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

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Collaborators

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PHYSICAL REVIEW C **84**, 015201 (2011)

Boundary between hadron and quark-gluon structure of nuclei

H. J. Pirner and J. P. Vary

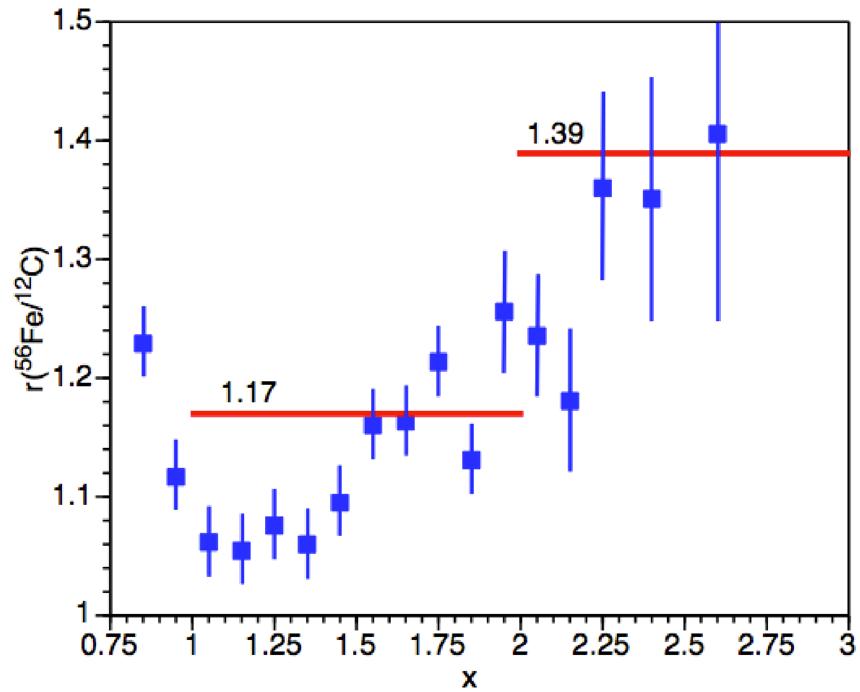


Figure 2: (Color online) JLAB data for the ratio of per nucleon responses of ^{56}Fe to ^{12}C over a range of Bjorken $x_B = x$ that exceeds unity [7], the limit for data on an isolated nucleon. We note there is a data point, $r = 2.2$ at $x = 2.8$, which is far off the vertical scale. Multi-quark clusters support a nuclear response above $x = 1$. The horizontal lines show the theoretical predictions (1.17, 1.39) for regions dominated by (6,9)-quark clusters respectively[4].

[4] M. Sato, S. A. Coon, H. J. Pirner and J. P. Vary, Phys. Rev. C 33, 1062(1986).

cluster probabilities are governed by intermediate range correlations evaluated with realistic correlated wavefunctions for A 4 nuclei

"cluster probability" is the probability that a quark chosen at random in the nucleus is found in a color singlet cluster consisting of 3,6,9,etc., quarks.

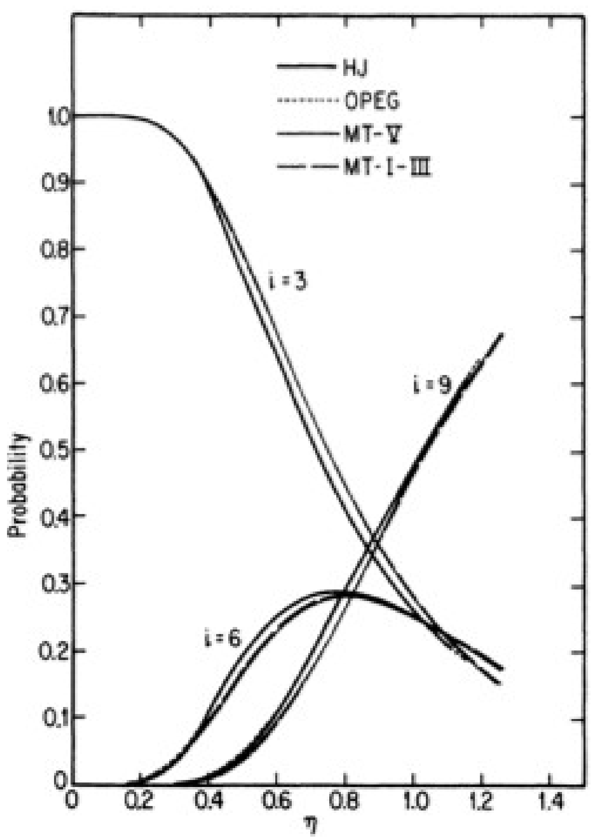


FIG. 4. *i*-quark cluster probabilities $\tilde{p}_i^{(3)}$ of Fig. 3 plotted as a function of $\eta = R_c/(r_m/A^{1/3})$. The MT potentials nearly coincide, and the HJ and OPEG have nearly the same $\tilde{p}_i^{(3)}$ as a function of η.

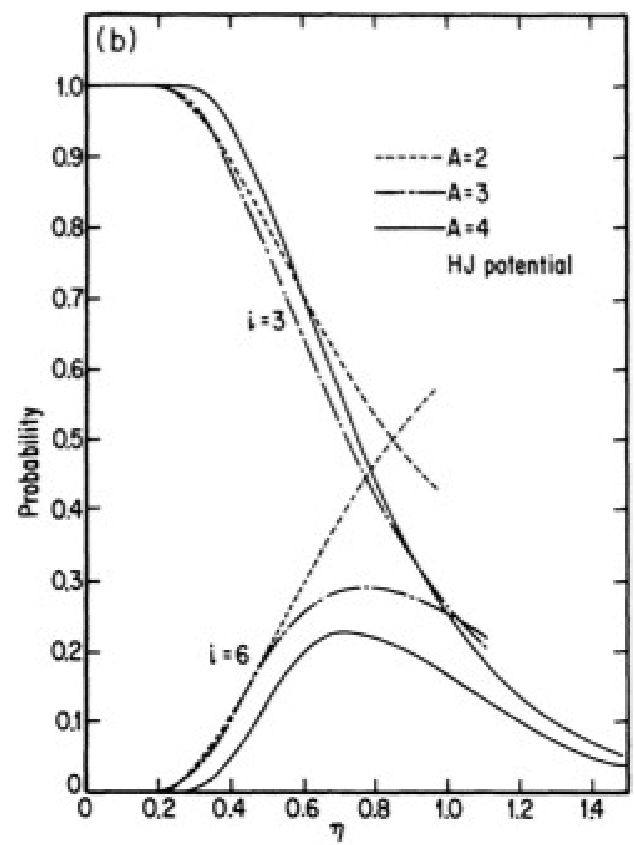


FIG. 8. *i*-quark cluster probabilities $\tilde{p}_3^{(A)}$ and $\tilde{p}_6^{(A)}$ in the series $A = 2$, 3, and 4 calculated with the Hamada-Johnston potential. (a) has R_c as the abscissa and (b) displays the same probabilities as a function of $\eta = R_c/(r_m/A^{1/3})$.

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:

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

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

$$E_v = \mathbf{a}^+ H_N \mathbf{a} / \mathbf{a}^+ N \mathbf{a} \tag{2.11}$$

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

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

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:

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

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 $E_1, \ldots, E_{N-1}$ of H; indeed we can show that

$$E_i(N) \geq E_i \qquad i = 0, \ldots, N-1 \tag{2.13}$$

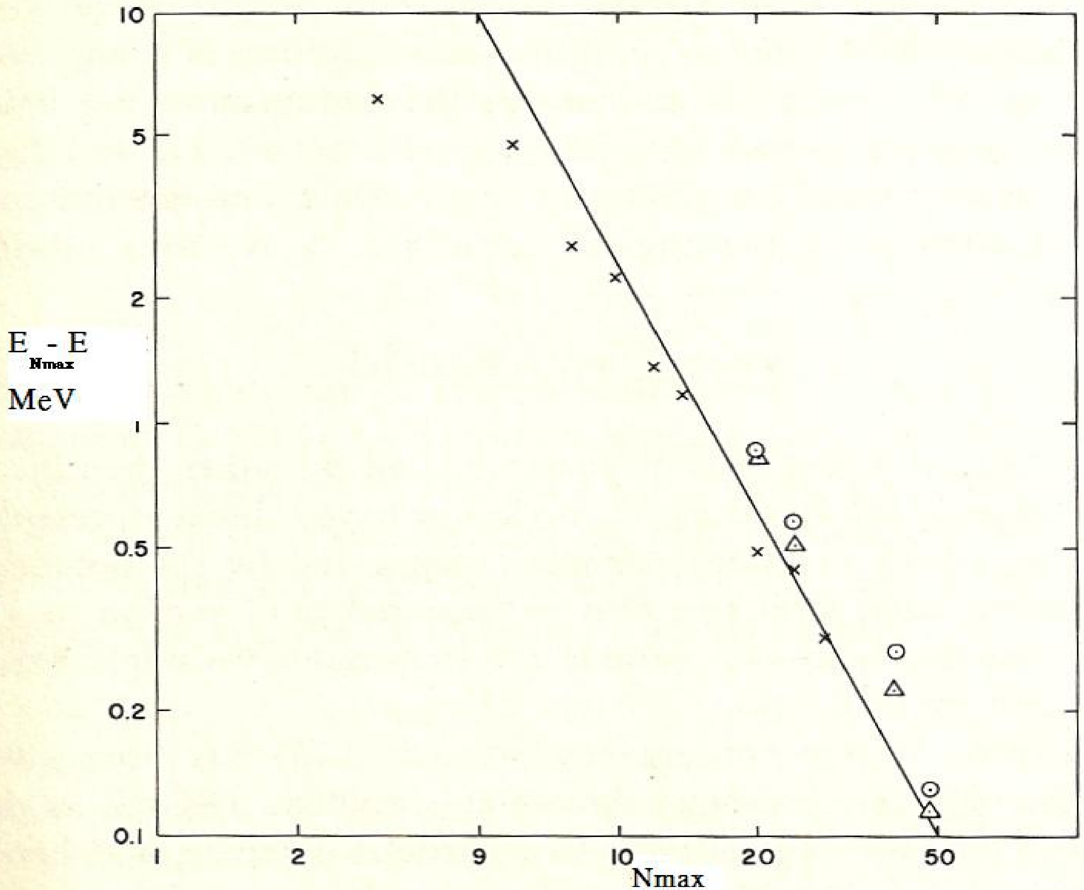


Fig. 8. Convergence rates for variational calculations with a harmonic oscillator basis. ⊙ Deuteron, Yamaguchi potential; × triton, Yamaguchi potential; and △ deuteron, Reid potential. Results taken from (JLS 70). The solid line has a slope of −2.0.

N_{max}

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

$$E_{N_{max}} = E + P(N_{max})^{-2}$$

"nonsmooth potentials" like Yukawa

"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

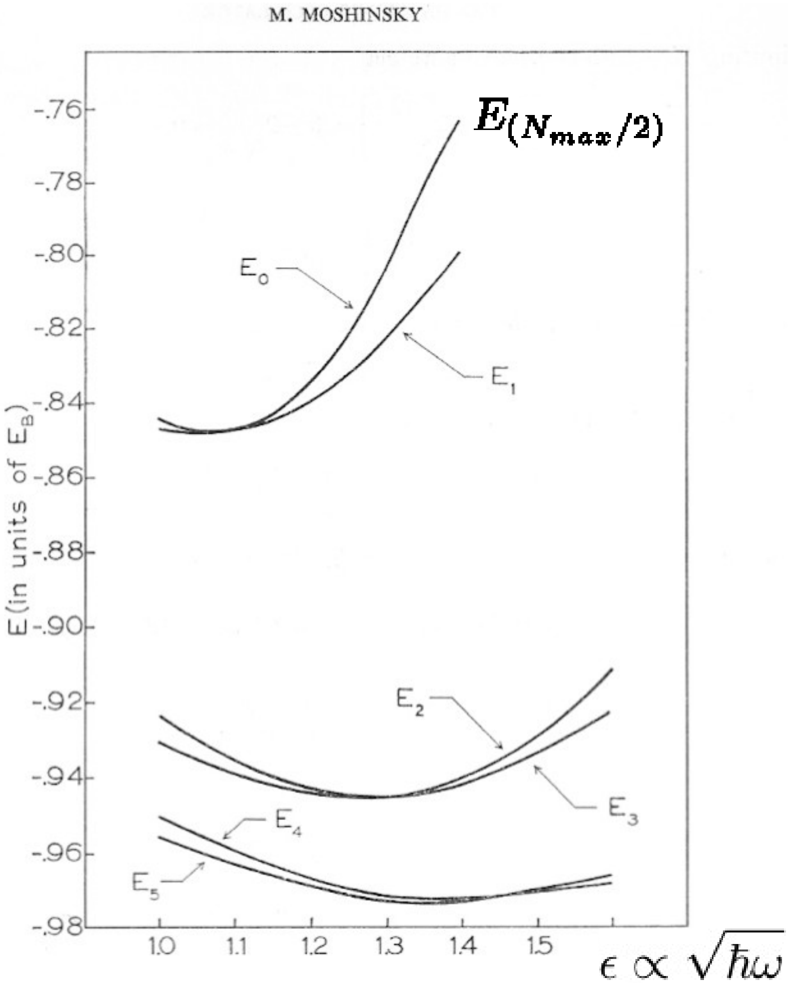
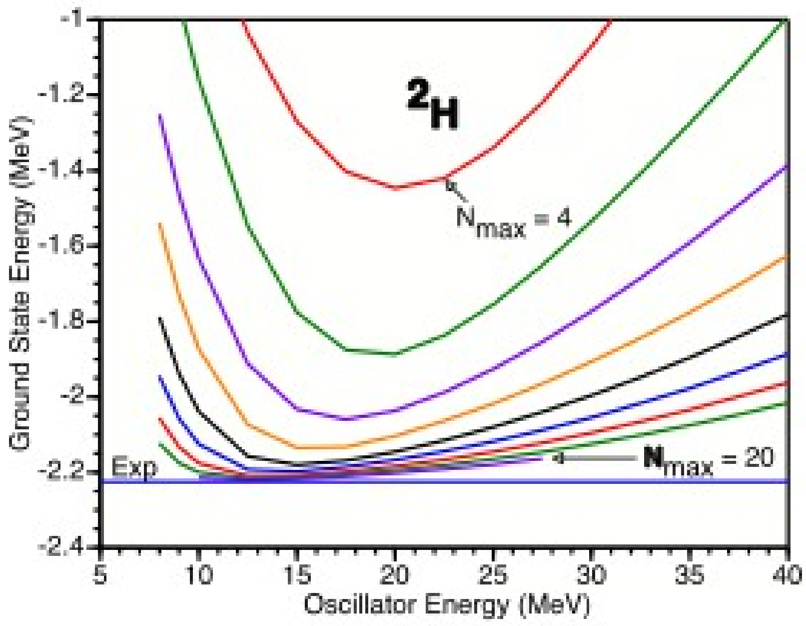


FIG. 1. Energy of the ground state of the H atom as a function of the parameter ε for the variational analysis discussed in Section 3. This energy $E_p(\varepsilon)$, $p = 0, 1, 2, 3, 4, 5$ is associated with a trial wave function $\psi_p = \Sigma_{n=0}^{p} a_n^{(p)} \mid n00\rangle$, where $\mid n00\rangle$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

2009 deuteron up to 20 quanta



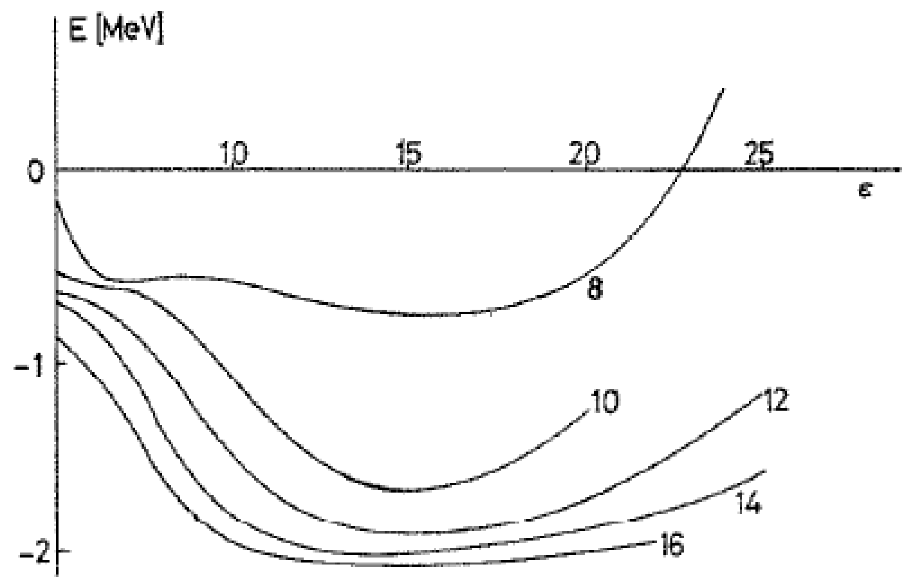
No-core full configuration method of Maris,Vary,Shirokov

ALPHA PARTICLE MODEL CALCULATIONS FOR ^{12}C AND ^{16}O†

R. M. MENDEZ-MORENO, M. MORENO and T. H. SELIGMAN††
Instituto de Fisica UNAM, México

Received 14 December 1973

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

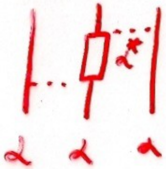


ε *is a scaled* $\hbar\omega$

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

include a 3α force in the Hamiltonian

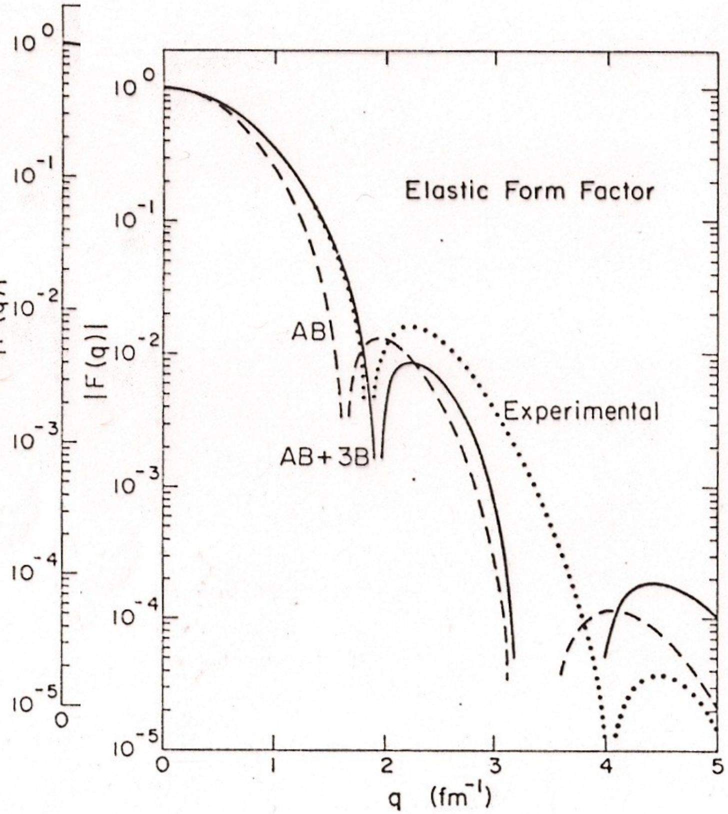
Portilho, Agrello, Coon PRC 27, 2923 (1983)

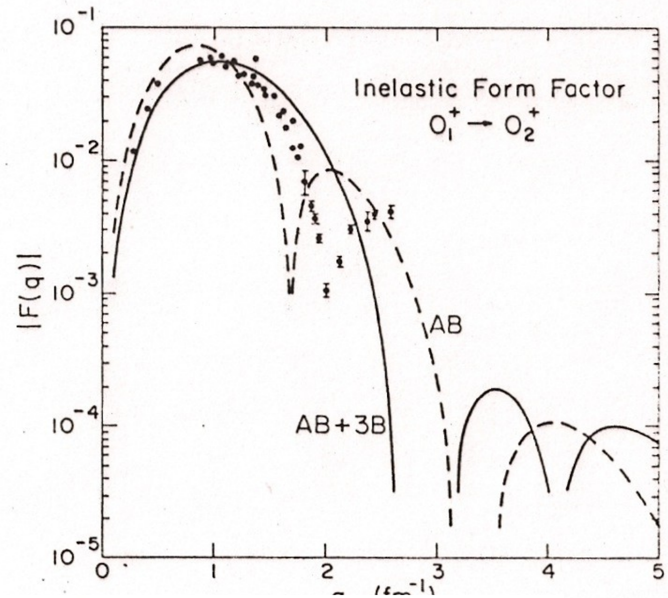


Convergence?

$N=10 \rightarrow N=12 \Rightarrow 5\%$ decrease in second maximum of elastic form factor

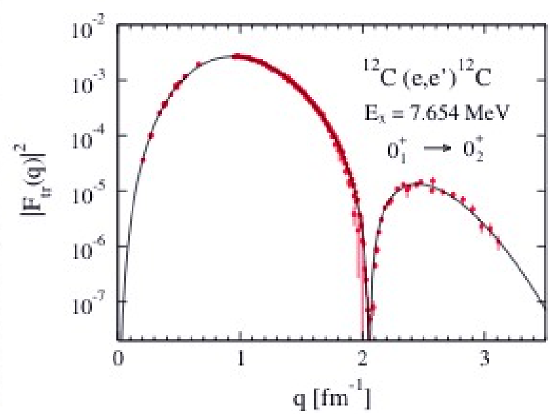
This calculation used $N=16$





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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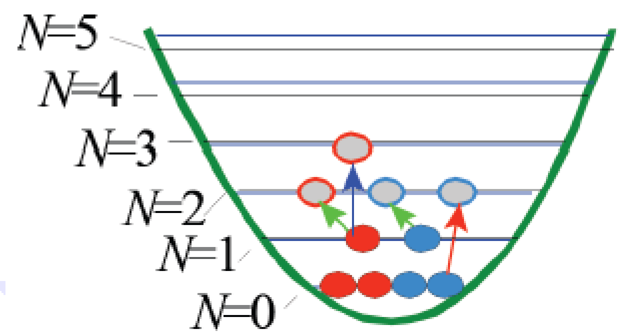
Delves, L. M. *Advances in Nuclear Physics*

The No-Core Shell Model (NCSM)

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

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

NCSM has two parameters: Nmax and Ω



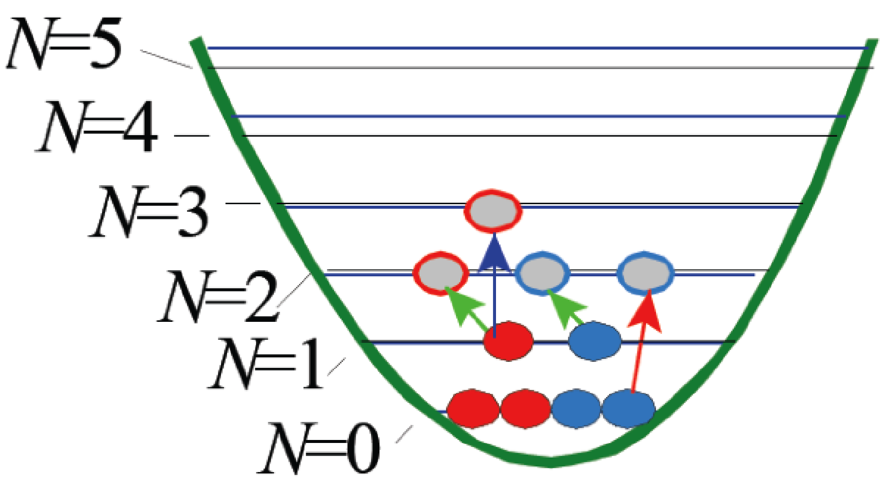
Provided interaction is "soft" we don't need to do any renormalization of interaction,

It's that "simple".

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

Slide from Michael Kruse



- 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 Nmax=2 configuration
- Two units of energy distributed among the six particles.

Extrapolating with N_{Max}

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

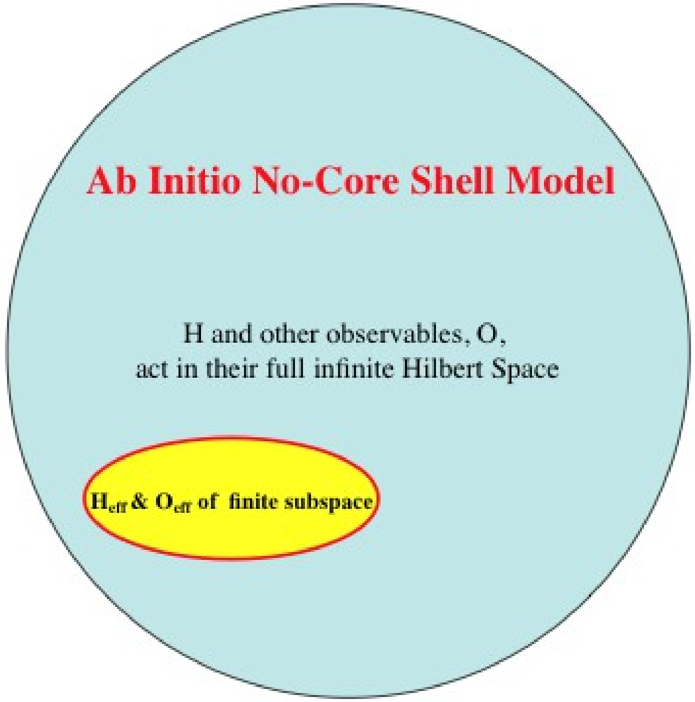
- Perform a series of calculations with increasing N_{max} truncation (while keeping everything else fixed)
- Extrapolate to infinite model space $\longrightarrow$ exact results
  - binding energy: exponential in N_{max}

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

  - use 3 or 4 consecutive N_{max} values to determine $E^{\infty}_{\text{binding}}$
  - use $\hbar\omega$ and N_{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_{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_{max} and $\hbar\omega$

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.

Slide by Matthew Avetian

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 Λ, 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 Λ in such a way that observables at momenta $Q \ll \Lambda$ are independent of how P is chosen, and in particular, independent of Λ.

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

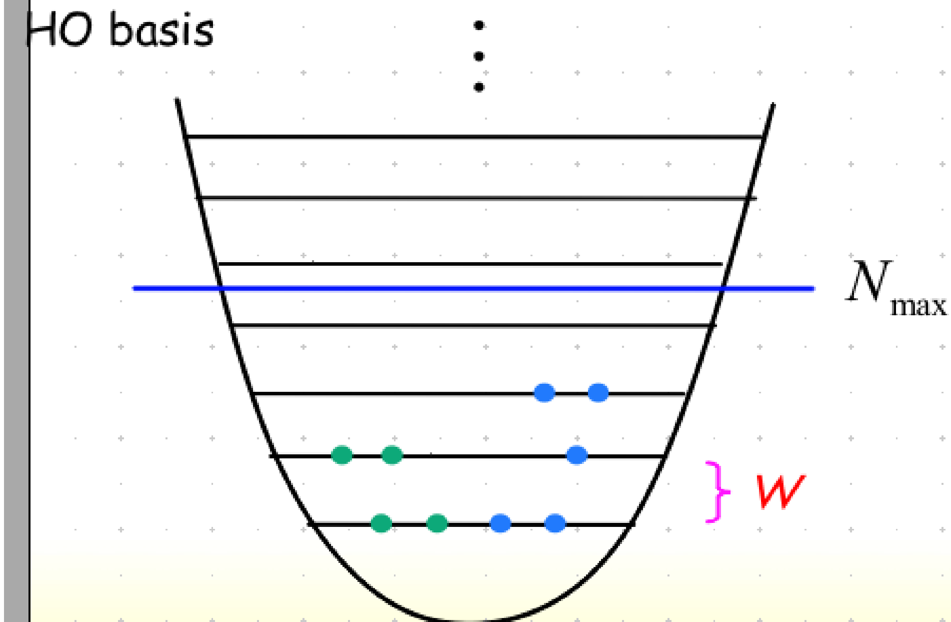
My more modest goal: can EFT motivate and shape an extrapolation to the infinite basis limit for the HO basis calculations called NCSM or NCFC which utilize “realistic” nuclear interactions fit to data, not in a clearly defined model space, but in free space?

~ 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



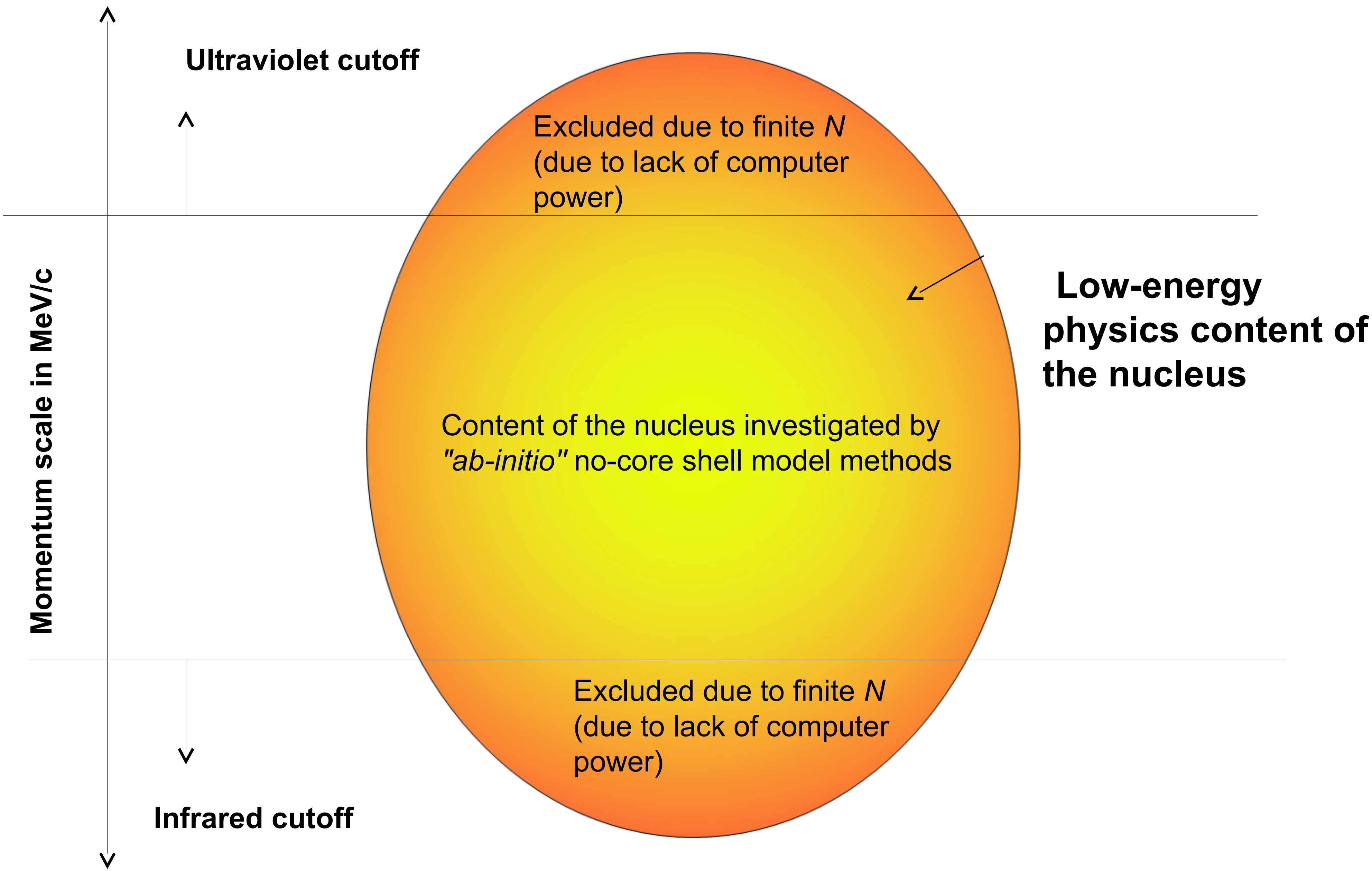
For lattice cutoffs:
Mueller, Koonin, Seki + v.K. '00
Lee *et al.* '03...

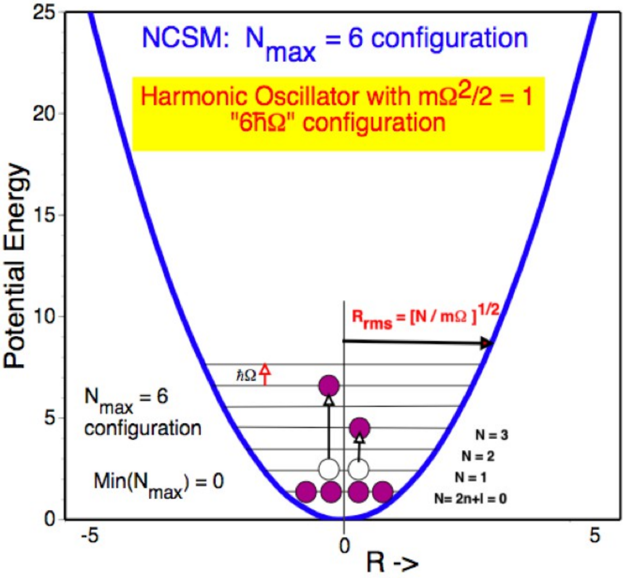
cutoffs

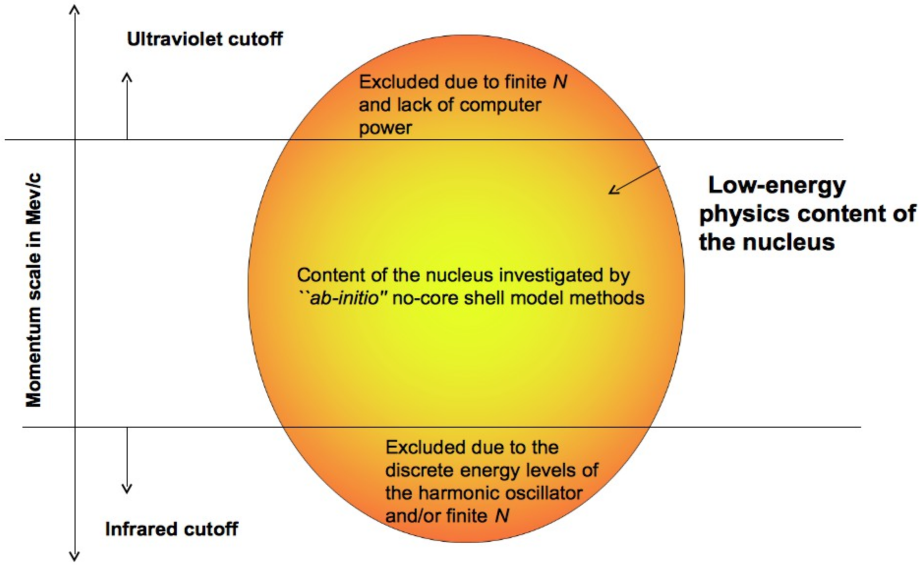
UV $\quad L = \sqrt{m_N \left(N_{max} + 3/2 \right) W}$

IR $\quad l = \sqrt{m_N W}$

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


Ultraviolet cutoff
Excluded due to finite N (due to lack of computer power)
Momentum scale in MeV/c
Low-energy physics content of the nucleus
Content of the nucleus investigated by "ab-initio" no-core shell model methods
Excluded due to finite N (due to lack of computer power)
Infrared cutoff





Define a UV momentum cutoff Λ equivalent to continuum Λ 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 λ.

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

λ 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

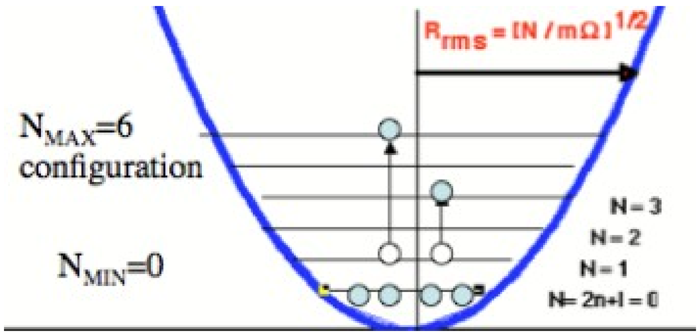
Continuum QCD simulated on a lattice has a model space with two cutoffs
UV cutoff $\Lambda \sim 1/a$ where a is lattice spacing
IR cutoff $\lambda \sim 1/L$ where L is the size of the lattice
a must be small enough to simulate the continuum
L must be large enough to contain the system

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?

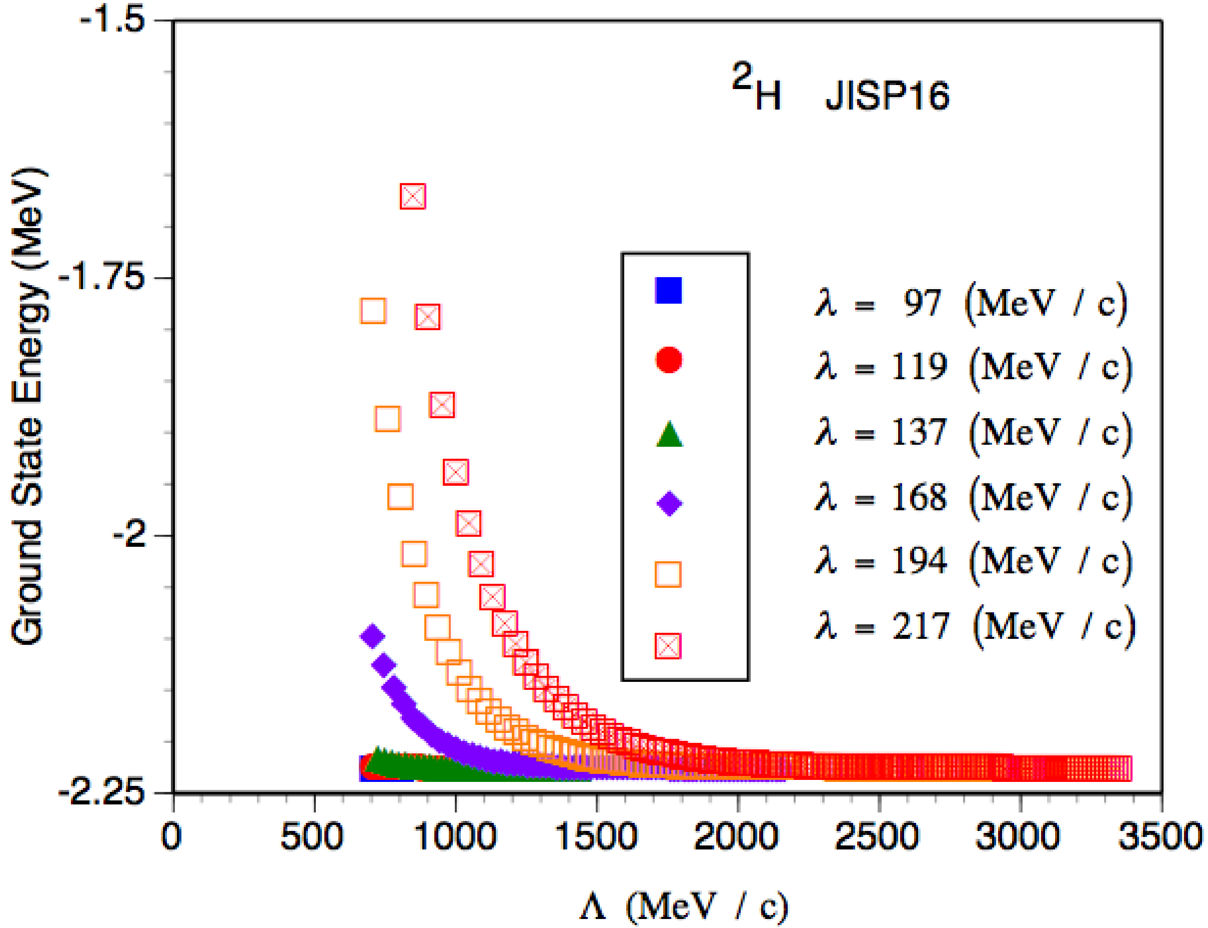
Note 1 $\lambda_{SC} = \lambda^2/\Lambda$

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 ħω convergence is clear as N_{max} goes to 238



Phenomeological NN interaction: JISP16

A.M. Shirokov, J.P. Vary, A.I. Mazur, T.A. Weber, PLB **644**, 33 (2007)

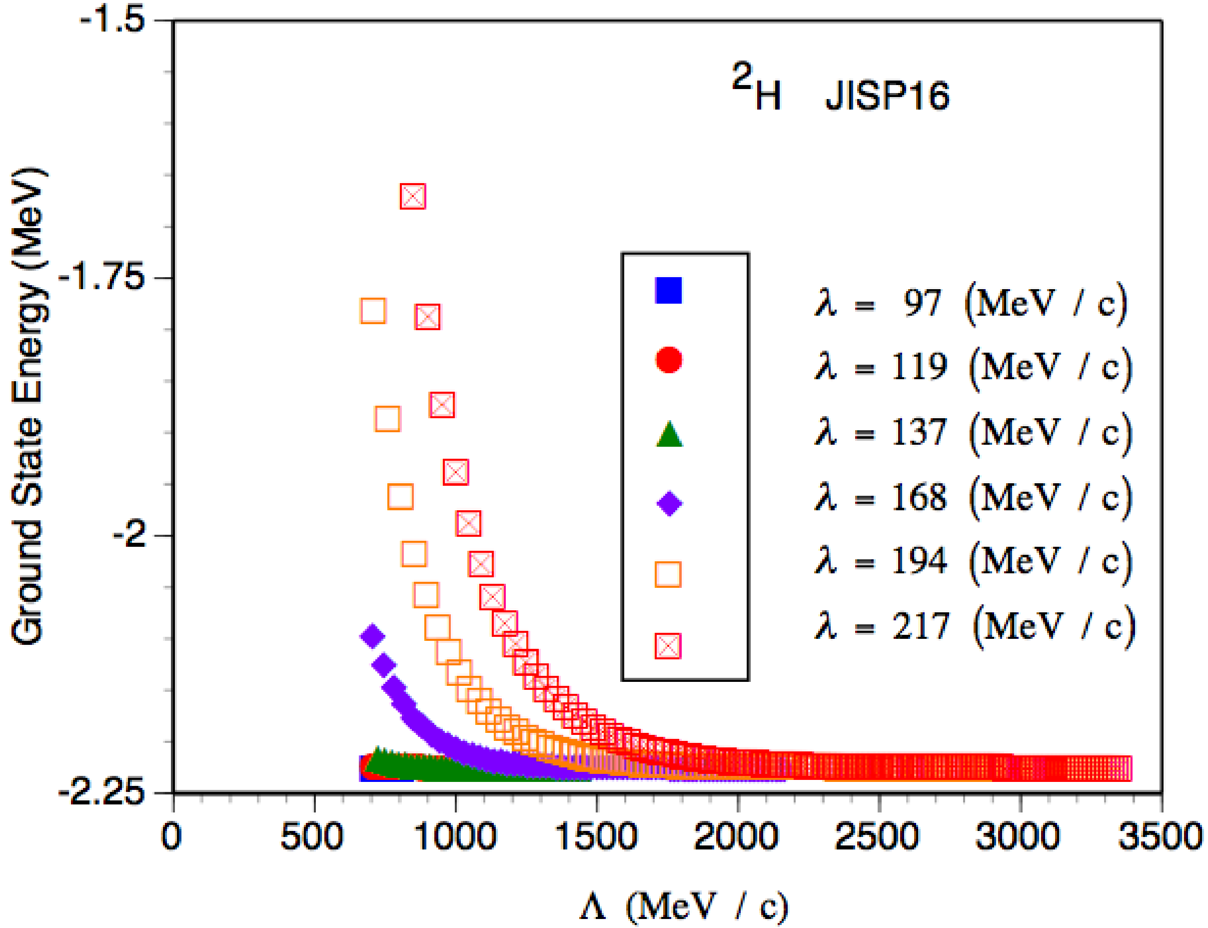
J-matrix Inverse Scattering Potential tuned up to ^{16}O

- finite rank seperable potential in H.O. representation
- fitted to available NN scattering data
- use unitary transformations to tune off-shell interaction to
  - binding energy of ^{3}He
  - low-lying spectrum of ^{6}Li (JISP6, precursor to JISP16)
  - binding energy of ^{16}O
- good fit to a range of light nuclear properties
- very soft potential compared to other NN potentials
- nonlocal potential (by construction)

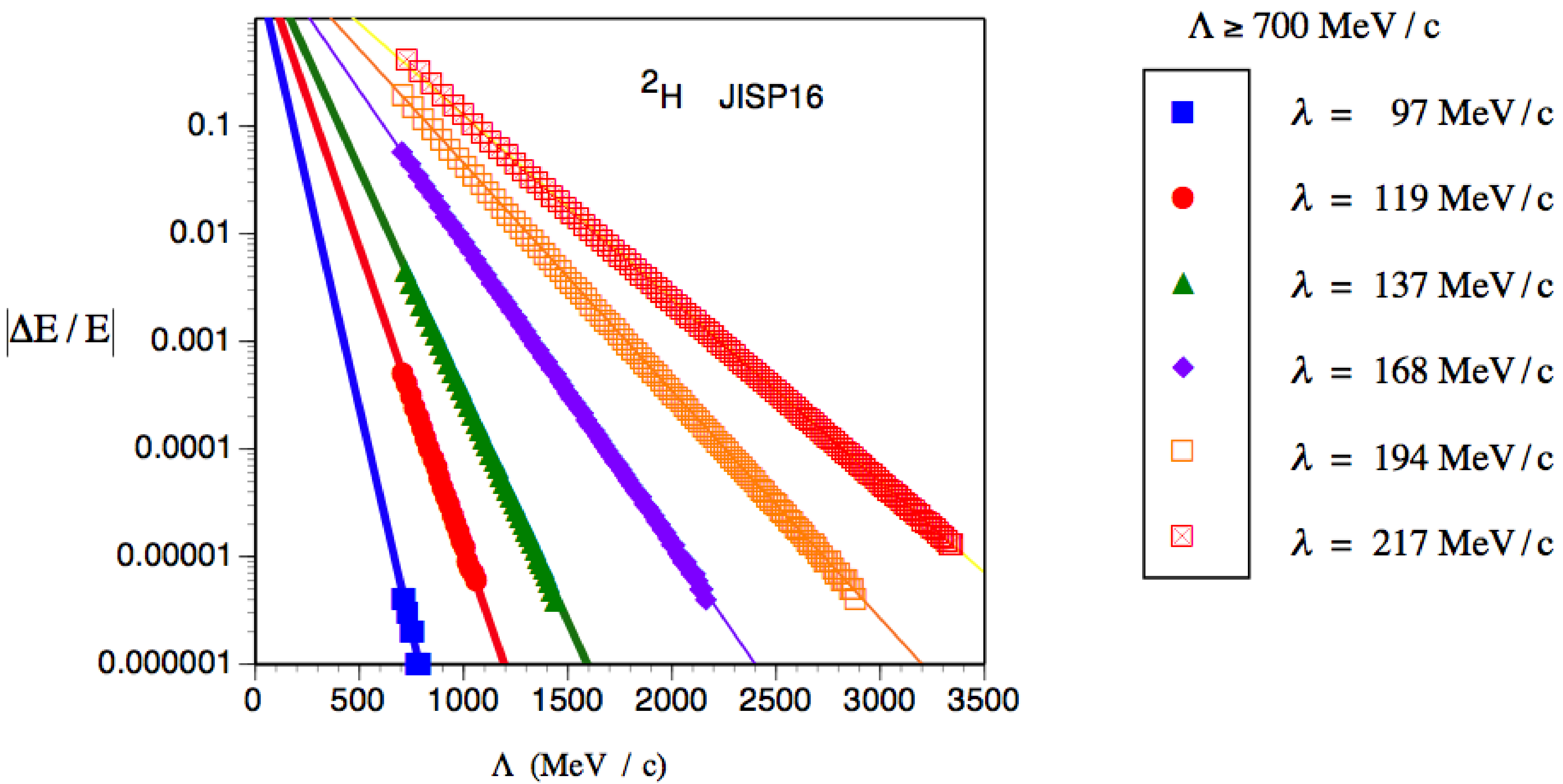
Fit was made for ħω=40 MeV and N_{max}=9 so that of JISP16 was fit in a model space of with cutoffs Λ~600-700 MeV/c and λ~194 MeV/c, Λ_{sc}~60 MeV/c

Test model space cutoffs with deuteron

E converges to -2.224574 MeV for all ħω as N_{max} goes as high as 238



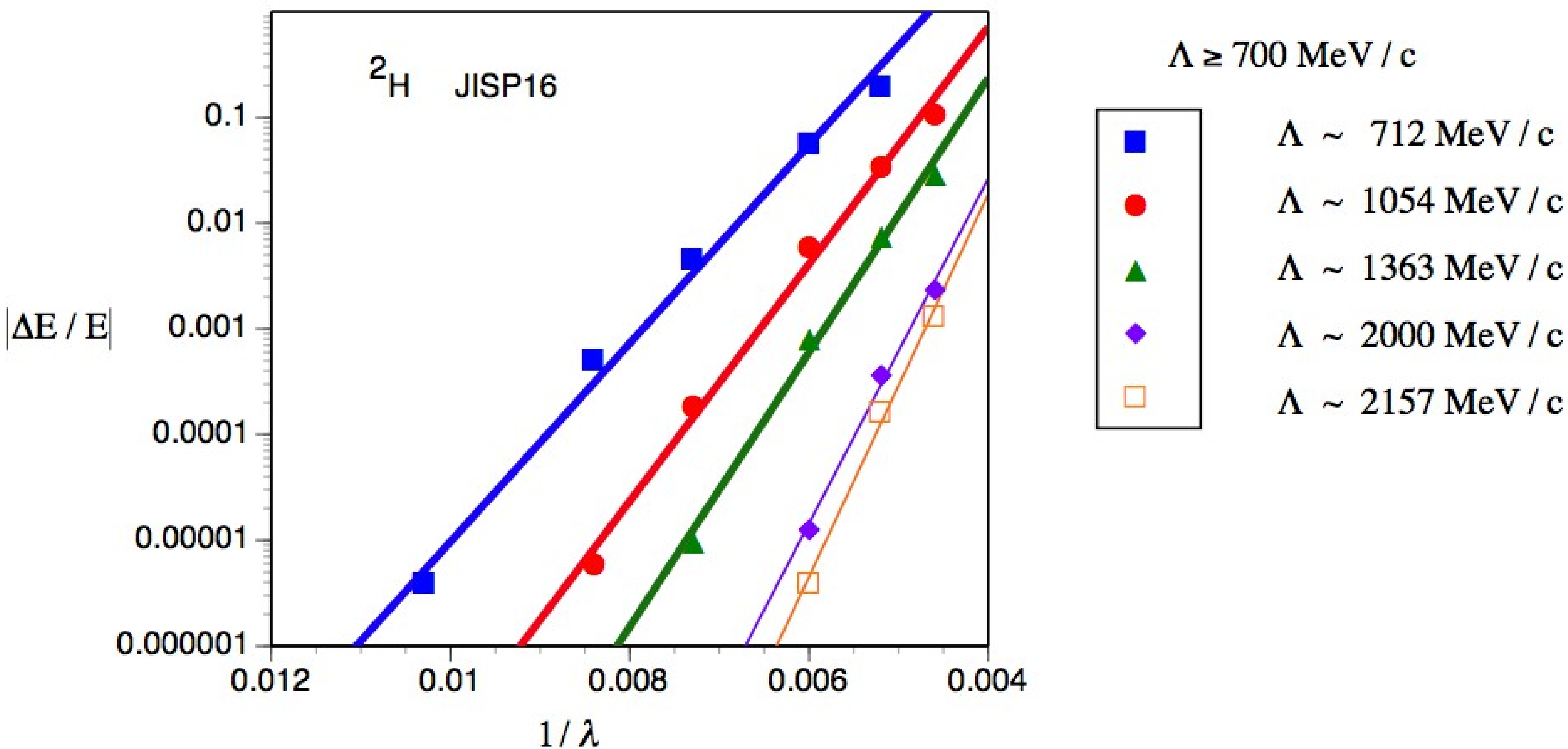
$\lambda_{IR} \equiv \lambda$ acts as an IR cutoff should!



As the ultraviolet cutoff increases, the fractional difference between calculated E(Λ, λ) and an accepted-as-converged E, lessens.

Alternatively, the plot can be read the other way, where if we fix the UV Λ, the results improve as we lower the IR cutoff λ.

Λ acts as an UV cutoff should!



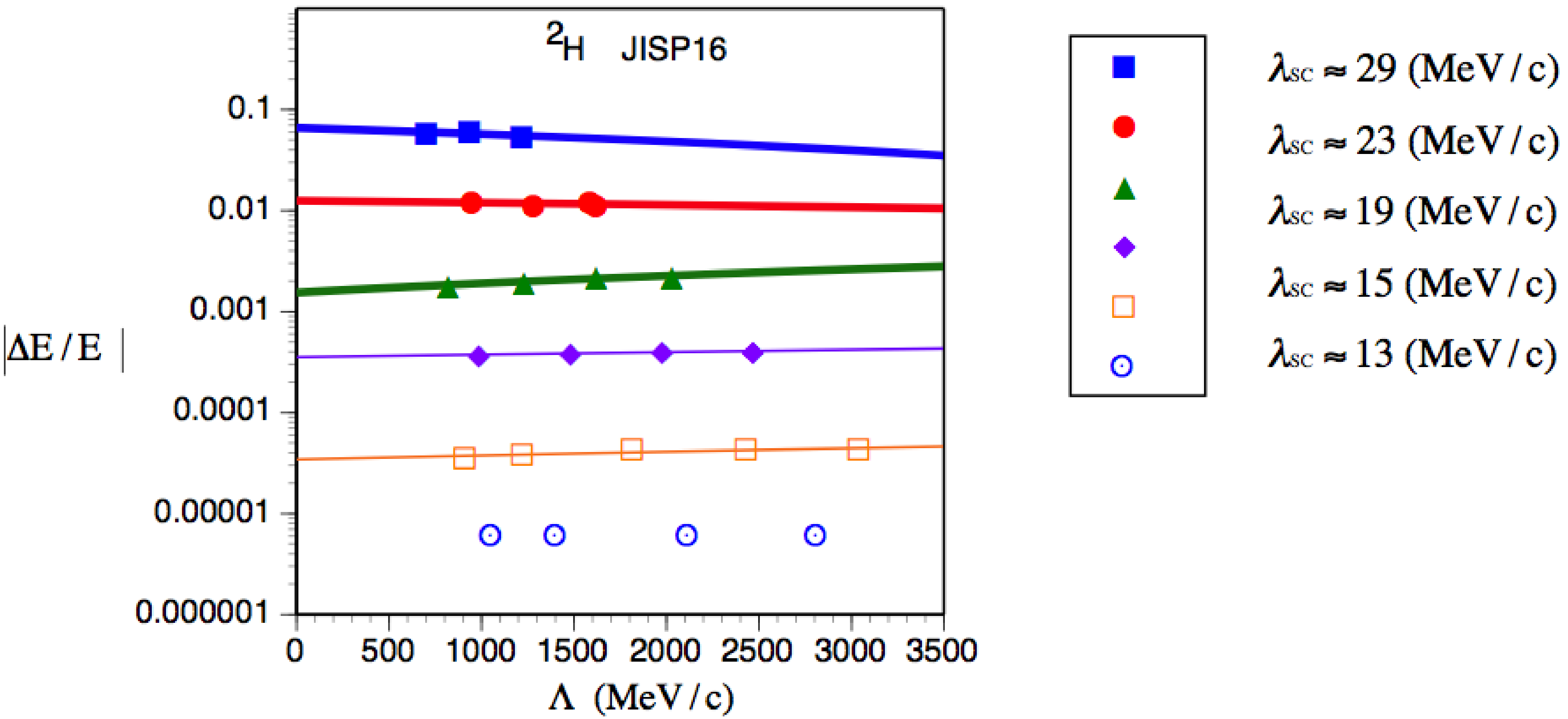
small λ

large λ

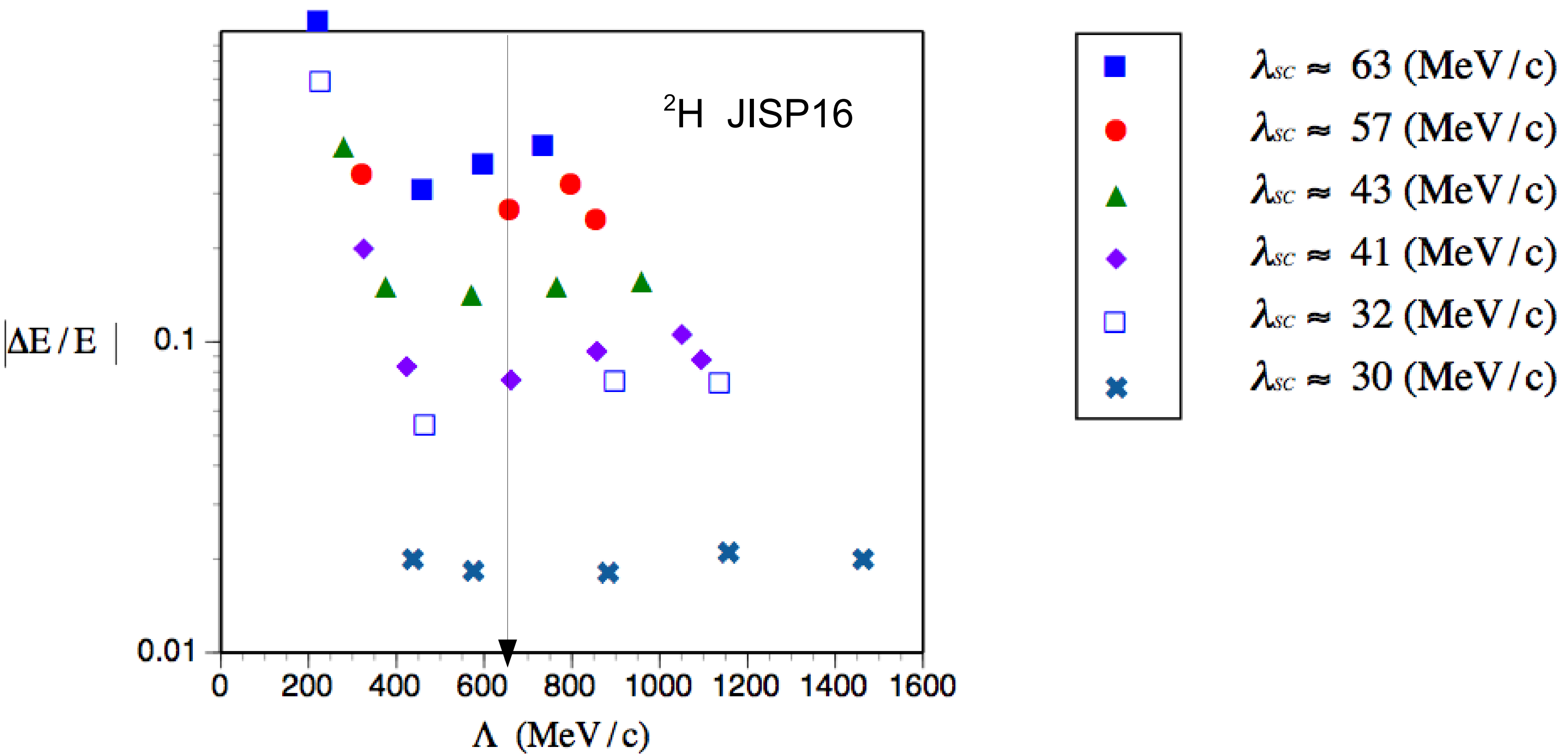
For fixed λ_{sc} result does NOT improve with increasing Λ if Λ≥700 MeV/c !

Why? answer a) λ_{sc} is NOT the correct IR cutoff!

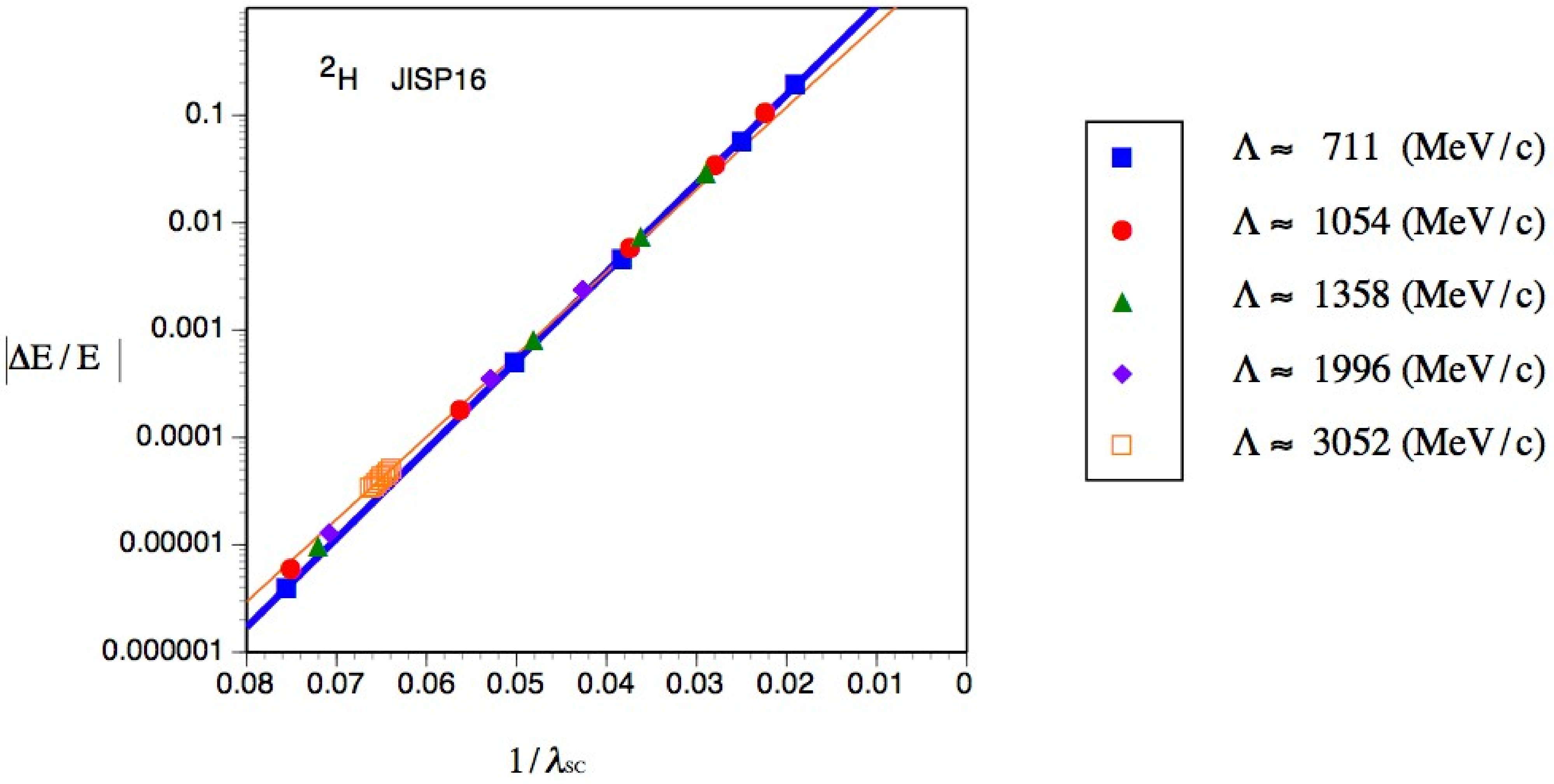
answer b) for JISP16 Λ is so large that the two cutoffs are already independent



Running of Λ below 700 MeV/c for λ_{sc} above 30 MeV/c has expected behavior



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

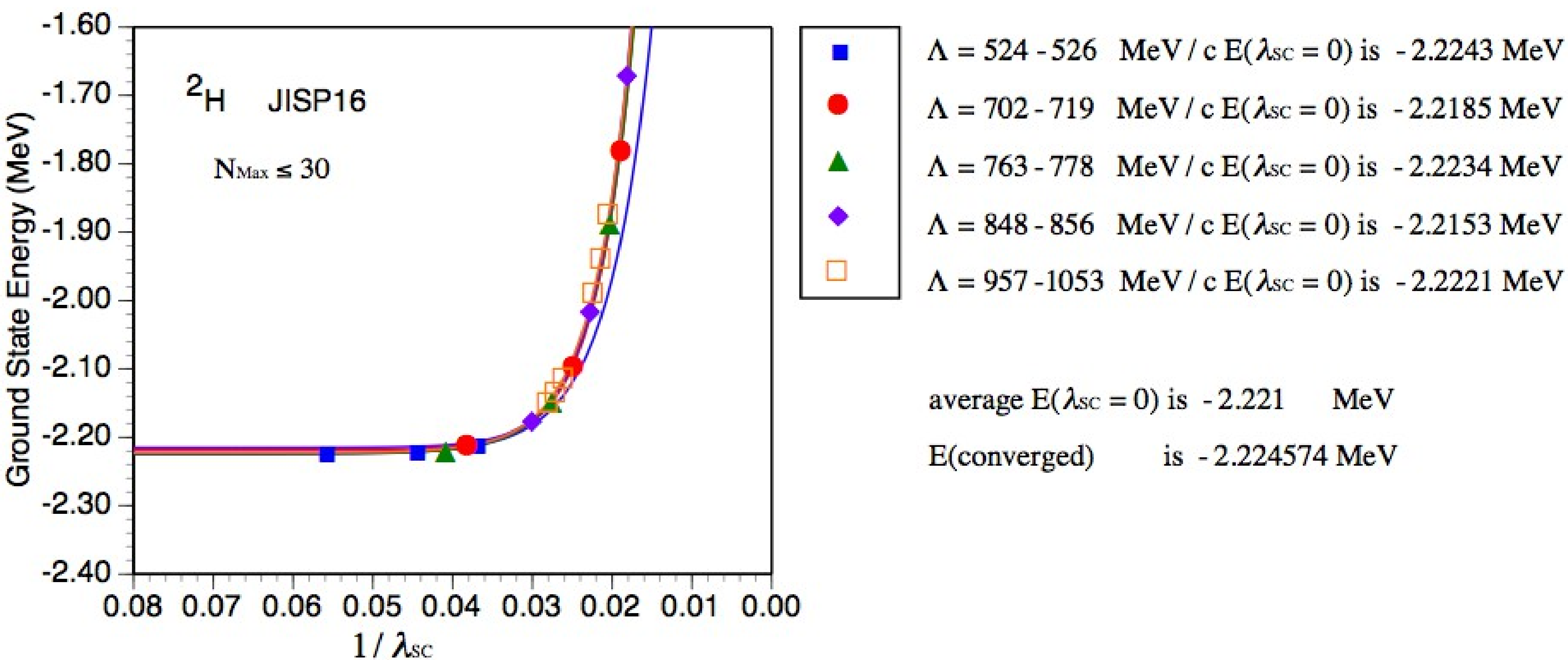


Success! UV and IR cutoffs identified as $N_{max} \rightarrow 238$

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

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

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



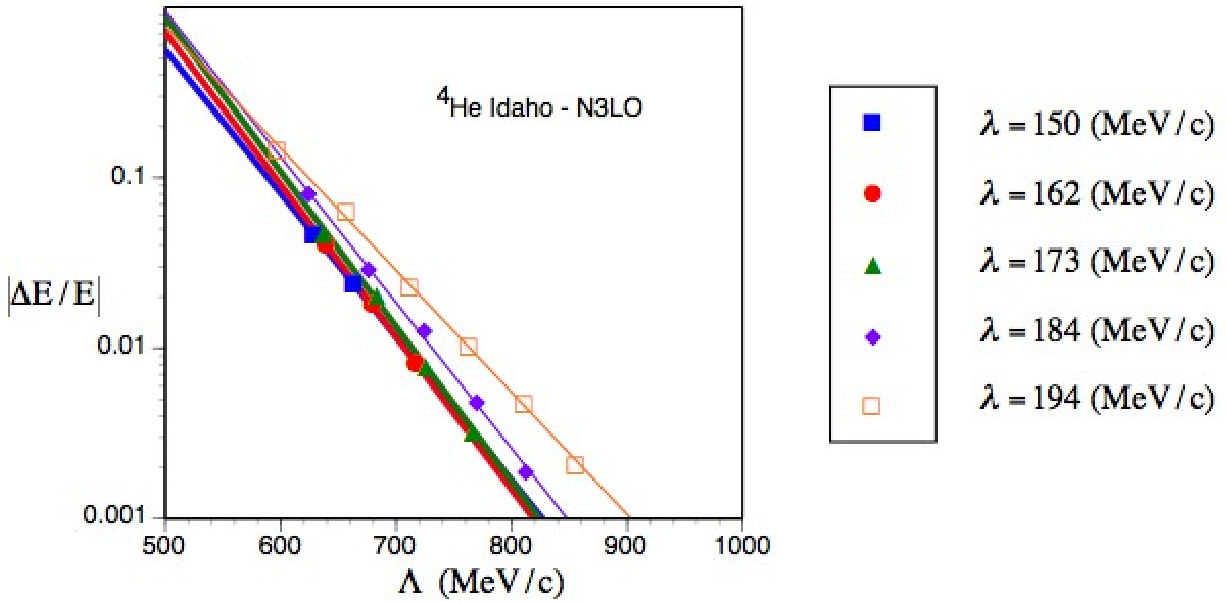
Note: This is not the usual extrapolation in N_{max} (with some prescription for ħω) because

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

N_{max} and ħω on an equal footing

Idaho-N3LO potential

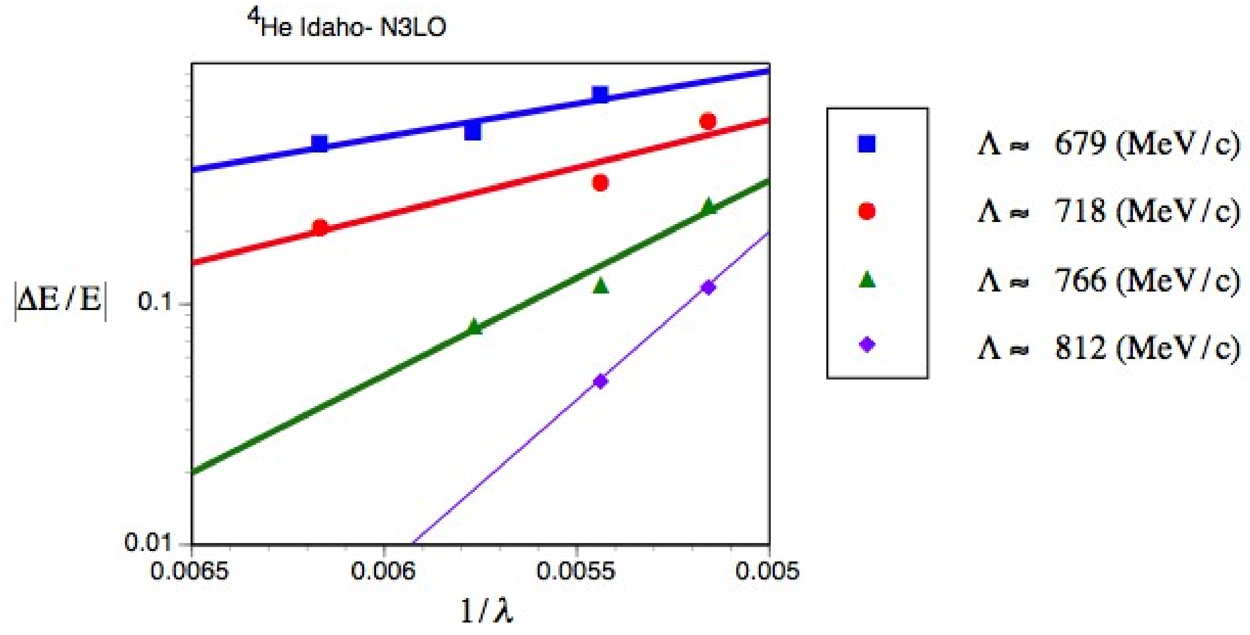
λ acts as an IR cutoff should



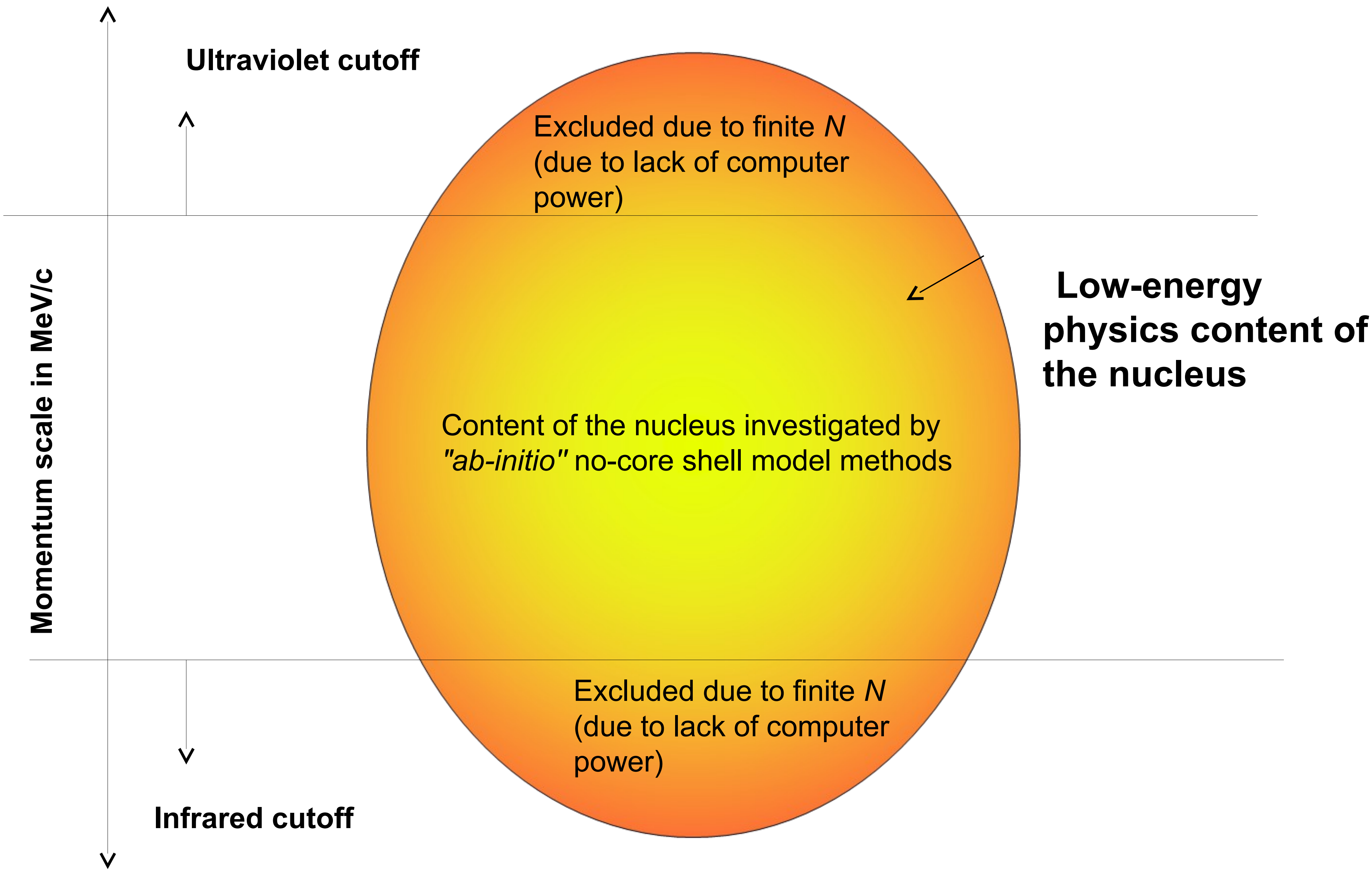
Replotted from calculations of Navratil and Caurier 2004

Idaho-N3LO potential

Λ acts as an UV cutoff should



Replotted from calculations of Navratil and Caurier 2004


Ultraviolet cutoff
Excluded due to finite N
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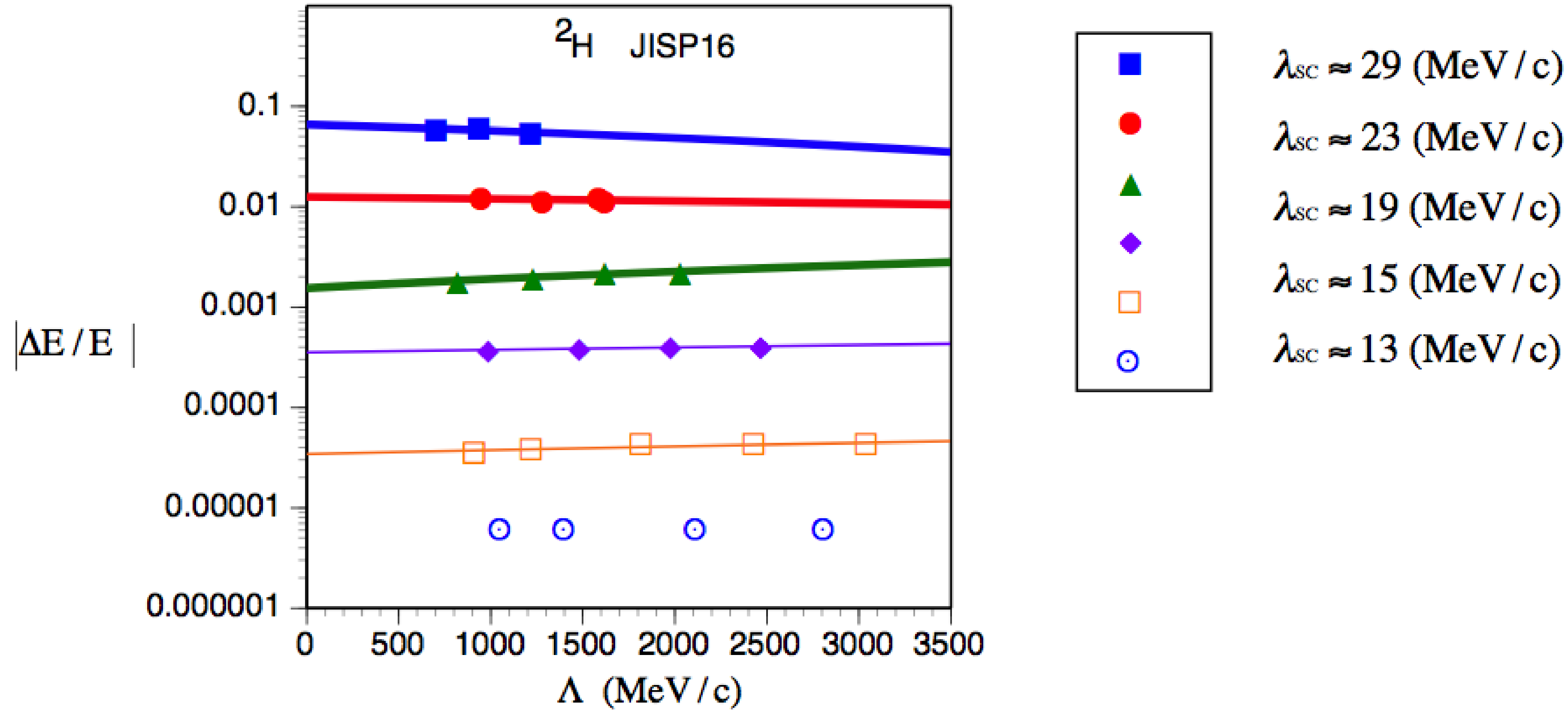
Momentum scale in MeV/c
Low-energy
physics content of
the nucleus
Content of the nucleus investigated by
"ab-initio" no-core shell model methods
Excluded due to finite N
(due to lack of computer
power)
Infrared cutoff

For fixed λ_{SC} result does NOT improve with increasing Λ if Λ≥700 MeV/c !

Why?

We need dedicated calculations

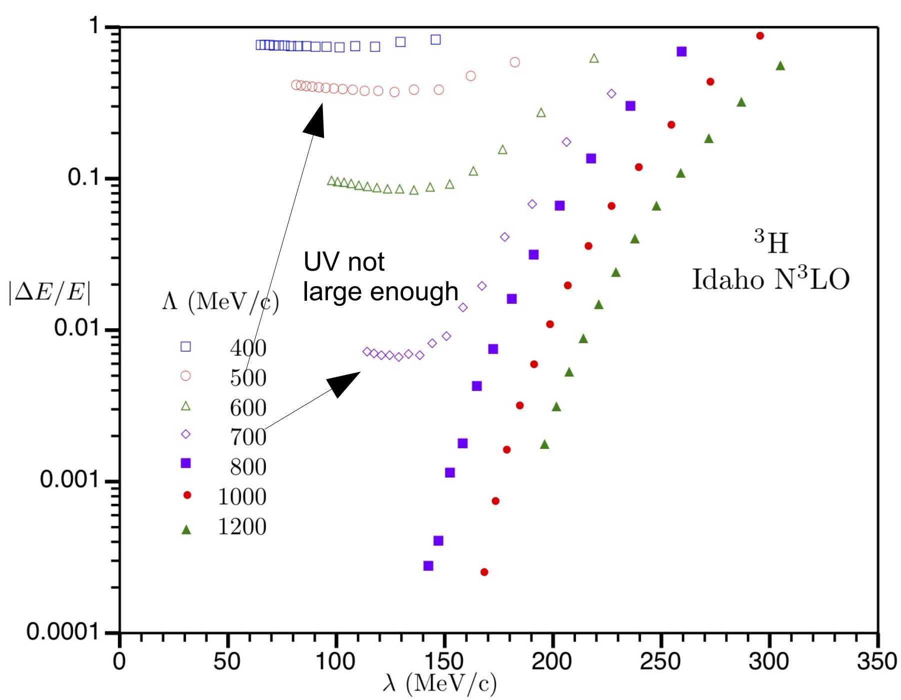
Binning and replotting archival calculations is not enough!

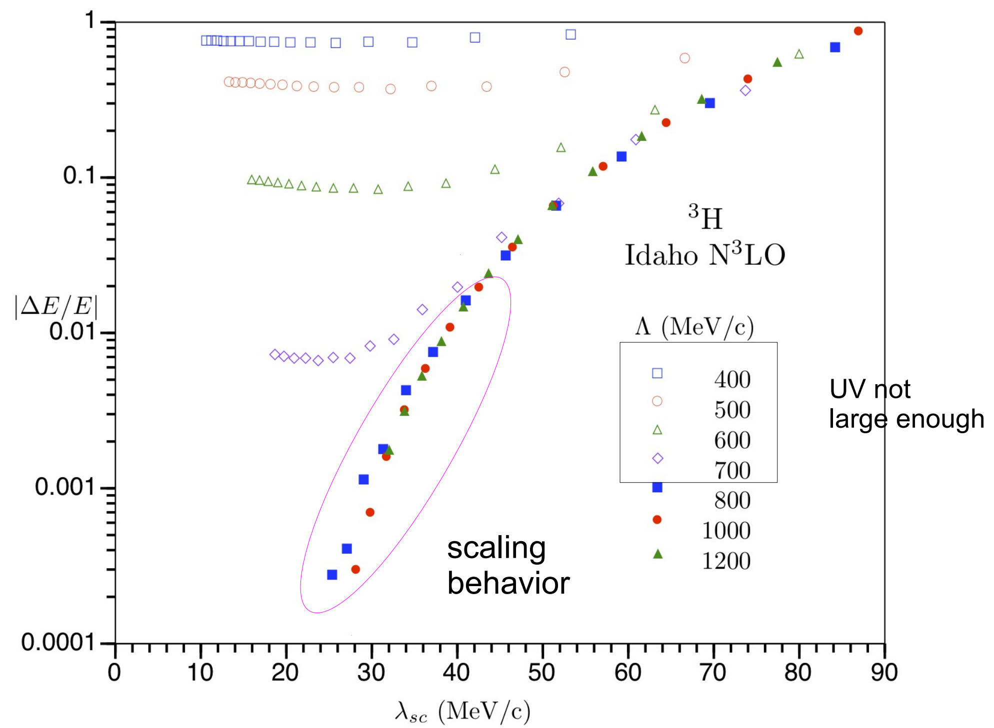


Fix UV regulator and take IR regulator toward zero

$\lambda_{IR} = \lambda$

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



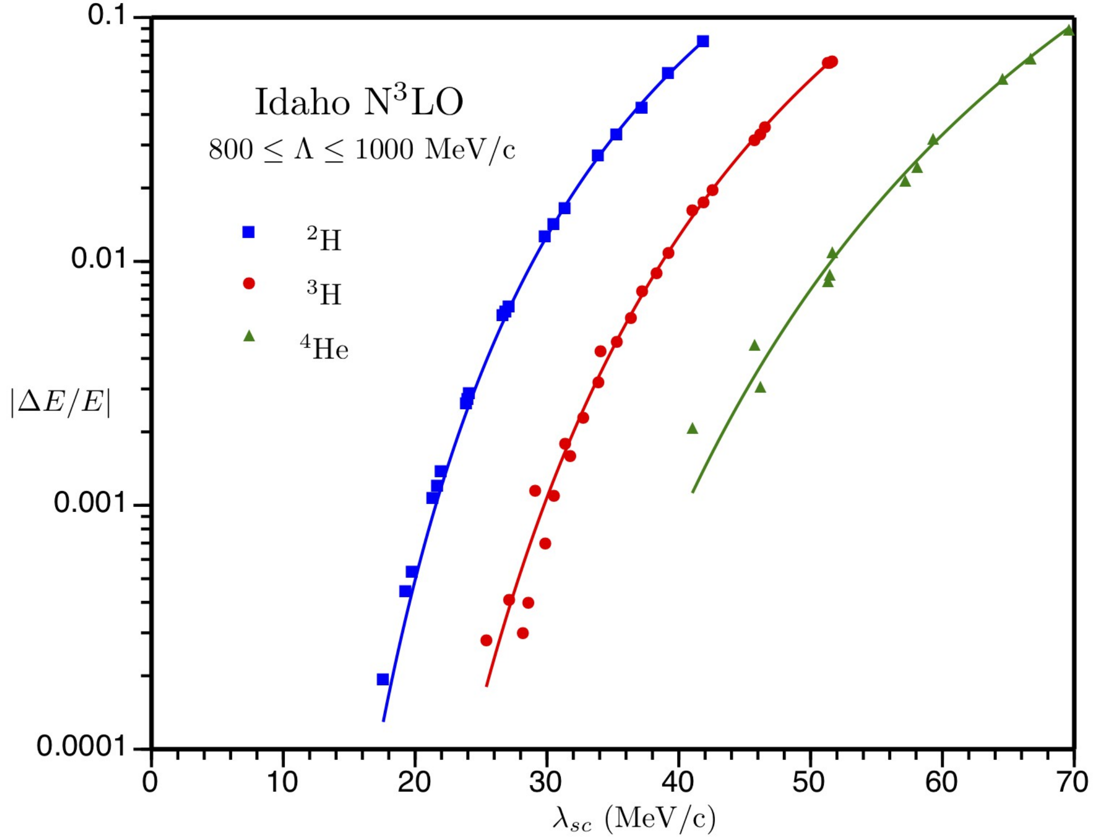


For a large enough ultraviolet cutoff, the fractional difference between calculated E(Λ, λ) and an accepted-as-converged E, lessens as the IR cutoff goes toward zero.

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

Slide by Michael Kruse

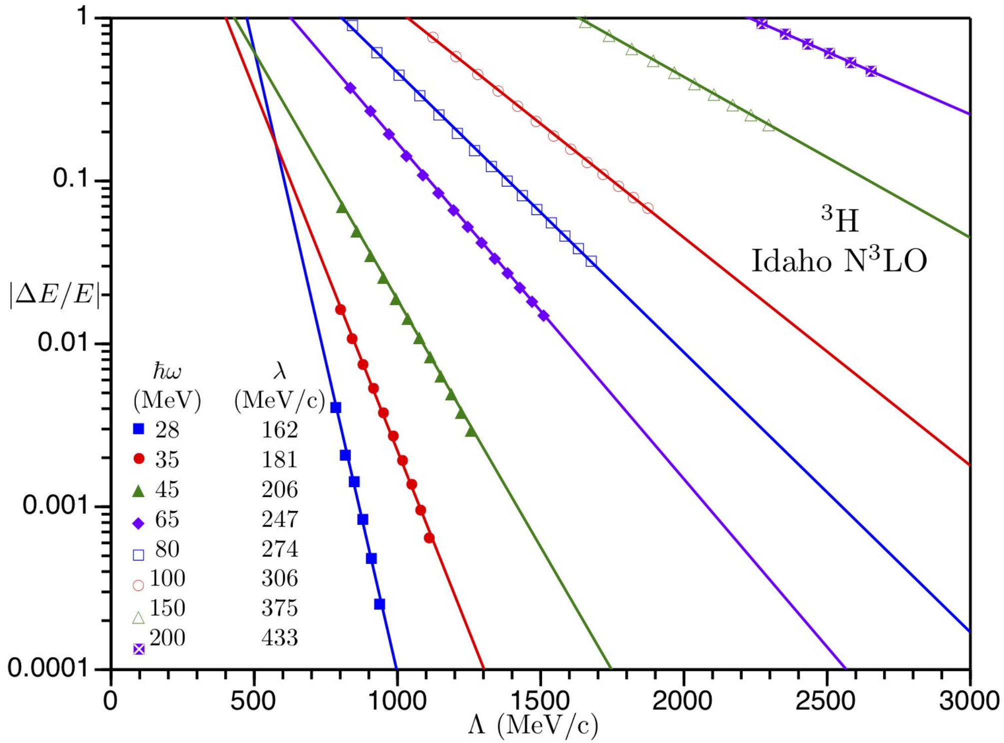
One can use this universal scaling behavior to make an extrapolation which is independent of particle number



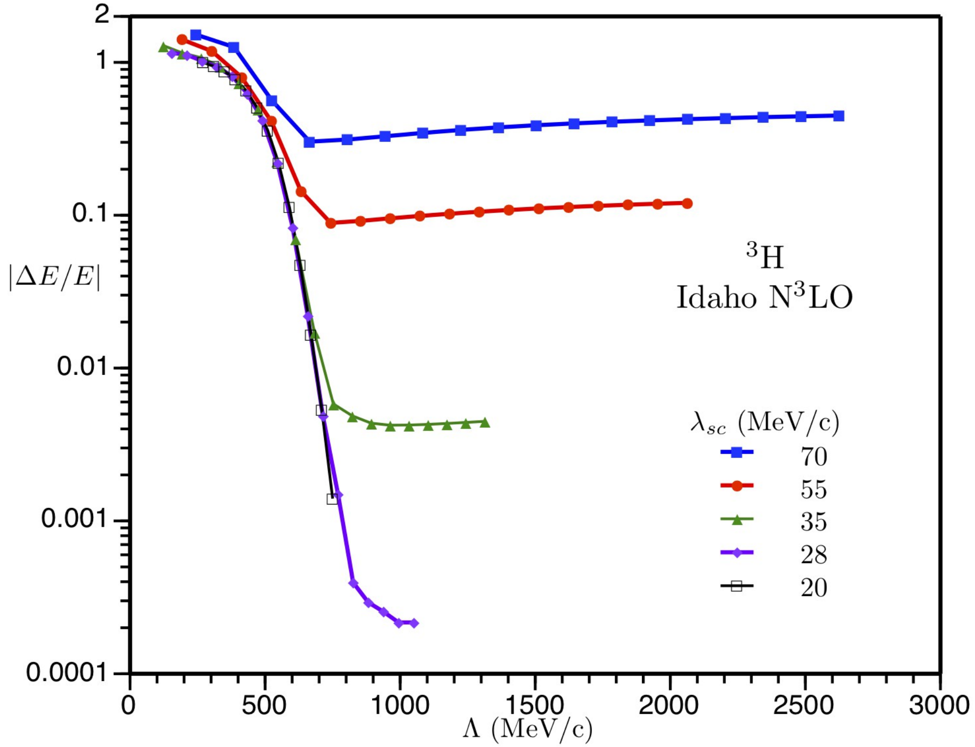
Data points are fit to $y = A\exp(-B/\lambda_{sc})$

Fix IR regulator and take UV regulator to infinity

$\lambda_{IR} = \lambda$



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



As the ultraviolet cutoff increases, the fractional difference between calculated E(Λ, λ) and an accepted-as-converged E, lessens.

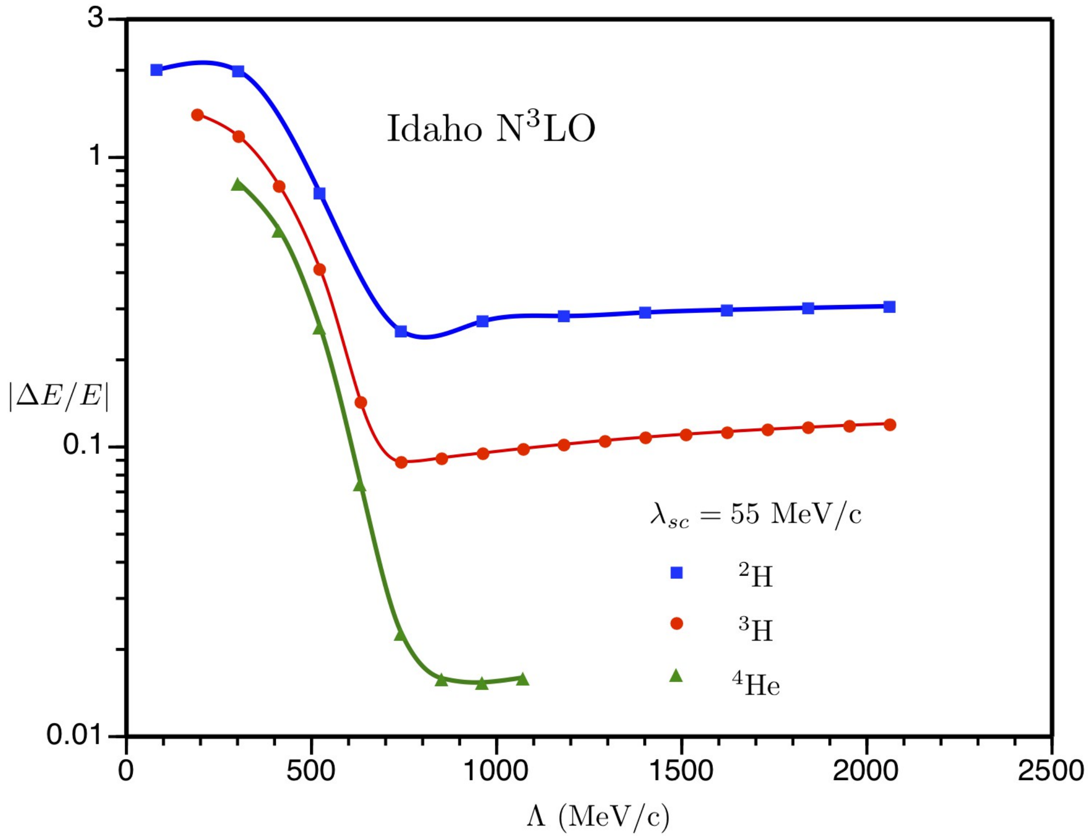
Alternatively, the plot can be read the other way, where if we fix the UV Λ, the results improve as we lower the IR cutoff λ.

For fixed λ_{sc} result does NOT improve with increasing Λ, if Λ≥800 MeV/c !

Small fixed λ_{sc} linked to small Λ, as N<36 and ħω/N must be constant

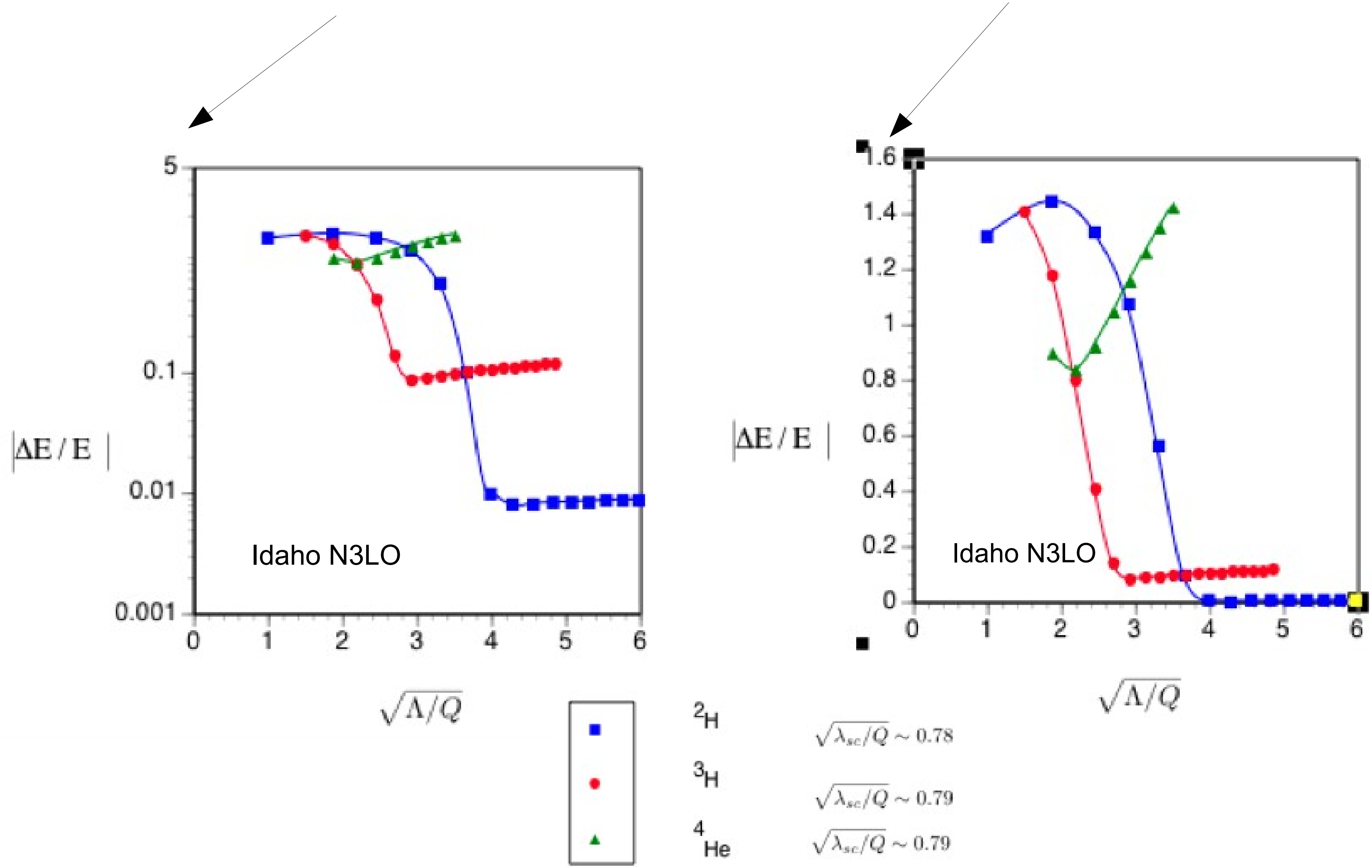
For fixed λ_{SC} result does NOT improve with increasing Λ, if Λ≥800 MeV/c !

Result independent of nucleus



Fix λ_{sc} and increase Λ (each are scaled by binding momentum Q)

y axis is logarithmic on left, linear on right



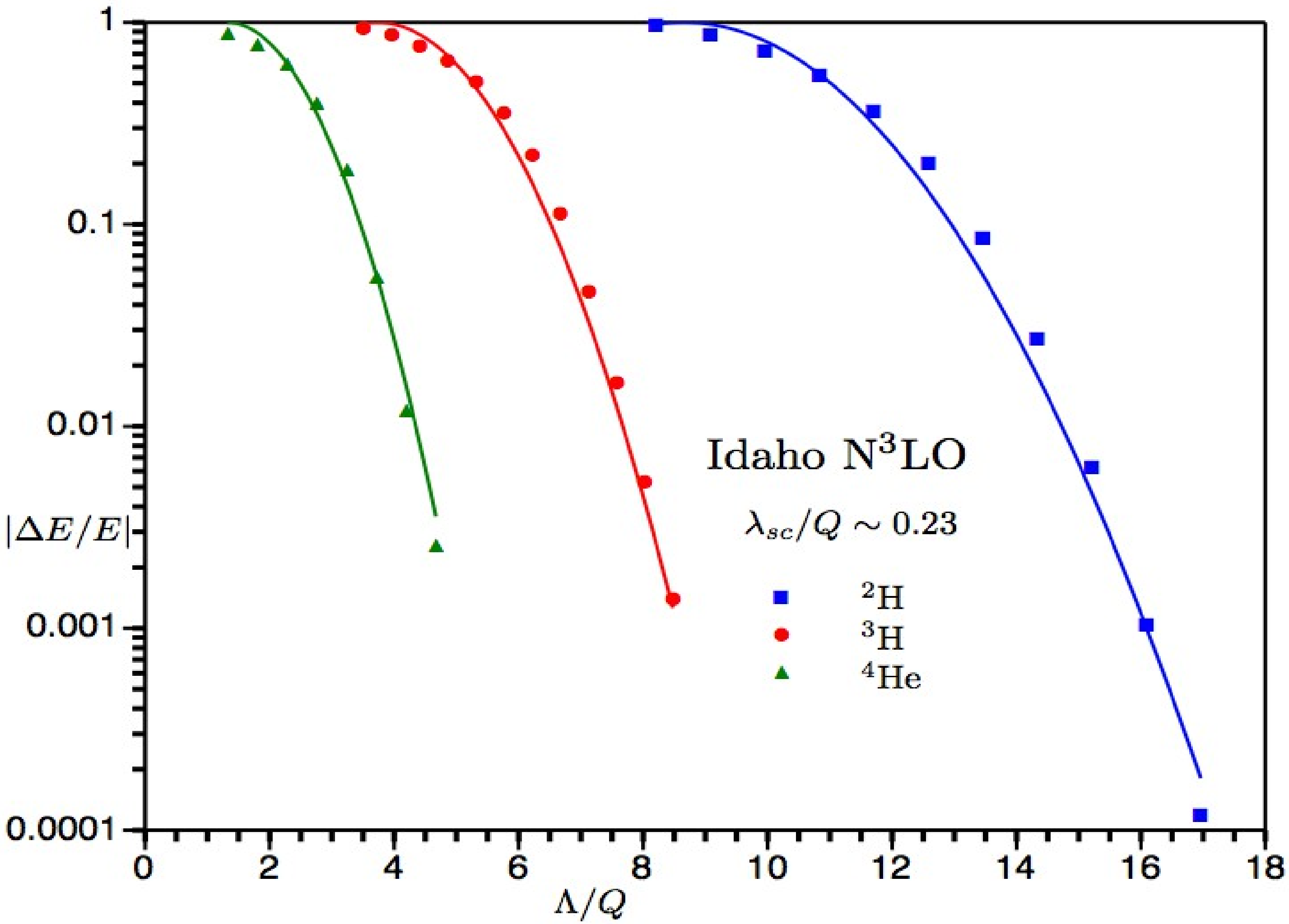
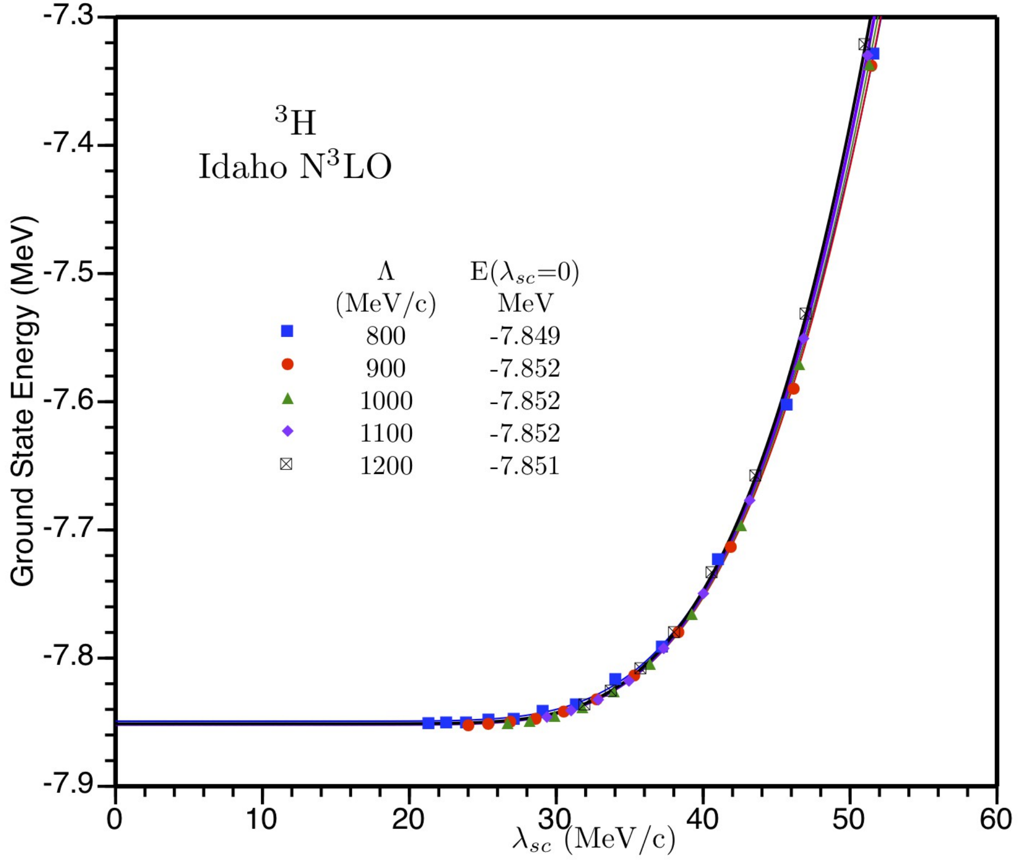


FIG. 9: (Color online) Dependence of the ground-state energy of three s-shell nuclei (compared to a converged value-see text) upon the uv momentum cutoff $\Lambda = \sqrt{m_N(N+3/2)\hbar\omega}$ for $\lambda_{sc} = \sqrt{(m_N\hbar\omega)/(N+3/2)}$ below the $\lambda_{sc}^{NN} \approx 36$ MeV/c set by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

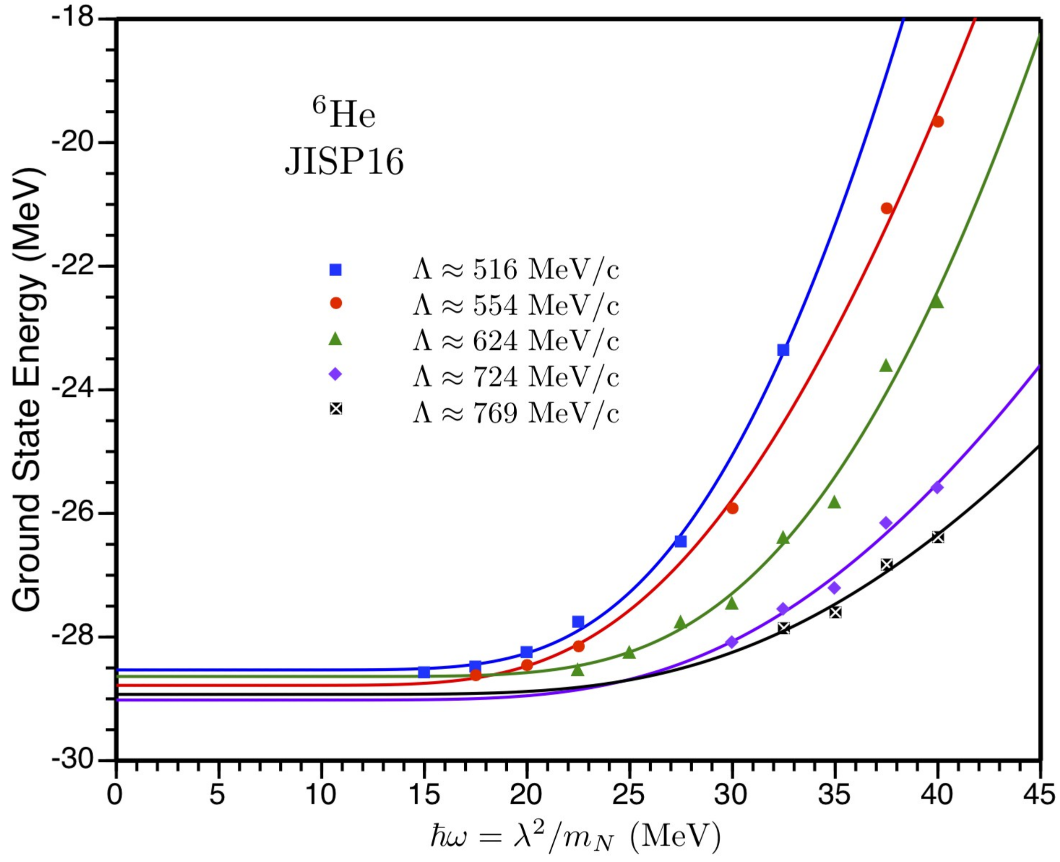
Extrapolations with λ_{sc}

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



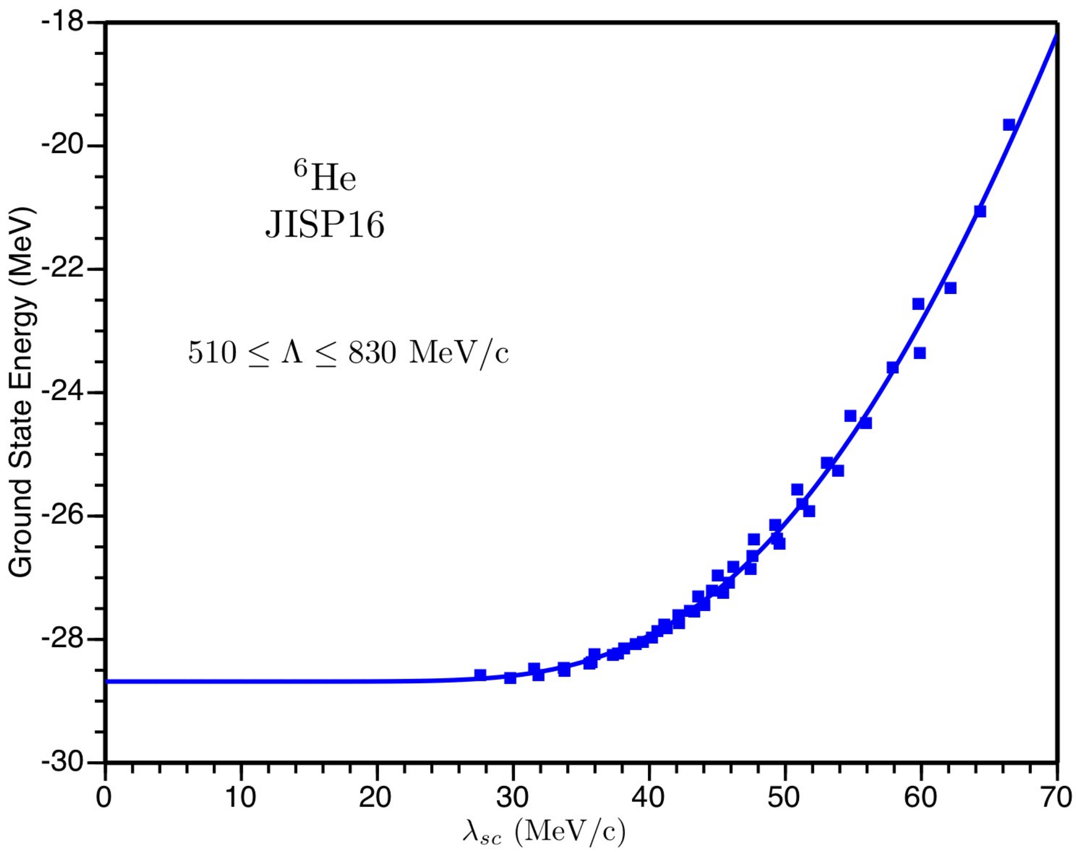
If UV cutoff is large enough, all extrapolations agree with each other and with the accepted value of -7.85 MeV

Extrapolations with 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 Λ. It is readily seen that one can indeed make an ir extrapolation by sending $\hbar\omega \to 0$ with fixed Λ 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.

Extrapolations with λ_{sc}



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

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 ħω for fixed number of quanta
Number of quanta increases by two for each curve

1969 H atom up to 10 quanta

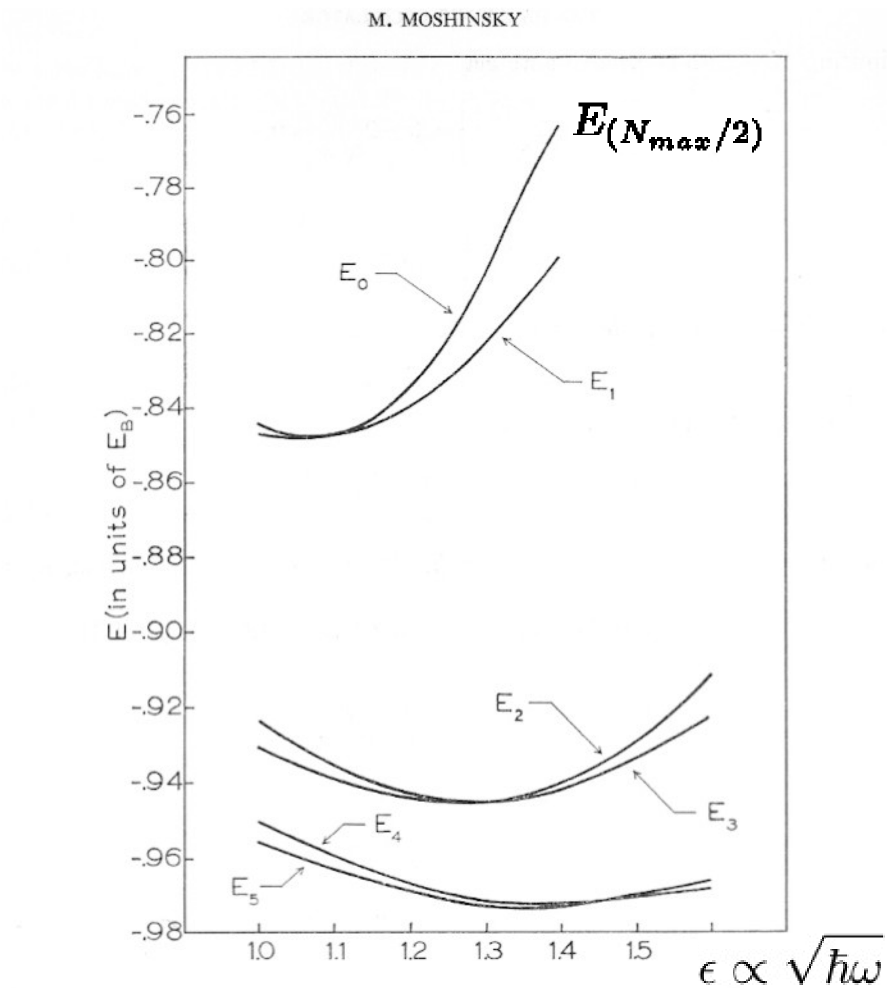
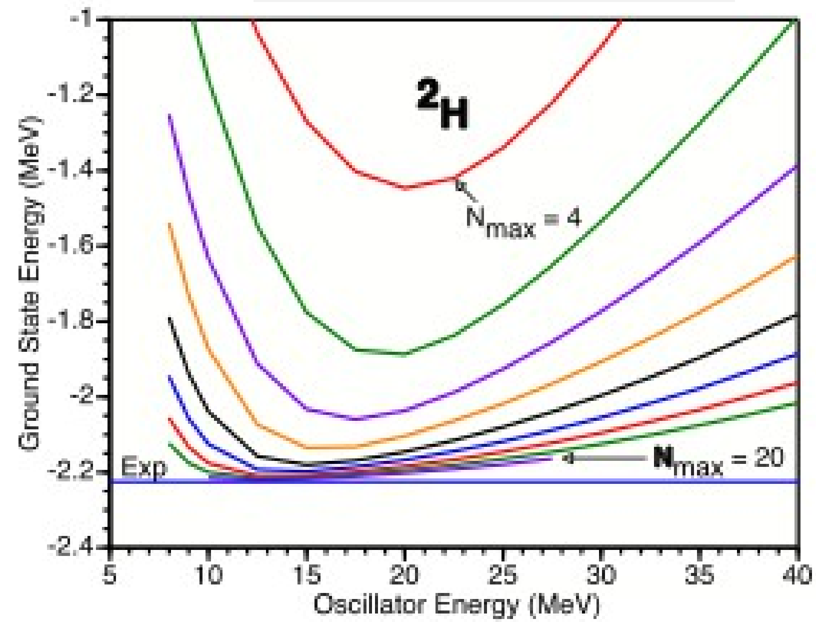


FIG. 1. Energy of the ground state of the H atom as a function of the parameter ε for the variational analysis discussed in Section 3. This energy $E_p(\varepsilon)$, $p = 0, 1, 2, 3, 4, 5$ is associated with a trial wave function $\psi_p = \Sigma_{n=0}^{p} a_n^{(p)} \mid n00\rangle$, where $\mid n00\rangle$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

2009 deuteron up to 20 quanta

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



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

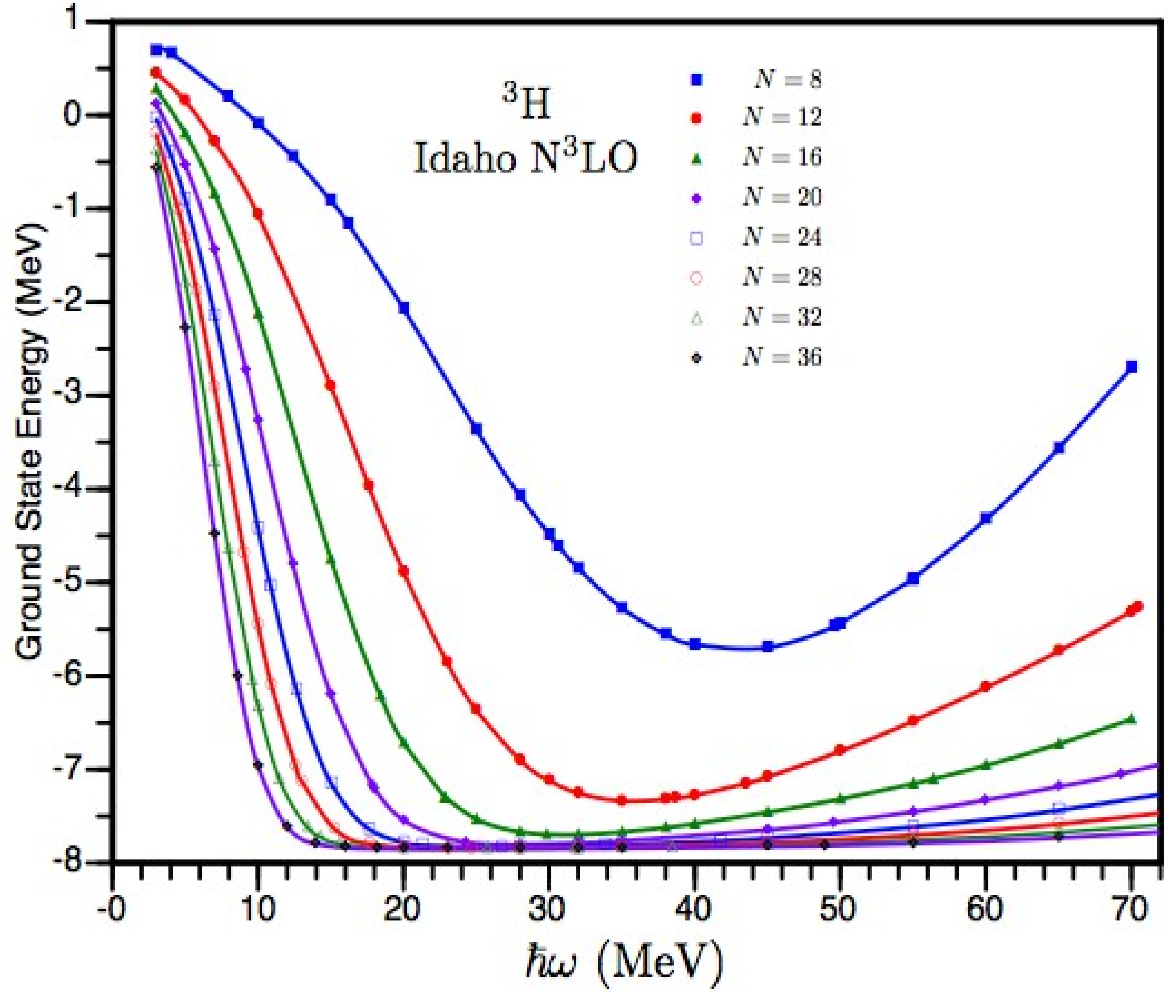
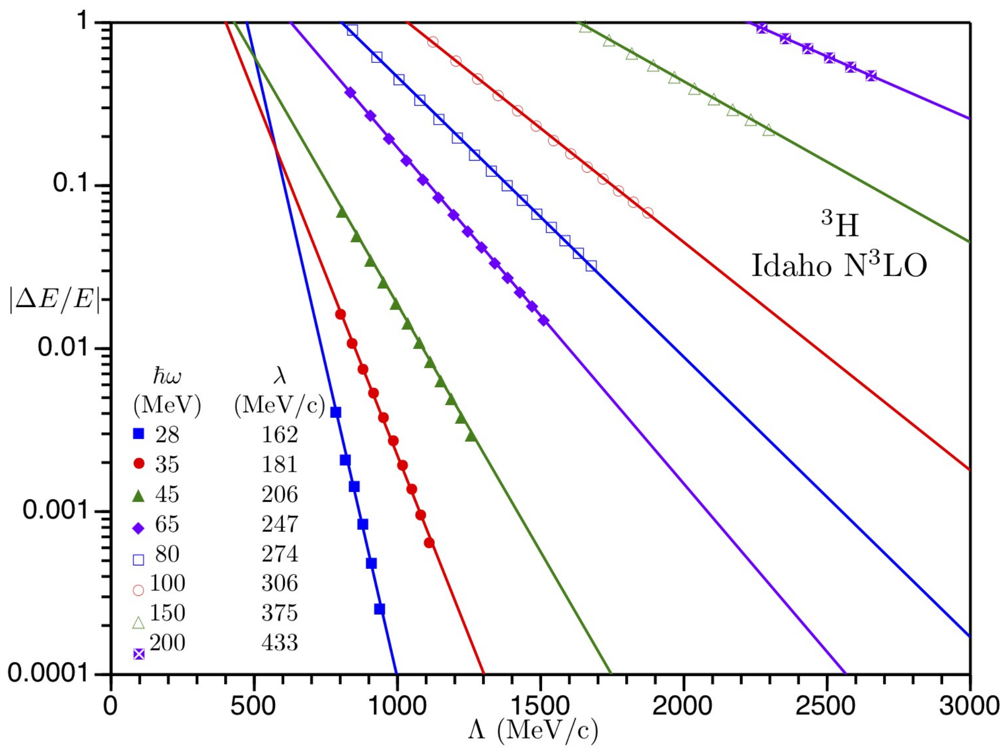


Figure 8: (Color online) Dependence of the ground-state energy of ^{3}H upon $\hbar\omega = \lambda^2/m_N = \lambda_{sc}^2/[m_N(N+3/2)]$ for fixed $N = \Lambda^2/\lambda^2 - 3/2 = \Lambda/\lambda_{sc} - 3/2$. Curves are not fits but spline interpolations to guide the eye.

Fix IR regulator and take UV regulator to infinity

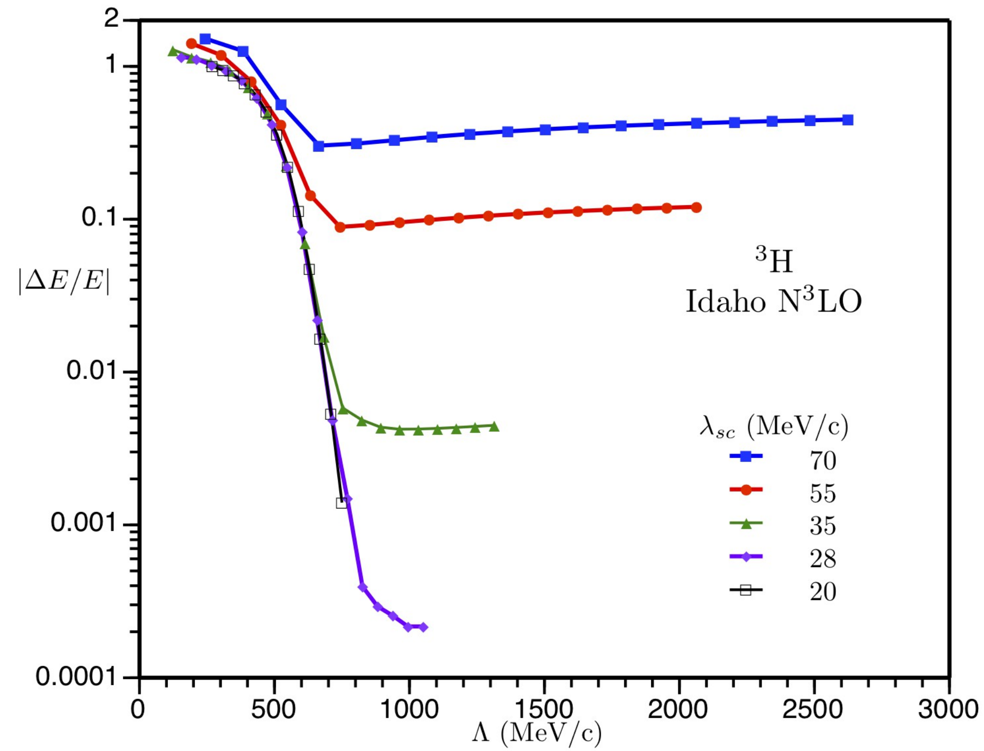
$\lambda_{IR} = \lambda$



As the ultraviolet cutoff increases, the fractional difference between calculated E(Λ, λ) and an accepted-as-converged E, lessens.

Alternatively, the plot can be read the other way, where if we fix the UV Λ, the results improve as we lower the IR cutoff λ.

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



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