field theory (EFT) [3] we have examined the dependence of the truncated results on two regulators: the HO ultraviolet (uv) regulator (related to the HO energy $\hbar\omega$ and N_{max}) associated with the maximum momentum included in the basis. There are two proposed definitions of the infrared (ir) momentum regulator inherent in a finite-dimensional HO basis. One definition is based upon the lowest momentum given by $\hbar\omega$ itself [3] and the other upon the infrared momentum which corresponds to the maximal radial extent needed to encompass the many-body system in coordinate space. Extending both the uv cutoff to infinity and the ir cutoff to zero is prescribed for a converged calculation. Our investigations with different Hamiltonians (i.e. different "realistic" NN interactions) show a significant tendency towards simple scaling in these two regulators as the calculation approaches separately the ir and uv limits. We have established a novel extrapolation parameter composed of the uv and the ir regulators of Ref. [3] which appears universal (that is, NN interaction and nucleus independent) and is useful even for modest model spaces. The robustness of these results to different interactions and to different light nuclei is quite striking. Other *ab initio* methods in a HO basis, such as the coupled-cluster approach in nuclear physics and configuration-interaction methods applied to quantum dots, may also be amenable to our EFT approach to truncation and extrapolation of finite basis results to the infinite matrix limit.

References

[1] S. A. Coon and O. Portilho, "Variational Methods for the Few-Body Bound State in a Harmonic Oscillator Basis", Lecture Notes in Physics 273, ed. L. S. Ferreira, A. C. Fonseca, and L. Streit, (Springer-Verlag 1987) pp 219-242.

[2] P. Maris, J. P. Vary, and A. M. Shirokov, "*Ab initio* no-core full configuration calculations of light nuclei", Phys. Rev. C79, 014308 (2009).

[3] I. Stetcu, B. R. Barrett, U. van Kolck "No-core shell model in an effective-field-theory frame-work", Physics Letters B **653**, 358 (2007).

Results obtained in collaboration with M. I. Avetian^{*a*}, M. K. G. Kruse^{*a*}, U. van Kolck^{*a,b*}, P. Maris^{*c*} and J. P. Vary^{*c*}

^a Department of Physics, University of Arizona, Tucson, Arizona 85721

^b Institut de Physique Nucléaire, Université Paris-Sud, IN2P3/CNRS, F-91406 Orsay Cedex, France

^c Department of Physics and Astronomy, Iowa State University, Ames, IA 50011