

# Infrared and ultraviolet cutoffs in variational calculations with a harmonic oscillator basis

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## Collaborators

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# 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 ground state energies.

### 2.1.2. Linear Trial Functions

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

$$\psi_T = \sum_{i=1}^N a_i \varphi_i \quad (2.10)$$

In (2.10) the  $a_i$  are parameters to be varied and the  $\varphi_i$  is a set of known functions. The  $\varphi_i$  may also contain parameters  $\beta_j$ , which will be varied, but it transpires that for fixed  $\beta_j$  the choice of the optimum  $a_i$  is very straightforward, and we do not display the  $\beta_j$  explicitly here. With the form (2.10) for  $\psi_T$ , equation (2.4) for  $E_v$  can be written

$$E_v = \mathbf{a}^+ H_N \mathbf{a} / \mathbf{a}^+ N \mathbf{a} \quad (2.11)$$

where  $H_N$  and  $N_N$  are the  $N \times N$  Hamiltonian and normalization matrices in the representation  $\{\varphi_i\}$ :

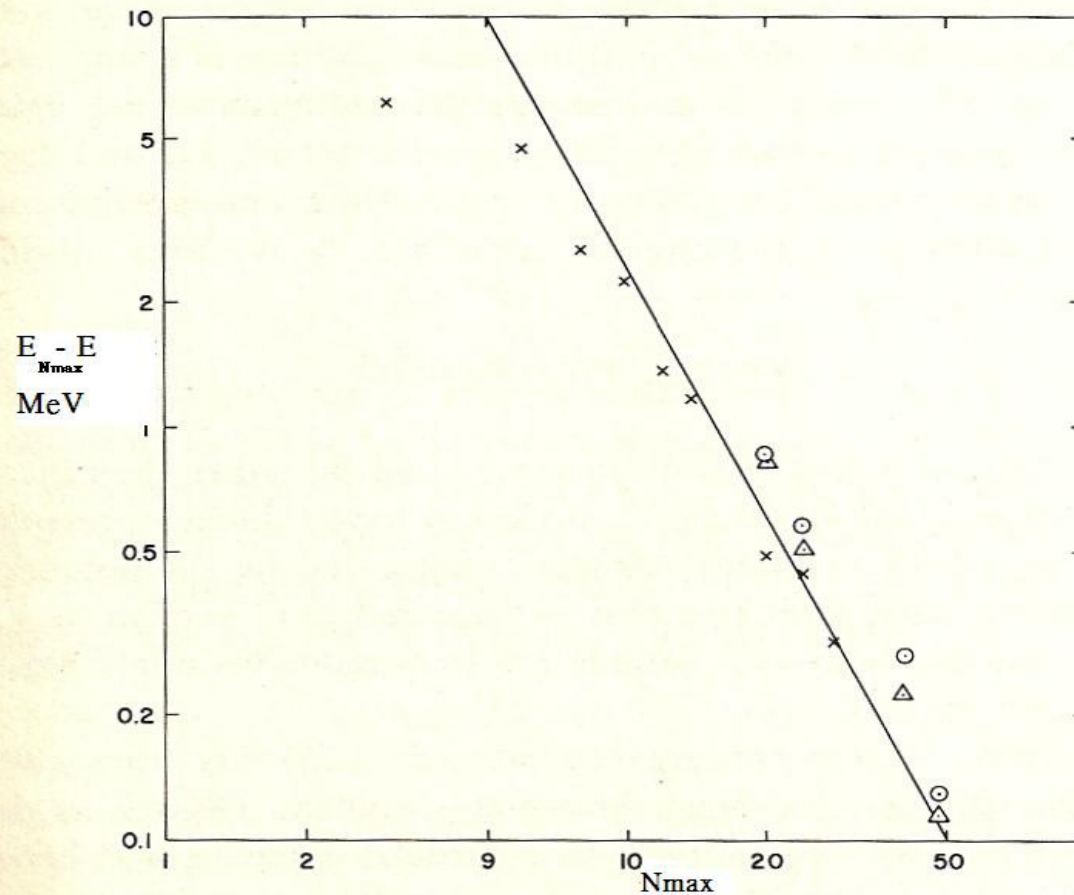
$$(H_N)_{ij} = (\varphi_i, H \varphi_j) \quad (N_N)_{ij} = (\varphi_i, \varphi_j) \quad i, j = 1, \dots, N$$

and  $\mathbf{a}$  is the vector of coefficients  $a_i$ .  $H_N$  and  $N_N$  are Hermitian matrices, and  $N_N$  is positive definite. From (2.11) or directly from (2.6) with  $\partial \psi_T / \partial a_i = \varphi_i$ , we obtain the defining equation for  $\mathbf{a}$  and  $E_v$ :

$$(H_N - E_v N_N) \mathbf{a} = 0 \quad (2.12)$$

Equation (2.11) has a number of attractive properties which help to make expansions of the form (2.10) popular. First, the minimum of  $E_v$  with respect to the parameter  $\mathbf{a}$  always exists, since a finite eigenvalue problem of the form (2.12) is guaranteed to have  $N$  real eigenvalues  $E_i(N)$ ,  $i = 1 - N$  and  $N$  independent eigenvectors. Second, as is well known, we obtain from (2.12) not only a bound on the lowest eigenvalue  $E_0$  but also on the higher eigenvalues  $E_1, \dots, E_{N-1}$  of  $H$ ; indeed we can show that

$$E_i(N) \geq E_i \quad i = 0, \dots, N - 1 \quad (2.13)$$



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  $\hbar\omega$  for fixed number of quanta  
 Number of quanta increases by two for each curve

1969 H atom up to 10 quanta

M. MOSHINSKY

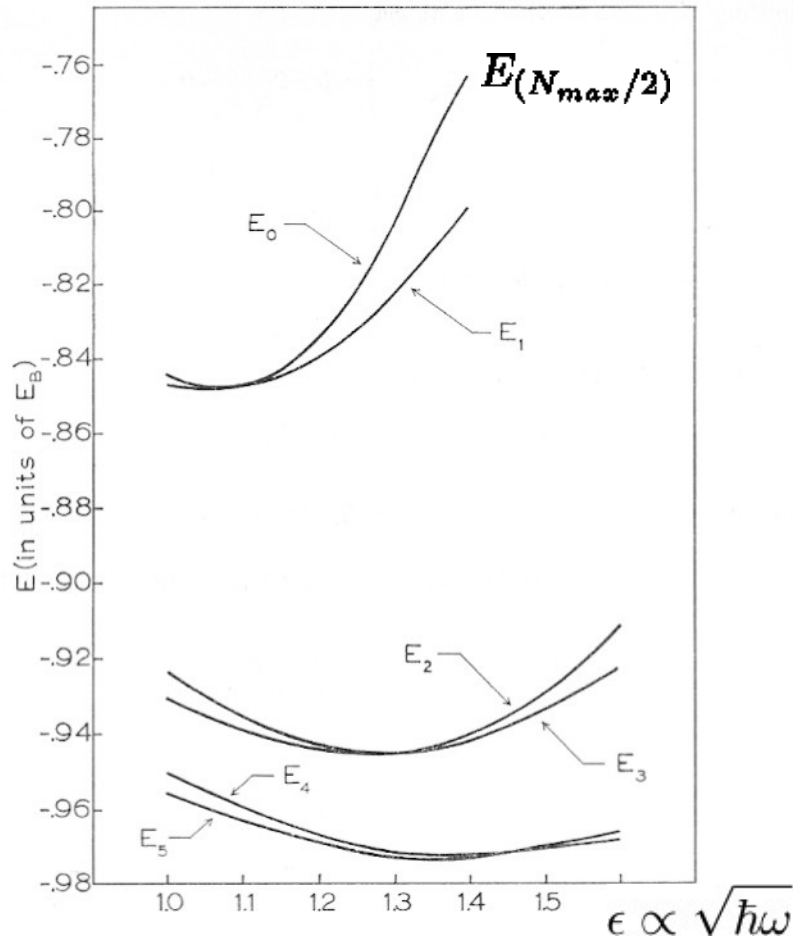
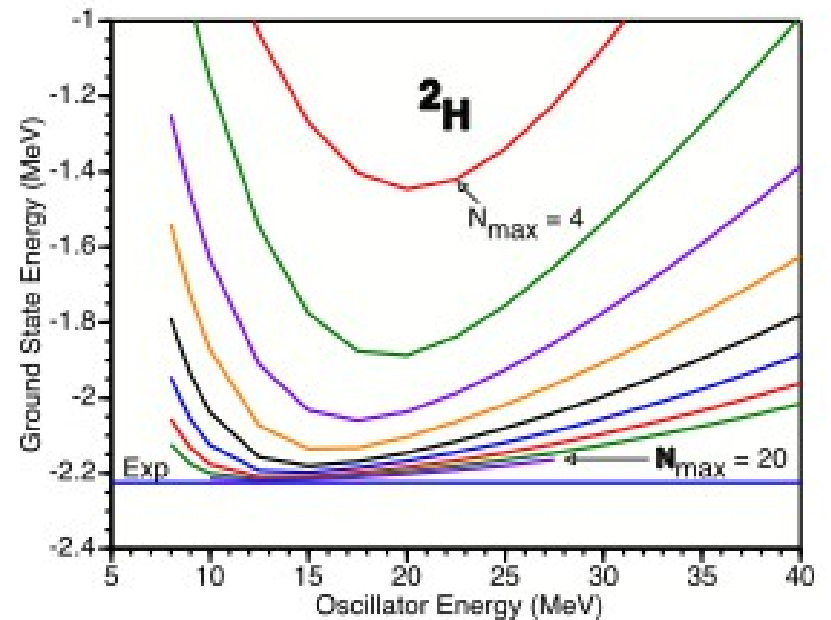


FIG. 1. Energy of the ground state of the H atom as a function of the parameter  $\epsilon$  for the variational analysis discussed in Section 3. This energy  $E_p(\epsilon)$ ,  $p = 0, 1, 2, 3, 4, 5$  is associated with a trial wave function  $\psi_p = \sum_{n=0}^p a_n^{(p)} |n00\rangle$ , where  $|n00\rangle$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

2009 deuteron up to 20 quanta



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



# ALPHA PARTICLE MODEL CALCULATIONS FOR $^{12}\text{C}$ AND $^{16}\text{O}$ <sup>†</sup>

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*Instituto de Física UNAM, México*

Received 14 December 1973

**Abstract:** Spectra and form factors of  $^{12}\text{C}$  and  $^{16}\text{O}$  are calculated in the  $\alpha$ -particle model. Empirical  $\alpha$ - $\alpha$  interactions are used in a variational calculation in a translationally invariant harmonic oscillator basis. The validity of the  $\alpha$ -particle model is discussed in view of the results, which show some nice qualitative features and fail quantitatively in some points.

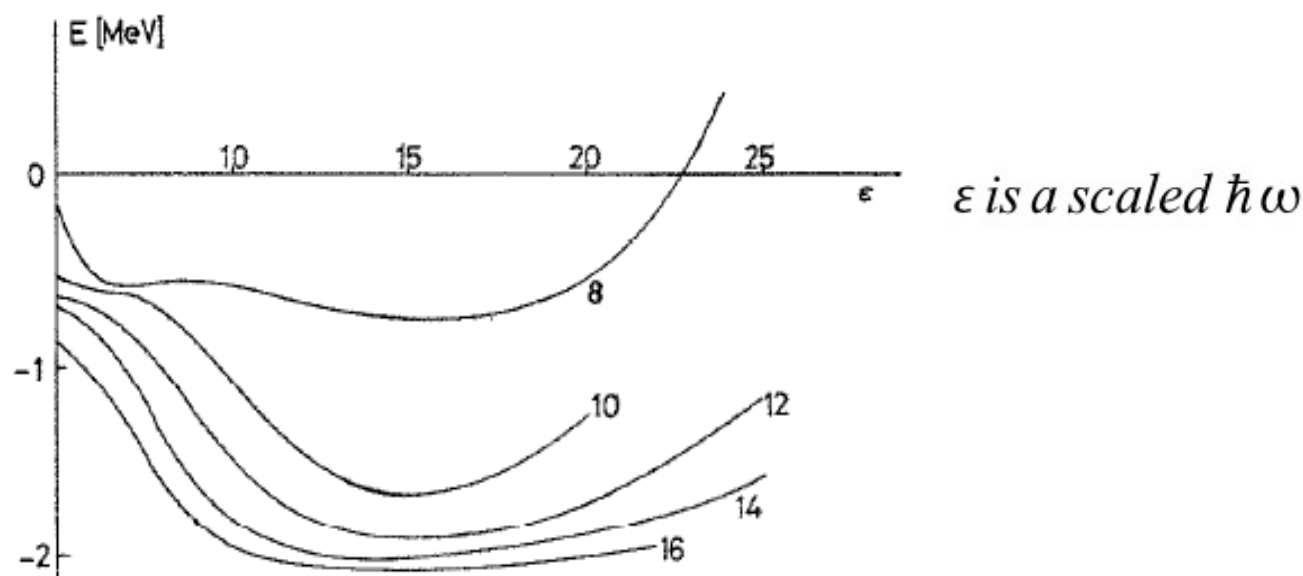
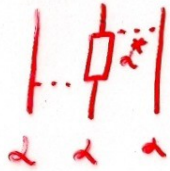


Fig. 2. Ground state energy of  $^{12}\text{C}$  for the potential A2 at 8, 10, 12, 14 and 16 quanta as a function of the oscillator width  $\epsilon$ .

include a 3d force in the Hamiltonian

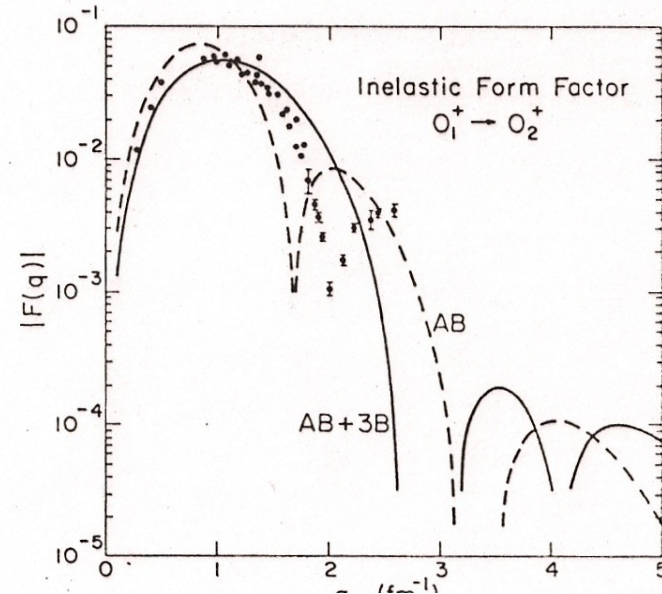
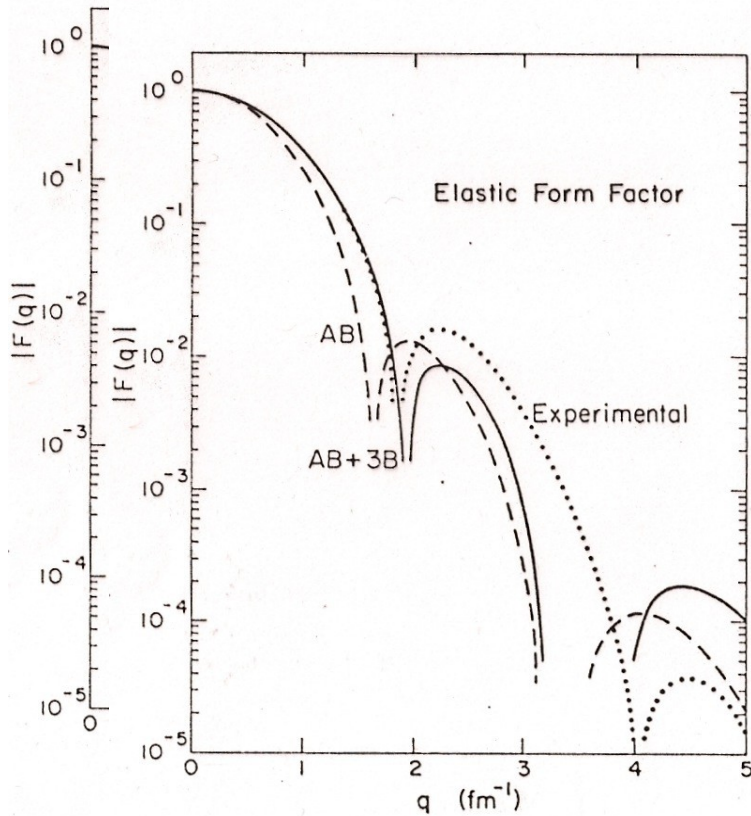
Portilho, Agrello, Coon PRC 27, 2923 (1983)

Convergence?



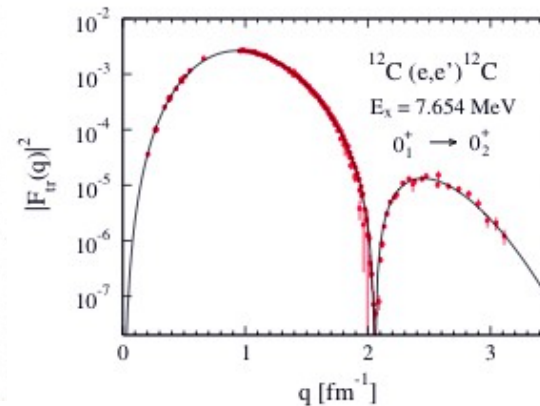
$N=10 \rightarrow N=12 \Rightarrow 57\%$  decrease  
in second maximum  
of elastic form factor

This calculation used  $N=16$



Hoyle state

1983  
data



2010  
data

# 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:

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# The No-Core Shell Model (NCSM)



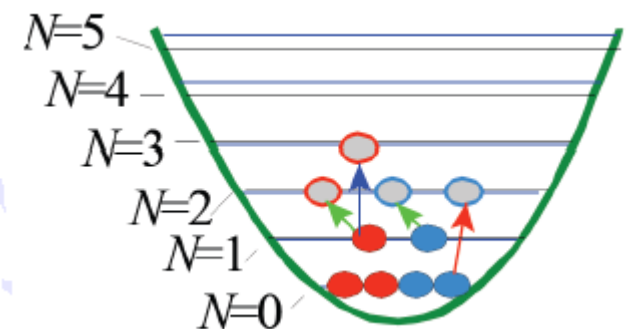
Starting Hamiltonian is translationally invariant.

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

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

It's that “simple”.

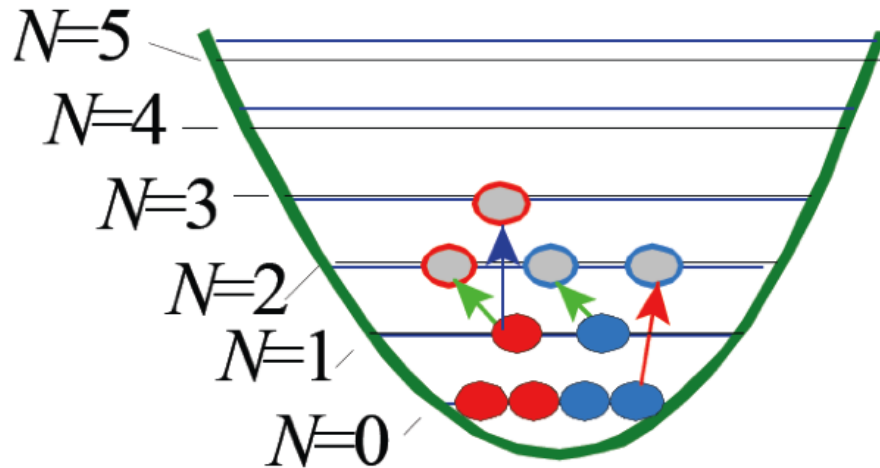
NCSM has two parameters:  
Nmax and  $\Omega$



If we now use a single-particle basis, we have to remove the spurious CM states.

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

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



- Each Slater determinant corresponds to a configuration of  $A$  particles distributed over  $A$  single-particle states.  
Irvine, J. M. et al. "Nuclear Shell-Model Calculations and Strong Two-Body Correlations"
- The picture to the left is for Li-6 (3 protons + 3 neutrons).
- Shows  $N_{\text{max}}=2$  configuration
- Two units of energy distributed among the six particles.

# Extrapolating with $N_{\text{Max}}$

Challenge: achieve numerical convergence for no-core Full Configuration calculations using finite model space calculations

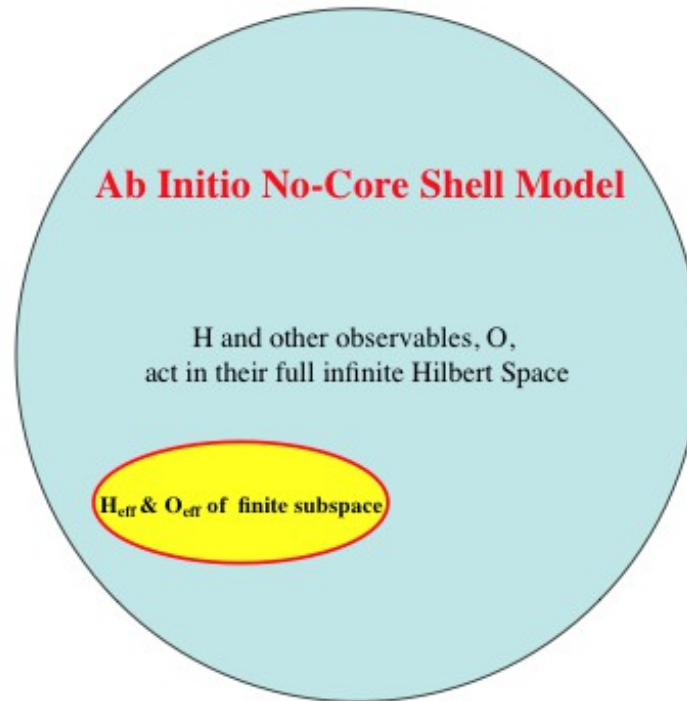
- Perform a series of calculations with increasing  $N_{\text{max}}$  truncation (while keeping everything else fixed)
- Extrapolate to infinite model space  $\longrightarrow$  exact results
  - binding energy: exponential in  $N_{\text{max}}$

$$E_{\text{binding}}^N = E_{\text{binding}}^{\infty} + a_1 \exp(-a_2 N_{\text{max}})$$

- use 3 or 4 consecutive  $N_{\text{max}}$  values to determine  $E_{\text{binding}}^{\infty}$
- use  $\hbar\omega$  and  $N_{\text{max}}$  dependence to estimate numerical error bars

Maris, Shirokov, Vary, Phys. Rev. C79, 014308 (2009)

Slide by Pieter Maris



This truncation/extrapolation scheme is essentially that of the earlier few-body variational studies  
 Assumes that the boundary of finite subspace is defined only by  $N_{\text{max}}$   
 implication:  $\hbar\omega$  is an inessential complication

**Not the case!** The use of HO single particle orbitals means that the many-fermion system is limited to a region whose size is governed by the parameter of the HO basis:  $\hbar\omega$

The finite model space is characterized by two parameters:  
 $N_{\text{max}}$  and  $\hbar\omega$



# Current Method is Unsatisfactory...

- ...from an effective field theory point of view.
- Results are oscillator frequency dependent.
- 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.

# Effective Field Theory (EFT)

In a field theory one *never* has access to the “full” Hilbert space. Interactions are only defined in the context of a model space—a truncation to *exclude* states with energies beyond those a physicist can access.

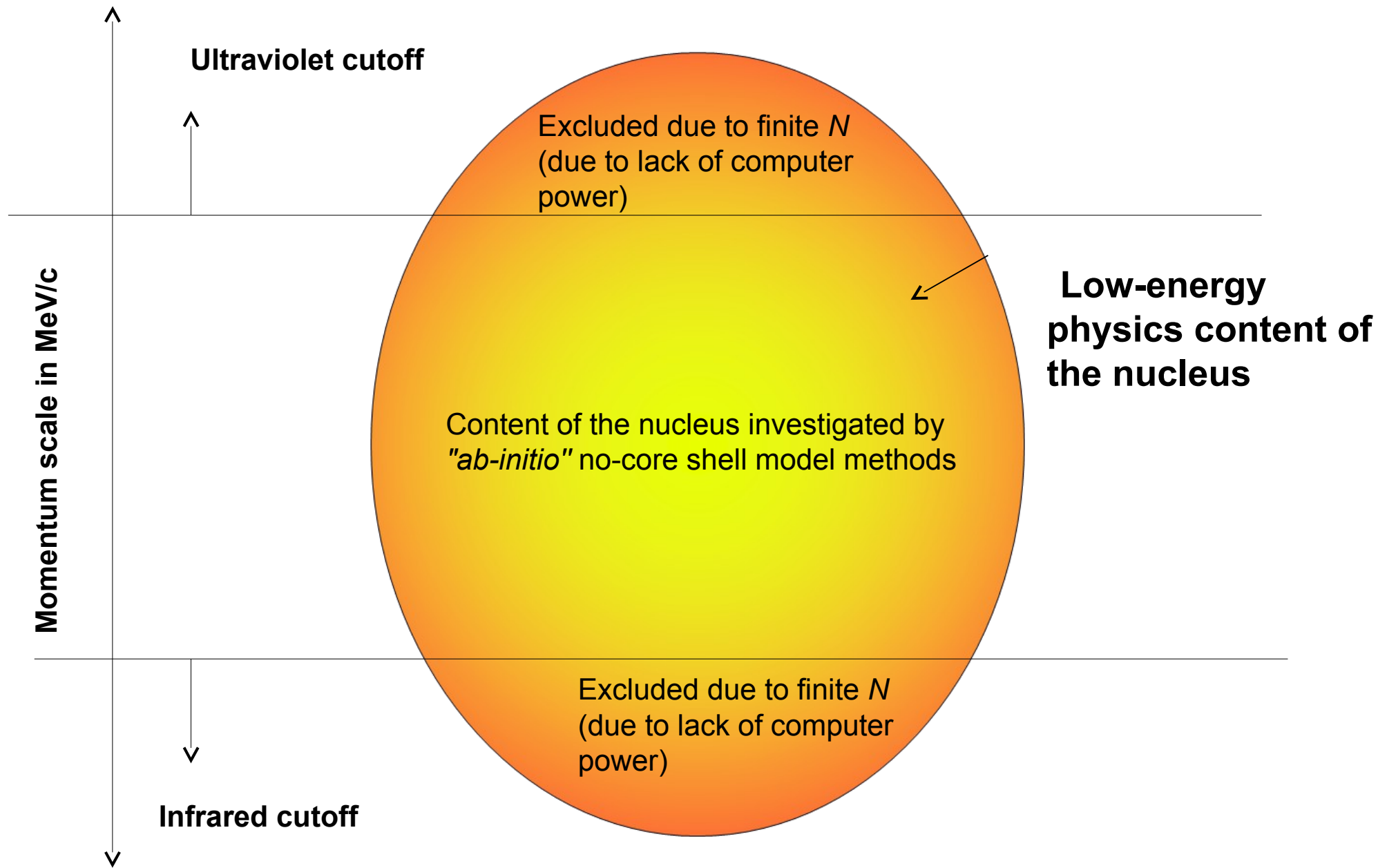
The parameter of the projection operator  $P$  onto the excluded states must have a dimension. Call the parameter  $\Lambda$ , the ultraviolet cutoff and take it to be a momentum.

**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  $Q \ll \Lambda$  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. Must deal with all interactions consistent with symmetries of problem, learn what is perturbative and what is not, arrange an organizational principle for perturbation theory (“power counting”) etc etc. 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 or NCFC which utilize “realistic” nuclear interactions fit to data, not in a clearly defined model space, but in free space?



~ larger nuclei?

As A grows, given computational power limits  
number of accessible one-nucleon states

## No-Core Shell Model!

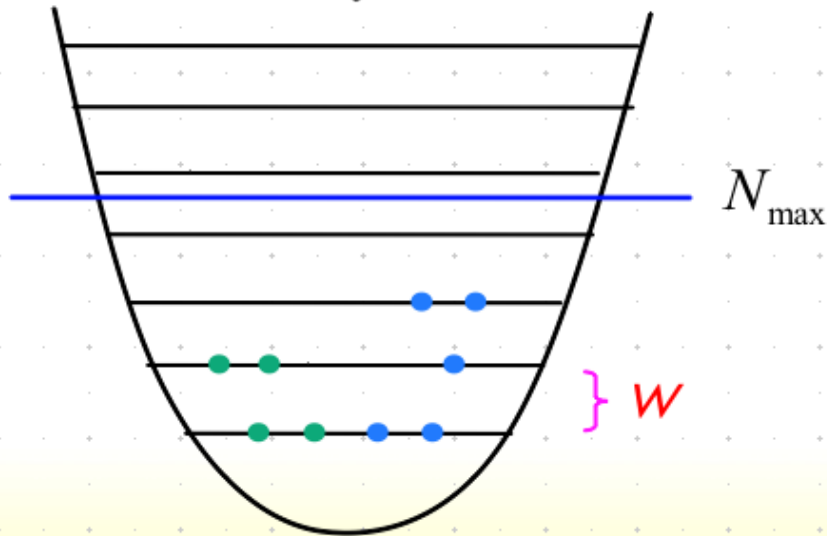
Stetcu, Barrett + v.K., '06

Stetcu, Barrett, Vary + v.K., '07

Stetcu, Rotureau, Barrett + v.K., in progress

HO basis

⋮



cutoffs

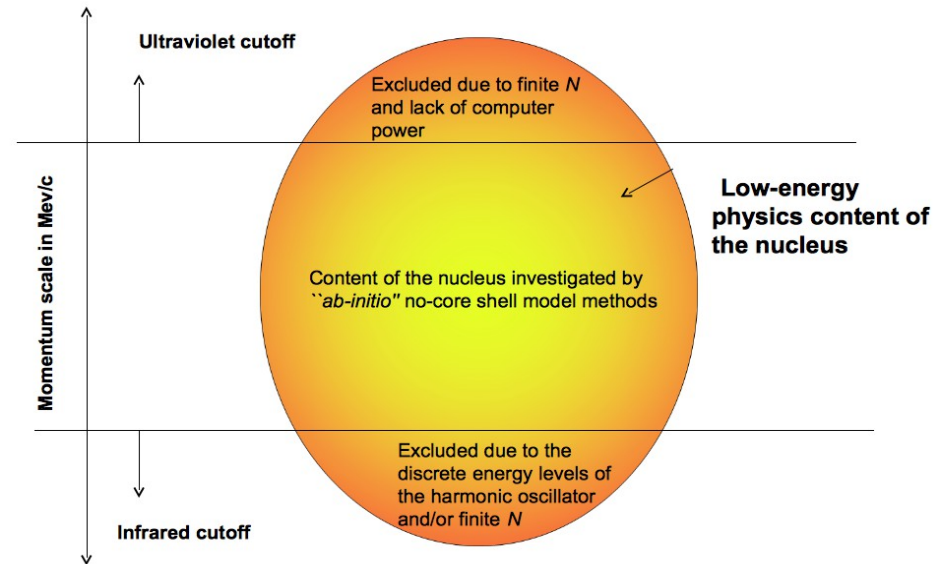
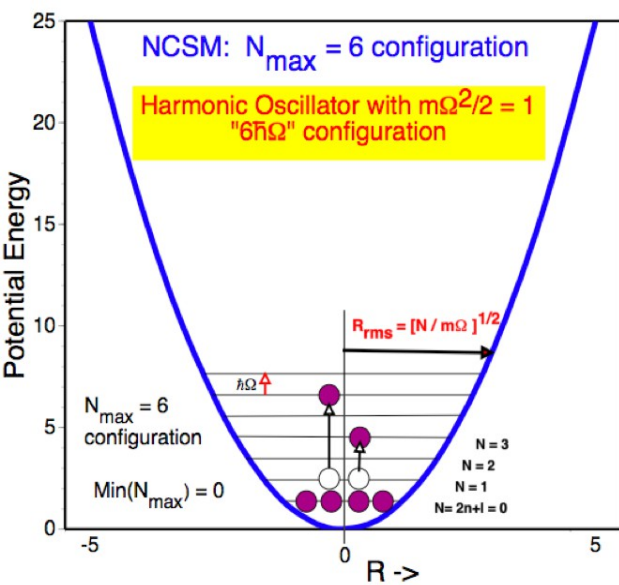
For lattice cutoffs:  
Mueller, Koonin, Seki + v.K. '00  
Lee et al. '03...

UV  $L = \sqrt{m_N (N_{\max} + 3/2) W}$

IR  $l = \sqrt{m_N W}$

**strategy:** at any given order, for each pair of cutoffs, fit parameters to binding energies of lightest nuclei, then predict other binding energies





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

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

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 means the energy levels are quantized. The associated momenta cannot take on continuous values so that the model space necessarily has an infrared (IR) momentum cutoff  $\lambda$ .

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

$\lambda$  is an artifact of the HO basis and must be removed as one extrapolates to an infinite basis

## Another discretization scheme: QCD on a 4-dimensional lattice

Continuum QCD simulated on a lattice has a model space with two cutoffs

UV cutoff  $\Lambda \sim 1/a$  where  $a$  is lattice spacing

IR cutoff  $\lambda \sim 1/L$  where  $L$  is the size of the lattice

$a$  must be small enough to simulate the continuum

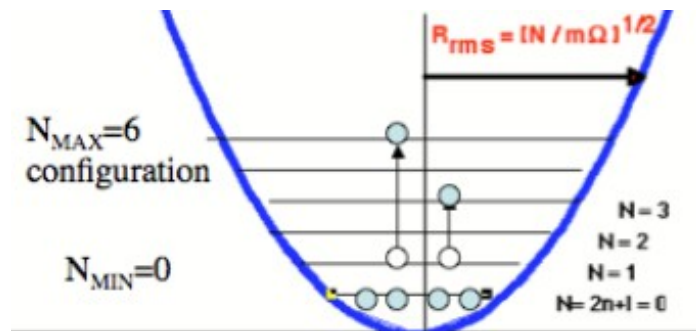
$L$  must be large enough to contain the system

Suggests another possible IR cutoff for a HO basis

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

This IR cutoff corresponds to the rms radius of the highest single particle state in the basis, i.e. the maximal radial extent needed to encompass the system

$$\lambda_{SC} = 1 / (\sqrt{N_{Max} + 3/2} b) \quad \text{where} \quad b = (m_N \hbar \omega)^{-1/2}$$



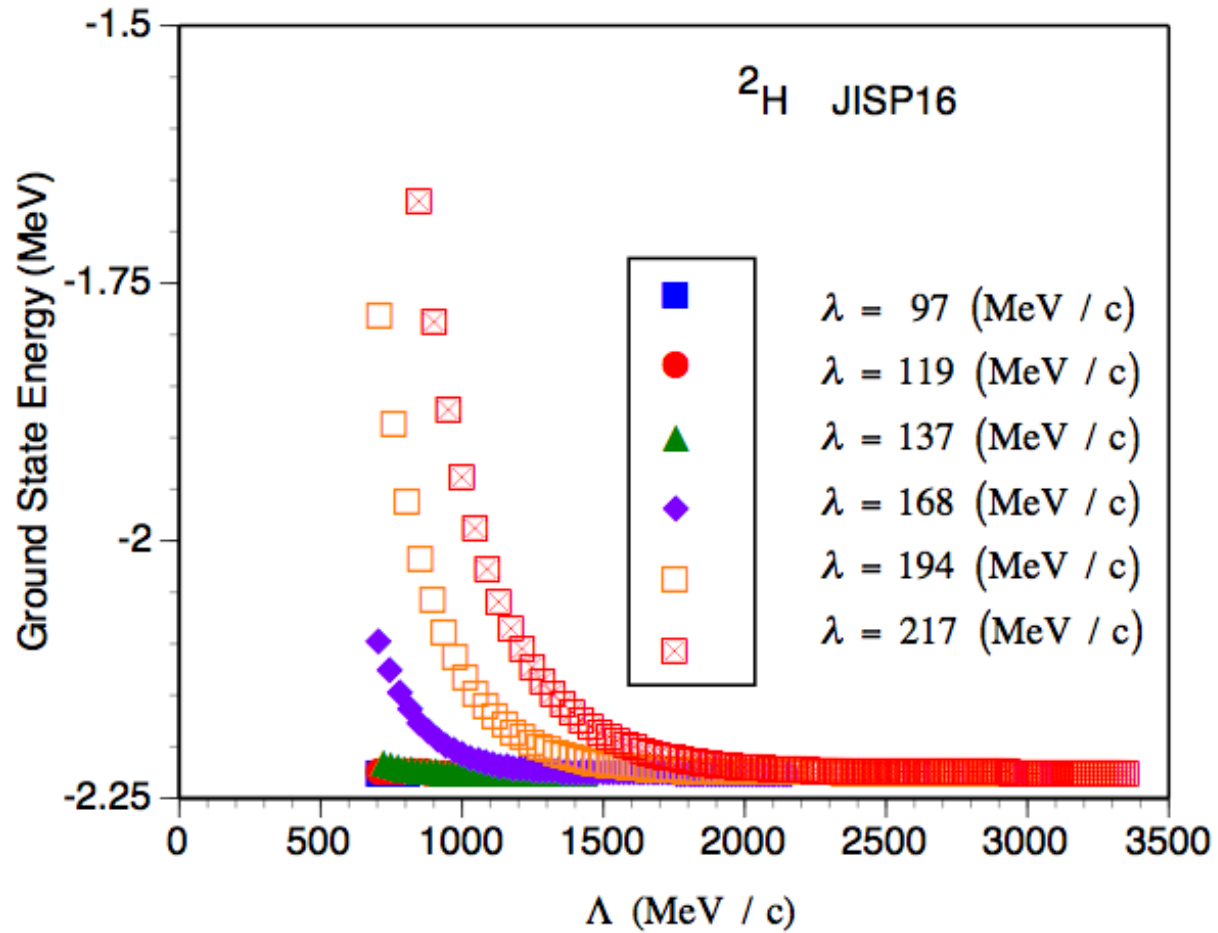
Which IR cutoff is it to be?

Note 1  $\lambda_{SC} = \lambda^2 / \Lambda$

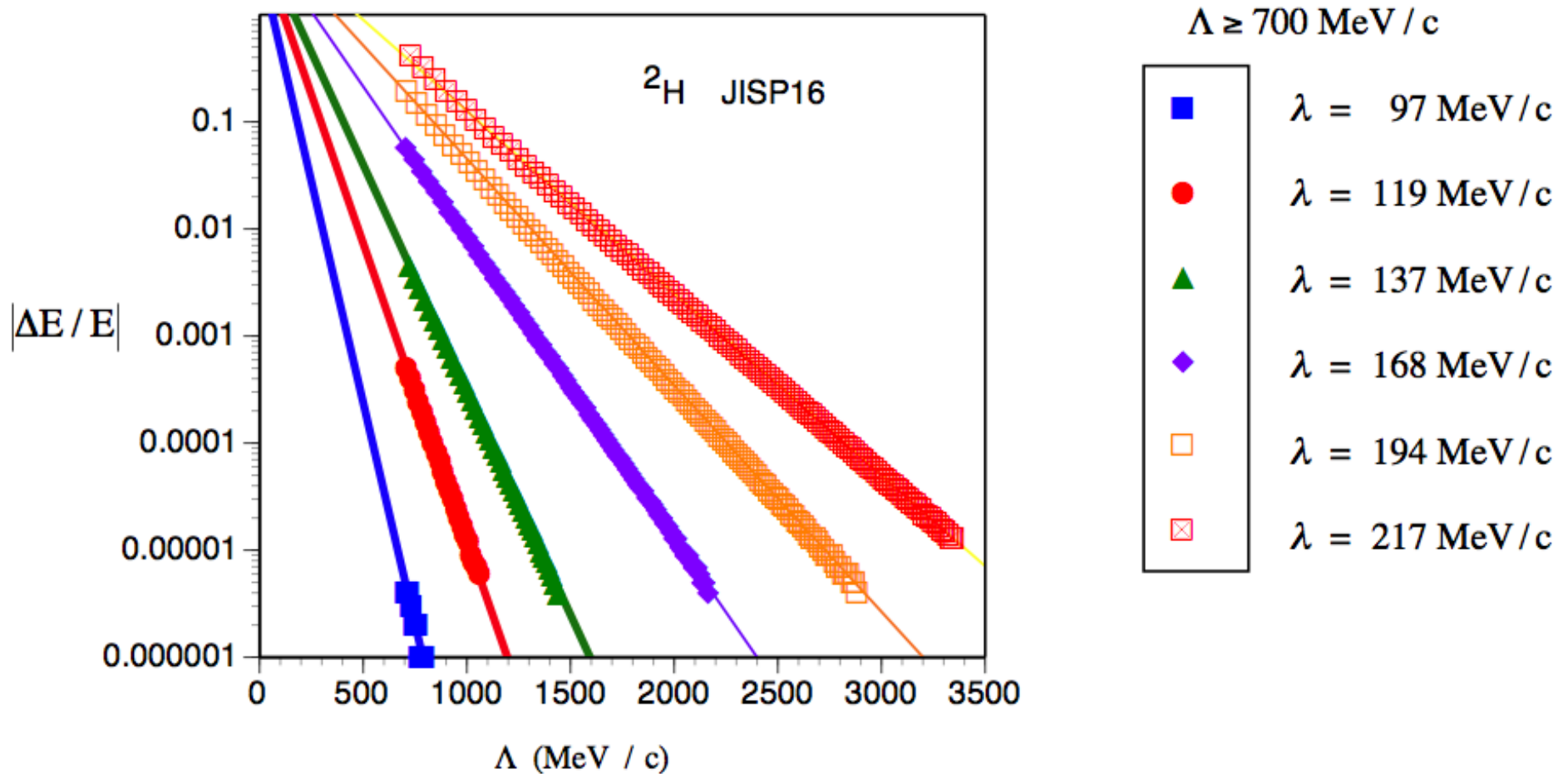
Note 2  $N_{Max} + 3/2 = \Lambda^2 / \lambda^2$   
 $= \Lambda / \lambda_{SC}$

Mixes up **two** dimensionful cutoffs

Test model space cutoffs with deuteron calculation done with defined  $N_{\max}$  and  $\hbar\omega$  convergence is clear as  $N_{\max}$  goes to 238



$\lambda_{\text{IR}} \equiv \lambda$  acts as an IR cutoff should!

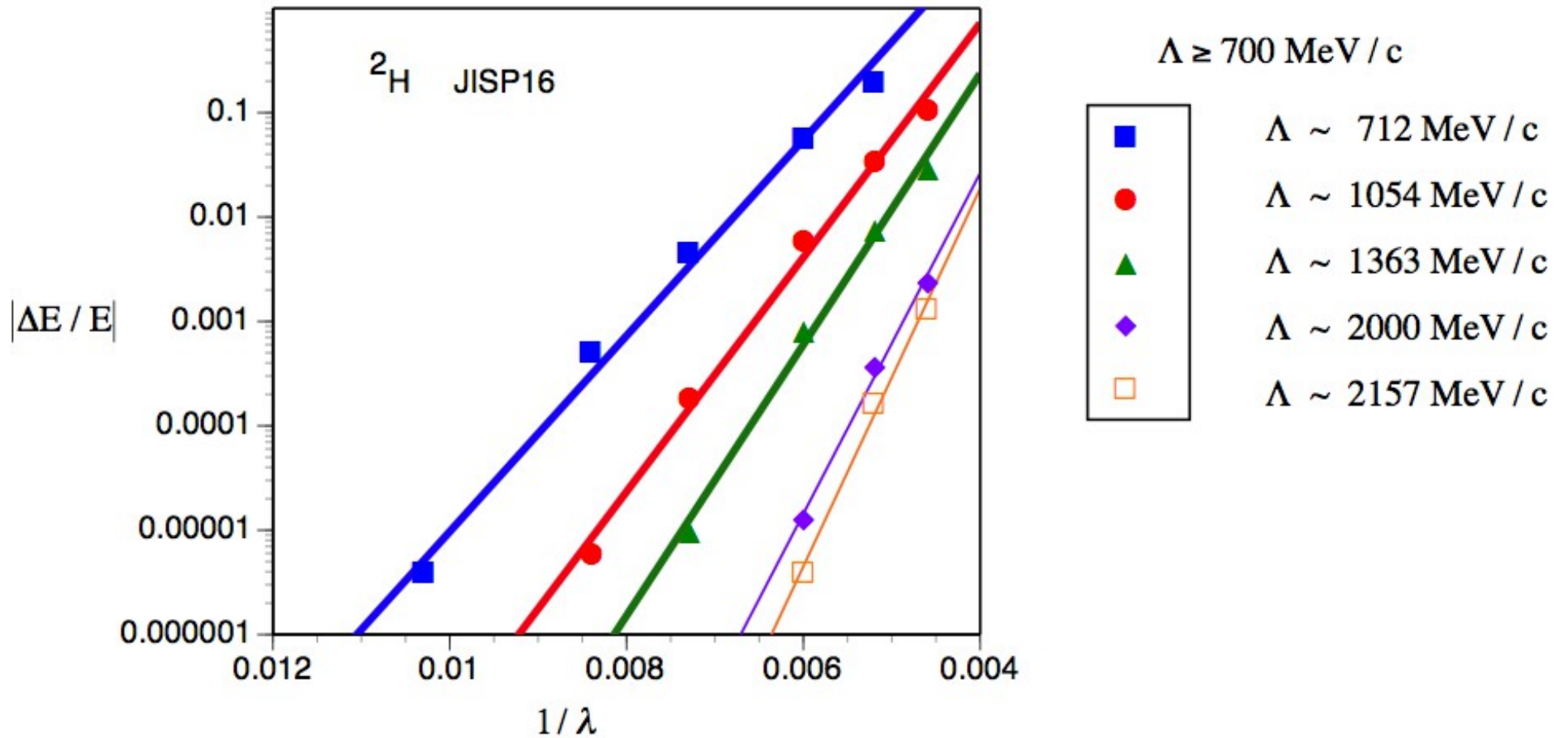


As the ultraviolet cutoff increases, the fractional difference between calculated  $E(\Lambda, \lambda)$  and an accepted-as-converged  $E$ , lessens.

Alternatively, the plot can be read the other way, where if we fix the UV  $\Lambda$ , the results improve as we lower the IR cutoff  $\lambda$ .



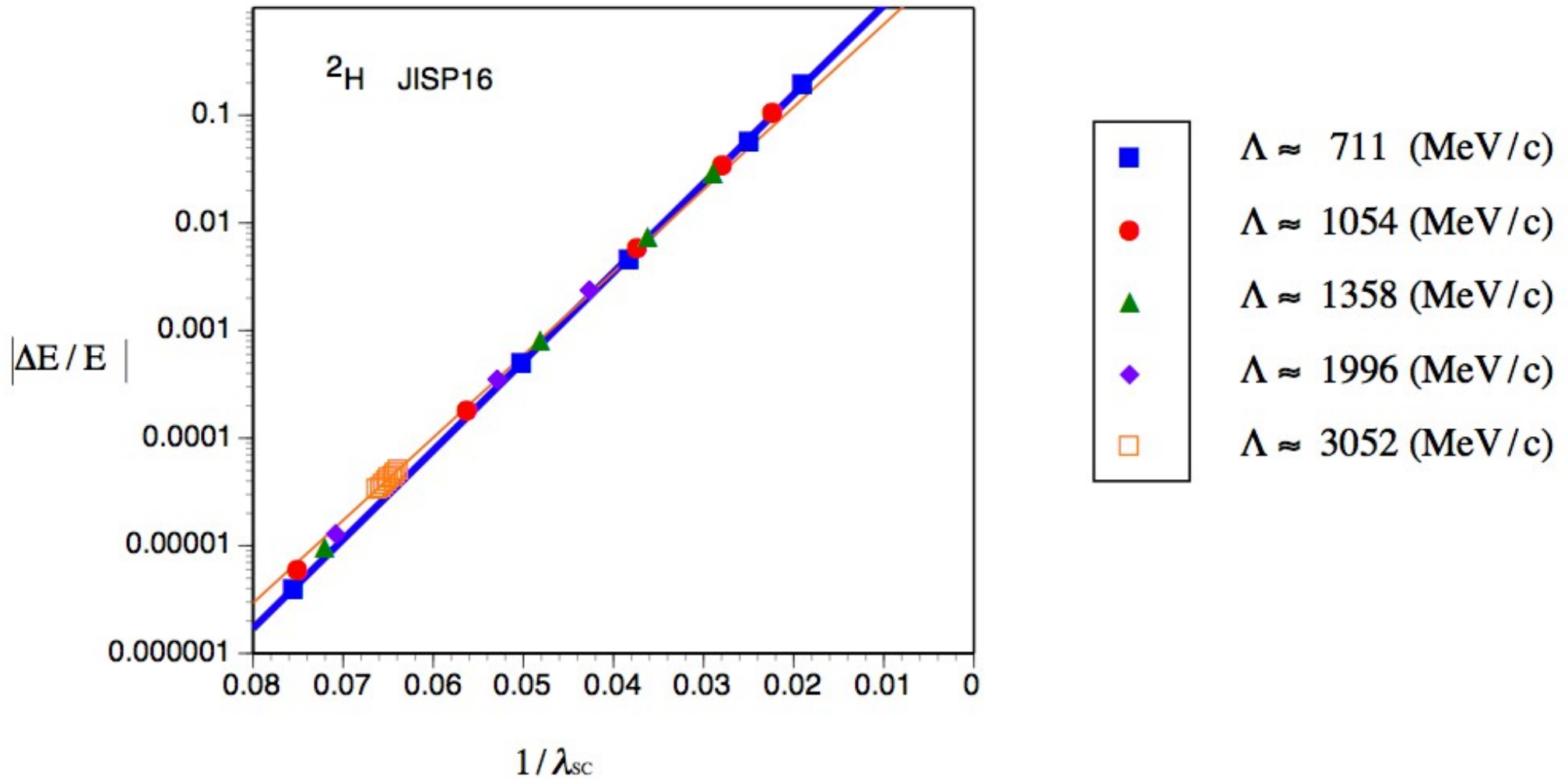
$\Lambda$  acts as an UV cutoff should!



small  $\lambda$

large  $\lambda$

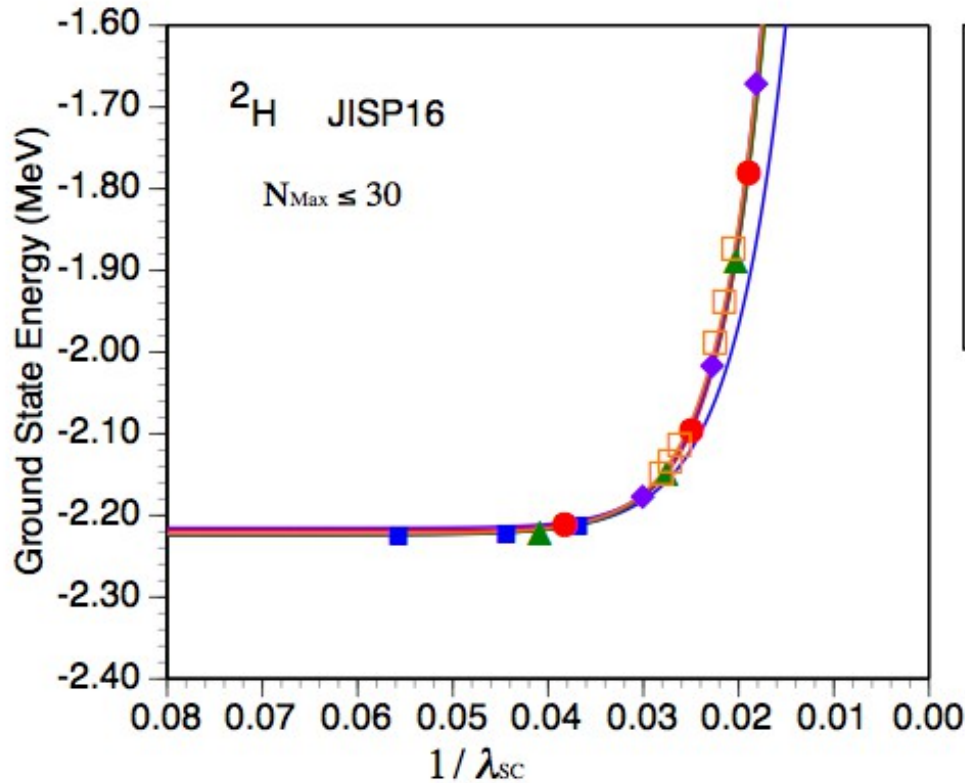
Result scales with  $1/\lambda_{sc} = \Lambda/\lambda^2$  , almost a universal behavior



Success! UV and IR cutoffs identified as  $N_{\max} \rightarrow 238$   
 $\lambda_{SC} = \lambda^2 / \Lambda$

Are cutoffs of any use for approachable  $N_{\max}$  ?

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



- $\Lambda = 524 - 526$  MeV / c  $E(\lambda_{sc} = 0)$  is -2.2243 MeV
- $\Lambda = 702 - 719$  MeV / c  $E(\lambda_{sc} = 0)$  is -2.2185 MeV
- ▲  $\Lambda = 763 - 778$  MeV / c  $E(\lambda_{sc} = 0)$  is -2.2234 MeV
- ◆  $\Lambda = 848 - 856$  MeV / c  $E(\lambda_{sc} = 0)$  is -2.2153 MeV
- $\Lambda = 957 - 1053$  MeV / c  $E(\lambda_{sc} = 0)$  is -2.2221 MeV

average  $E(\lambda_{sc} = 0)$  is -2.221 MeV

$E(\text{converged})$  is -2.224574 MeV

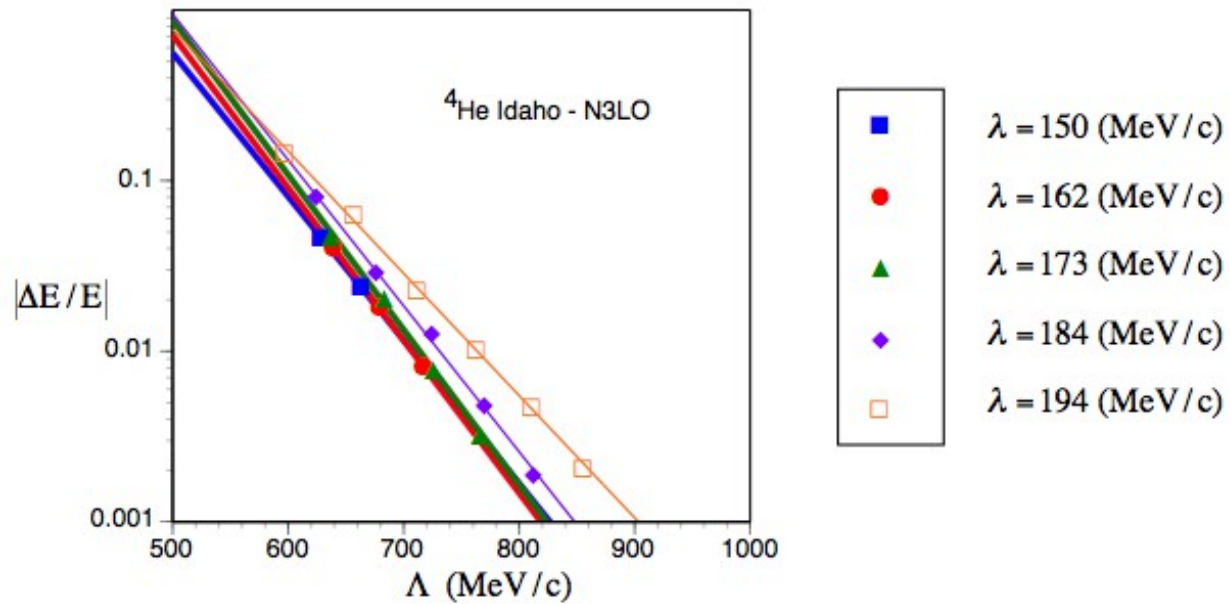
Note: This is not the usual extrapolation in  $N_{\max}$  (with some prescription for  $\hbar\omega$ ) because

$$\begin{aligned} 1/\lambda_{sc} &= \Lambda/\lambda^2 \\ &= \sqrt{(N_{\max} + 3/2)/(m_N \hbar\omega)} \\ &\propto \sqrt{N_{\max}/(m_N \hbar\omega)} \end{aligned}$$

$N_{\max}$  and  $\hbar\omega$  on an equal footing

# Idaho-N3LO potential

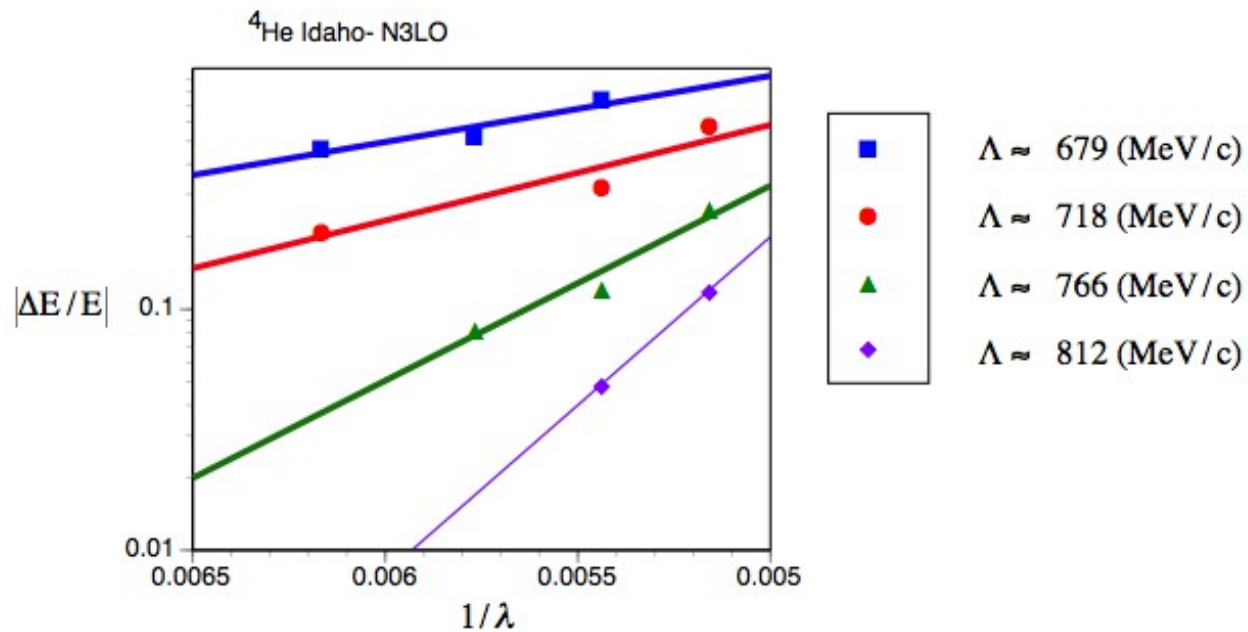
$\lambda$  acts as an IR cutoff should



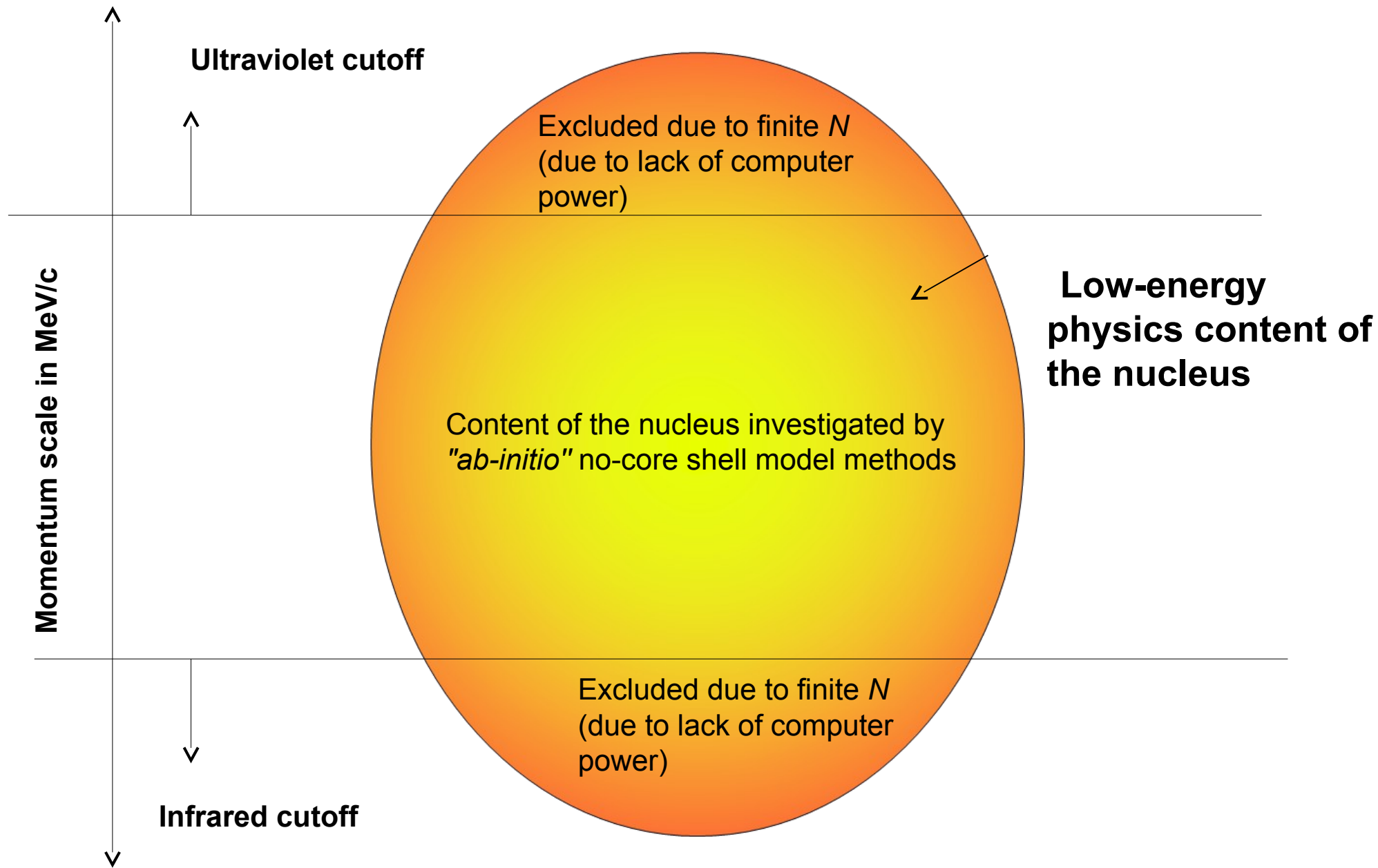
Replotted from calculations of Navratil and Caurier 2004

# Idaho-N3LO potential

$\Lambda$  acts as an UV cutoff should



Replotted from calculations of Navratil and Caurier 2004



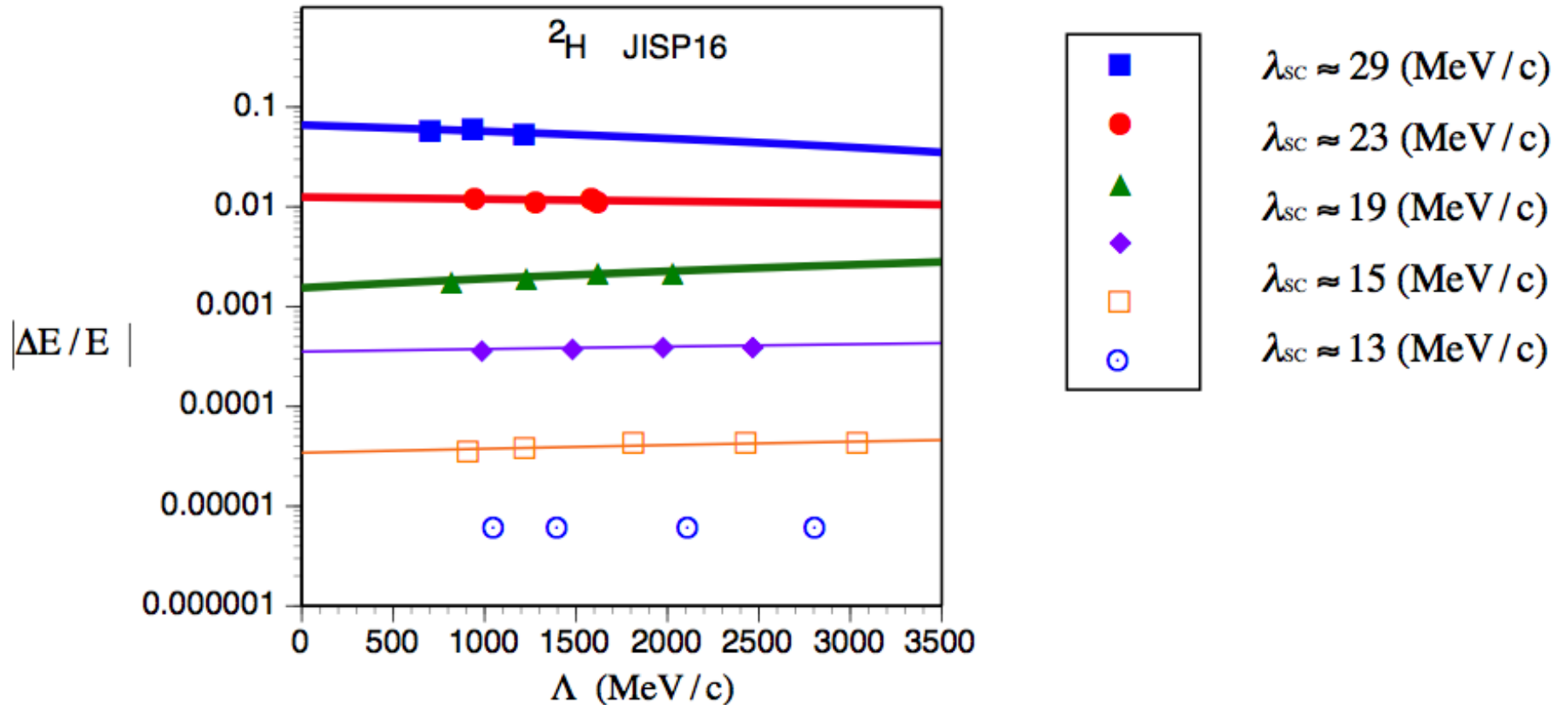


For fixed  $\lambda_{sc}$  result does NOT improve with increasing  $\Lambda$  if  $\Lambda \geq 700$  MeV/c !

Why?

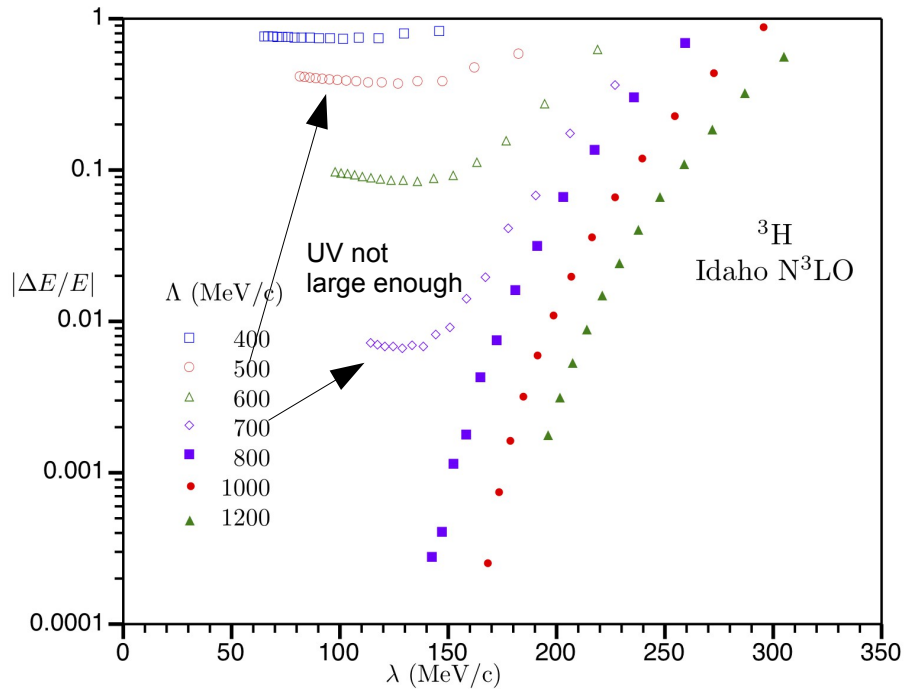
We need dedicated calculations

Binning and replotting archival calculations is not enough!

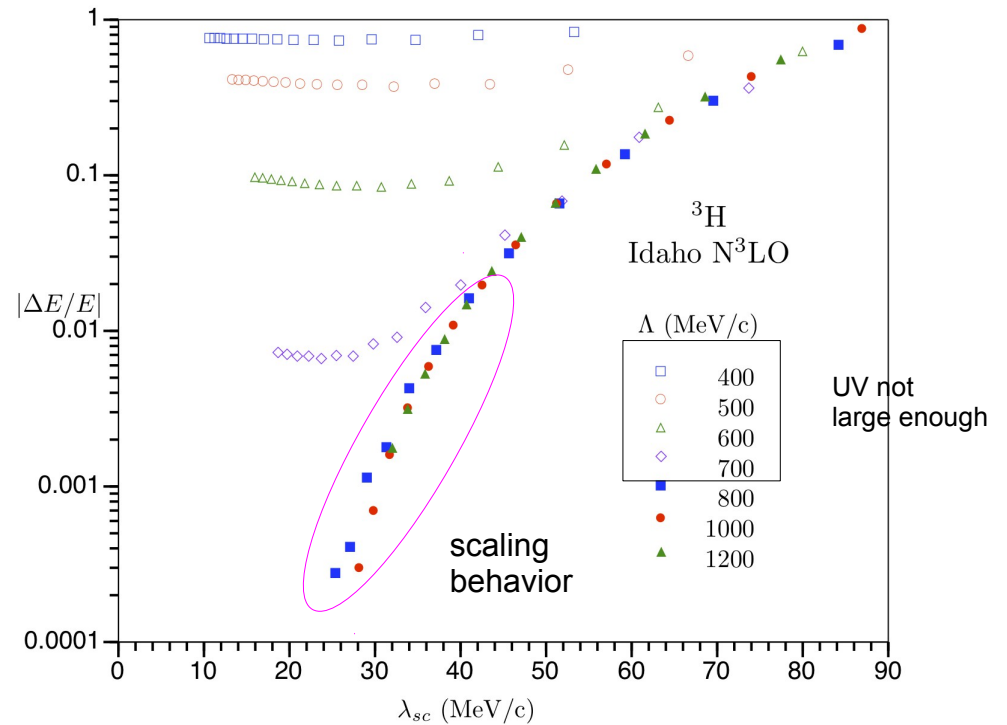


# Fix UV regulator and take IR regulator toward zero

$$\lambda_{IR} = \lambda$$



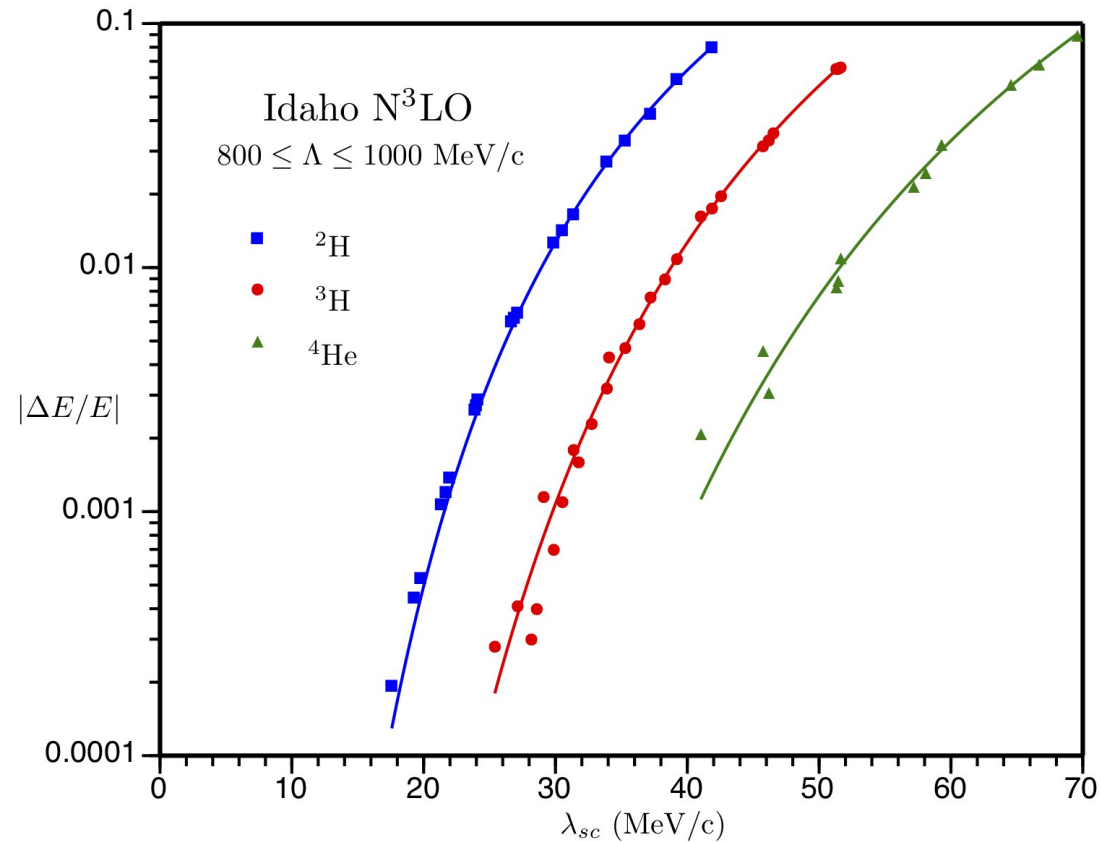
$$\lambda_{IR} = \lambda_{sc}$$



For a large enough ultraviolet cutoff, the fractional difference between calculated  $E(\Lambda, \lambda)$  and an accepted-as-converged  $E$ , lessens as the IR cutoff goes toward zero.

For a large enough UV cutoff,  $\lambda_{sc}$  displays an almost universal scaling behavior

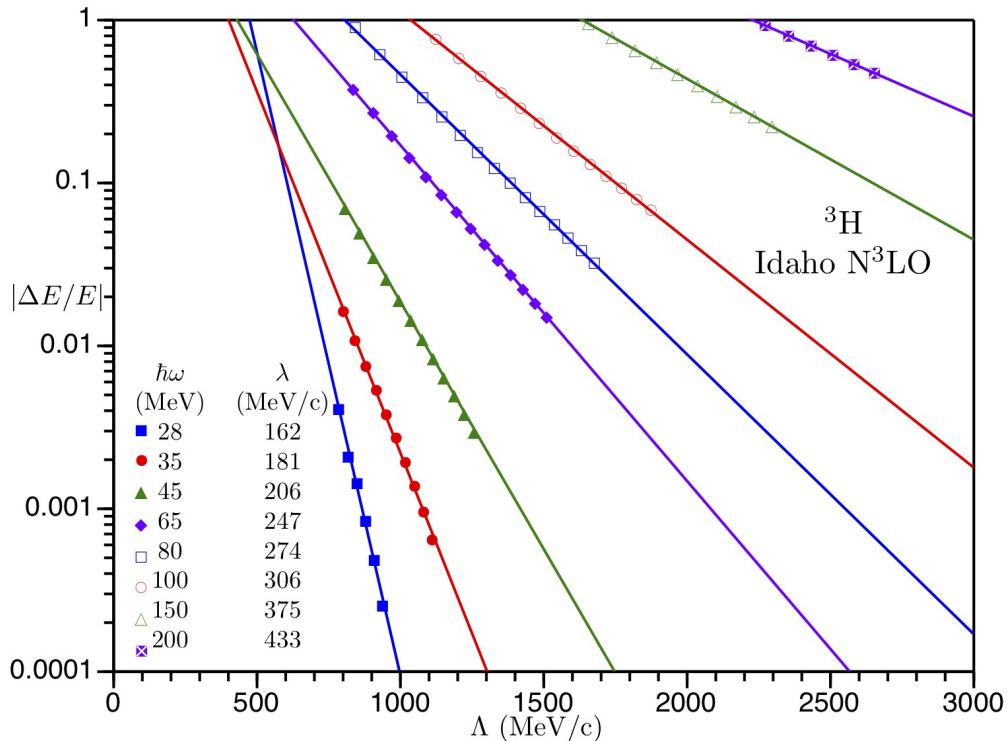
One can use this universal scaling behavior to make an extrapolation which is independent of particle number



Data points are fit to  $y = A \exp(-B/\lambda_{sc})$

# Fix IR regulator and take UV regulator to infinity

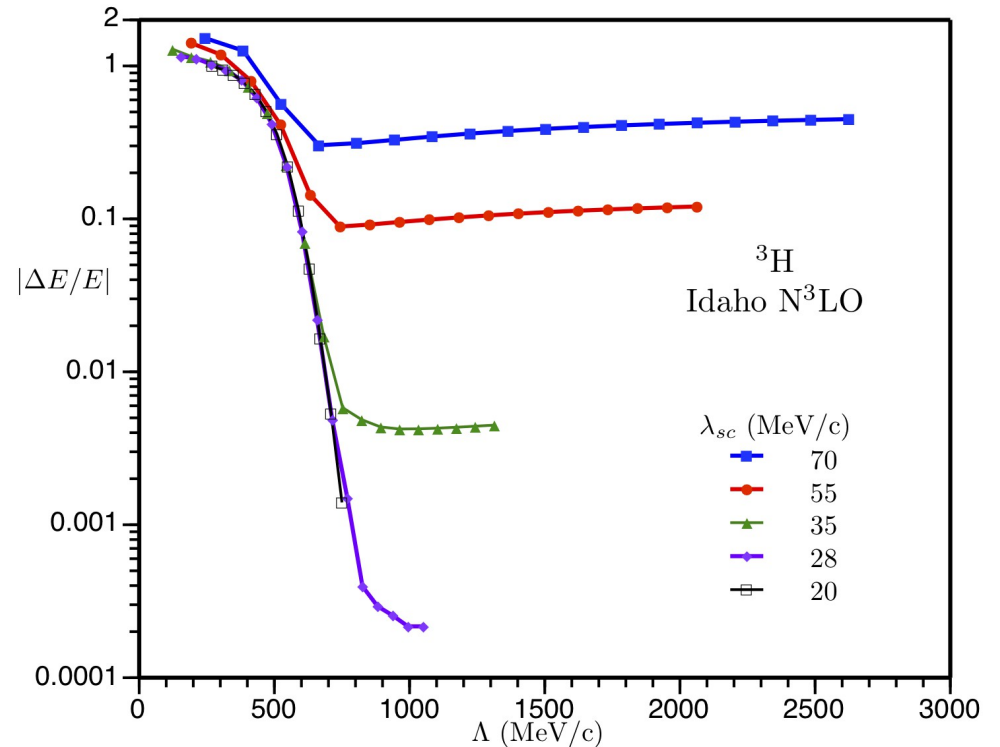
$$\lambda_{IR} = \lambda$$



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Alternatively, the plot can be read the other way, where if we fix the UV  $\Lambda$ , the results improve as we lower the IR cutoff  $\lambda$ .

$$\lambda_{IR} = \lambda_{sc}$$

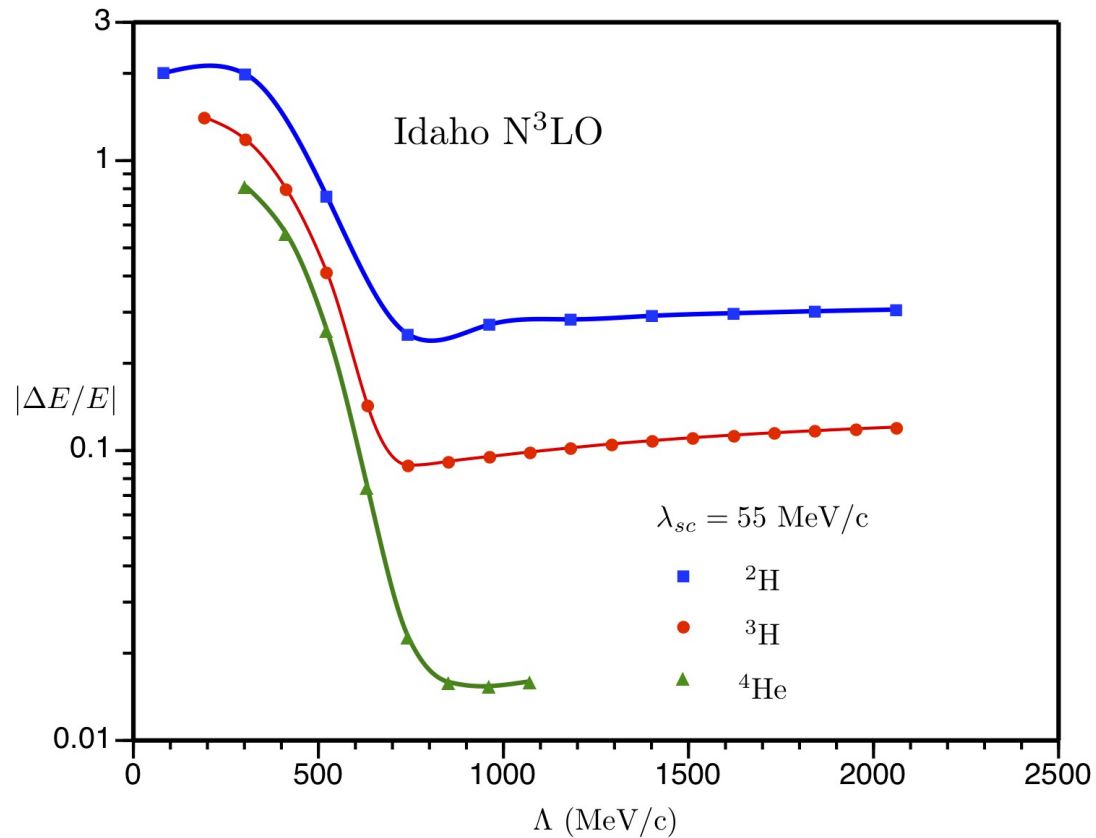


For fixed  $\lambda_{sc}$  result does NOT improve with increasing  $\Lambda$ , if  $\Lambda \geq 800$  MeV/c !

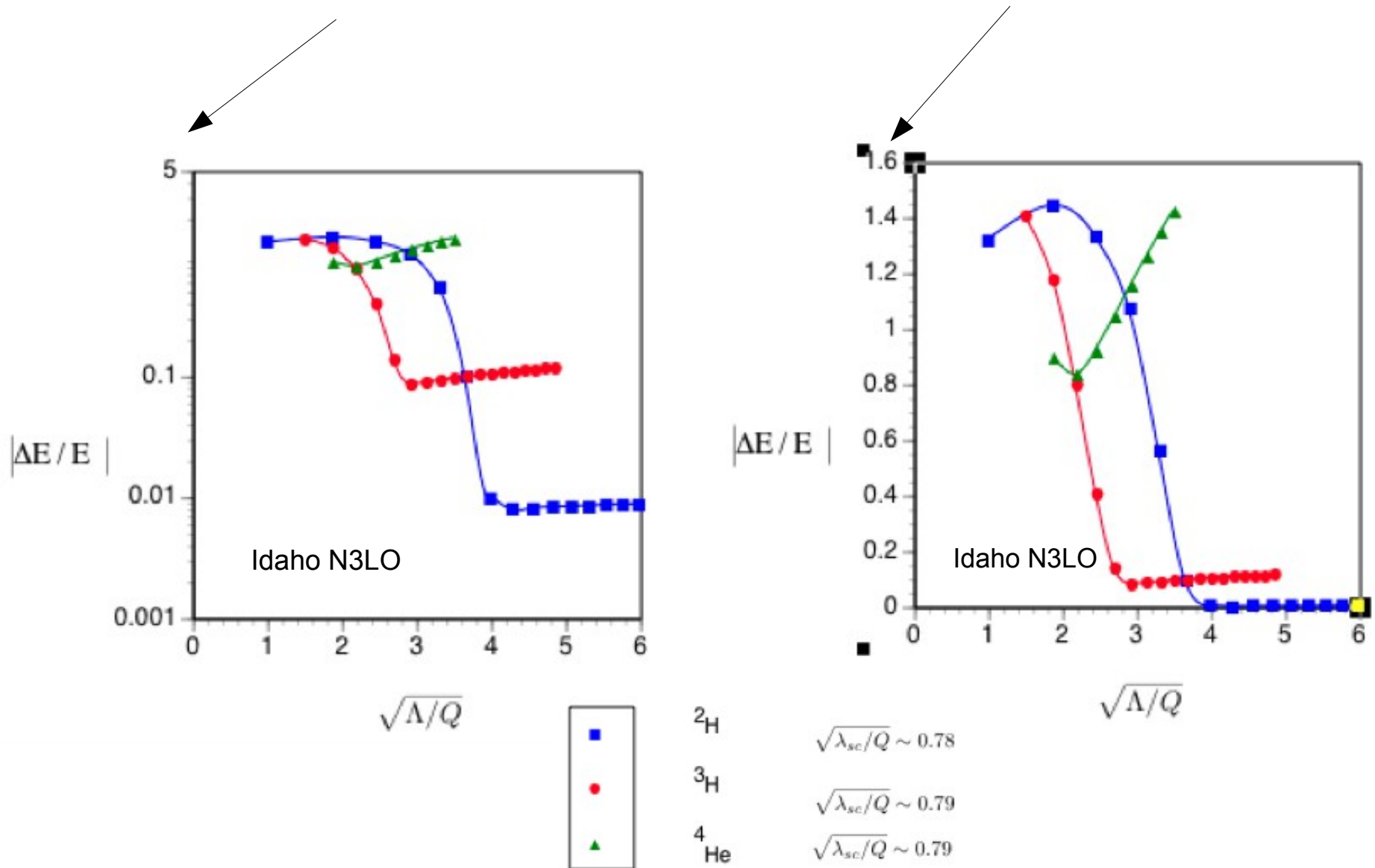
Small fixed  $\lambda_{sc}$  linked to small  $\Lambda$ , as  $N < 36$  and  $\hbar\omega/N$  must be constant

For fixed  $\lambda_{sc}$  result does NOT improve with increasing  $\Lambda$ , if  $\Lambda \geq 800$  MeV/c !

Result independent of nucleus



Fix  $\lambda_{sc}$  and increase  $\Lambda$  (each are scaled by binding momentum  $Q$ )  
 y axis is logarithmic on left, linear on right





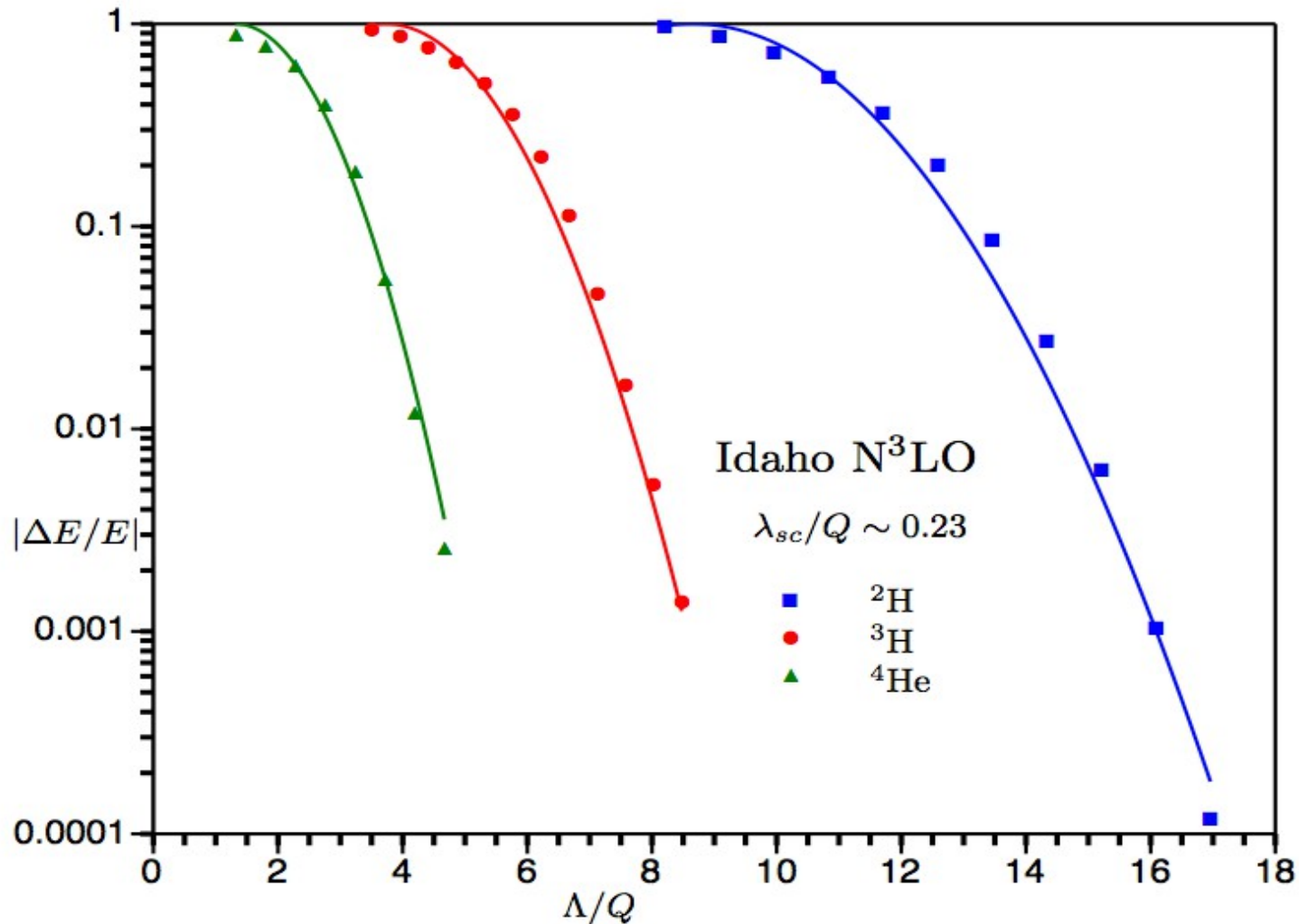
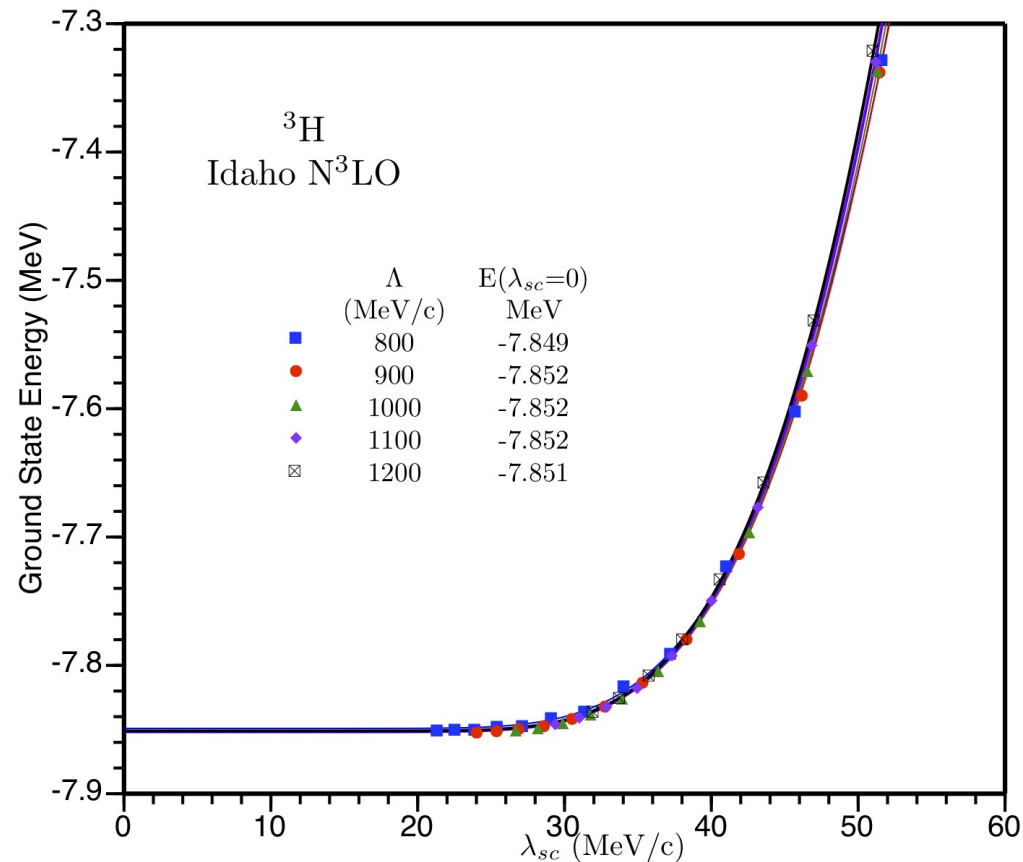


FIG. 9: (Color online) Dependence of the ground-state energy of three  $s$ -shell nuclei (compared to a converged value-see text) upon the uv momentum cutoff  $\Lambda = \sqrt{m_N(N+3/2)\hbar\omega}$  for  $\lambda_{sc} = \sqrt{(m_N\hbar\omega)/(N+3/2)}$  below the  $\lambda_{sc}^{NN} \approx 36$  MeV/c set by the  $NN$  potential. The data are fit to Gaussians.

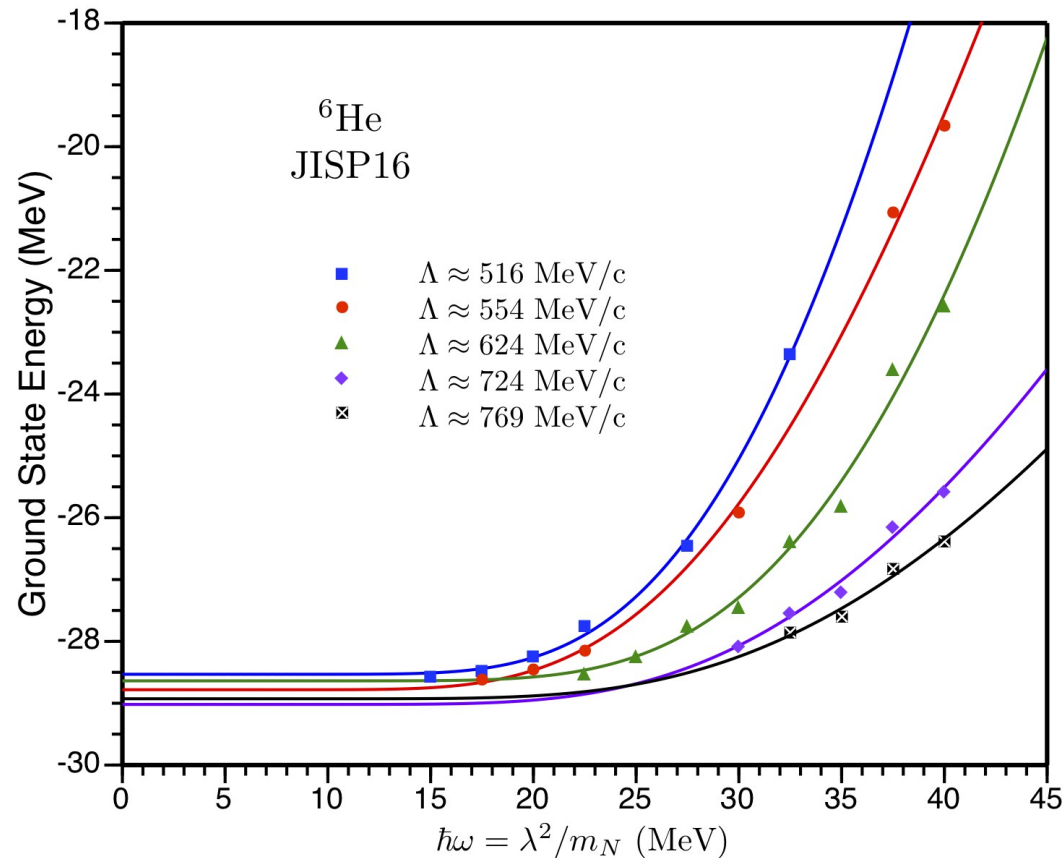
# Extrapolations with $\lambda_{sc}$

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



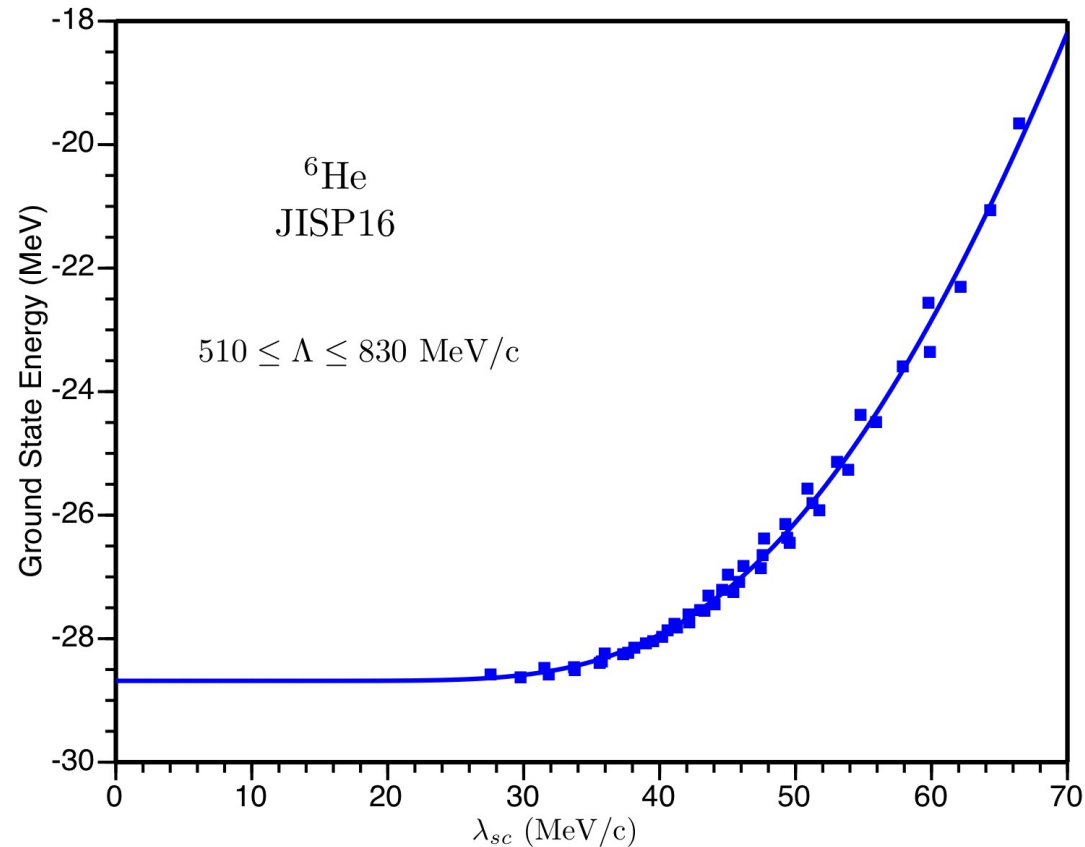
If UV cutoff is large enough, all extrapolations agree with each other and with the accepted value of -7.85 MeV

# Extrapolations with $\lambda$



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  $\hbar\omega \rightarrow 0$  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  $-28.78 \text{ MeV}$ . The standard deviation is 200 keV.

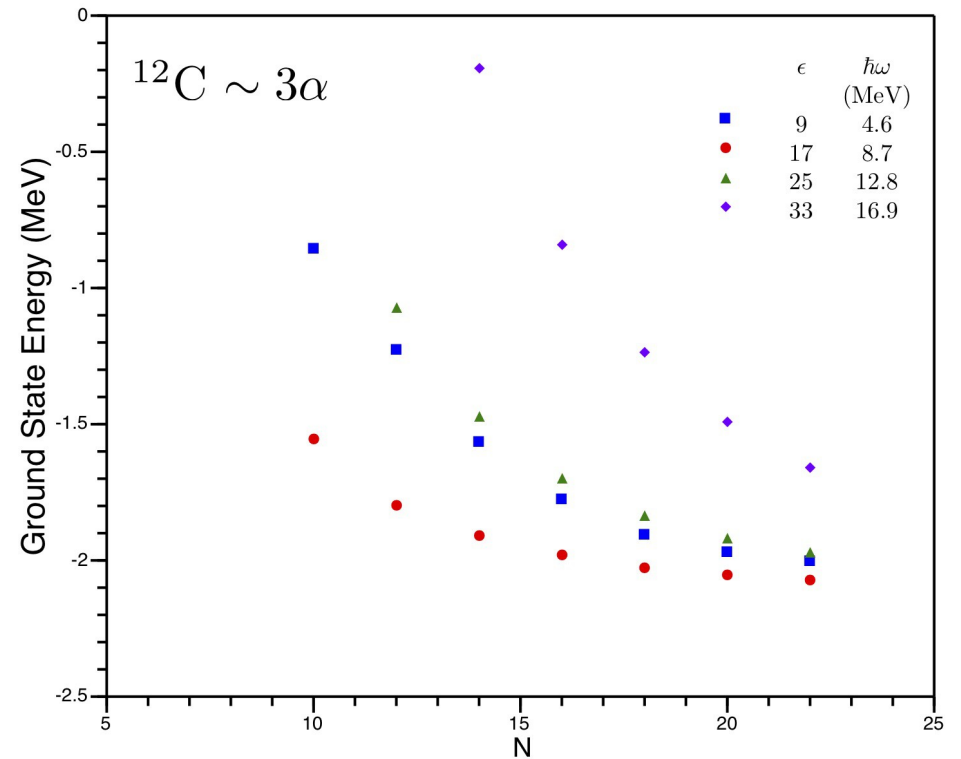
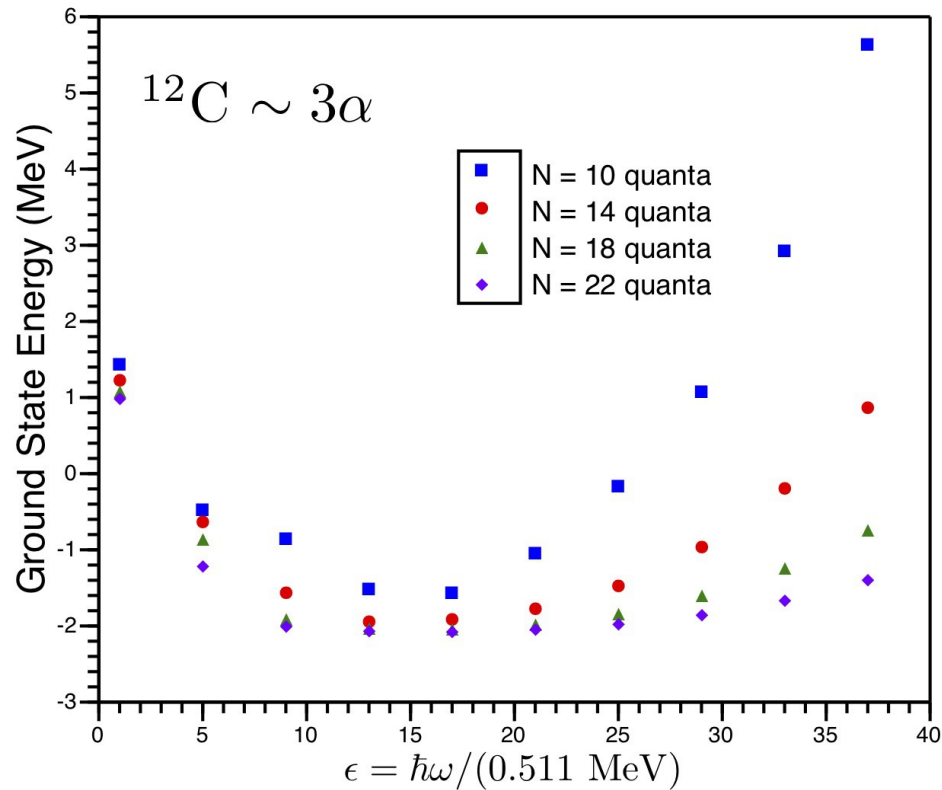
# Extrapolations with $\lambda_{sc}$

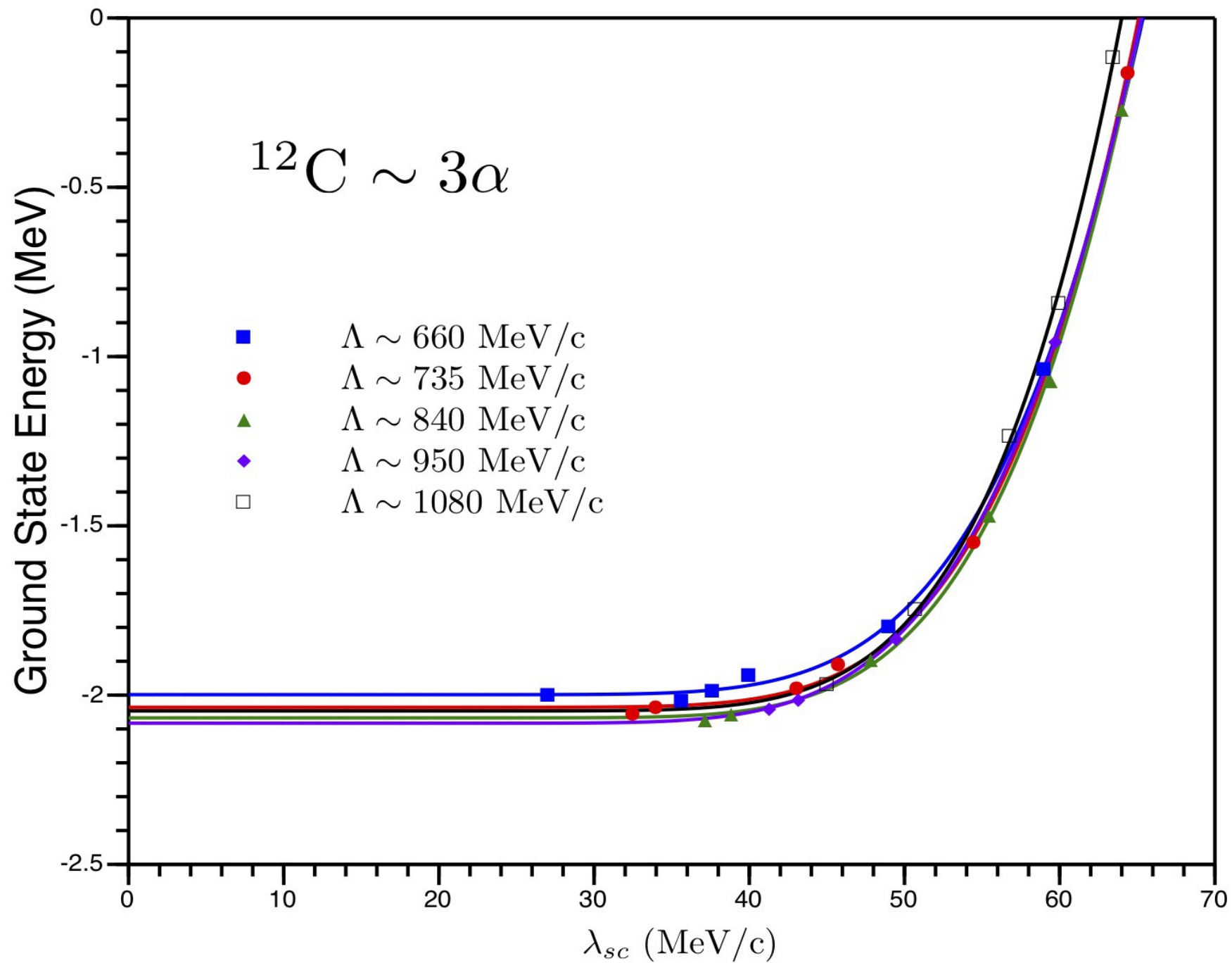


In conclusion, our extrapolations in the ir cutoff  $\lambda$  of  $-28.78(50)$  MeV or the ir cutoff  $\lambda_{sc}$  of  $28.68(22)$  MeV are consistent with each other and with the independent calculations.

# Carbon-12 as a three alpha bound state

functions of basis are transitionally invariant, symmetric, coupled to  $J=L$







# 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 ground state energies. Can it be extended to other observables?**

# Extra slides

Variational energy as a function of oscillator energy  $\hbar\omega$  for fixed number of quanta  
 Number of quanta increases by two for each curve

1969 H atom up to 10 quanta

M. MOSHINSKY

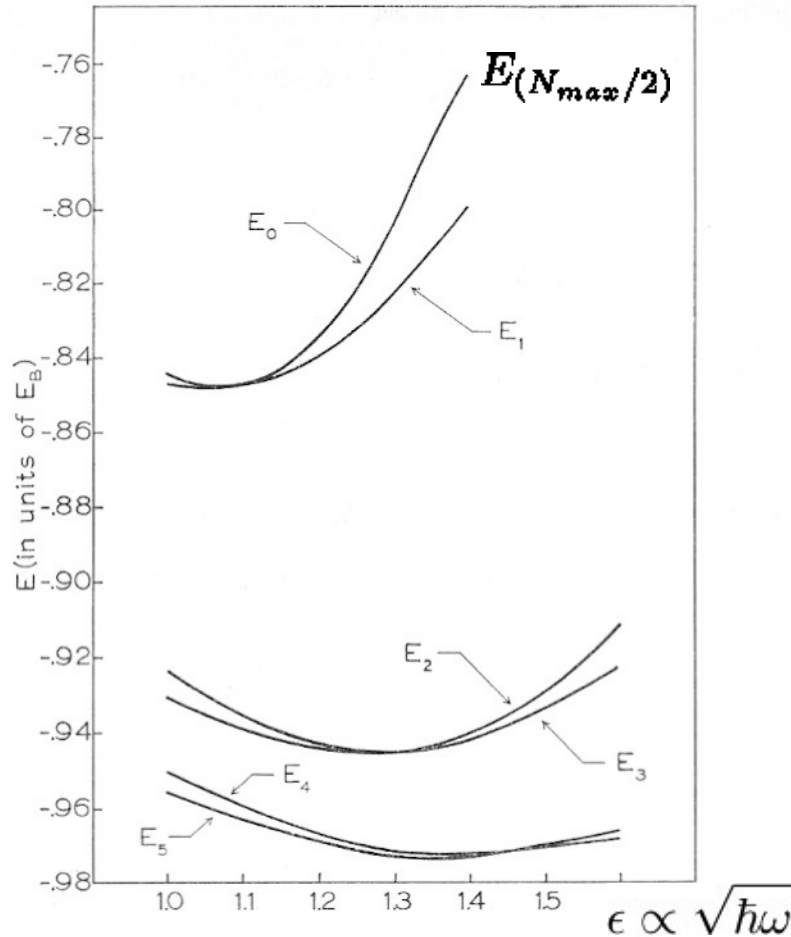
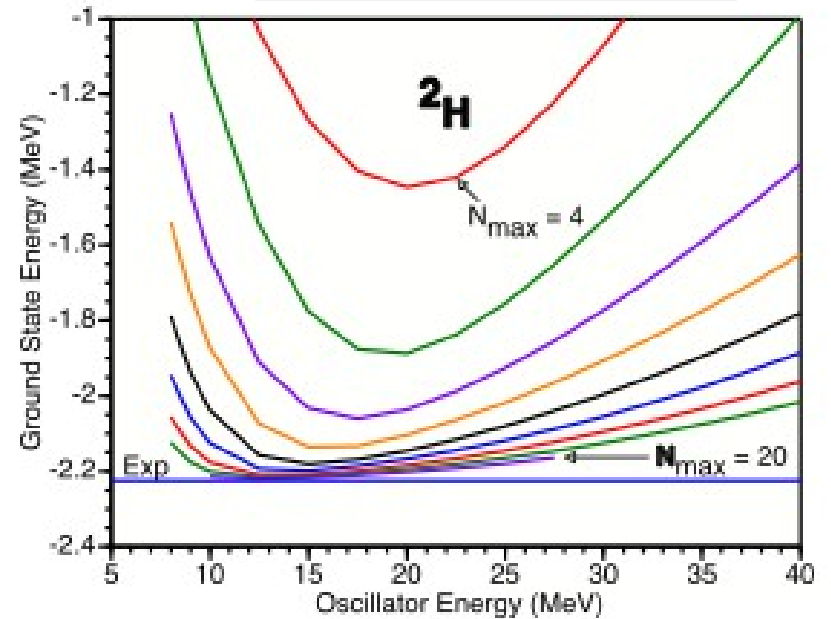


FIG. 1. Energy of the ground state of the H atom as a function of the parameter  $\epsilon$  for the variational analysis discussed in Section 3. This energy  $E_p(\epsilon)$ ,  $p = 0, 1, 2, 3, 4, 5$  is associated with a trial wave function  $\psi_p = \sum_{n=0}^p a_n^{(p)} |n00\rangle$ , where  $|n00\rangle$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

2009 deuteron up to 20 quanta

$$N_{Max} + 3/2 = \Lambda^2 / \lambda^2$$

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



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

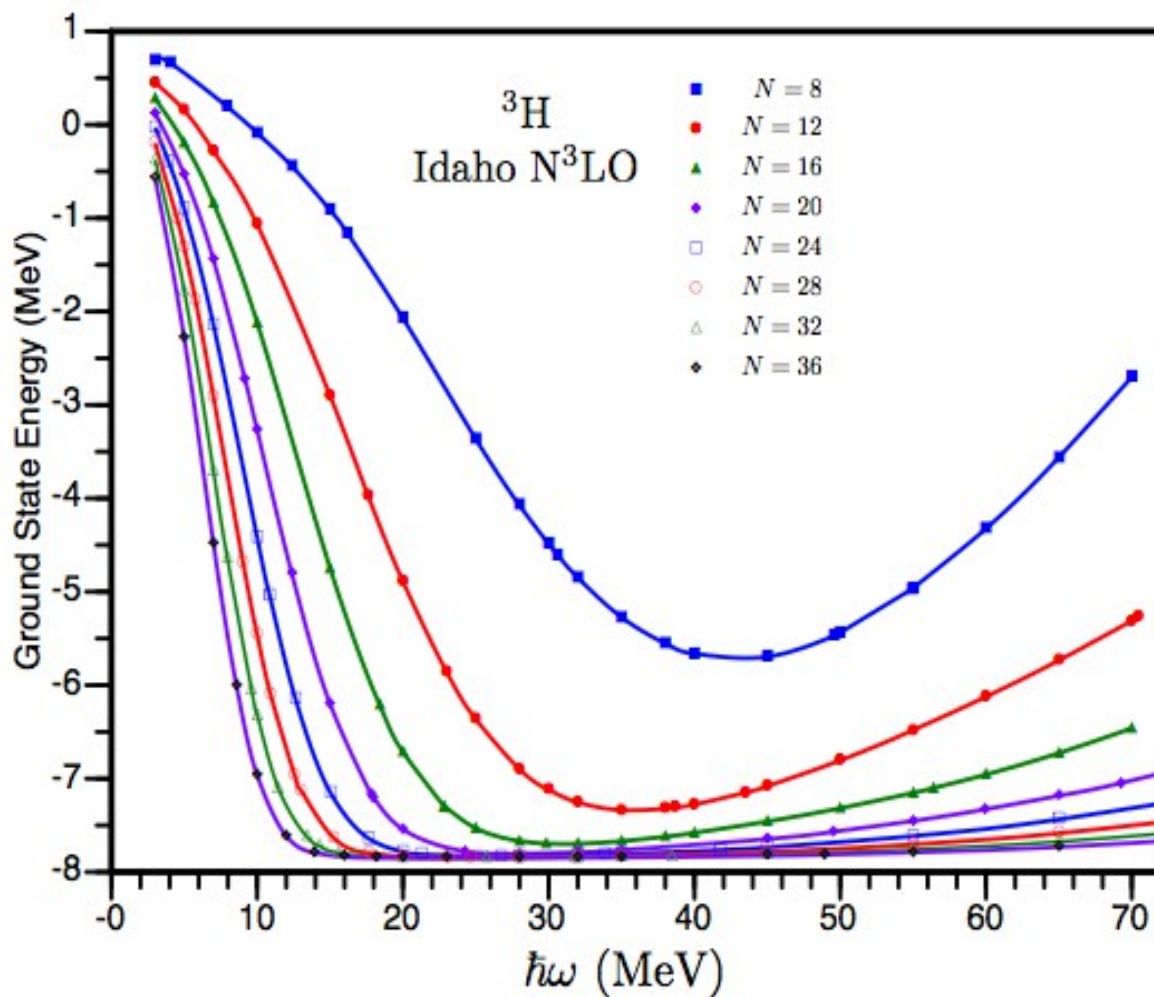
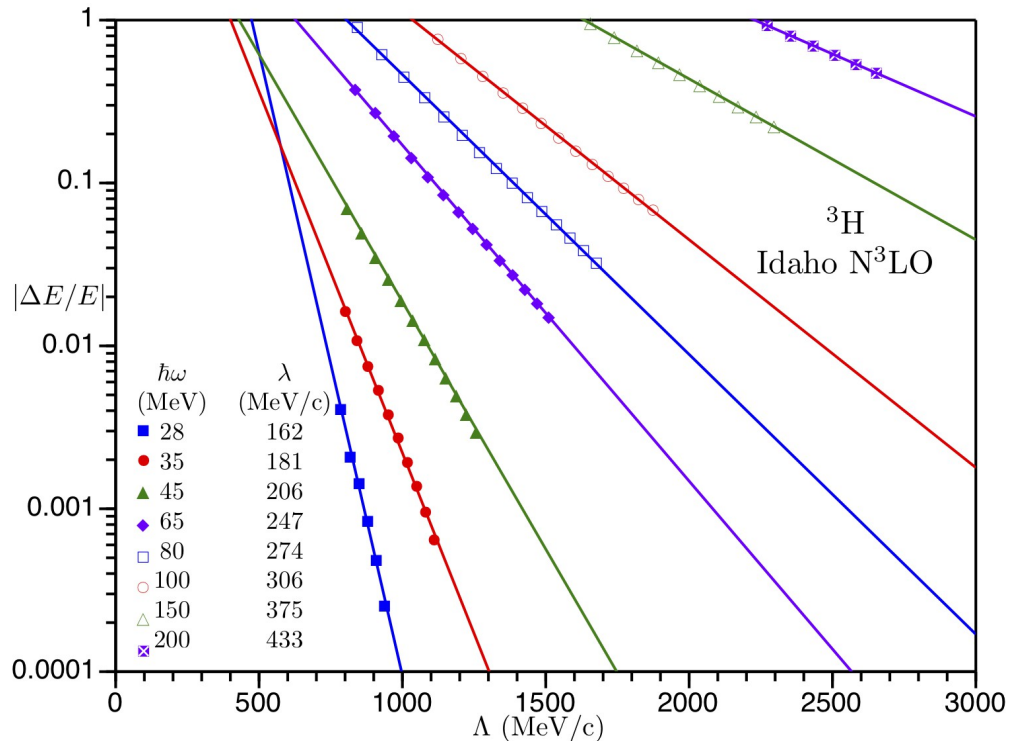


Figure 8: (Color online) Dependence of the ground-state energy of  ${}^3\text{H}$  upon  $\hbar\omega = \lambda^2/m_N = \lambda_{sc}^2/[m_N(N + 3/2)]$  for fixed  $N = \Lambda^2/\lambda^2 - 3/2 = \Lambda/\lambda_{sc} - 3/2$ . Curves are not fits but spline interpolations to guide the eye.

# Fix IR regulator and take UV regulator to infinity

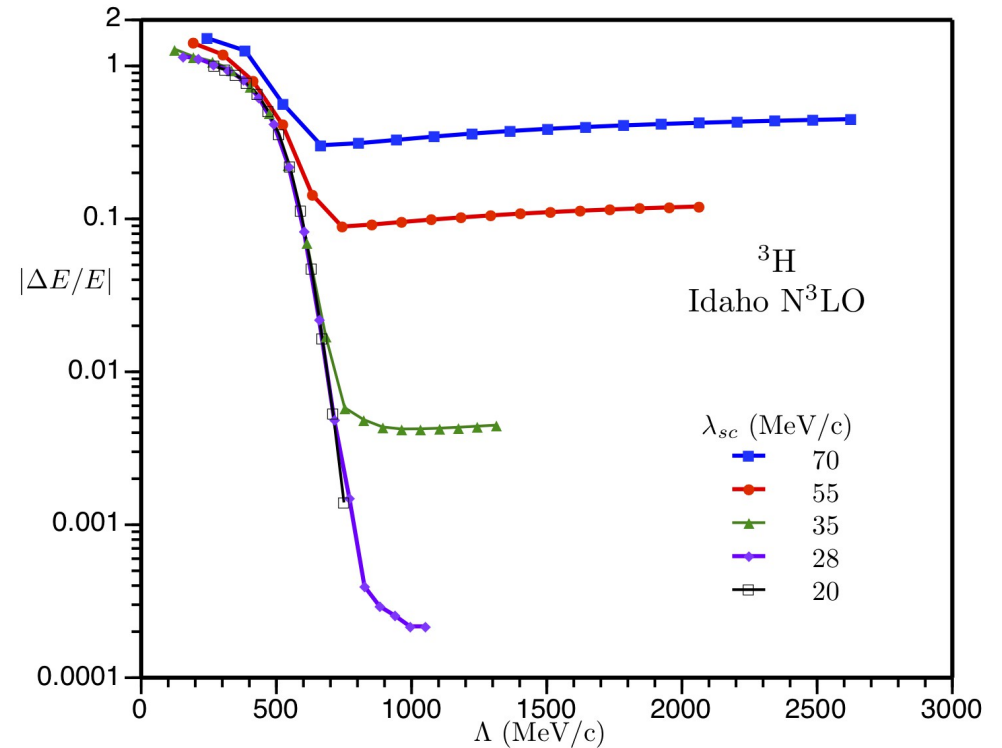
$$\lambda_{IR} = \lambda$$



As the ultraviolet cutoff increases, the fractional difference between calculated  $E(\Lambda, \lambda)$  and an accepted-as-converged  $E$ , lessens.

Alternatively, the plot can be read the other way, where if we fix the UV  $\Lambda$ , the results improve as we lower the IR cutoff  $\lambda$ .

$$\lambda_{IR} = \lambda_{sc}$$



As the ultraviolet cutoff increases, the results get worse for large fixed  $\lambda_{sc}$ .

