

# Universal Properties of Infrared Extrapolations in a Harmonic Oscillator Basis

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## Abstract

We continue our studies of infrared (ir) and ultraviolet (uv) regulators of no-core shell model calculations. We extend our results that an extrapolation in the ir cutoff with the uv cutoff above the intrinsic uv scale of the interaction is quite successful, not only for the eigenstates of the Hamiltonian but also for expectation values of operators considered long range. The latter results are obtained with Hamiltonians transformed by the similarity renormalization group (SRG) evolution. On the other hand, a suggested extrapolation in the uv cutoff when the ir cutoff is below the intrinsic ir scale is neither robust nor reliable.

**Keywords:** *No-core shell model; convergence of expansion in harmonic oscillator functions; ultraviolet regulator; infrared regulator*

## 1 Introduction

Variational calculations based upon a harmonic oscillator (HO) basis expansion have a long history in nuclear structure physics. If one views a shell-model calculation as a variational calculation, expanding the configuration space merely serves to improve the trial wave function [1]. A parallel program uses the HO eigenfunctions as a basis of a finite linear expansion to make a straightforward variational calculation of the properties of light nuclei [2]. Theorems based upon functional analysis established the asymptotic convergence rate of these calculations as a function of the counting number ( $\mathcal{N}$ ) which characterizes the size of the expansion basis (or model space) [3,4]. The convergence rates of these theorems (inverse power laws in  $\mathcal{N}$  for “non smooth” potentials such as Yukawa’s with strong short range correlations and exponential in  $\mathcal{N}$  for “smooth” potentials such as gaussians) were demonstrated numerically in Ref. [3] for the HO expansion and in Ref. [5] for the analogous expansion in hyperspherical harmonics. These convergence theorems are used to extrapolate to the “infinite” basis in few-body studies [6] and in “*ab initio*” “no-core shell model” (NCSM) calculations of *s*- and *p*-shell nuclei [7]. However, the HO expansion basis has an intrinsic scale parameter  $\hbar\omega$  which does not naturally fit into an extrapolation scheme based upon  $\mathcal{N}$  as discussed in Refs. [3,4,8]. Indeed the model spaces of these NCSM approaches are characterized by the ordered pair  $(\mathcal{N}, \hbar\omega)$ . Here the basis truncation parameter  $\mathcal{N}$  and the HO energy parameter  $\hbar\omega$  are variational parameters [7,9,10]. With the HO basis in the nuclear structure problem, convergence has been discussed, in practice, with an emphasis on obtaining those parameters which appear linearly in the trial function (i. e. convergence with  $\mathcal{N}$ ). In an early example,  $\hbar\omega$  is simply fixed at a value which gives the fastest convergence in  $\mathcal{N}$  [6]. Later, for each  $\mathcal{N}$  the non-linear parameter  $\hbar\omega$  is varied to obtain the minimal energy [9,11] for a fixed  $\mathcal{N}$  and then

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*<http://www.ntse-2013.khb.ru/Proc/Coon.pdf>.*

the convergence with  $\mathcal{N}$  is examined at that fixed value of  $\hbar\omega$ . Other extrapolation schemes have been proposed and used [10, 12].

It is the purpose of this contribution to continue an investigation of the extrapolation tools introduced in Ref. [13] which use  $\mathcal{N}$  and  $\hbar\omega$  on an equal footing. These tools are based upon the pair of ultraviolet (uv) and infrared (ir) cutoffs (each a function of both  $\mathcal{N}$  and  $\hbar\omega$ ) of the model space. These regulators were first introduced to the NCSM by Ref. [14] in the context of an effective field theory (EFT) approach. For a recent review of this program see Ref. [15].

The early *ab initio* calculations, both of the “no-core” shell model in which all nucleons are active [1] and of the Moshinsky program attempted to overcome the challenges posed by “non-smooth” two-body potentials by including Jastrow type two-body correlations in the trial wave function. Nowadays, the  $NN$  potentials are tamed by unitary transformations within the model space [16] or in free space by either the similarity renormalization group (SRG) evolution [17] or the  $V_{low k}$  truncation [18, 19]. In all three cases, this procedure generates effective many-body interactions in the new Hamiltonian. Neglecting these destroys the variational aspect of the calculation (and changes the physics contained in the calculation, of course). We retain the variational nature of our NCSM investigation by choosing a realistic smooth nucleon-nucleon ( $NN$ ) interaction Idaho N<sup>3</sup>LO [20] which has been used previously without renormalization within the model space for light nuclei ( $A \leq 6$ ) [9]. The Idaho N<sup>3</sup>LO potential is a rather soft one, with heavily reduced high-momentum components (“super-Gaussian falloff in momentum space”) as compared to earlier realistic  $NN$  potentials with a strongly repulsive core. Alternatively, in coordinate space, the contact interaction and the Yukawa singularity at the origin are regulated away so that this potential would be considered “smooth” by Delves and Schneider and the convergence in  $\mathcal{N}$  would be expected to be exponential [3, 4]. Even without the construction of an effective interaction, convergence with the Idaho N<sup>3</sup>LO  $NN$  potential is exponential in  $\mathcal{N}$ , as numerous studies have shown [9, 17].

We refer the reader to a comprehensive review article [7] on the no-core shell model (NCSM) for details and references to the literature. Inspired by EFT, one uses a truncation parameter  $\mathcal{N}$  which refers, not to the many-body system, but to the properties of the HO single-particle states. The many-body truncation parameter  $N_{max}$  is the maximum number of oscillator quanta shared by all nucleons above the lowest HO configuration for the chosen nucleus. One unit of oscillator quanta is one unit of the quantity  $(2n + l)$  where  $n$  is the principle quantum number and  $l$  is the angular quantum number. If the highest HO single-particle state of this lowest HO configuration has  $N_0$  HO quanta, then  $N_{max} + N_0 = N$  identifies the highest HO single-particle states that can be occupied within this many-body basis. Since  $N_{max}$  is the maximum of the *total* HO quanta above the minimal HO configuration, we can have at most one nucleon in such a highest HO single-particle state with  $N$  quanta. Note that  $N_{max}$  characterizes the many-body basis space, whereas  $N$  is a label of the corresponding single particle space. Let us illustrate this distinction with two examples. <sup>6</sup>He is an open shell nucleus with  $N_0 = 1$  since the valence neutron occupies the  $0p$  shell in the lowest many-body configuration. Thus if  $N_{max} = 4$  the single particle truncation  $N$  is 5. On the other hand, the highest occupied orbital of the closed shell nucleus <sup>4</sup>He has  $N_0 = 0$  so that  $N = N_{max}$ .

## 2 Ultraviolet and infrared cutoffs inherent to the finite HO basis

We begin by thinking of the finite single-particle basis space defined by  $N$  and  $\hbar\omega$  as a model space characterized by two momenta associated with the basis functions themselves. We follow Ref. [14] and define  $\Lambda = \sqrt{m_N(N + 3/2)\hbar\omega}$  as the momentum

(in units of MeV/c) associated with the energy of the highest HO level. The nucleon mass is  $m_N = 938.92$  MeV. To arrive at this definition one applies the virial theorem to this highest HO level to establish kinetic energy as one half the total energy [i. e.,  $(N + 3/2)\hbar\omega$ ] and solves the non-relativistic dispersion relation for  $\Lambda$ . Thus, the usual definition of an ultraviolet cutoff  $\Lambda$  in the continuum has been extended to discrete HO states. It is then quite natural to interpret the behavior of the variational energy of the system with addition of more basis states as the behavior of this observable with the variation of the ultraviolet cutoff  $\Lambda$ . Because the energy levels of a particle in a HO potential are quantized in units of  $\hbar\omega$ , the momentum difference between single-particle orbitals is  $\lambda = \sqrt{m_N\hbar\omega}$  and that has been taken to be an infrared cutoff [14]. That is, there is a low-momentum cutoff  $\lambda = \hbar/b$  where  $b = \sqrt{\frac{\hbar}{m_N\omega}}$  plays the role of a characteristic length of the HO potential and basis functions. Note however that there is *no* external confining HO potential in place. Instead the only  $\hbar\omega$  dependence is due to the scale parameter of the underlying HO basis. In Ref. [14] the influence of the infrared cutoff is removed by extrapolating to the continuum limit, where  $\hbar\omega \rightarrow 0$  with  $N \rightarrow \infty$  so that  $\Lambda$  is fixed. Clearly, one cannot achieve both the ultraviolet limit and the infrared limit by taking  $\hbar\omega$  to zero in a fixed- $N$  model space as this procedure takes the ultraviolet cutoff to zero. Other studies define the ir cutoff as the infrared momentum which corresponds to the maximal radial extent needed to encompass the many-body system we are attempting to describe by the finite basis space (or model space). These studies find it natural to define the ir cutoff by  $\lambda_{sc} = \sqrt{(m_N\hbar\omega)/(N + 3/2)}$  [17, 21]. Note that  $\lambda_{sc}$  is the inverse of the root-mean-square (rms) radius of the highest single-particle state in the basis;  $\langle r^2 \rangle^{1/2} = b\sqrt{N + 3/2}$ . We distinguish the two definitions by denoting the first (historically) definition by  $\lambda$  and the second definition by  $\lambda_{sc}$  because of its scaling properties demonstrated in the next Section.

### 3 Running of variational energies with cutoffs and establishment of intrinsic regulator scales

We display in the next two figures the running of the ground-state eigenvalue of the nucleus,  ${}^2\text{H}$ , on the truncated HO basis by holding one cutoff of  $(\Lambda, \lambda_{ir})$  fixed and letting the other vary. In Fig. 1 and the following figures,  $|\Delta E/E|$  is defined as  $|(E(\Lambda, \lambda_{ir}) - E)/E|$  where  $E$  reflects a consensus ground-state energy from benchmark calculations with this  $NN$  potential, this nucleus, and different few-body methods.

In Fig. 1 we hold fixed the uv cutoff of  $(\Lambda, \lambda_{ir})$  to display the running of  $|\Delta E/E|$  upon the suggested ir cutoff  $\lambda_{sc}$ . For fixed  $\lambda_{sc}$ , a larger  $\Lambda$  implies a smaller  $|\Delta E/E|$  since more of the uv region is included in the calculation. But we immediately see a qualitative change in the curves between the transition  $\Lambda = 700$  MeV and  $\Lambda = 900$  MeV; for smaller  $\Lambda$ ,  $|\Delta E/E|$  does not go to zero as the ir cutoff is lowered and more of the infrared region is included in the calculation. This behavior suggests that  $|\Delta E/E|$  does not go to zero unless  $\Lambda \geq \Lambda^{NN}$ , where  $\Lambda^{NN}$  is some uv regulator scale of the  $NN$  interaction itself. From this figure one estimates  $\Lambda^{NN} \sim 900$  MeV/c for the Idaho  $N^3\text{LO}$  interaction. For  $\Lambda < \Lambda^{NN}$  there will be missing contributions so “plateaus” develop as  $\lambda_{ir} \rightarrow 0$ , revealing this missing contribution to  $|\Delta E/E|$ . The “plateaus” that we do see are not flat as  $\lambda_{ir} \rightarrow 0$  and, indeed, rise significantly with decreasing  $\Lambda < \Lambda^{NN}$ . This suggests that corrections are needed to  $\Lambda$  and  $\lambda_{ir}$  which are presently defined only to leading order in  $\lambda_{ir}/\Lambda$ .

Around  $\Lambda \sim 700$  MeV/c and above the plot of  $|\Delta E/E|$  versus  $\lambda_{sc}$  in Fig. 1 begins to suggest a universal pattern, especially at large  $\lambda_{sc}$ . For  $\Lambda \sim 900$  MeV/c and above the pattern defines a universal curve for all values of  $\lambda_{sc}$ . This is the region where  $\Lambda \geq \Lambda^{NN}$  indicating that nearly all of the ultraviolet physics set by the potential

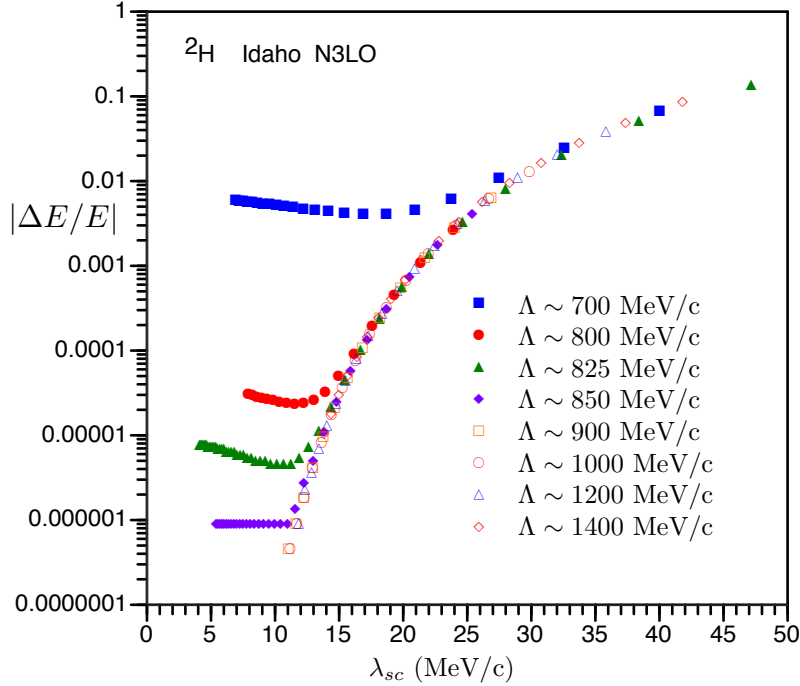


Figure 1: Dependence of the ground-state energy of  ${}^2\text{H}$  (compared to a converged value; see text) upon the ir momentum cutoff  $\lambda_{sc} = \sqrt{(m_N \hbar \omega)/(N + 3/2)}$  for fixed  $\Lambda = \sqrt{m_N(N + 3/2)\hbar\omega}$ .

has been captured. The universal curve can be fit by the  $|\Delta E/E| = a \exp(-b/\lambda_{sc})$  which suggests immediately that  $\lambda_{sc}$  could be used for extrapolation to the ir limit, provided that  $\Lambda$  is kept large enough to capture the uv region of the calculation, i. e.  $\Lambda \geq \Lambda^{NN}$ . Figure 1 is also the motivation for our appellation  $\lambda_{sc}$ , which we read as “lambda scaling”, since this figure exhibits the attractive scaling properties of this regulator.

The originally suggested ir cutoff  $\lambda = \sqrt{m_N \hbar \omega}$ , corresponding to the non-zero energy spacing between HO levels, gives not a universal curve for  $\Lambda \geq \Lambda^{NN}$  but instead a set of curves fit by  $|\Delta E/E| = a \exp(-B(\Lambda)/\lambda)$  (see Fig. 3 of Ref. [13]). That is,  $B$  is not a constant and independent of the uv cutoff  $\Lambda$ , as it should be in an EFT framework. One can remove the dependence of  $B$  upon  $\Lambda$  to a large extent by noting that  $\lambda = \sqrt{\Lambda \lambda_{sc}}$  so that  $\exp(-B/\lambda)$  becomes  $\exp\left(\frac{-B/\sqrt{\Lambda}}{\sqrt{\lambda_{sc}}}\right)$  and this multiplier of  $1/\sqrt{\lambda_{sc}}$  is constant to within a few per cent. This trivial manipulation demonstrates that the ir regulator which is independent of the uv cutoff is a function of  $\lambda_{sc}$ . The point is not that the ir regulator  $\lambda$  cannot be used to remove ir effects by extrapolating it to zero; indeed it works equally well to remove ir artifacts from a calculation as does  $\lambda_{sc}$  [13]. Indeed, any momentum cutoff  $\lambda_{sc} \leq \lambda_{ir} \leq \Lambda$  will remove ir artifacts, but the ir regulator which is independent of the uv cutoff is some function of  $\lambda_{sc}$ . It is  $\lambda_{sc}$  which causes the ir effects and one does not need to decrease an ir cutoff below that of  $\lambda_{sc}$  to remove ir effects (i. e. extrapolate to zero).

In Fig. 2 we hold fixed the ir cutoff of  $(\Lambda, \lambda_{ir})$  to display the running of  $|\Delta E/E|$  upon the cutoff  $\Lambda$ . Again plateaus are evident. Such a plateau-like behavior was attributed in Fig. 1 to a uv regulator scale characteristic of the  $NN$  interaction. Another “missing contributions” argument leads to a universal behavior at low  $\Lambda$  only if  $\lambda_{sc} \leq \lambda_{sc}^{NN}$  where  $\lambda_{sc}^{NN}$  is a second characteristic ir regulator scale implicit in the  $NN$  interaction itself. One can envisage such an ir cutoff as related to the lowest

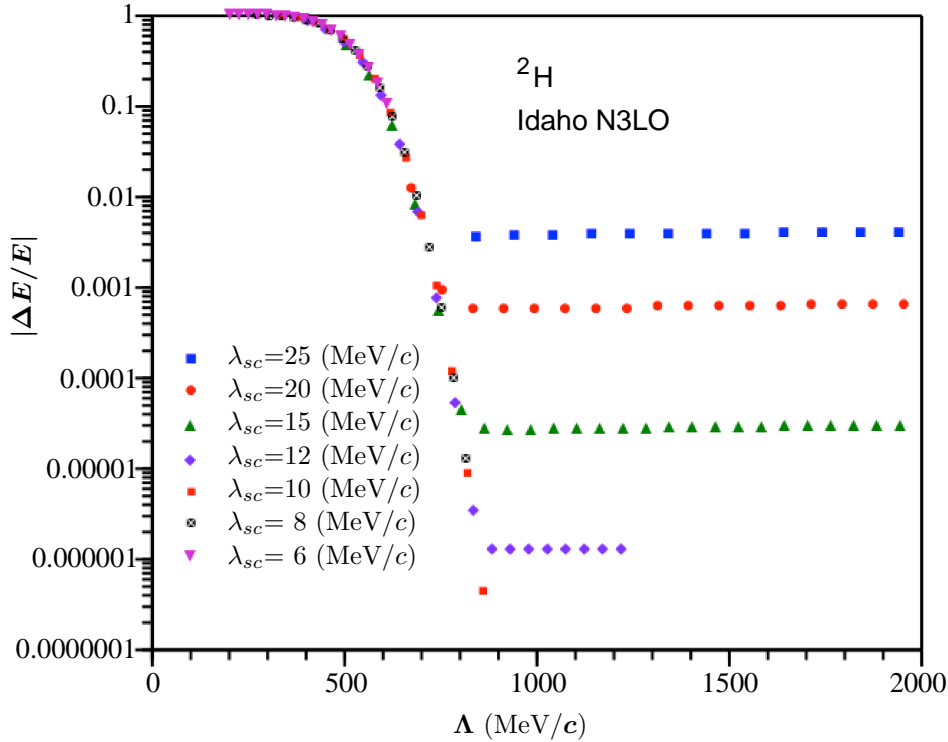


Figure 2: Dependence of the ground-state energy of  ${}^2\text{H}$  (compared to a converged value; see text) upon the uv momentum cutoff  $\Lambda$  for different values of the ir momentum cutoff  $\lambda_{sc}$ .

energy configuration that the  $NN$  potential could be expected to describe. This would be in the range of the deuteron binding momentum  $Q = 45$  MeV/c down to about 16 MeV/c which is the average of the four inverse scattering lengths. However the behavior of the running as  $\Lambda \geq \Lambda^{NN}$  again suggests that corrections are needed to  $\Lambda$  and  $\lambda_{ir}$  which are presently defined only to leading order in  $\lambda_{ir}/\Lambda$ .

Can one make an estimate of the uv and ir regulator scales of the  $NN$  interactions used in nuclear structure calculations? It is easy with the JISP16 potential [22]. The  $S$  wave parts of JISP16 potential are fit to data in a HO space of  $N = 8$  and  $\hbar\omega = 40$  MeV. Nucleon-nucleon interactions are defined in the relative coordinates of the two-body system so one should calculate  $\Lambda^{NN} = \sqrt{m(N + 3/2)\hbar\omega}$  with the *reduced* mass  $m$  rather than the nucleon mass  $m_N$  appropriate for the single-particle states of the model space. Taking this factor into account, one finds  $\Lambda^{\text{JISP16}} \sim 600$  MeV/c and  $\lambda_{sc}^{\text{JISP16}} \sim 63$  MeV/c. In practice, the uv region seems already captured at  $\Lambda > 500$ – $550$  MeV/c [13]. The Idaho N<sup>3</sup>LO interaction was fit to data with a high-momentum cutoff of the “super-Gaussian” regulator set at  $\Lambda_{\text{N}^3\text{LO}} = 500$  MeV/c [20]. What is the uv regulator scale of the Idaho N<sup>3</sup>LO interaction appropriate to the discrete HO basis of this study? A published emulation of this interaction in a harmonic oscillator basis uses  $\hbar\omega = 30$  MeV and  $N_{max} \approx 2n = 40$ . A more systematic study of emulations gave a few more sets of  $(N, \hbar\omega)$  which described  ${}^3\text{He}$  ground state energy equally well [23]. The successful emulation of the Idaho N<sup>3</sup>LO interaction in a HO basis suggests that  $\Lambda^{\text{N}^3\text{LO}} \sim 900$ – $1100$  MeV/c and  $\lambda_{sc}^{\text{N}^3\text{LO}} \sim 21$ – $42$  MeV/c, consistent with Figs. 2 and 3. In practice from calculations of a variety of light nuclei the uv region seems already captured at  $\Lambda > 800$  MeV/c [13].

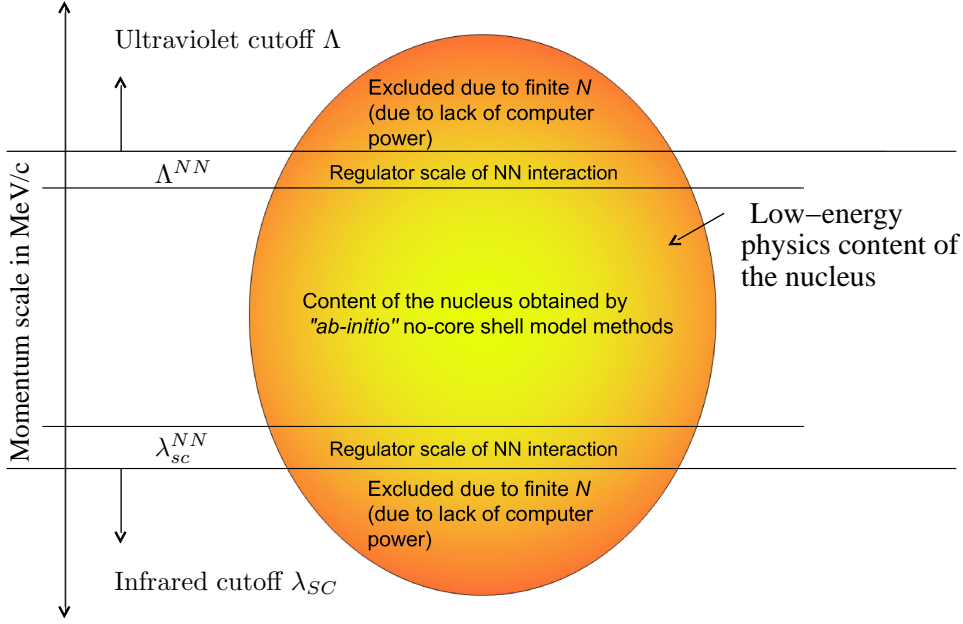


Figure 3: Schematic view of a finite model space (limited by the basis truncation parameter  $N$  as described in the text), in which the uv and ir momentum cutoffs are arbitrary. To reach the full many-body Hilbert space, symbolized by the complete oval, one expects to let the uv cutoff  $\rightarrow \infty$  and the ir cutoff  $\rightarrow 0$ .

## 4 Extrapolations

The extrapolation scheme proposed in [13] gives  $N$  and  $\hbar\omega$  equal roles by employing uv and ir cutoffs which should be taken to infinity and to zero, respectively to achieve a converged result (see Fig. 3).

From Fig. 1 we conclude uv cutoff  $\Lambda = \sqrt{m_N(N + 3/2)\hbar\omega}$  should be greater than the intrinsic  $\Lambda^{NN}$  of the  $NN$  interaction. Figure 2 suggests that the ir cutoff  $\lambda_{sc} = \sqrt{(m_N\hbar\omega)/(N + 3/2)}$  should be less than the intrinsic  $\lambda_{sc}^{NN}$  of the chosen  $NN$  interaction. Noting that  $N = \Lambda/\lambda_{sc} - 3/2$  and  $\hbar\omega = (\Lambda\lambda_{sc})/m_N$ , one can establish the minimum values of  $N$  and  $\hbar\omega$  needed for a converged result (see Table 1). The intrinsic  $\lambda_{sc}^{NN}$  corresponding to the lowest energy configuration of two nucleons is not well determined by numerical investigations (see Figs. 4 and 8 of Ref. [13]) so we include a range of values in Table 1. It is a computational challenge to increase  $N$  which gets harder the more particles there are in the nucleus. From this Table one

Table 1: Intrinsic regulator scales determine  $N$  and  $\hbar\omega$  for a converged result.

$\Lambda \geq \Lambda^{NN} = 800 \text{ MeV}/c$		
$\lambda_{sc}^{NN} \approx 10 \text{ MeV}/c$	$\lambda_{sc}^{NN} \approx 20 \text{ MeV}/c$	$\lambda_{sc}^{NN} \approx 40 \text{ MeV}/c$
$N \geq 80$	$N \geq 40$	$N \geq 20$
$\hbar\omega \geq 8 \text{ MeV}$	$\hbar\omega \geq 16 \text{ MeV}$	$\hbar\omega \geq 32 \text{ MeV}$
$\Lambda \geq \Lambda^{NN} = 500 \text{ MeV}/c$		
$\lambda_{sc}^{NN} \approx 10 \text{ MeV}/c$	$\lambda_{sc}^{NN} \approx 20 \text{ MeV}/c$	$\lambda_{sc}^{NN} \approx 40 \text{ MeV}/c$
$N \geq 50$	$N \geq 25$	$N \geq 12$
$\hbar\omega \geq 5 \text{ MeV}$	$\hbar\omega \geq 10 \text{ MeV}$	$\hbar\omega \geq 20 \text{ MeV}$

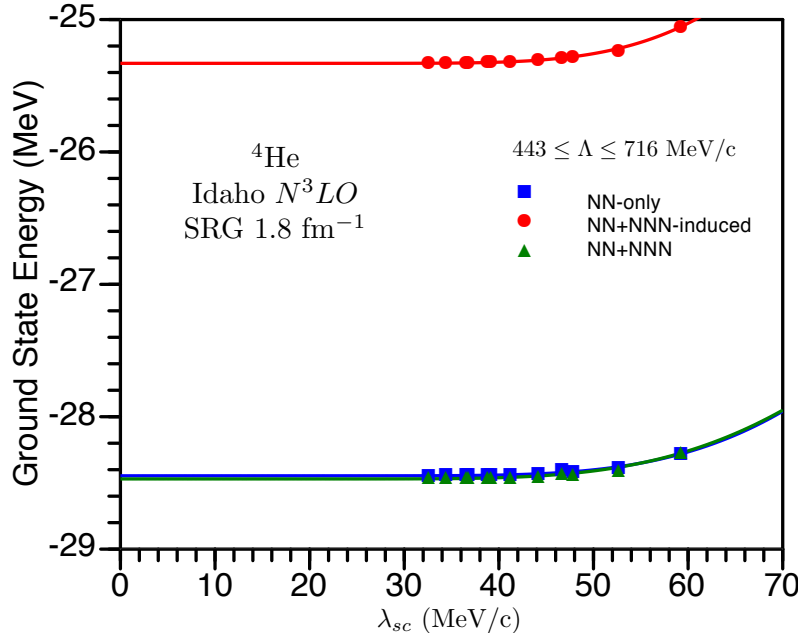


Figure 4: The ground state energy of  ${}^4\text{He}$  calculated at values of  $\Lambda \geq 443$  MeV/ $c$  and variable  $\lambda_{sc}$ . The curves are a fit to the points and the function fitted is used to extrapolate to the ir limit  $\lambda_{sc} = 0$ . The three SRG transformed Hamiltonians are described in the text.

concludes that one must extrapolate for all but the lightest nuclei and the softest of interactions.

We now utilize the scaling behavior displayed on Fig. 1 to suggest an extrapolation procedure which we illustrate in Figs. 4, 5, and 6. We plot the ground state energy eigenvalue, the root mean square radius, and the total dipole strength of  ${}^4\text{He}$  obtained by a NCSM calculation [24], done in a translationally invariant basis which depends only on Jacobi coordinates [25]. The  $NN$  interaction is the Idaho  $N^3\text{LO}$  [20] softened by the similarity renormalization group (SRG) evolution according to the method described in Ref. [17]. Transforming the Hamiltonian induces the appearance of higher order many-body forces which should be kept to preserve the unitary nature of the transformation. If they are not kept results become dependent on the SRG flow parameter. It is of interest to learn if the scaling behavior apparent in Fig. 1 and the many examples in Ref. [13] is also true for the induced many-body forces and the three-body forces added to the Hamiltonian (see Refs. [17, 24] for a full description of the SRG scheme and nomenclature). For this exercise, we utilized calculations with  $\hbar\omega = 22$  and 28 MeV and  $N \leq 18$ . The SRG parameter was  $1.8$  fm $^{-1}$  and our own study of the results suggest that the intrinsic uv cutoff of this SRG transformed interaction is less than 440 MeV/ $c$  (see Figures). Then according to Table 1, the calculations should be fully converged with this model space.

The extrapolation is performed by a fit of an exponential plus a constant to each set of results at fixed  $\Lambda$ . That is, we fit the ground state energy with three adjustable parameters using the relation  $E_{gs}(\lambda_{sc}) = a \exp(-b/\lambda_{sc}) + E_{gs}(\lambda_{sc} = 0)$ . The rms radius and the total dipole strength are obtained by similar fits:  $r(\lambda_{sc}) = a \exp(-b/\lambda_{sc}) + r(\lambda_{sc} = 0)$  and  $D^2(\lambda_{sc}) = a \exp(-b/\lambda_{sc}) + D^2(\lambda_{sc} = 0)$ . The extrapolation formulae work equally well for the induced three-body forces and the added three-body forces. It should be noted that our extrapolations in these figures employ an exponential function whose argument  $1/\lambda_{sc} = \sqrt{(N + 3/2)/(m_N \hbar\omega)}$  is proportional to  $\sqrt{N/(\hbar\omega)}$ . This extrapolation procedure of taking  $\lambda_{sc}$  downward from the

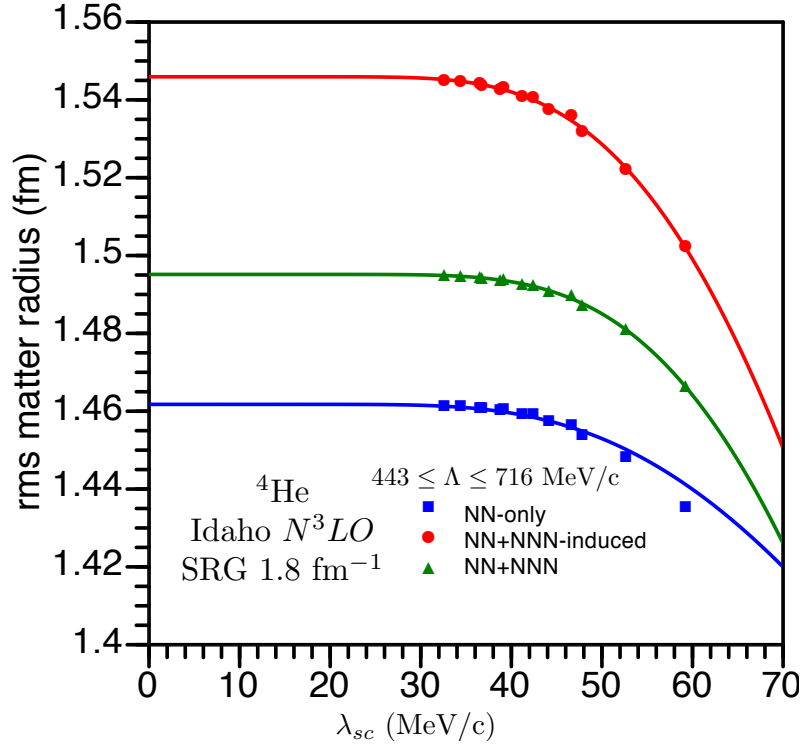


Figure 5: The rms radius  $\langle 0|r^2|0\rangle^{1/2}$  of  ${}^4\text{He}$  calculated as in Fig. 4.

smallest value allowed by computational limitations treats both  $N$  and  $\hbar\omega$  on an equal basis. The exponential extrapolation in  $\sqrt{N/(\hbar\omega)}$  is therefore distinct from the popular extrapolation which employs an exponential in  $N_{max}$  ( $= N$  for this  $s$ -shell

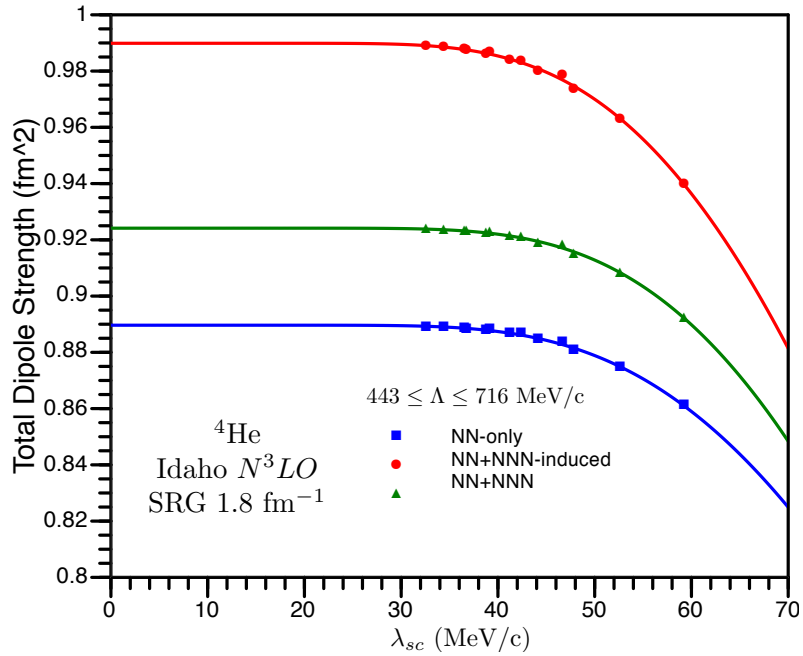


Figure 6: (Color online) The total dipole strength  $\langle 0|\mathbf{D} \cdot \mathbf{D}|0\rangle$  of  ${}^4\text{He}$  calculated as in Fig. 4. Here  $\mathbf{D}$  is the unretarded dipole operator defined in Ref. [24].



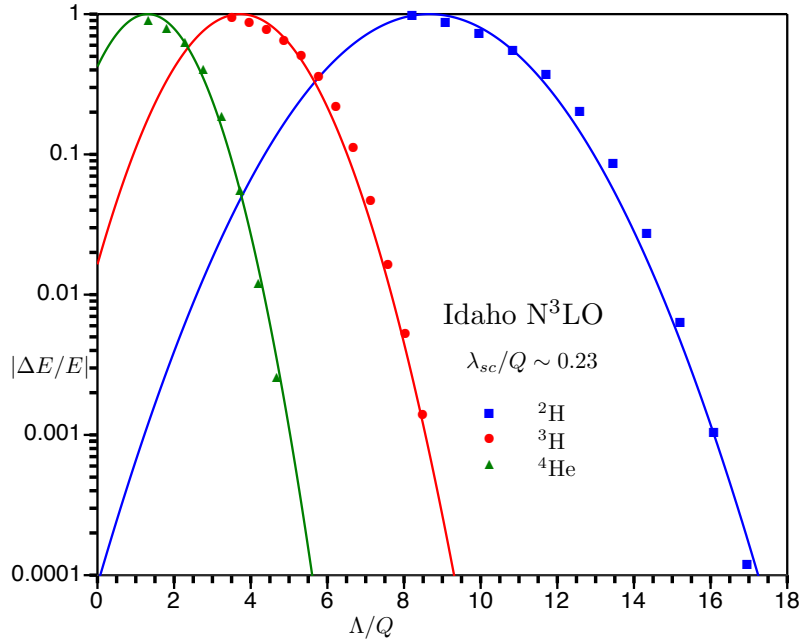


Figure 7: Dependence of the ground-state energy of three  $s$ -shell nuclei (compared to a converged value; see text) upon the uv momentum cutoff  $\Lambda \leq \Lambda^{N^3LO}$ . The data are fit to Gaussians. Both uv and ir cutoffs are scaled to  $Q$ , the binding momentum of each nucleus, so that the  $s$ -state nuclei can be fit on a single plot. The unscaled values are  $\lambda_{sc} = 10$  MeV/ $c$  for  ${}^2\text{H}$ ,  $\lambda_{sc} = 20$  MeV/ $c$  for  ${}^3\text{H}$  and  $\lambda_{sc} = 40$  MeV/ $c$  for  ${}^4\text{He}$ .

case) [7, 9, 10, 17]. The convergence of all three operators is the same with the  $\lambda_{sc}$  extrapolation, in contrast to the traditional extrapolation for the same data which found slower and slower convergence for the ground state energy eigenvalue, the root mean square radius, and the total dipole strength [24]. As the model space is large and the intrinsic uv cutoff is small, the extrapolated results obtained here agree with those of the traditional extrapolation of Ref. [24].

Finally, we return to Fig. 2 and restrict our attention to the sector  $\Lambda \leq \Lambda^{NN}$ . The universal curve in that sector is generalized to three  $s$ -shell nuclei in Fig. 7 where all momenta are scaled by the binding momentum  $Q$  of the considered nucleus in order to put them on the same plot. For such low fixed momenta  $\lambda_{sc}$ ,  $|\Delta E/E|$  does go to zero with increasing  $\Lambda$  because  $\lambda_{sc} \leq \lambda_{sc}^{NN}$ . The “high”  $\Lambda$  tails of these curves were fit by Gaussians (shifted from the origin) in the variable  $\Lambda/Q$  in Ref. [13]. This behavior suggests another possible extrapolation scheme; fixing the ir physics first and then extrapolating in the uv cutoff. A later paper did advocate such an extrapolation with  $\Lambda^2$  in the exponential fit function [26]. We have tried to fit our data with the ansatz,  $E_{gs}(\Lambda) = A \exp(-2\Lambda^2/\Lambda^{NN^2}) + E(\Lambda = \infty)$ , of that paper and failed. Because the Gaussians are shifted from the origin, a fit requires  $E_{gs}(\Lambda/Q) = a \exp[-(\Lambda/Q - b)^2/2c^2] + E(\Lambda/Q = \infty)$ , provided that one restricts to values of  $\Lambda/Q \leq \Lambda^{NN}/Q$ . Such fits are shown in Fig. 8.

Unfortunately, the extrapolated energies of Fig. 8 do not agree with those obtained from independent calculations. The extrapolated energies are always lower: 2 keV for the deuteron, 300 keV (or 4%) for the triton and 20 keV (or 2.4 %) for the alpha particle. It is difficult to achieve consistent extrapolations with different values of fixed (low)  $\lambda_{sc}$ . For example, if one takes  $\lambda_{sc} = 12$  MeV/ $c$ , seemingly closer to the ir limit so that even more of the ir physics is captured, the extrapolated triton energy is  $-10.149$  MeV; 2.3 MeV below the accepted value. Only with the SRG transformed potentials does the extrapolation illustrated in Fig. 8 agree with other independent

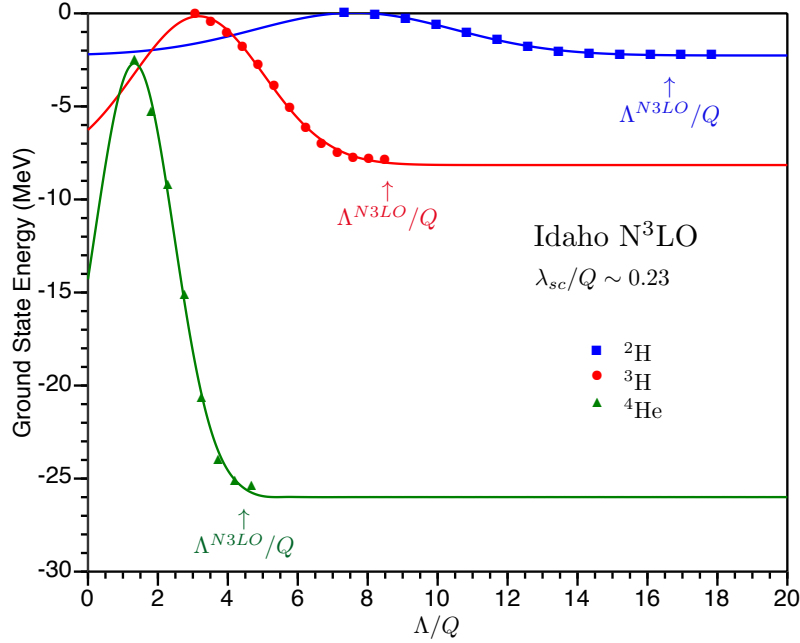


Figure 8: Extrapolation at fixed  $\lambda_{sc} \leq \lambda_{sc}^{N^3LO}$ . Both uv and ir cutoffs are scaled to  $Q$ , the binding momentum of each nucleus, so that the  $s$ -state nuclei can be fit on a single plot. The unscaled values are  $\lambda_{sc} = 10$  MeV/ $c$  for  ${}^2\text{H}$ ,  $\lambda_{sc} = 20$  MeV/ $c$  for  ${}^3\text{H}$  and  $\lambda_{sc} = 40$  MeV/ $c$  for  ${}^4\text{He}$ . The arrows indicate that the UV extrapolation uses only points for which  $\Lambda \leq \Lambda^{N^3LO}$ .

calculations.

In conclusion, we have established that an extrapolation in the ir cutoff with the uv cutoff above the intrinsic uv scale of the interaction is quite successful, not only for the eigenstates of the Hamiltonian but also for expectation values of operators considered long range. On the other hand, the suggested extrapolation [26] in the uv cutoff when the ir cutoff is below the intrinsic ir scale is neither robust nor reliable.

## 5 Acknowledgements

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