### Properties of infrared extrapolations in a harmonic oscillator basis

Sidney A Coon Michael K G Kruse University of Arizona LLNL

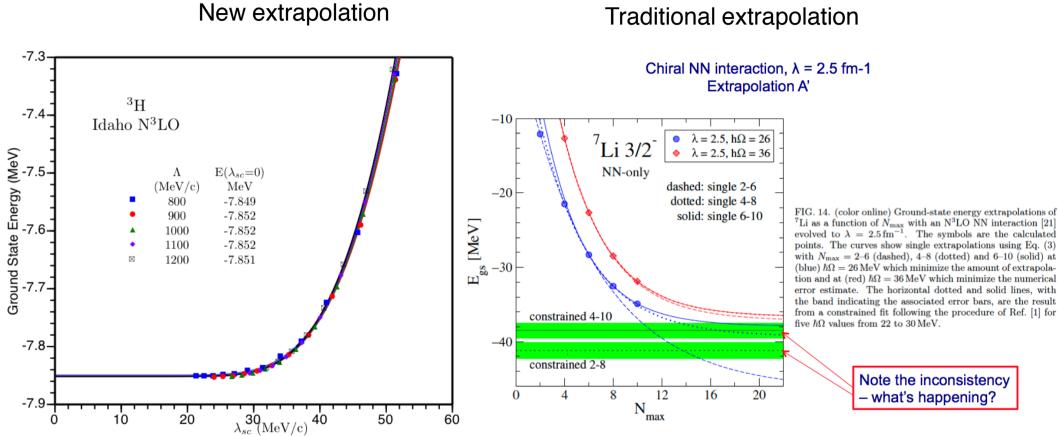
#### Collaborators

Bira van Kolck University of Arizona
Institut de Physique Nucléaire d'Orsay
Michael Kruse University of Arizona
Matthew Avetian University of Arizona
James Vary Iowa State University
Pieter Maris

PHYSICAL REVIEW C 86, 054002 (2012)

Convergence properties of ab initio calculations of light nuclei in a harmonic oscillator basis

S. A. Coon, M. I. Avetian, M. K. G. Kruse, U. van Kolck, P. Maris, and J. P. Vary



S. A. Coon, M. I. Avetian, M. K. G. Kruse, U. Van Kolck, P. Maris, J. P. Vary Archive:1205.3230, PRC 86, 054002 (2012)

E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary, submitted to PRC; arXiv: 1302:5473

#### Outline

- History: HO shell model can provide a linear trial function for a variational calculation of few-body systems (energies, etc.)
- Review: How to extrapolate to infinite number of terms, based on functional analysis theorems
- Effective Field Theory concepts applied to a discrete basis suggest an alternative extrapolation approach respecting ultraviolet (UV) and infrared (IR) running of the results as the basis is extended.
- Examples:Two alternate proposals for IR running, two soft NN potentials (Idaho N3LO and JISP16), light nuclei A=2-6
- Conclusion: Extrapolation method is successful for energies and lo range operators such as radius and total dipole moment.

### The No-Core Shell Model (NCSM)



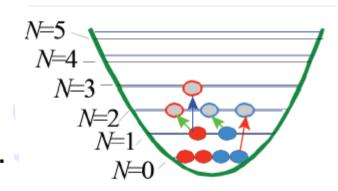
**Starting Hamiltonian is <u>translationally invariant.</u>** 

$$H_A = \frac{1}{A} \sum_{i < j}^{A} \frac{(\vec{p_i} - \vec{p_j})^2}{2m} + \sum_{i < j}^{A} V_{\text{NN},ij}$$

Provided interaction is "soft" we don't need to do any renormalization of interaction,

It's that "simple".

### NCSM has two parameters: Nmax and $\Omega$

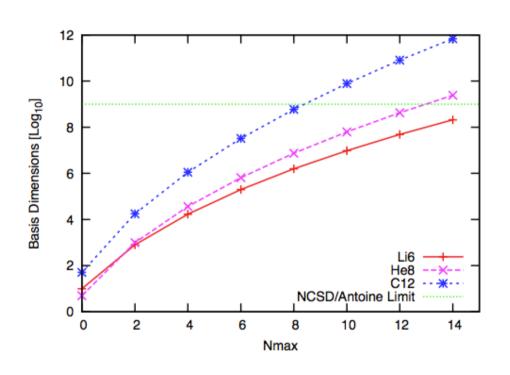


If we now use a single-particle basis, we have to remove the spurious CM states. Translational invariance is automatic if HO basis depends on Jacobi coordinates.

Advantage in m-scheme: Antisymmetry is easy to implement.

Disadvantage in m-scheme: Number of basis states is much larger than JT basis

### M-scheme basis dimensions



- Size of the m-scheme basis grows rapidly with increasing Nmax.
- Switch to HO JT coupled basis? Possibly, but painful.
- Difficulties with such an approach, e.g. Jacobi coordinates or rewrite codes.
- Even if techniques like SRG potentials are used, you still can't perform converged calculations all the time.
- But why stick with the HO basis?
- Only basis where center of mass and intrinsic states can be completely decoupled.

### The Variational Approach

- One can view a shell model calculation as a variational calculation, and is thus expanding the configuration space merely serves to improve the trial wavefunction.
- The traditional shell-model calculation involves trial wavefunctions which are linear combinations of Slater determinants.

Irvine, J. M. et al. "Nuclear Shell-Model Calculations and Strong Two-Body Correlations"

#### 2.1.2. Linear Trial Functions

We next consider a trial function in the form of a linear expansion:

$$\psi_T = \sum_{i=1}^N a_i \varphi_i \tag{2.10}$$

Delves, L. M. Advances in Nuclear Physics Vol 5 1972 (N → Nmax)

The traditional shell-model calculation involves trial variational wave functions which are linear combinations of Slater determinants. Expanding the configuration space merely serves to improve the trial wave function.

• J. M. Irvine, et al "Nuclear shell-model calculations and strong two-body correlations", Ann. Phys. 102, 129 (1976). early appearance of the term "no-core shell model" (NCSM)

Use the HO eigenfunctions as a basis of a finite linear expansion to make a straightforward variational calculation of the properties of light nuclei.

M. Moshinsky, "The Harmonic Oscillator in Modern Physics: from Atoms to Quarks" (Gordon and Breach, New York, 1969).

$$\Psi_T = \sum_{
u} a_{
u}^{(\mathcal{N})} h_{
u}$$

where  $a_{\nu}^{(\mathcal{N})}$  are the parameters to be varied and  $h_{\nu}$  are many-body states based on a summation over products of HO functions.

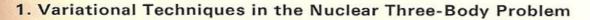
Theorems based upon functional analysis established the asymptotic convergence rate of these calculations as a function of the counting number N which characterizes the size of the expansion basis (or model space)

- inverse power laws in N for ``non smooth" potentials with strong short range correlations
- exponential in N for ``smooth" potentials such as gaussians

HO basis: I. M. Delves, "Variational Techniques in the Nuclear Three-body Problem" in Advances in Nuclear Physics, Volume 5, ed. M. Baranger and E. Vogt (Plenum Press, New York, 1972) p.1-224, Simen Kvaal, "Harmonic oscillator eigenfunction expansions, quantum dots, and effective interactions", Phys. Rev. B 80, 045321 (2009).

Hyperspherical Harmonics basis: T. R. Schneider, "Convergence of generalized spherical harmonic expansions in the three nucleon bound state", Phys. Lett. 40B, 439 (1972).

However, the HO expansion basis has an intrinsic scale parameter  $\hbar\omega$  which does not naturally fit into an extrapolation scheme based upon  $\mathcal{N}$ . Indeed the model spaces of these NCSM approaches are characterized by the ordered pair  $(\mathcal{N}, \hbar\omega)$  where the basis truncation parameter  $\mathcal{N}$  and the HO energy parameter  $\hbar\omega$  are variational parameters. It is the purpose of this talk to summarize the properties of another ordered pair which more physically describes the nature of the model spaces and provides extrapolation tools which use  $\mathcal{N}$  and  $\hbar\omega$  on an equal footing





L.M Delves; in Advances In Nuclear Physics vol 5 1972

$$E_{N_{max}} = E + P(N_{max})^{-2}$$
 "nonsmooth potentials" like Yukawa

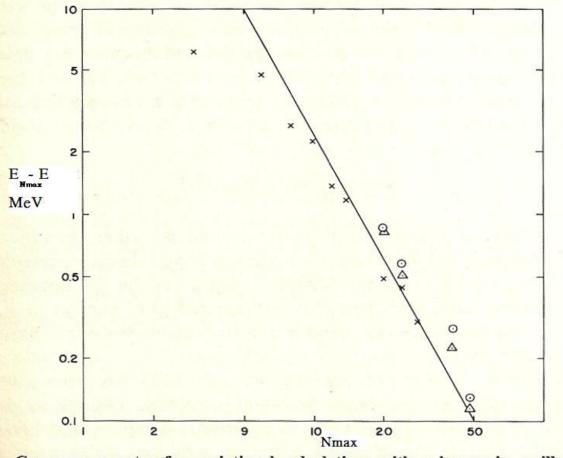


Fig. 8. Convergence rates for variational calculations with a harmonic oscillator basis.  $\odot$  Deuteron, Yamaguchi potential;  $\times$  triton, Yamaguchi potential; and  $\triangle$  deuteron, Reid potential. Results taken from (JLS 70). The solid line has a slope of -2.0.

"These results are independent of the dimensionality of the problem, that is, of the number of particles, provided that the appropriate  $N_{max}$  is used. ... The extrapolated results of these authors have been used for E. On the logarithmic scale used, these differences are predicted by our crude theory to lie on a straight line of slope 2 for the Reid potential; it is not clear to what extent we should expect the nonlocal [separable] Yamaguchi potential to be `smooth'."

### Variational energy as a function of oscillator energy ħω for fixed number of quanta Number of quanta increases by two for each curve

#### 1969 H atom up to 10 quanta

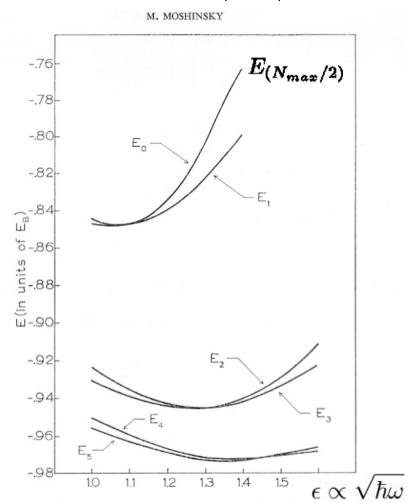
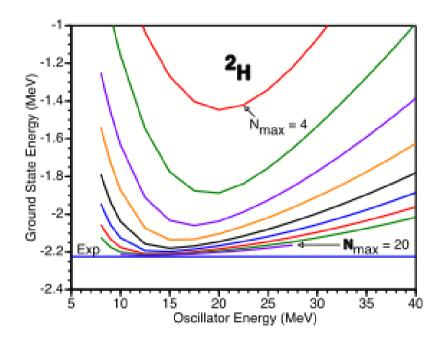


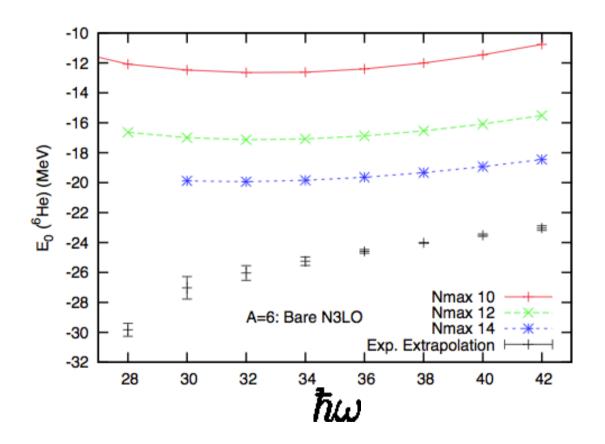
Fig. 1. Energy of the ground state of the H atom as a function of the parameter  $\varepsilon$  for the variational analysis discussed in Section 3. This energy  $E_p(\varepsilon)$ , p=0,1,2,3,4,5 is associated with a trial wave function  $\psi_p = \sum_{n=0}^p a_n^{(p)} \mid n00\rangle$ , where  $\mid n00\rangle$  is a harmonic-oscillator state of frequency  $\hbar\omega = (me^4/2\hbar^2)\varepsilon^2$ .

2009 deuteron up to 20 quanta



No-core full configuration method of Maris, Vary, Shirokov

The current method is to seek the minimum of E(Nmax,  $\hbar\omega$ ).



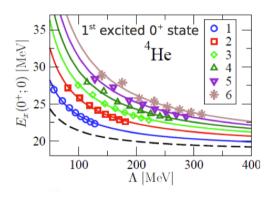
Extrapolation A of Maris et al PRC 79, 014308 (2009)

### Current Method is Unsatisfactory...

- ...from an effective field theory point of view.
- Results are <u>oscillator frequency dependent</u>.
- No clear control of ultra-violet or infra-red nuclear physics.
- The goal is to investigate an alternate way from a more formal view point.

### UV & IR CUTOFFS INTRODUCED

Construction of an effective field theory within the No Core Shell Model



#### -> calculation at Leading

#### order:

two N-N contact interactions in the  ${}^3S_{_{1,}}{}^1S_{_0}$  channel and a three-body contact interaction in the 3-nucleon  $S_{_{1/2}}$  channel

-> coupling constants fitted to the binding energy of the deuteron, triton and <sup>4</sup>He.



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No-core shell model in an effective-field-theory framework

I. Stetcu a,b,\*, B.R. Barrett a, U. van Kolck a

Department of Physics, University of Arizona, Tucson, AZ 85721, USA
 Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
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#### **Effective Field Theory (EFT)**

In a field theory one **never** has access to the "full" Hilbert space. Experiments only probe a region of momenta. Nature is quantum mechanical. So to develop a theory for such a region we must pose a model space. For smallest errors the model space should be as big, if possible, as the region one is interested in.

The parameter of the projection operator P into the model space must have a dimension. Call the parameter  $\Lambda$ , the ultraviolet cutoff and take it to be a momentum.

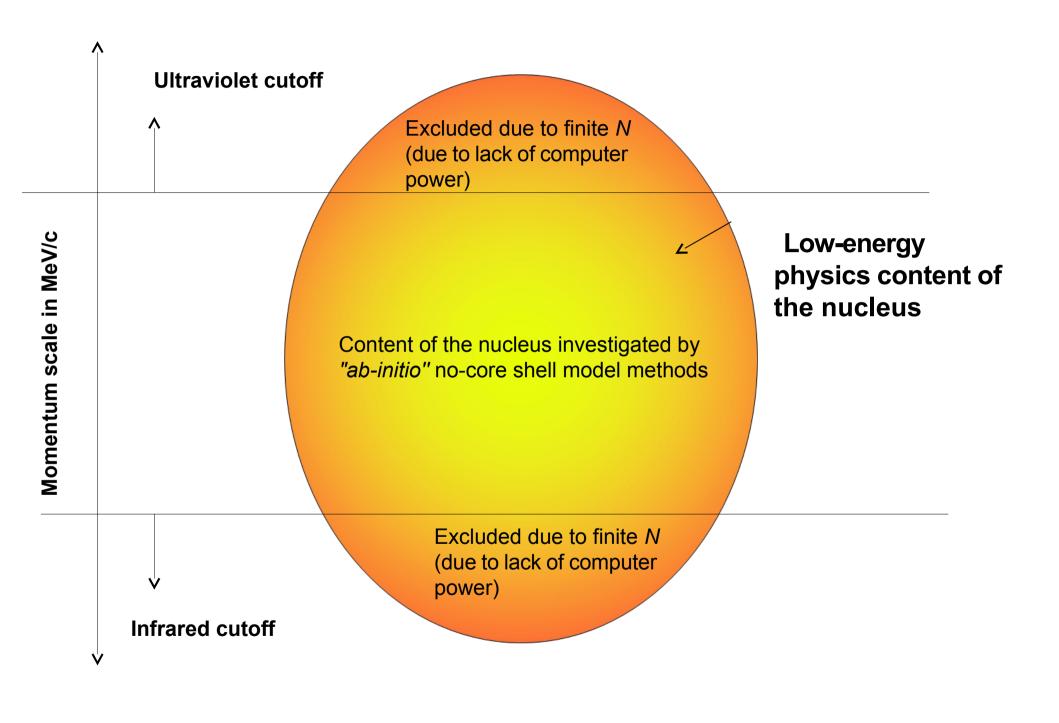
#### Model space can be arbitrary but observables calculated within it cannot.

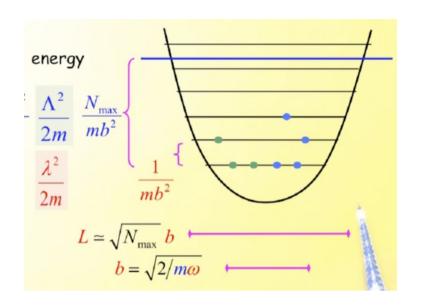
The Hamiltonian operator of the model space must depend on  $\Lambda$  in such a way that observables at momenta Q<< $\Lambda$  are independent of how P is chosen, and in particular, independent of  $\Lambda$ .

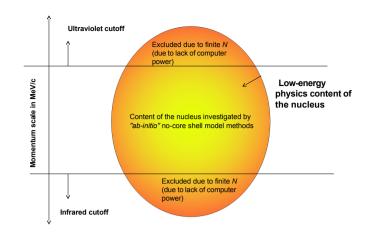
**Arizona program:** formulate a nuclear EFT in an HO basis as an efficient way of reaching larger nuclei. The HO basis also introduces into the model space a parameter  $\lambda$ , an infrared cutoff in addition to  $\Lambda$ , so that observables at momenta Q>>  $\lambda$  are independent of  $\lambda$ . That is, the values of  $\Lambda$  and  $\lambda$  control the size of the model space and the projection operators P( $\Lambda$ ) and P( $\lambda$ ) define the boundaries of the model space.

van Kolck, Barrett, Stetcu, Rotureau, Yang

**My more modest goal:** can EFT motivate and shape an extrapolation to the infinite basis limit for the HO basis calculations called NCSM which utilize "realistic" nuclear interactions fit to data, not in a clearly defined model space, but in free space?







Define a UV momentum cutoff  $\Lambda$  analogous to continuum  $\Lambda$  in which the particles are not confined:

$$\Lambda = \sqrt{m_N(N_{Max} + 3/2)\hbar\omega}$$

A high momentum cutoff corresponding to the maximal non-infinite momentum in the bound system.

Interpret behavior of variational energy of system as more basis states are added as the running of an observable with the variation (increase) of the UV cutoff of model space

Confinement to a volume because  $\hbar\omega>0$  means the energy levels are quantized. The associated momenta cannot take on continuous values so that the model space has an infrared (IR) momentum cutoff  $\lambda$ .

Define 
$$\lambda = \sqrt{(m_N \hbar \omega)}$$

A low momentum cutoff corresponding to the minimal non-zero momentum in the bound system.

### Definition of Momentum Cutoffs

#### Ultraviolet momentum cutoff

$$\Lambda = \sqrt{m_N(N+3/2)\hbar\omega}$$

Stetcu et al. PLB **653** (2007)

"Kallio momentum"  $\Lambda_a = \sqrt{2}\Lambda$ 

JPVary lectures (2012) Furnstahl et al. PRC **86** (2012)

Infrared momentum cutoff defined by discrete energy levels of the HO

$$\lambda = \sqrt{(m_N \hbar \omega)}$$
  
Stetcu et al. PLB **653** (2007)

Alternate infrared cutoff defined by maximal radial extent of highest sp state of model space

$$\lambda_{SC}=\sqrt{(m_N\hbar\Omega)/(N+3/2)}$$
  $\lambda_{SC}=\lambda^2/\Lambda$  Jurgenson et al. PRC (2011)

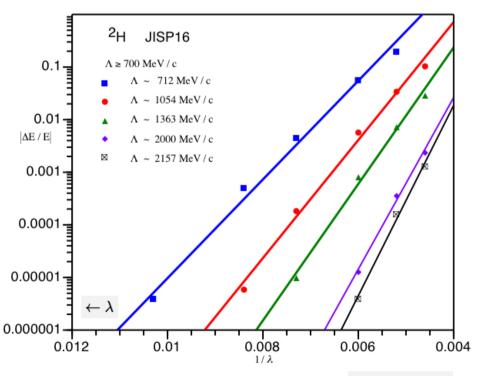
Strategy: minimize  $E(\Lambda,\lambda)$  or  $E(\Lambda,\lambda)$ 

Works only if the answer improves as we lower the infrared cutoff at a fixed ultraviolet cutoff

Or if answer improves as we raise UV cutoff at a fixed ir cutoff

Alternate  $\lambda_{sc}$  in Furnstahl et al. PRC **86** (2012), More et al. PRC **87** (2013), Furnstahl et al. ArXiv:1312.6876

# Remove IR effects by decreasing value of IR momentum cutoff in the function chosen as an extrapolator whilst keeping the UV cutoff undisturbed.



Extrapolator is clearly the exponential function.

• 
$$\frac{E(\lambda)-E(\lambda=0)}{E(\lambda=0)} \equiv \frac{\Delta E}{E} = A \exp(-B/\lambda)$$

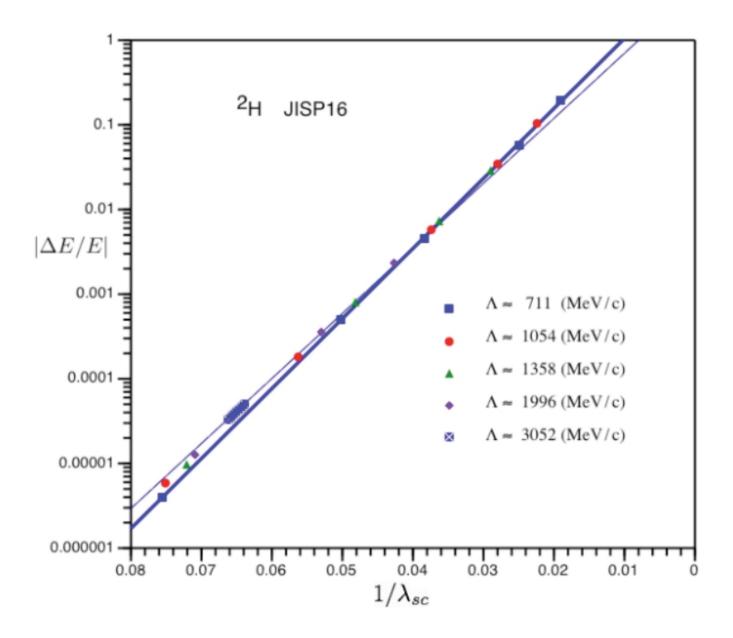
- B is a function of the UV cutoff
- The IR cutofcannotbe aware of the UV cutoff.
- Remove dependence upon

• 
$$\lambda = \sqrt{\Lambda \lambda_{sc}} \Longrightarrow$$
•  $\exp(-B/\lambda) = \exp(-B/\sqrt{\Lambda \lambda_{sc}}) = \exp\left(-\frac{B/\sqrt{\Lambda}}{\sqrt{\lambda_{sc}}}\right)$ 
•

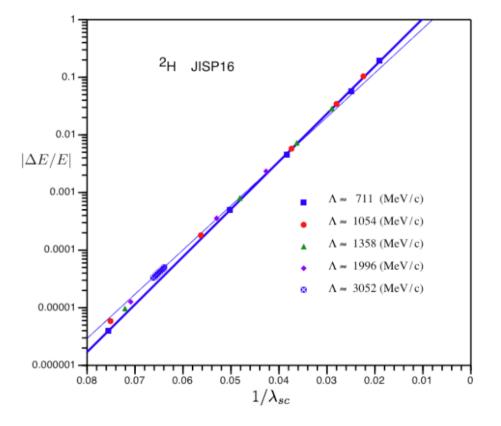
 $B/\sqrt{\Lambda}$  (i.e., multiplier of  $1/\sqrt{\lambda_{sc}}$  ) is constant to within 5 %.

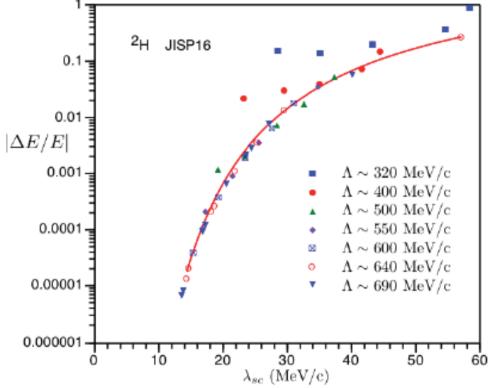
The momentum cutoff  $\lambda$  will remove IR effects. Indeed, any momentum cutoff  $\lambda_{sc} \leq \lambda_{IR} \leq \Lambda$  will remove IR effects, but the IR regulator which is independent of the UV cutoff is some function of  $\lambda_{sc}$ . It is  $\lambda_{sc}$  which causes the IR effects and one does not need to decrease a IR cutoff below that of  $\lambda_{sc}$  to remove IR effects (i.e. extrapolate to zero).

#### Result scales with $1/\lambda_{sc} = \Lambda/\lambda^2$ almost a universal behavior



 $1/\lambda_{sc}$  has units of a length.  $1/\lambda_{SC}$  is the maximal radial extent needed to encompass the system. One could call this radius ``L'' if one wanted a different name for  $1/\lambda_{sc}$ .

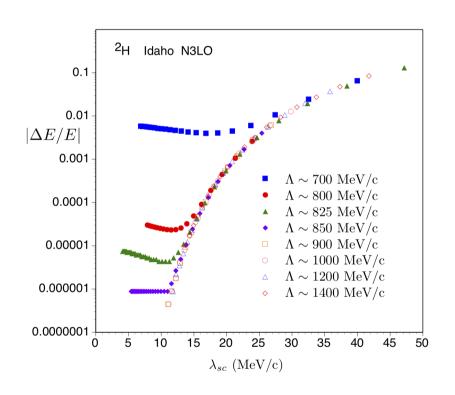


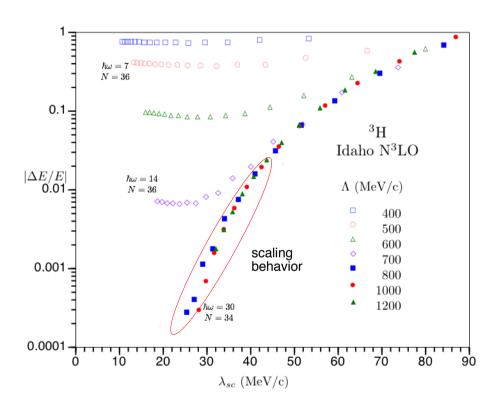


 $\Lambda > 700 \text{ MeV}$ 

 $\Lambda$  < 700 MeV

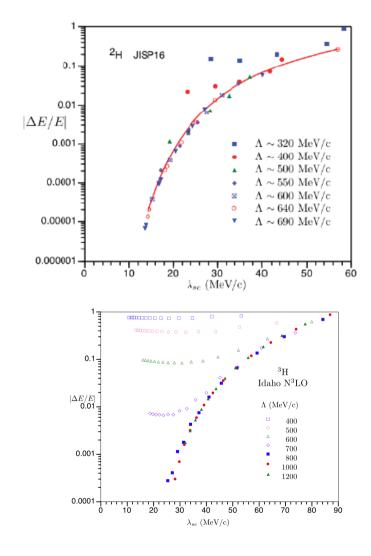
### Running of $|\Delta E/E|$ with IR cutoff suggests an intrinsic UV scale of the NN interaction

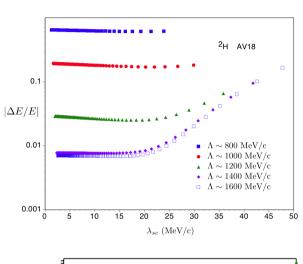


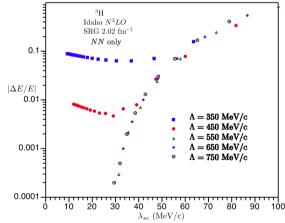


 $|\Delta E/E|$  does not go to zero unless  $\Lambda > \Lambda^{NN}$  where  $\Lambda^{NN}$  is some uv regulator scale of the NN interaction For  $\Lambda < \Lambda^{NN}$  there are missing contributions of size  $|\Lambda - \Lambda^{NN}|/\Lambda^{NN}$  so "plateaus" appear as ir cutoff approaches 0. Rise of plateaus suggests corrections are needed to  $\Lambda$  and  $\lambda_{sc}$ , which are defined only to leading order in  $\lambda_{sc}/\Lambda$ .

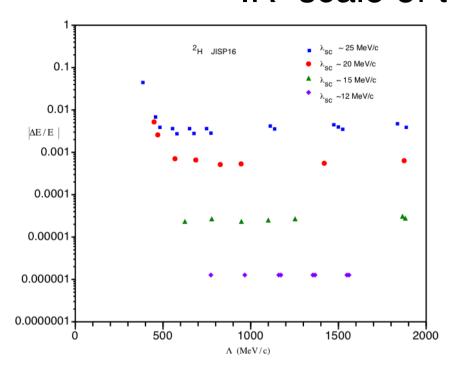
### Intrinsic UV scale depends on the NN interaction







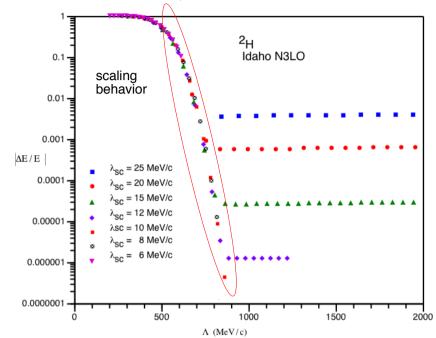
### Running of $|\Delta E/E|$ with UV cutoff suggests an intrinsic IR scale of the NN interaction

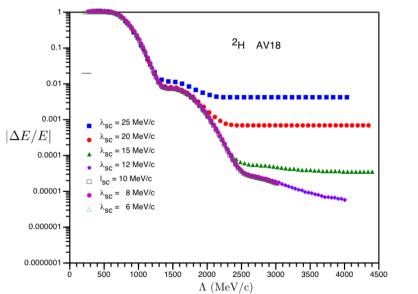


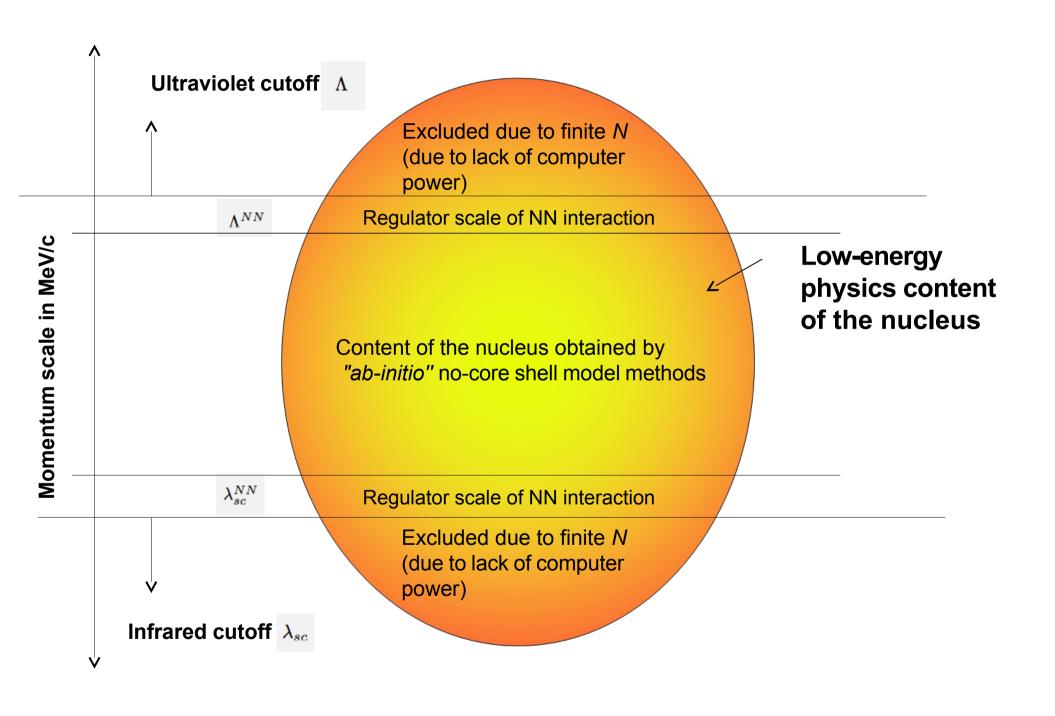
Plateau's ascribed to another "missing contributions" argument.

 $|\Delta E/E|$  does not go to zero unless  $\lambda_{sc} \leq \lambda_{sc}^{NN}$  where  $\lambda_{sc}^{NN}$  is some ir regulator scale of the NN interaction.

Value of  $\lambda_{sc}^{NN}$  is consistent with lowest energy configuration described by NN interaction; e.g. deuteron binding momentum Q = 45 MeV/c, or average of inverse scattering lengths  $\approx 16 \text{ MeV/c}$ 







# How do intrinsic regulator scales control needed values of N and hbar-omega for a converged result?

$$\Lambda/\lambda_{sc} = N + 3/2$$
 $(\Lambda\lambda_{sc})/m_N = \hbar\omega$ 

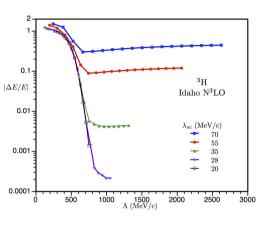
$$egin{aligned} \Lambda \geq \Lambda^{NN} = 800 \ \lambda_{sc} pprox 10 & \lambda_{sc} pprox 20 & \lambda_{sc} pprox 40 \ N \geq 80 & N \geq 40 & N \geq 20 \ \hbar\omega \succeq 8 & \hbar\omega \succeq 16 & \hbar\omega \succeq 32 \end{aligned}$$

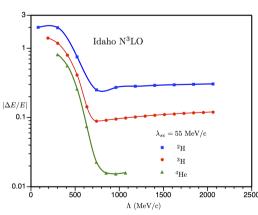
$$egin{aligned} \Lambda \geq \Lambda^{NN} = 500 \ \lambda_{sc} pprox 10 & \lambda_{sc} pprox 20 & \lambda_{sc} pprox 40 \ N \geq 50 & N \geq 25 & N \geq 12 \ \hbar\omega \succeq 5 & \hbar\omega \succeq 10 & \hbar\omega \succeq 20 \end{aligned}$$

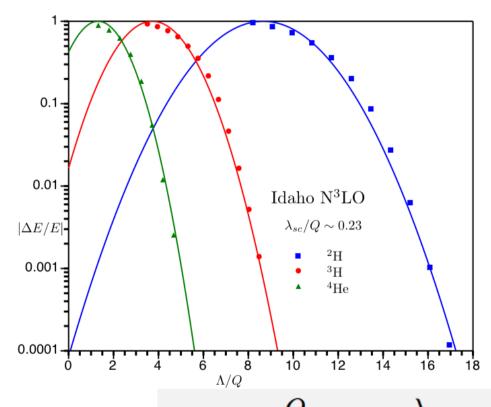
Conclusion: One must extrapolate for all but the lightest nuclei

#### Single curve for $\lambda_{sc} \leq \lambda_{sc}^{NN}$ and $\Lambda \leq \Lambda^{NN}$

$$\lambda_{sc} \le \lambda_{sc}^{NN}$$



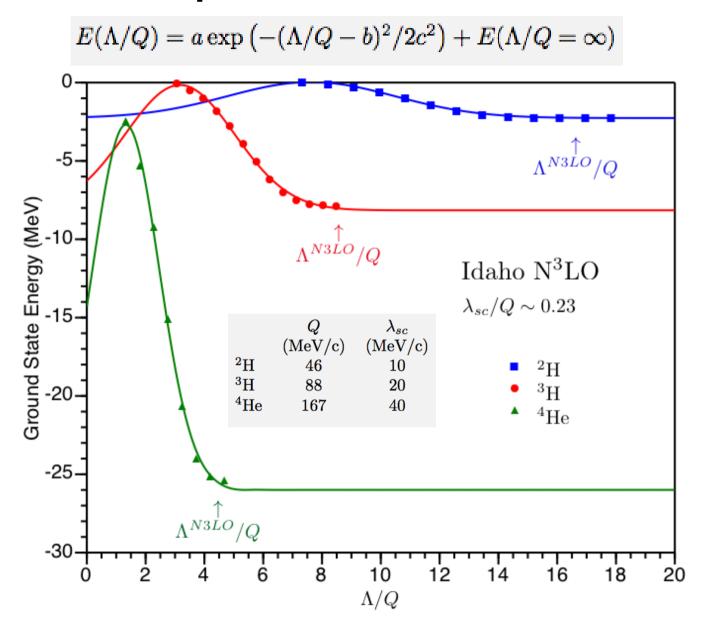




Scale each model space cutoff by binding Momentum of nucleus Q to demonstrate universal (i.e., independent of particle number) nature of the Gaussian fits to low values of UV cutoff A

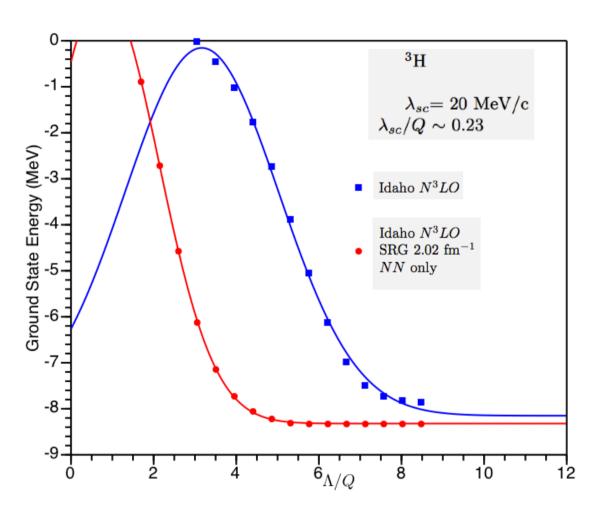
	Q	$\lambda_{sc}$	
	(MeV/c)	(MeV/c)	
$^2\mathrm{H}$	46	10	
$^3\mathrm{H}$	88	20	
$^4{ m He}$	167	40	

### UV extrapolations with $\Lambda < \Lambda^{\text{NN}}$



Extrapolated energies do NOT agree with independent calculations but are *lower*: 2 keV for deuteron, 300 keV (or 4%) for triton and 620 keV (or 2.4%) for alpha

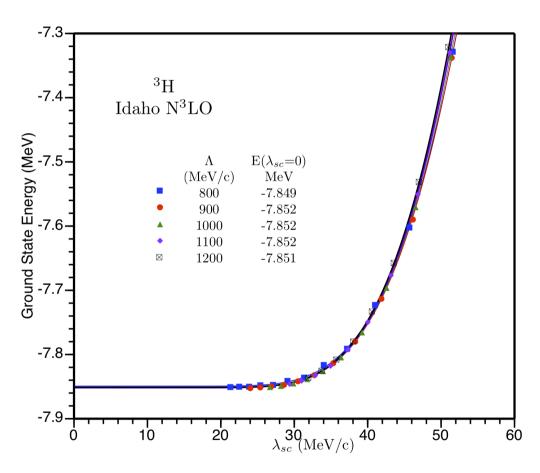
# UV extrapolations with $\Lambda < \Lambda^{NN}$



- 1) Extrapolation agrees with independent calculations only for SRG transformed potential.
- 2) Extrapolation with other values of fixed  $\lambda_{sc}$  is neither reliable nor robust.

### IR extrapolations with $\lambda_{s}$

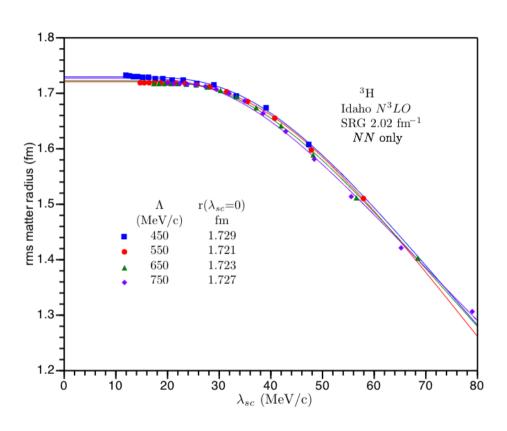
$$E(\lambda_{sc}) = A \exp(-B/\lambda_{sc}) + E(\lambda_{sc} = 0)$$

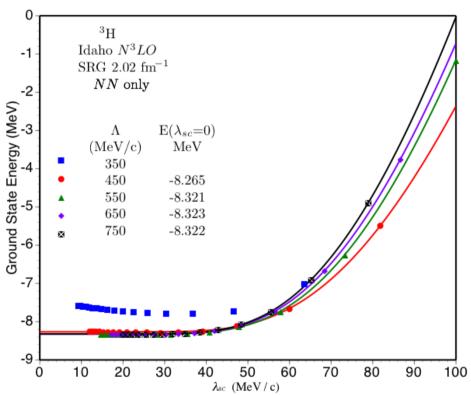


If UV cutoff is large enough, all extrapolations agree with each other and with the accepted value of -7.85 MeV

### IR extrapolations with $\lambda_{sc}$

 $\Lambda > \Lambda^{NN} \sim 500$  MeV/c for this SRG transformed interaction





Radius extrapolation

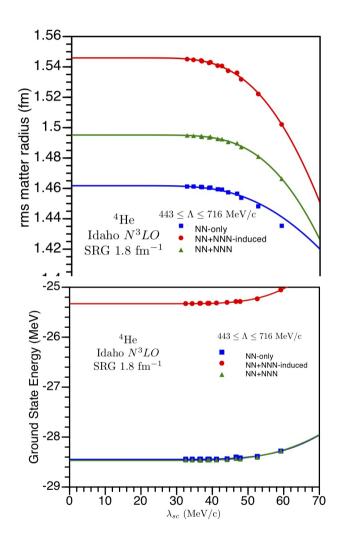
$$r(\lambda_{sc}) = -A \exp(-B/\lambda_{sc}) + r(\lambda_{sc} = 0)$$

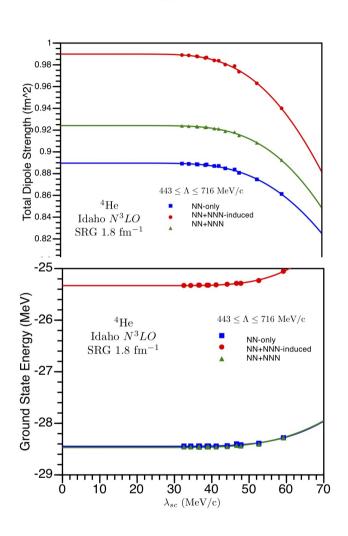
**Energy extrapolation** 

$$E(\lambda_{sc}) = A \exp(-B/\lambda_{sc}) + E(\lambda_{sc} = 0)$$

#### IR extrapolations of energy, radius, and total dipole moment operator

Convergence of all three operators is the same with  $\lambda_{_{\text{sc}}}$  extrapolation

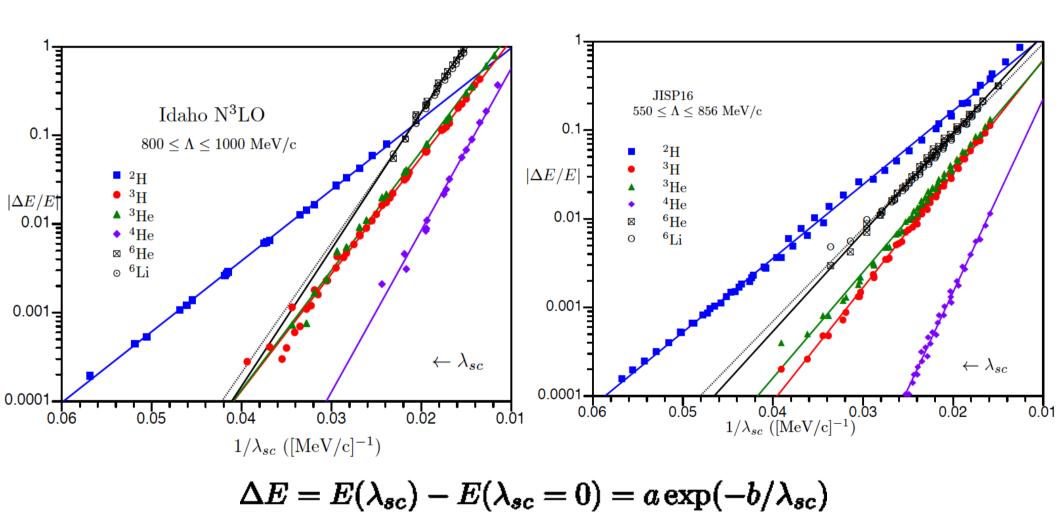




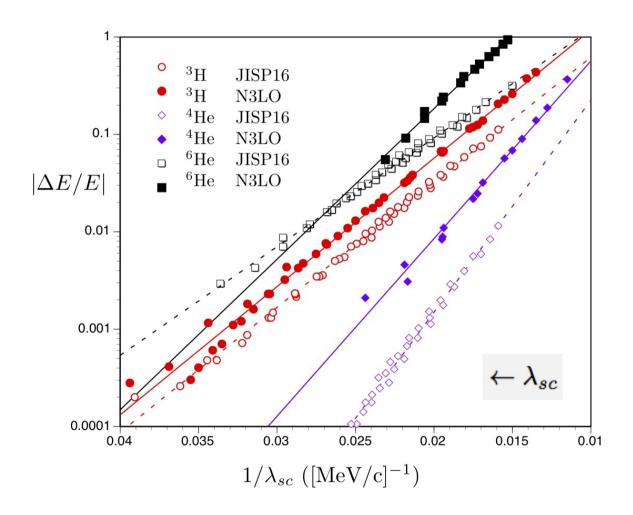
Plot all results at  $\hbar\omega$  = 22 and 28 MeV and Nmax up to 18

Data from M. D. Schuster, S. Quaglioni, C. W. Johnson and P. Navratil, ArXiv:1304:5491 "Ab Initio many-body calculation of the 4He photo-absorbtion cross section"

#### Universal property of IR extrapolation is nucleus dependent



#### Universal property of IR extrapolation is potential dependent



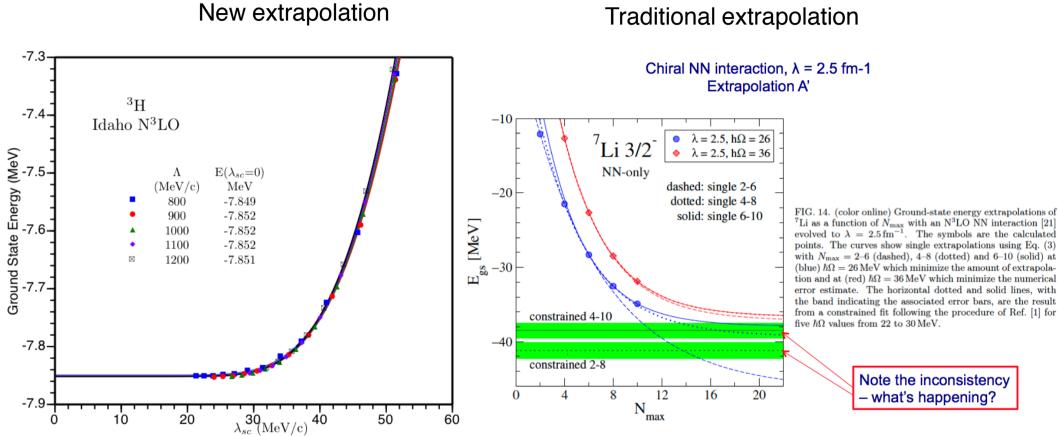
$$\Delta E = E(\lambda_{sc}) - E(\lambda_{sc} = 0) = a \exp(-b/\lambda_{sc})$$

Single nucleon separation energies and slopes of  $\Delta E/E$  vs  $1/\lambda_{sc}$  plots

nucleus	exp.		JISP16	$N^3LO$
	S	$4\sqrt{m_Nc^2S}$	bc	bc
	(MeV)	(MeV)	(MeV)	(MeV)
$^{2}\mathrm{H}$	2.22457	183	192	184
$^{3}\mathrm{H}$	6.25723	307	296	304
$^3{ m He}$	5.49348	287	275	310
$^4\mathrm{He}$	20.2 (ave)	551	502	420
$^6\mathrm{He}$			257	356
<sup>6</sup> Li	5.0 (ave)	275	240	336

Alternate defs of  $\lambda_{sc}$  in Furnstahl et al. PRC **86** (2012), More et al. PRC **87** (2013), Furnstahl et al. ArXiv:1312.6876

model the slope "b" in the table by the momentum which corresponds to the separation energy of a single nucleon from the nucleus.



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E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary, submitted to PRC; arXiv: 1302:5473

### Summary

HO shell model provides a linear trial function for a variational calculation of few-body systems.

Traditional extrapolation from finite model space (N,  $\hbar\omega$ ) is based upon extension of basis (N) "guided by" considerations of non-linear scale parameter ( $\hbar\omega$ ).

Effective Field Theory concepts applied to a discrete basis suggest an alternative extrapolation approach based upon  $(\Lambda, \lambda_{sc})$  which respects ultraviolet (UV) and infrared (IR) running of the results as the basis is extended.

Intrinsic UV and IR scales of the NN interaction are identified.

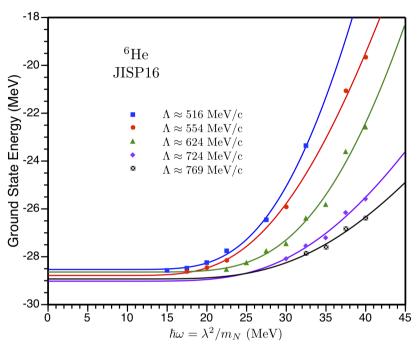
Extrapolation in UV with IR cutoff of model space below intrinsic IR scale is neither robust nor reliable.

Extrapolation in IR with UV cutoff of model space above intrinsic UV scale is quite successful.

Continuing need for higher order (in  $\lambda_{\rm sc}/\Lambda$ ) corrections to these lowest order  $\lambda_{\rm IR}$  and  $\Lambda_{\rm UV}$ 

### Extra Slides

### IR extrapolations with λ



We fit the ground state energy with three adjustable parameters using the relation  $E_{gs}(\hbar\omega) = a \exp(-b/\hbar\omega) + E_{gs}(\hbar\omega = 0)$  five times, once for each "fixed" value of  $\Lambda$ . It is readily seen that one can indeed make an ir extrapolation by sending  $\hbar\omega \to 0$  with fixed  $\Lambda$  as first advocated in Ref. [35] and that the five ir extrapolations are consistent. The spread in the five extrapolated values is about 500 keV or about 2% about the mean of -28.78 MeV. The standard deviation is 200 keV.

S. A. Coon, M. I. Avetian, M. K. G. Kruse, U. Van Kolck, P. Maris, J. P. Vary Archive:1205.3230, PRC 86, 054002 (2012)

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\Lambda =700 MeV/c E(0) = -7.798 MeV 

\Lambda =800 eV/c E(0) = -7.844 MeV 

\Lambda =900 MeV/c E(0) = -7.844 MeV 

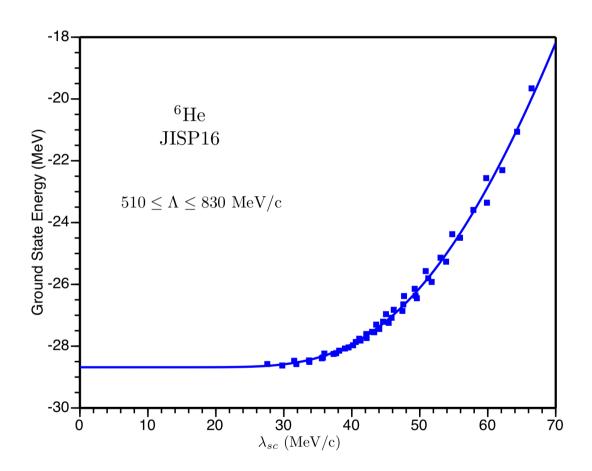
\Lambda =1000 MeV/c E(0) = -7.843 MV 

\Lambda =1100 MeV/c E(0) = -7.841 MeV 

\Lambda =1200 MeV/c E(0) = -7.847 MeV
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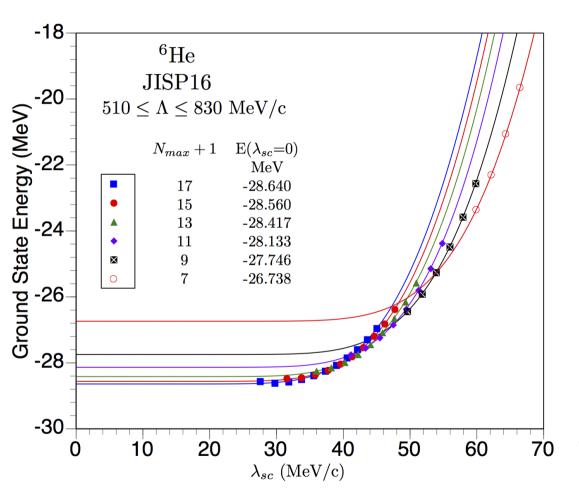
NCSM (Navratil) E= -7.85(1) MeV Faddeev (Machleidt) E= -7.85 MeV HH (Pisa) E= -7.854 MeV

### IR extrapolations with $\lambda_{sc}$



In conclusion, our extrapolations in the ir cutoff  $\lambda$  of -28.78(50) MeV or the ir cutoff  $\lambda_{sc}$  of 28.68(22) MeV are consistent with each other and with the independent calculations.

### Map (N,ħω) onto $(\Lambda, \lambda_{sc})$ holding N fixed



Accepted extrapolation is -28.68(22) MeV

Of the 6 extrapolations only the three with N≥13 are consistent with this number.

But mean of these three large N extrapolations is -28.54 MeV with standard deviation of 0.11 MeV.

Naively concentrating on large N gives a worse extrapolation than using all points with  $\Lambda > 500$  MeV/c.

Moral: results with low N can usefully stabilize and bound an extrapolation to the IR limit.

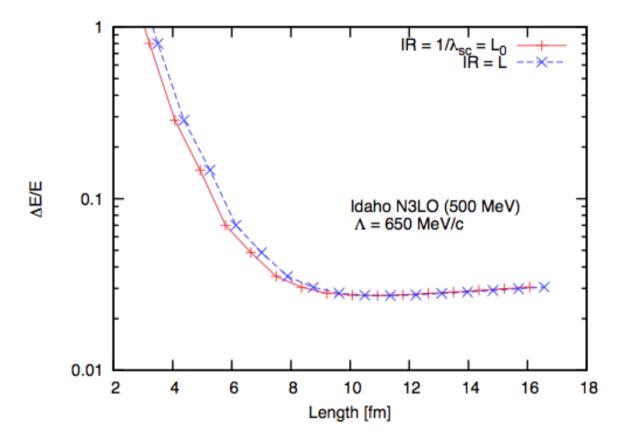


Figure 1: The plot shows the famous plateaus for  $\Lambda = 650 \text{ MeV/c}$ . Note that there is no difference between using the original IR definition  $L_0$  or the 'corrected' IR L.