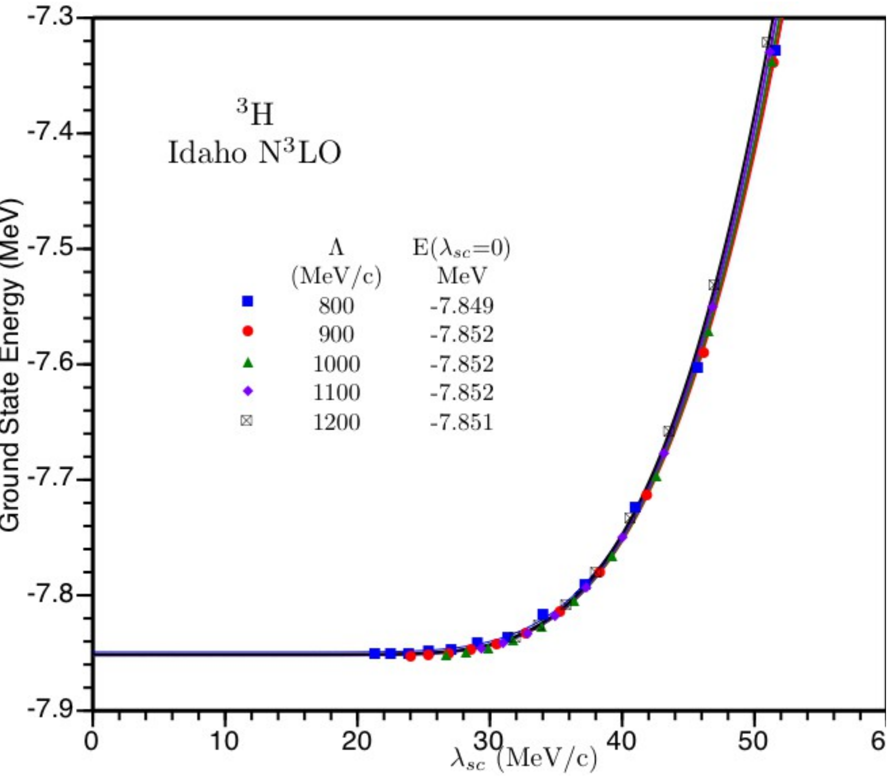
Universal properties of infrared extrapolations in a harmonic oscillator basis

Sidney A Coon and Michael K.G. Kruse



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)

Chiral NN interaction, λ = 2.5 fm-1
Extrapolation A'

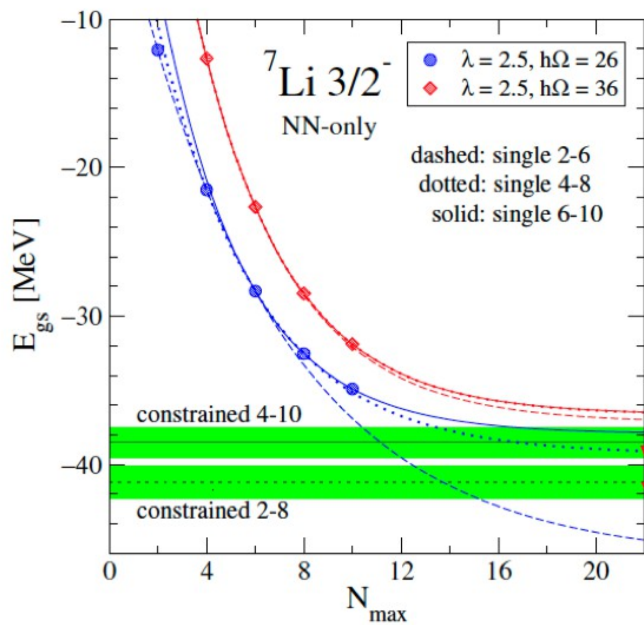
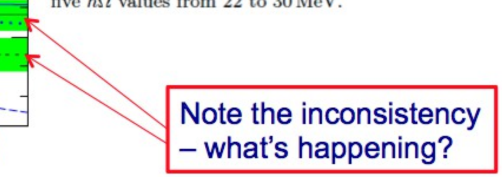


FIG. 14. (color online) Ground-state energy extrapolations of ^{7}Li as a function of N_{max} with an N^{3}LO NN interaction [21] evolved to $\lambda = 2.5\,\mathrm{fm}^{-1}$. The symbols are the calculated points. The curves show single extrapolations using Eq. (3) with N_{max} = 2–6 (dashed), 4–8 (dotted) and 6–10 (solid) at (blue) $\hbar\Omega$ = 26 MeV which minimize the amount of extrapolation and at (red) $\hbar\Omega$ = 36 MeV which minimize the numerical error estimate. The horizontal dotted and solid lines, with the band indicating the associated error bars, are the result from a constrained fit following the procedure of Ref. [1] for five $\hbar\Omega$ values from 22 to 30 MeV.



Slide by James Vary

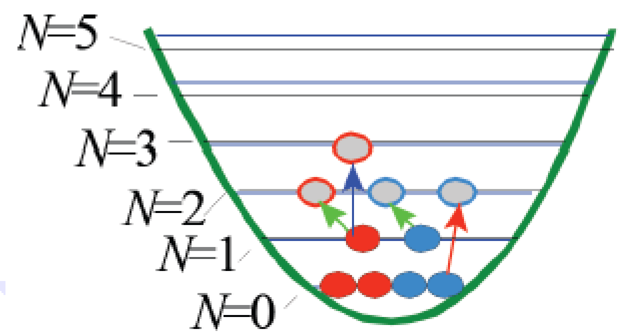
E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary, submitted to PRC; arXiv: 1302:5473

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,

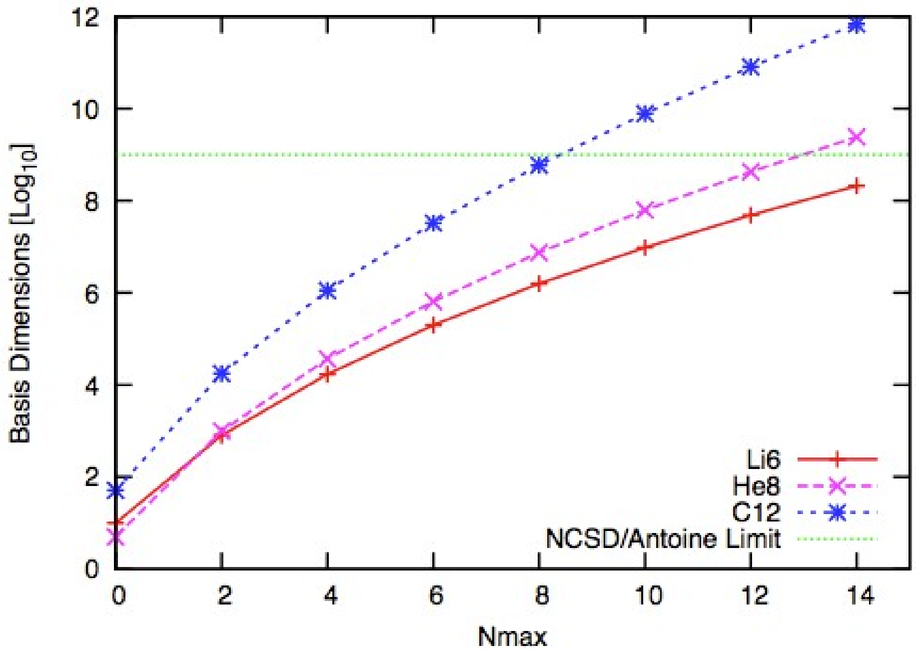
It's that "simple".

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

Slide from Michael Kruse

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 co-ordinates 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.

Slide from Michael Kruse

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:

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

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

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

2009 deuteron up to 20 quanta

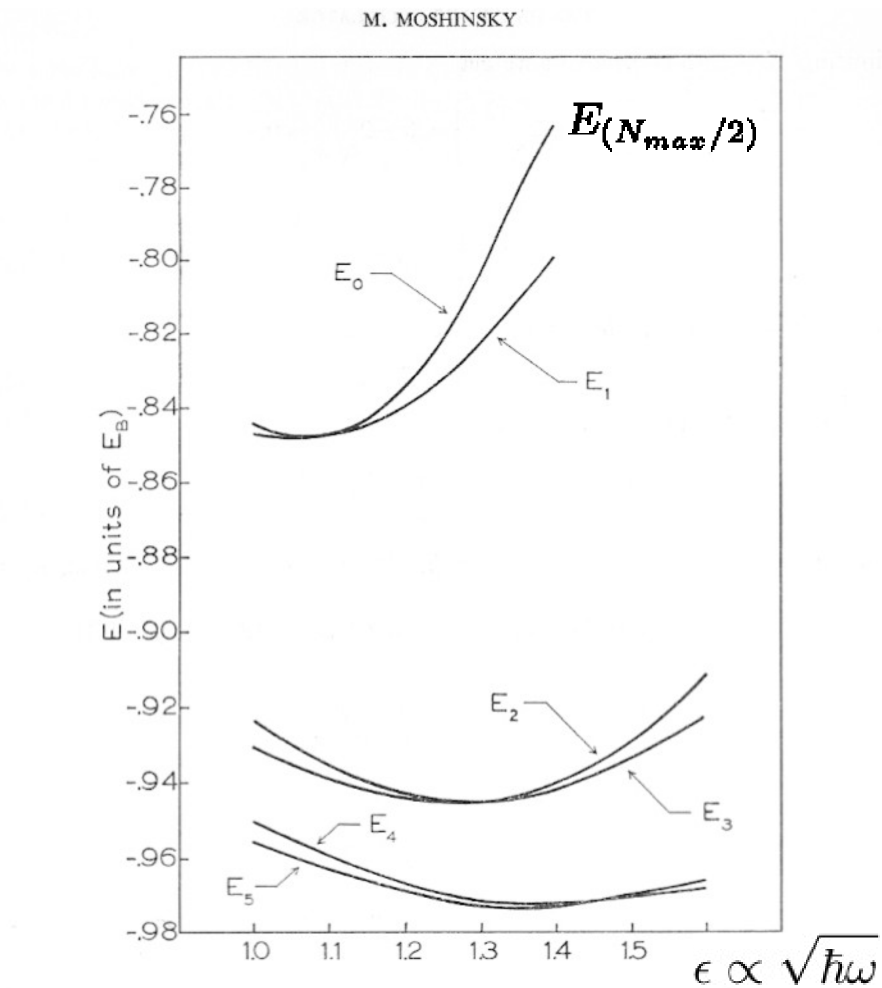
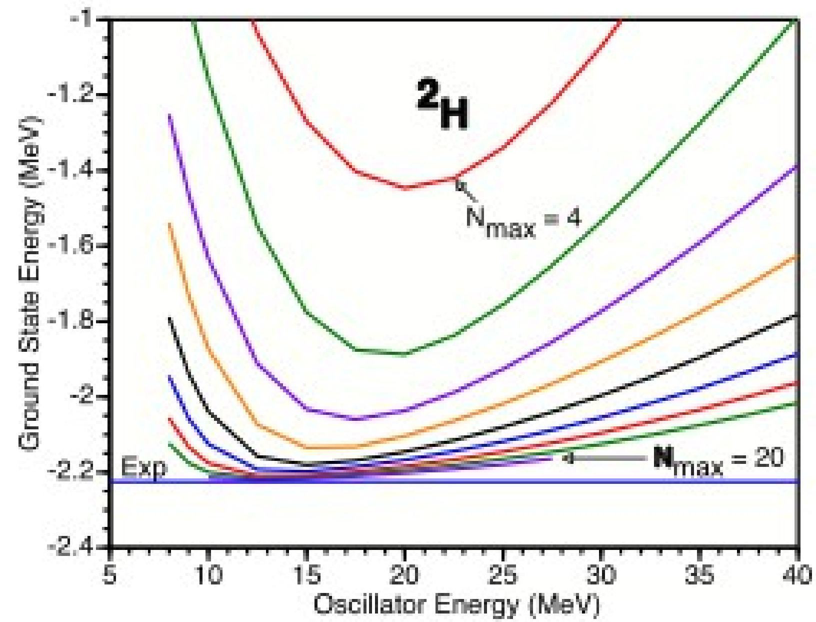
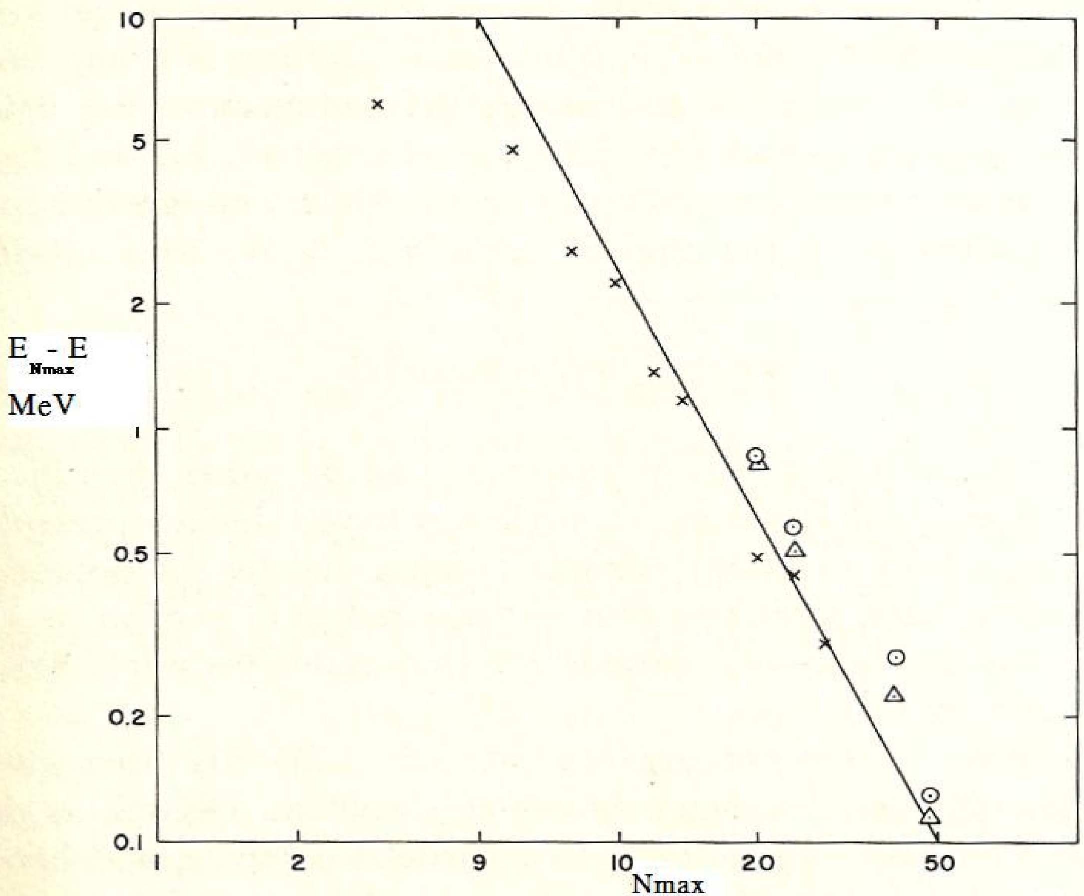


FIG. 1. Energy of the ground state of the H atom as a function of the parameter ε for the variational analysis discussed in Section 3. This energy $E_p(\varepsilon)$, $p = 0, 1, 2, 3, 4, 5$ is associated with a trial wave function $\psi_p = \Sigma_{n=0}^{p} a_n^{(p)} \mid n00\rangle$, where $\mid n00\rangle$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



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

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



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

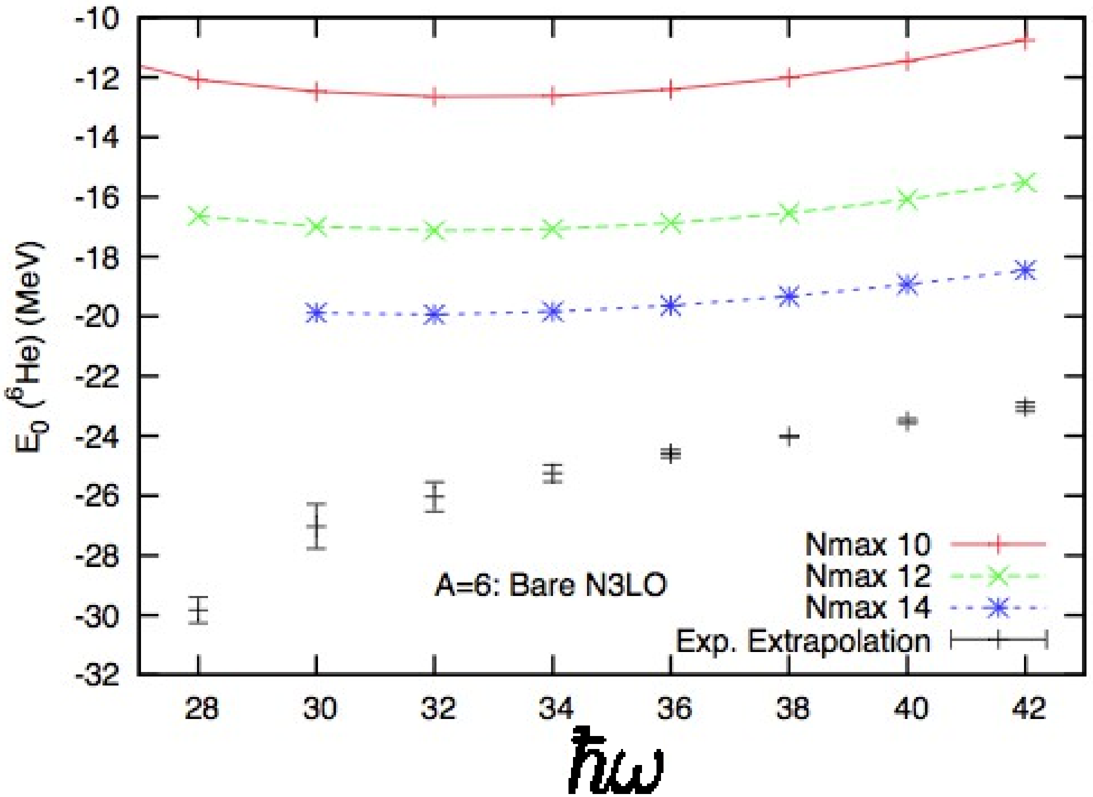
"nonsmooth potentials" like Yukawa

Fig. 8. Convergence rates for variational calculations with a harmonic oscillator basis. ⊙ 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}

"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'."

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



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

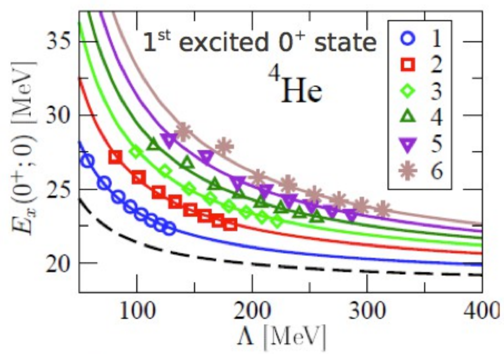
Current Method is Unsatisfactory…

- …from an effective field theory point of view.
- Results are 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.

Slide by Matthew Avetian undergraduate honors thesis 2011

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 ^{4}He.

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PHYSICS LETTERS B

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

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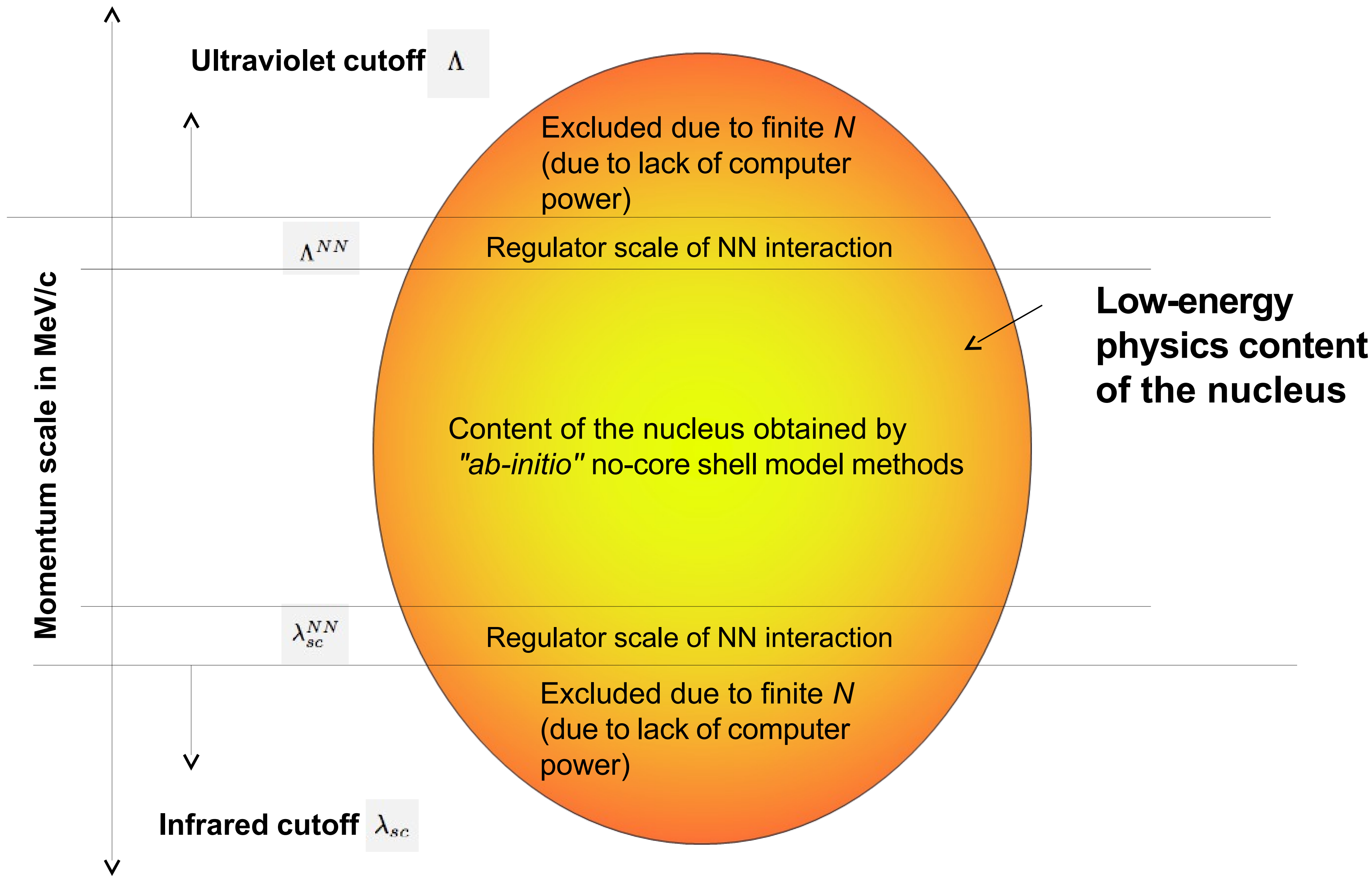


Ultraviolet cutoff Λ
Excluded due to finite *N*
(due to lack of computer
power)
Λ^{NN}
Regulator scale of NN interaction
Momentum scale in MeV/c
Low-energy
physics content
of the nucleus
Content of the nucleus obtained by
"ab-initio" no-core shell model methods
λ_{sc}^{NN}
Regulator scale of NN interaction
Excluded due to finite *N*
(due to lack of computer
power)
Infrared cutoff λ_{sc}

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)

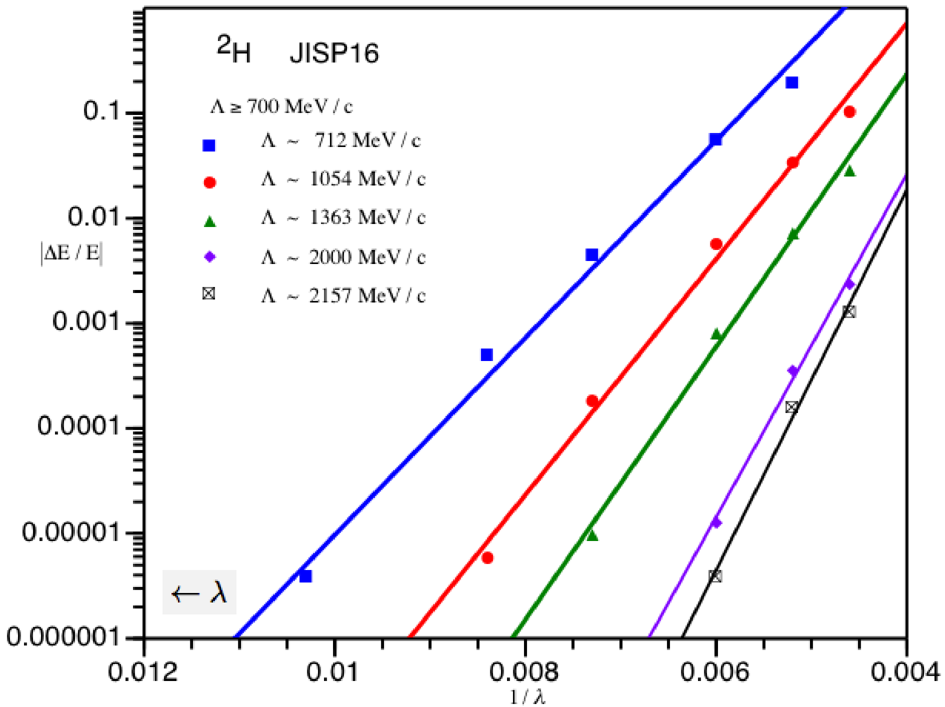
Alternate λ_{sc} in Furnstahl et al. PRC **86** (2012),
More et al. PRC **87** (2013),
Furnstahl et al. ArXiv:1312.6876

Strategy:
minimize $E(\Lambda,\lambda)$ or $E(\Lambda,\lambda_{sc})$

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

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

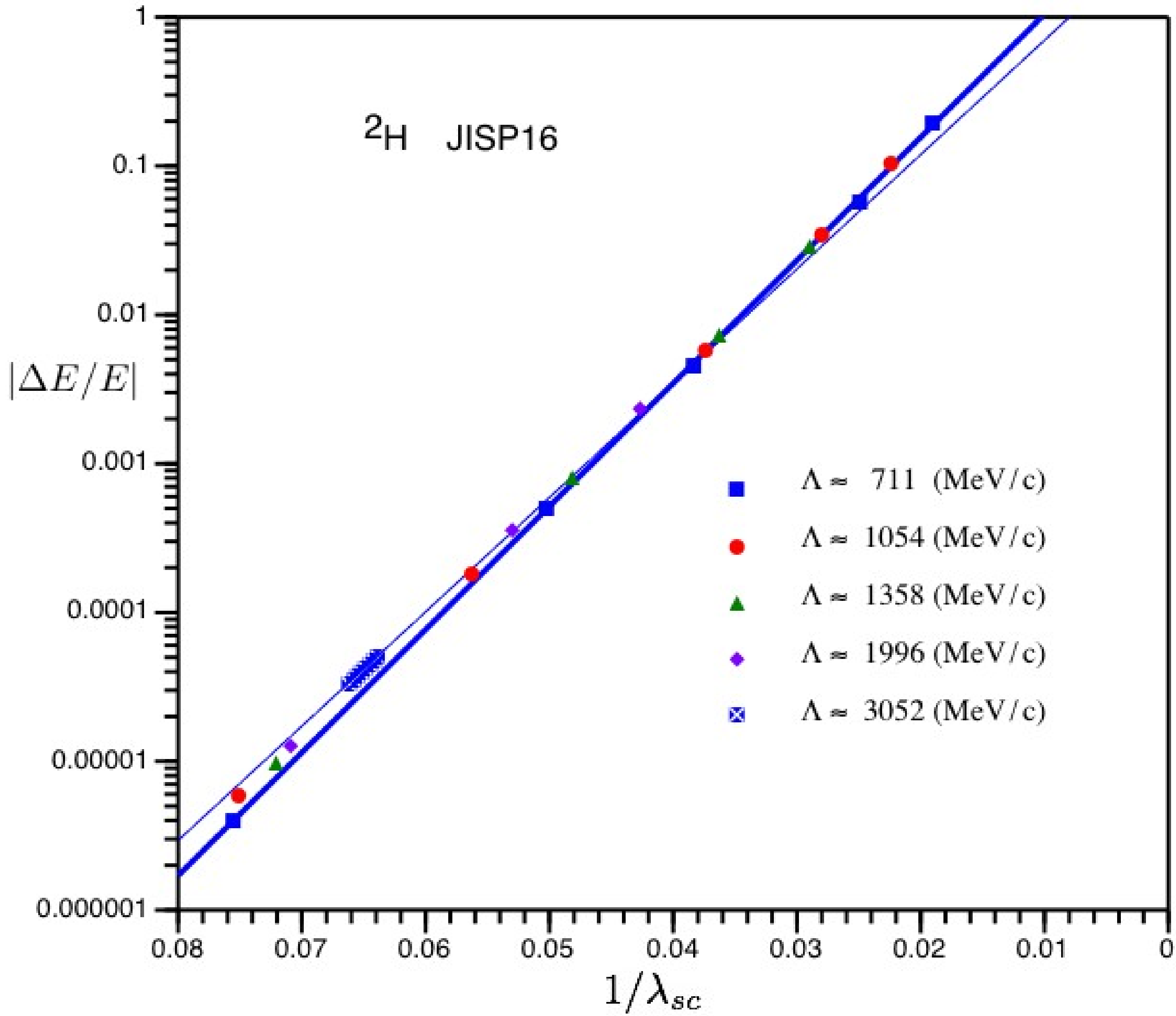


- Extrapolator is clearly the exponential function.
- $\frac{E(\lambda)-E(\lambda=0)}{E(\lambda=0)} \equiv \frac{\Delta E}{E} = A\exp(-B/\lambda)$
- *B* is a function of the UV cutoff Λ
- The IR cutoff *cannot* be aware of the UV cutoff.
- Remove dependence upon Λ
- $\lambda = \sqrt{\Lambda\lambda_{sc}} \Longrightarrow$
- $\exp(-B/\lambda) = \exp(-B/\sqrt{\Lambda\lambda_{sc}}) = \exp\left(-\frac{B/\sqrt{\Lambda}}{\sqrt{\lambda_{sc}}}\right)$
-

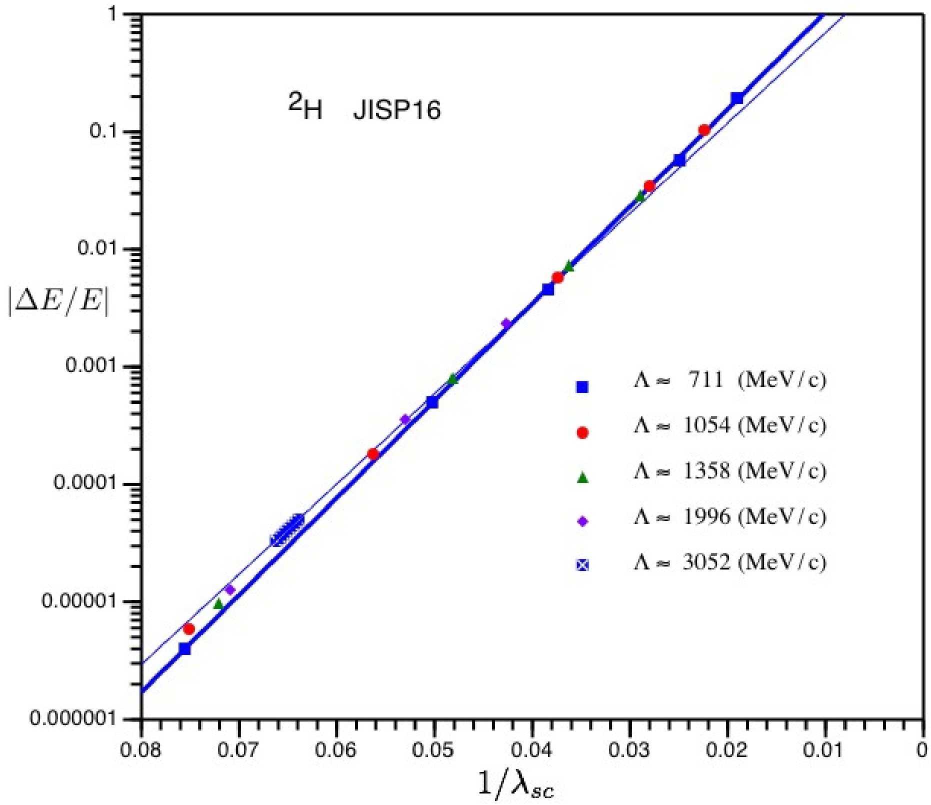
$B/\sqrt{\Lambda}$ (i.e., multiplier of $1/\sqrt{\lambda_{sc}}$) is constant to within 5 %.

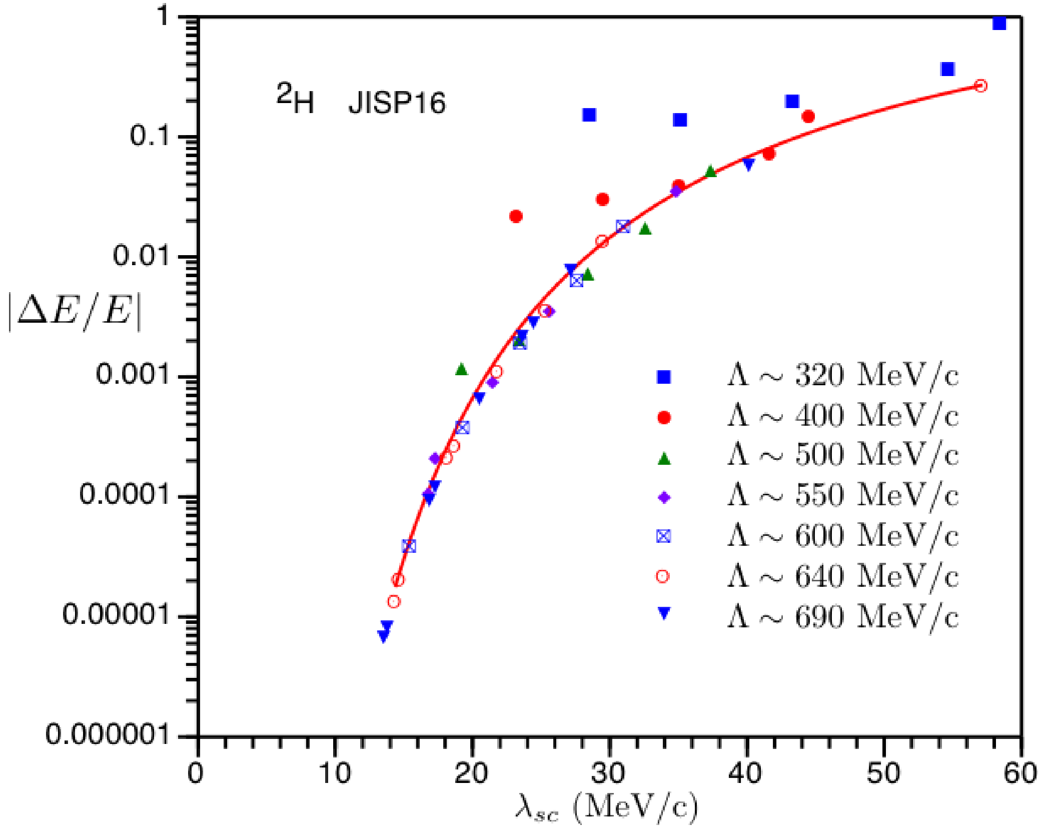
The momentum cutoff λ will remove IR effects. Indeed, any momentum cutoff $\lambda_{sc} \leq \lambda_{IR} \leq \Lambda$ will remove IR effects, but the IR regulator which is independent of the UV cutoff is some function of λ_{sc}. It is λ_{sc} which causes the IR effects and one does not need to decrease a IR cutoff below that of λ_{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 $1/\lambda_{sc}$.

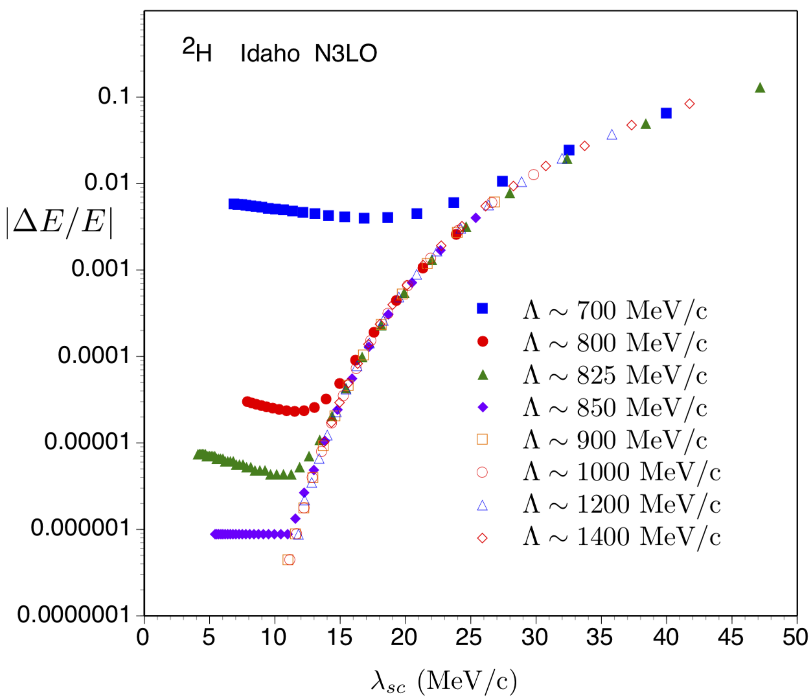


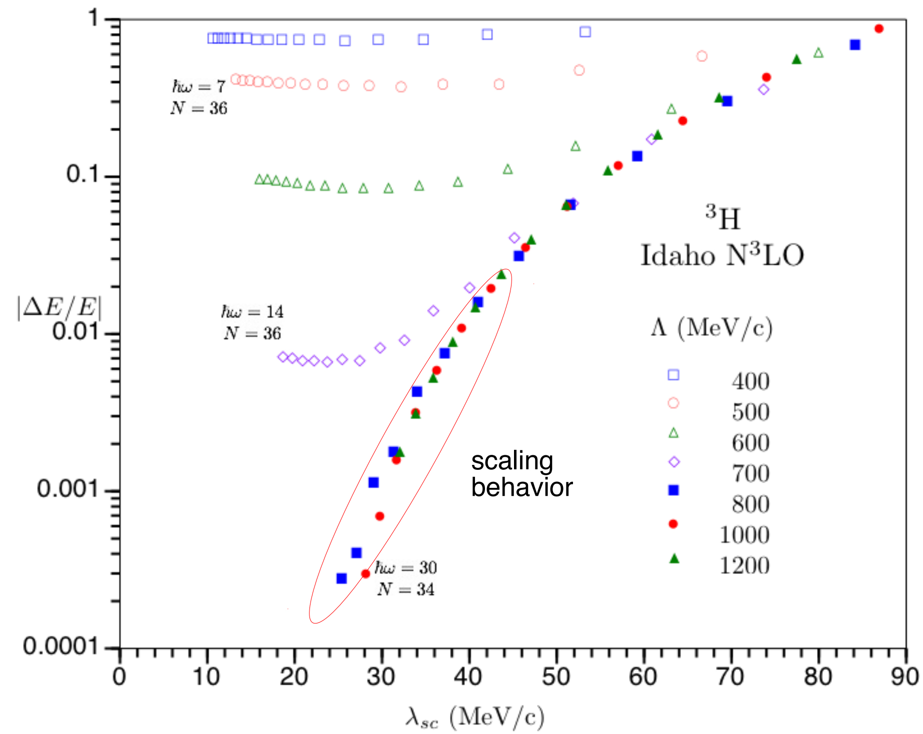


$\Lambda > 700$ MeV/c

$\Lambda < 700$ MeV/c

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



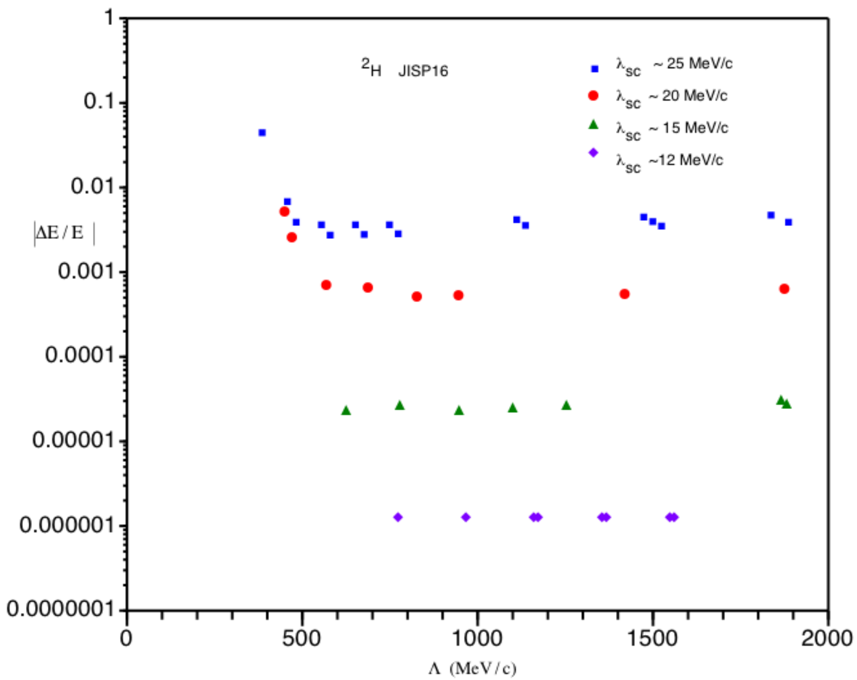


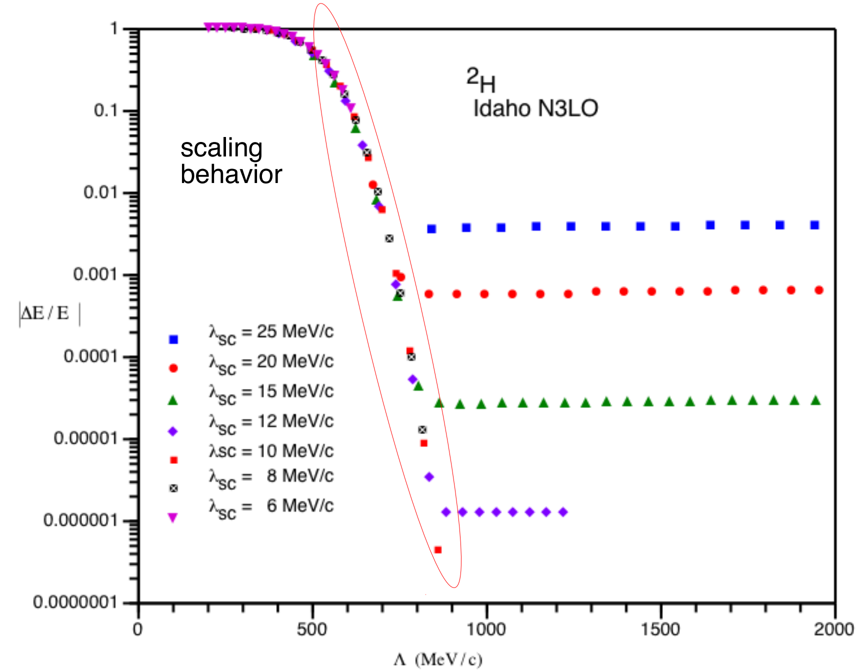
$|\Delta E/E|$ does not go to zero unless $\Lambda > \Lambda^{NN}$ where Λ^{NN} is some uv regulator scale of the NN interaction

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 Λ and λ, which are defined only to leading order in λ/Λ.

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

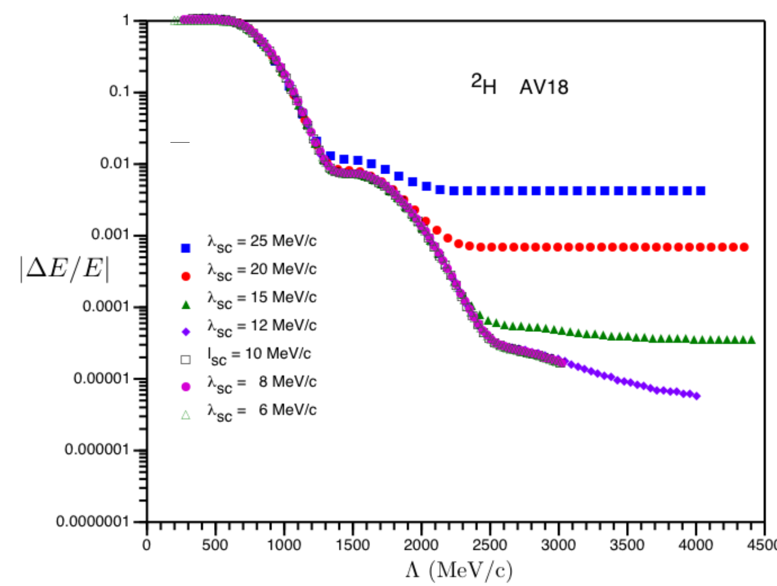


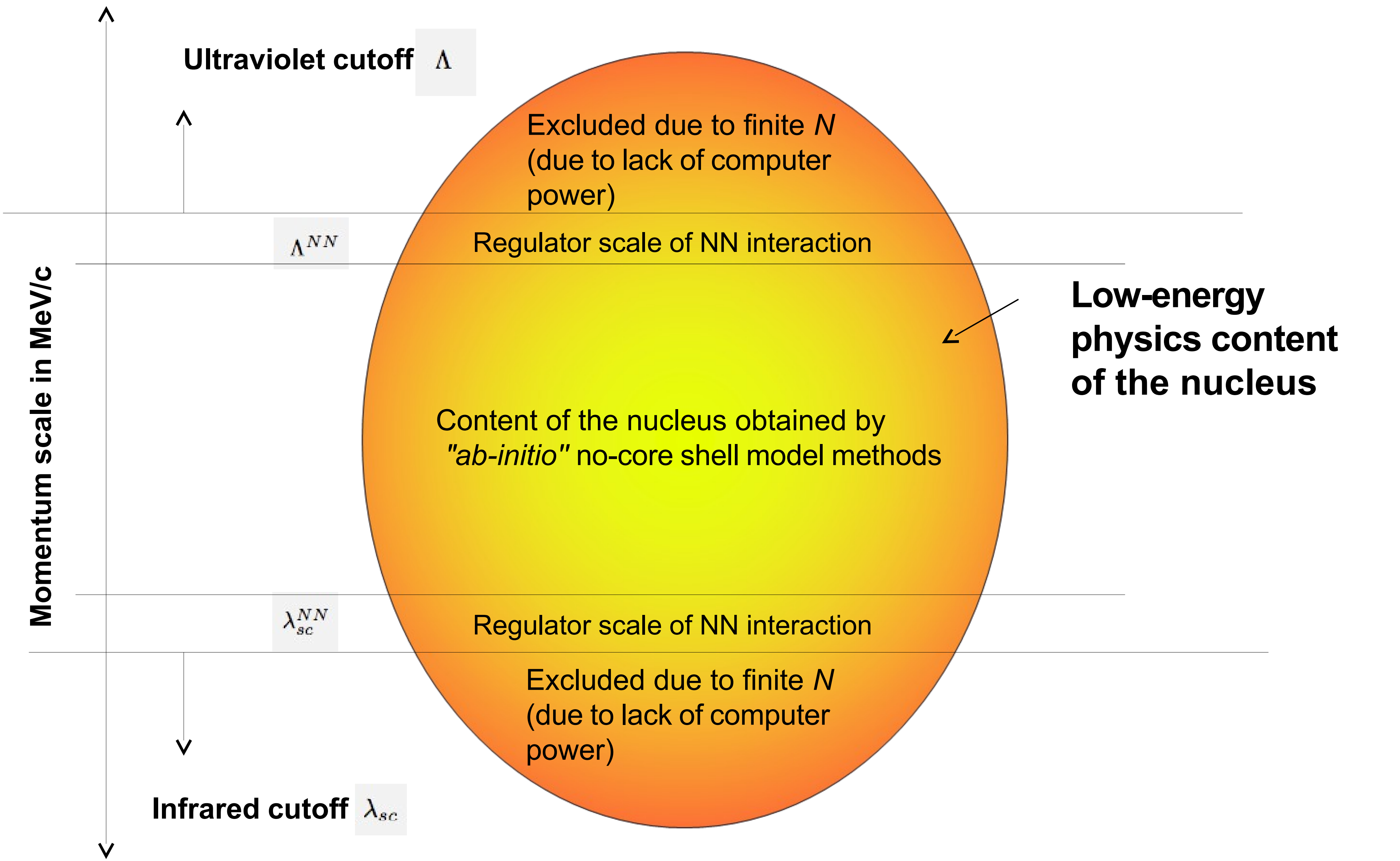


Plateau's ascribed to another “missing contributions” argument.

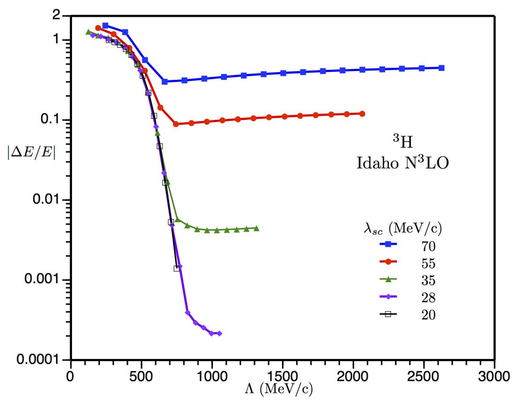
$|\Delta E/E|$ does not go to zero unless $\lambda_{sc} \leq \lambda_{sc}^{NN}$
where λ_{sc}^{NN} is some ir regulator scale of the NN interaction.

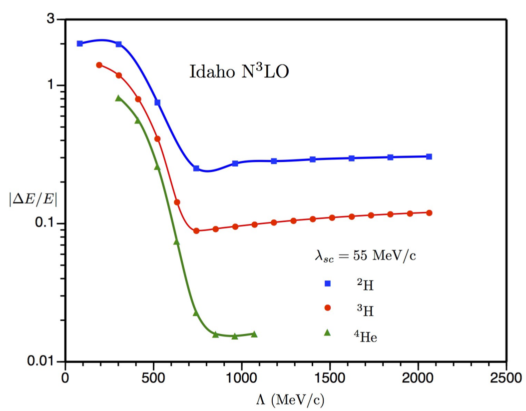
Value of λ_{sc}^{NN} is consistent with lowest energy configuration described by NN interaction;
e.g. deuteron binding momentum Q = 45 MeV/c,
or average of inverse scattering lengths ≈ 16 MeV/c

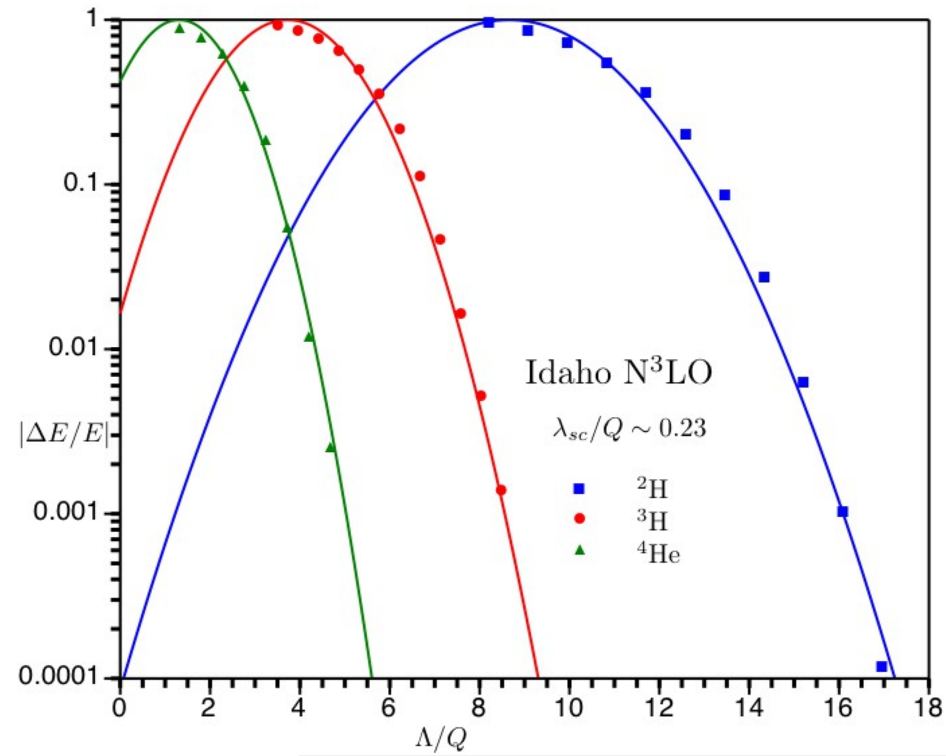



Ultraviolet cutoff Λ
Excluded due to finite *N* (due to lack of computer power)
Λ^{NN}
Regulator scale of NN interaction
Low-energy physics content of the nucleus
Momentum scale in MeV/c
Content of the nucleus obtained by *"ab-initio"* no-core shell model methods
λ_{sc}^{NN}
Regulator scale of NN interaction
Excluded due to finite *N* (due to lack of computer power)
Infrared cutoff λ_{sc}

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





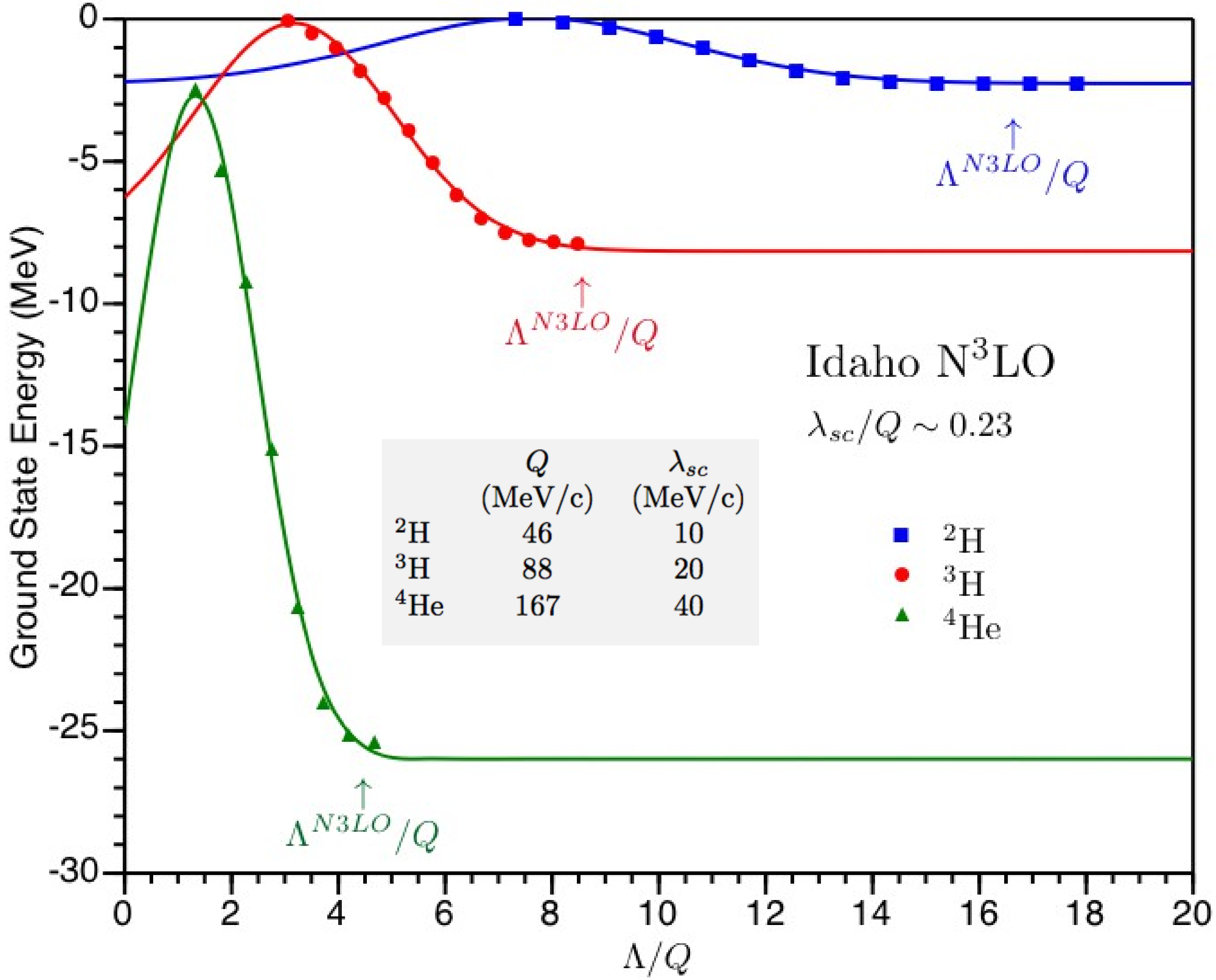


	Q (MeV/c)	λ_{sc} (MeV/c)
^{2}H	46	10
^{3}H	88	20
^{4}He	167	40

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 Λ

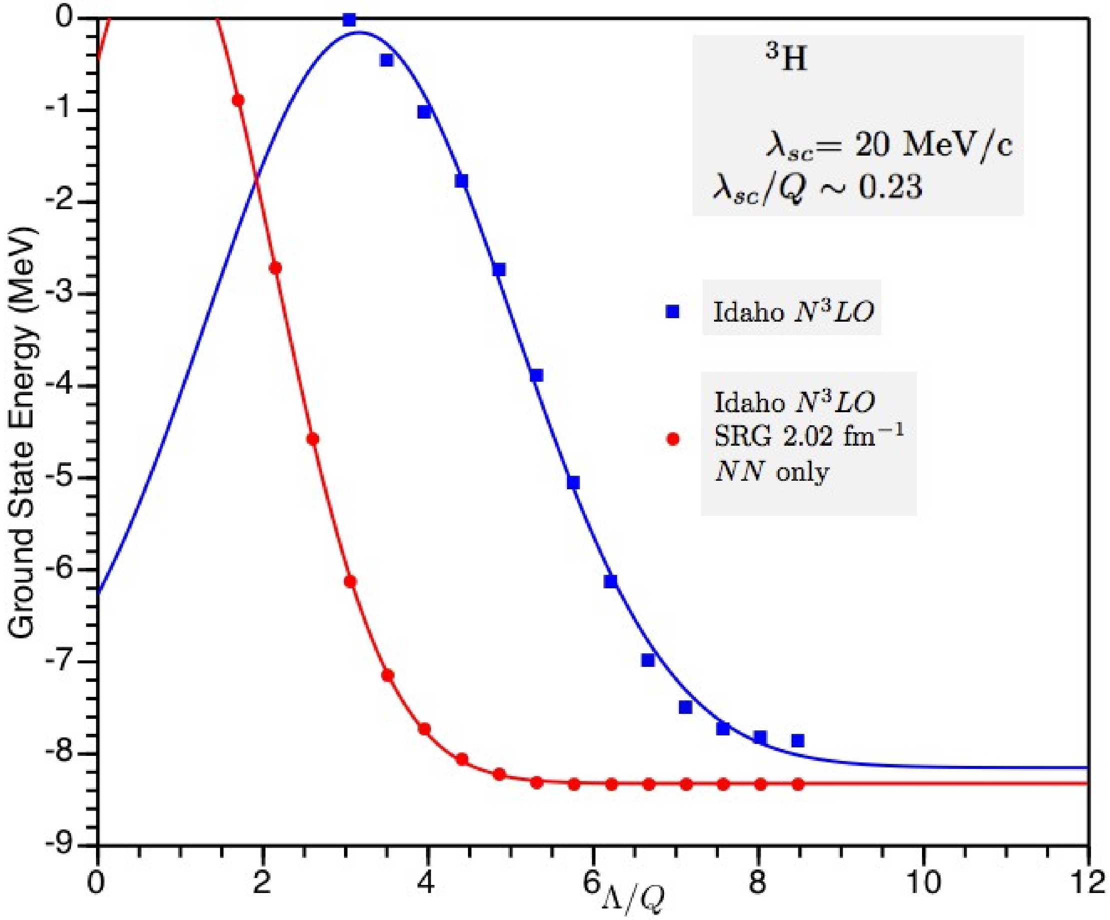
UV extrapolations with $\Lambda < \Lambda^{NN}$

$$E(\Lambda/Q) = a \exp\left(-(\Lambda/Q - b)^2/2c^2\right) + E(\Lambda/Q = \infty)$$



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 $\Lambda < \Lambda^{NN}$

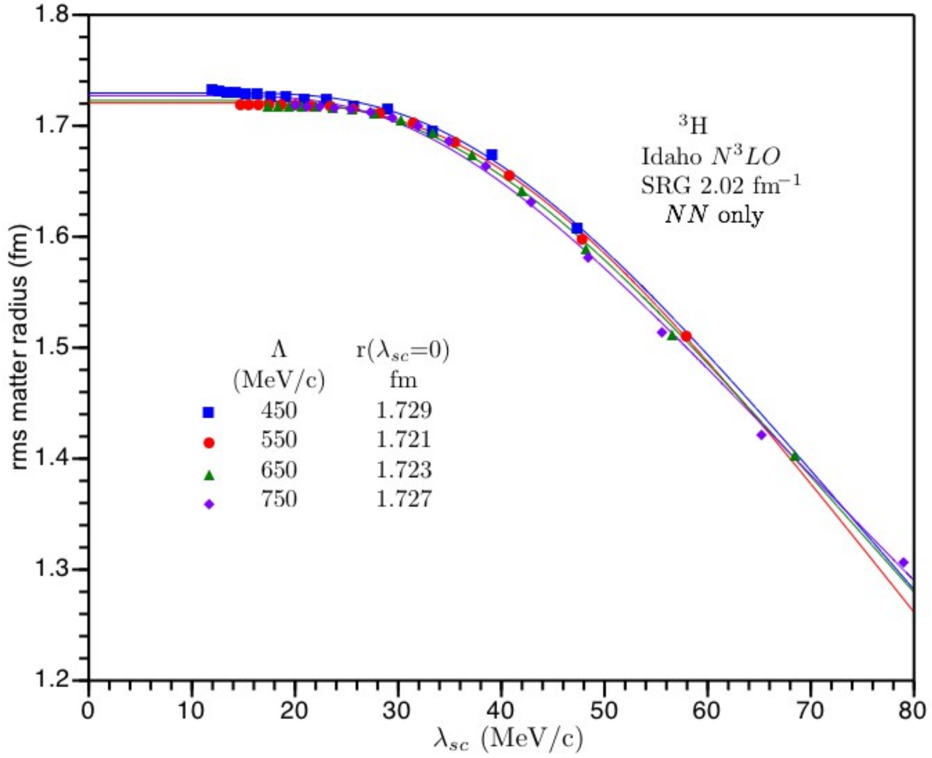


1) Extrapolation agrees with independent calculations only for SRG transformed potential.

2) Extrapolation with other values of fixed λ_{sc} is neither reliable nor robust.

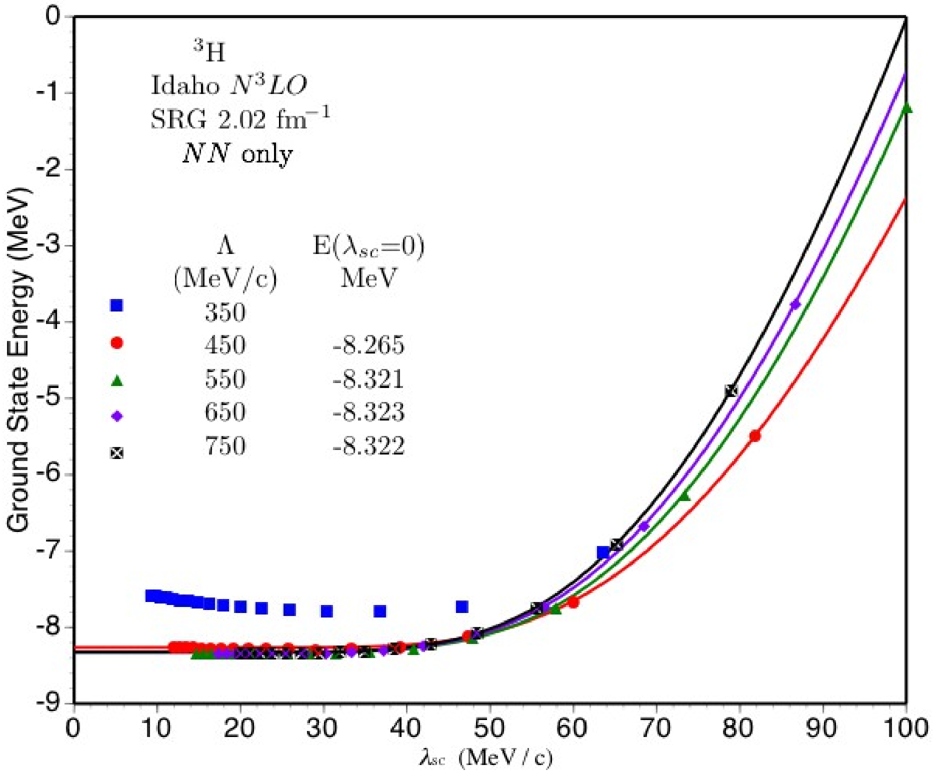
IR extrapolations with λ_{sc}

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



Radius extrapolation

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

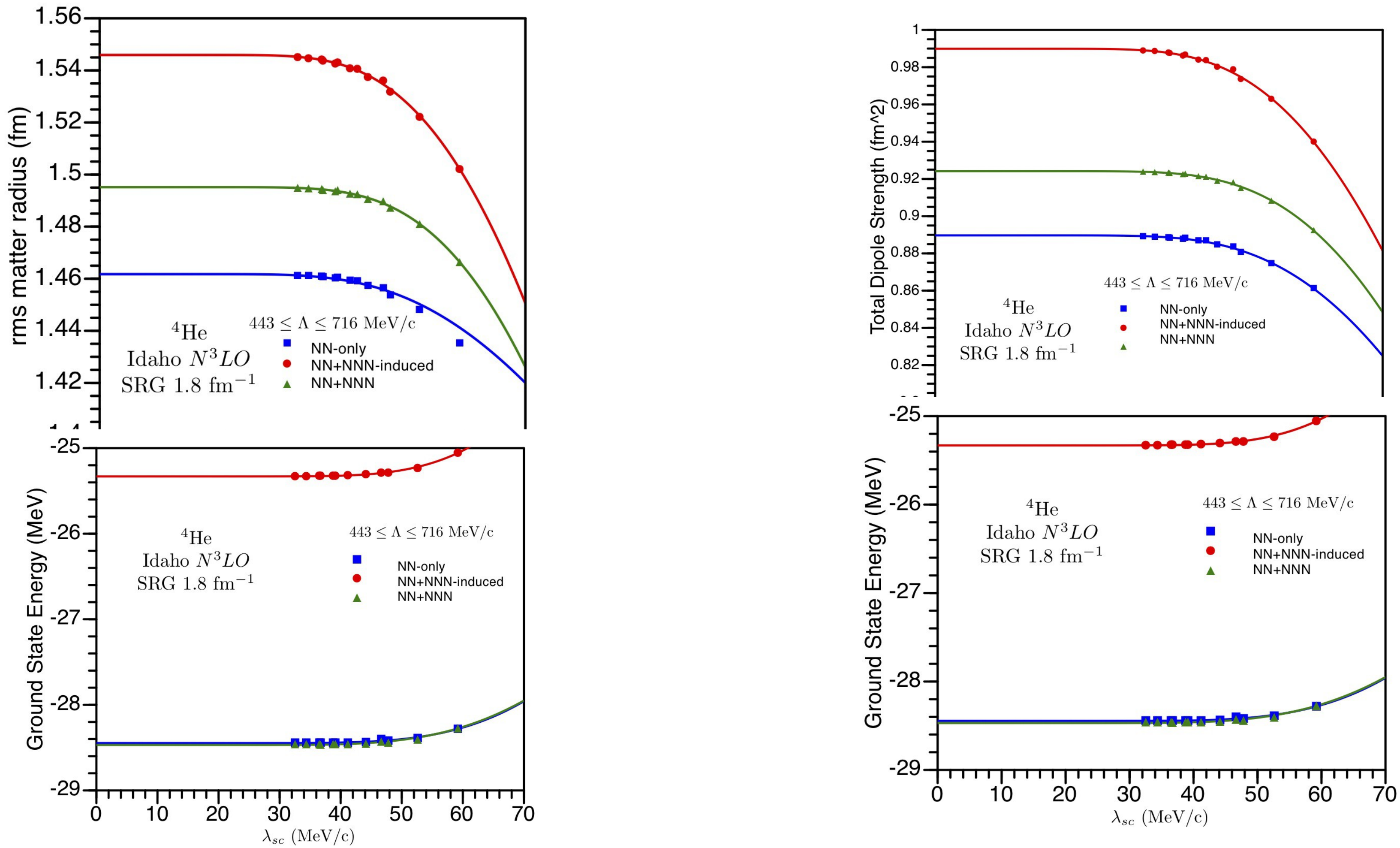


Energy extrapolation

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

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

Convergence of all three operators is the same with λ_{sc} extrapolation



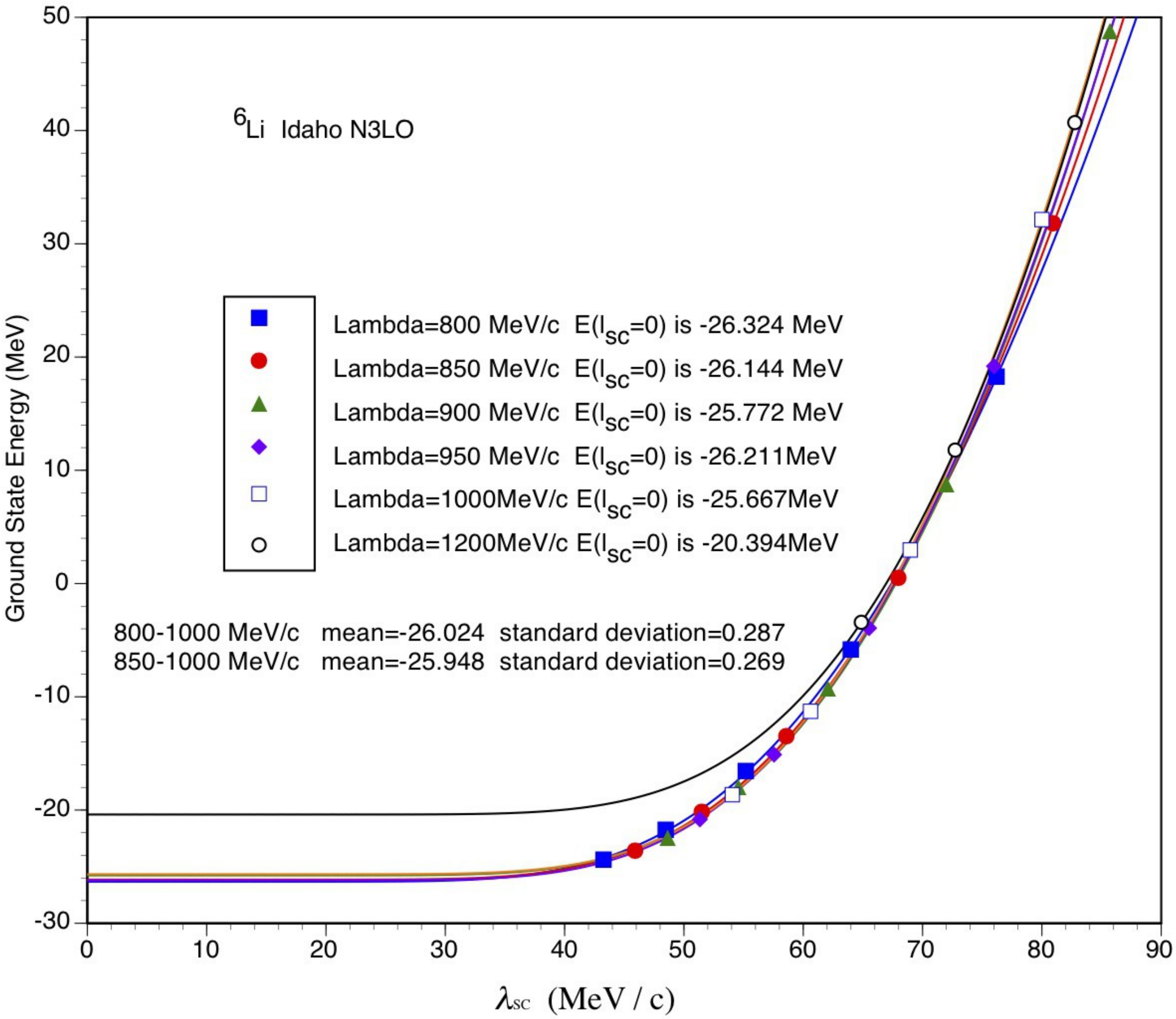
Plot all results at $\hbar\omega$ = 22 and 28 MeV and Nmax up to 18

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"

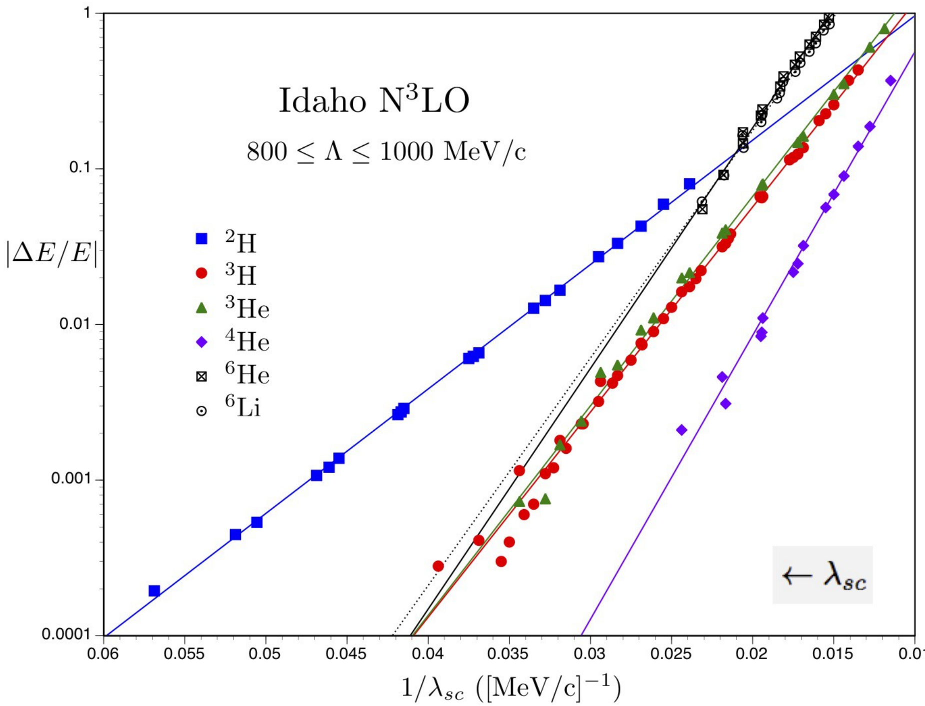
Basis: Nmax up through 16

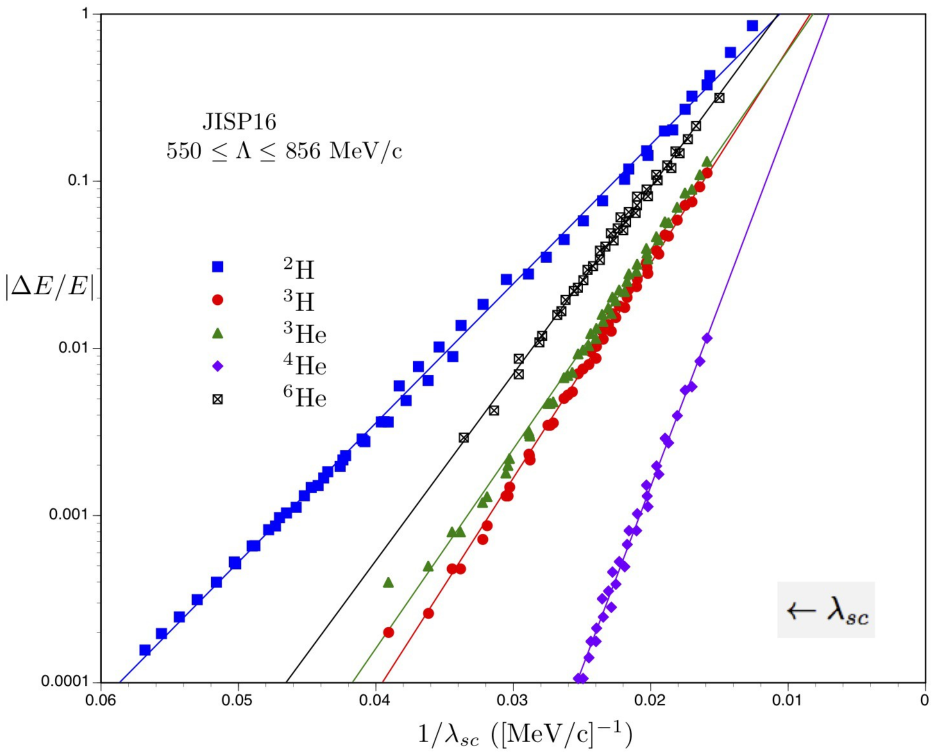
2004 fixed $\hbar\omega$ extrapolation yields E_{gs} = -28.2 MeV

We think IR extrapolation E_{gs} = -26.0 is correct



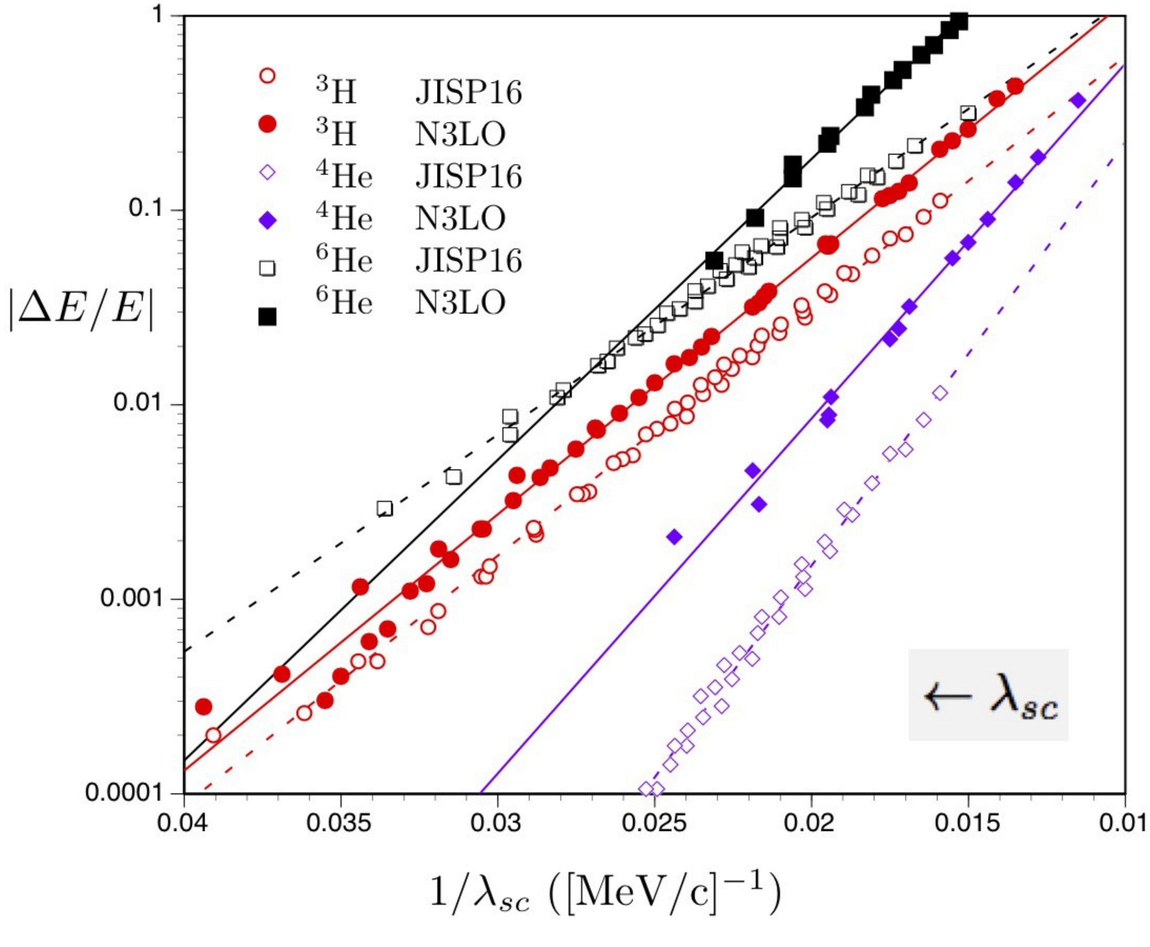
Universal property of IR extrapolation is nucleus dependent





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

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 (MeV)	$4\sqrt{m_N c^2 S}$ (MeV)	bc (MeV)	bc (MeV)
^2H	2.22457	183	192	184
^3H	6.25723	307	296	304
^3He	5.49348	287	275	310
^4He	20.2 (ave)	551	502	420
^6He			257	356
^6Li	5.0 (ave)	275		336

Alternate λ_{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.

Extra Slides

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

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

$$\Lambda \geq \Lambda^{NN} = 800$$

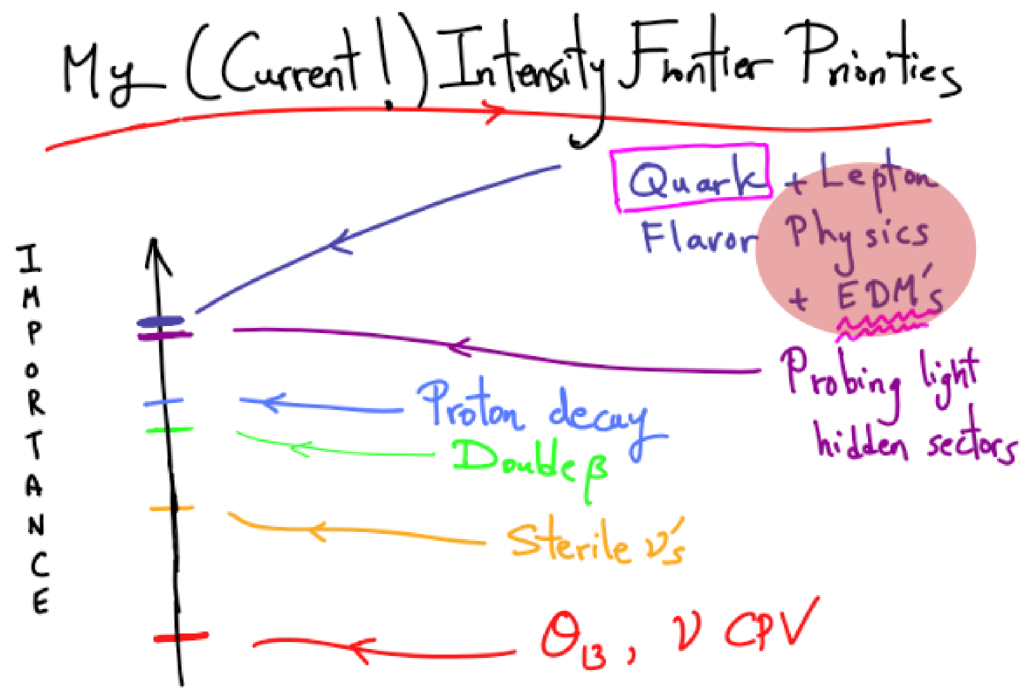
$\lambda_{sc} \approx 10$	$\lambda_{sc} \approx 20$	$\lambda_{sc} \approx 40$
$N \geq 80$	$N \geq 40$	$N \geq 20$
$\hbar\omega \succeq 8$	$\hbar\omega \succeq 16$	$\hbar\omega \succeq 32$

$$\Lambda \geq \Lambda^{NN} = 500$$

$\lambda_{sc} \approx 10$	$\lambda_{sc} \approx 20$	$\lambda_{sc} \approx 40$
$N \geq 50$	$N \geq 25$	$N \geq 12$
$\hbar\omega \succeq 5$	$\hbar\omega \succeq 10$	$\hbar\omega \succeq 20$

Conclusion: One must extrapolate for all but the lightest nuclei

Physics: Potential of EDMs



N. Arkani-Hamed (IAS, Princeton) at Intensity Frontier WS, USA (2011)

EDMs of d, ^{3}H, ^{3}He, ^{6}Li

The key role of LFV and EDMs

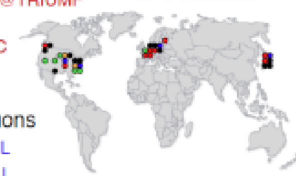
The search for Electric Dipole Moments of fundamental particles (n, e, μ, … *and, more generally, atoms or heavy nuclei*), share the three main virtues of LFV searches:

- We know CP is not an exact symmetry of nature => non-vanishing EDMs
- Virtually no problems of SM backgrounds
- EDMs close to the present bounds in several realistic models

Observable	Exp. Current
$\vert d_{Tl}\vert$ [e cm]	$< 9.0 \times 10^{-25}$
$\vert d_{Hg}\vert$ [e cm]	$< 3.1 \times 10^{-29}$
$\vert d_n\vert$ [e cm]	$< 2.9 \times 10^{-26}$

Rough estimate of numbers of researchers, in total ~500 (with some overlap)

- Neutrons (~200)
  - @ILL
  - @ILL,@PNPI
  - @PSI
  - @FRM-2
  - @RCNP,@TRIUMF
  - @SNS
  - @J-PARC
- Molecules (~50)
  - YbF@Imperial
  - PbO@Yale
  - ThO@Harvard
  - HfF+@JILA
  - WC@UMich
  - PbF@Oklahoma
- Atoms (~100)
  - Hg@UWash
  - Xe@Princeton
  - Xe@TokyoTech
  - Xe@TUM
  - Xe@Mainz
  - Cs@Penn
  - Cs@Texas
  - Fr@RCNP/CYRIC
  - Rn@TRIUMF
  - Ra@ANL
  - Ra@KVI
  - Yb@Kyoto
- Ions-Muons (~200)
  - @BNL
  - @FZJ
  - @FNAL
  - @JPARC
- Solids (~10)
  - GGG@Indiana
  - ferroelectrics@Yale



world-wide effort in trying to improve the limits by ~ 1 order of magnitude

G. Isidori at ESPP Open Symposium, Cracow (Sept. 2012)

EDM of charged particles: use of storage rings

PROCEDURE

- Place particles in a storage ring
- Align spin along momentum (→freeze horizontal spin precession)
- Search for time development of vertical polarization