Corrections to nuclear energies and radii in finite oscillator spaces

Thomas Papenbrock

and

OAK RIDGE NATIONAL LABORATORY

R. J. Furnstahl, G. Hagen, TP, Phys. Rev. C 86, 031301(R) (2012)

Sushant N. More, A. Ekström, R. J. Furnstahl, G. Hagen, TP, Phys. Rev. C 87, 044326 (2013)

SciDAC
Scientific Discovery through Advanced Computing

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Lüscher's formula

[Comm. Math. Phys. 104, 177 (1986)]

Two-particle bound state on a lattice of size L with periodic boundary conditions [Beane, Bedaque, Parreno, Savage, Phys. Lett. B 585, 106 (2004)]:

• computed energy is too low (because of tunneling between boxes)

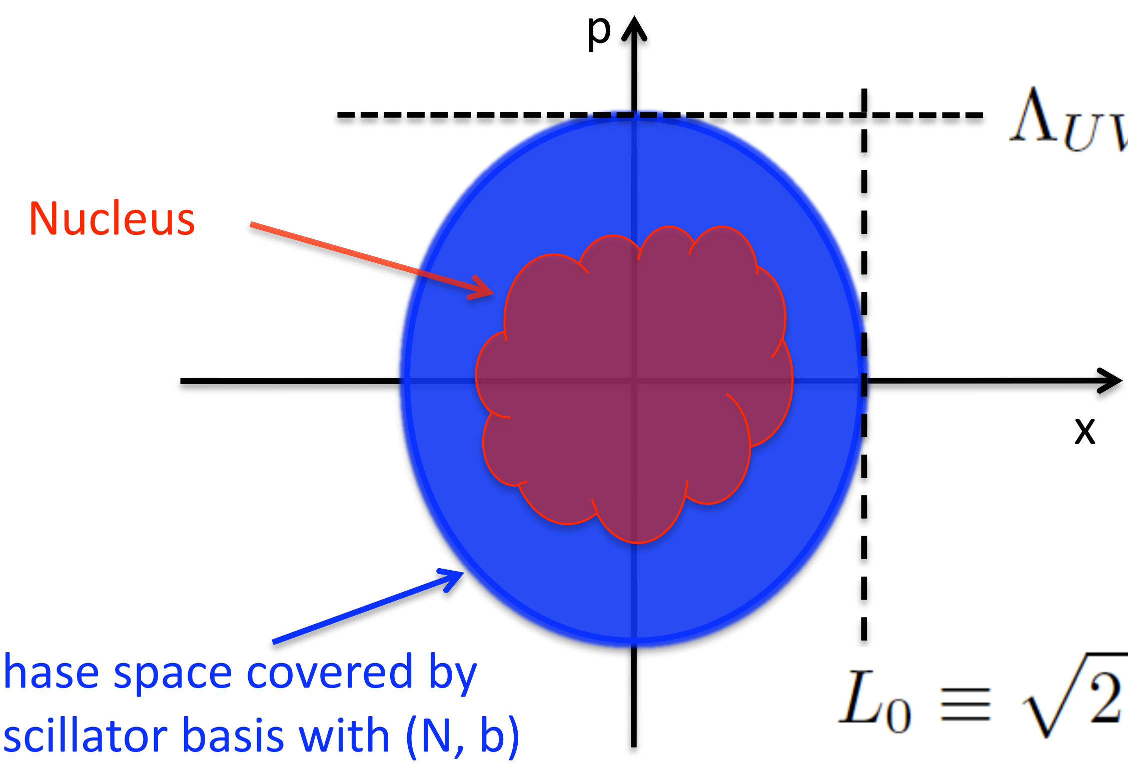
$$E_{-1} = -\frac{\gamma^2}{M}\left[1 + \frac{12}{\gamma L}\,\frac{1}{1-2\gamma(p\cot\delta)'}\,e^{-\gamma L} + \ldots\right]$$

What is the equivalent of Lüscher's formula for the harmonic oscillator basis?

Convergence in finite oscillator spaces

Calculations are performed in finite oscillator spaces. How can one reliably extrapolate to infinity?

Convergence in momentum space (UV) and in position space (IR) needed
[Hagen *et al*., PRC 82, 034330 (2010); Jurgenson *et al*., PRC 83, 034301 (2011)]



$$\Lambda_{UV} \equiv \sqrt{2(N+3/2)}\hbar/b$$

$$L_0 \equiv \sqrt{2(N+3/2)}b$$

Nucleus needs to "fit" into basis:

- Nuclear radius R < L
- cutoff of interaction $\Lambda < \Lambda_{UV}$

Infrared cutoff in the HO basis

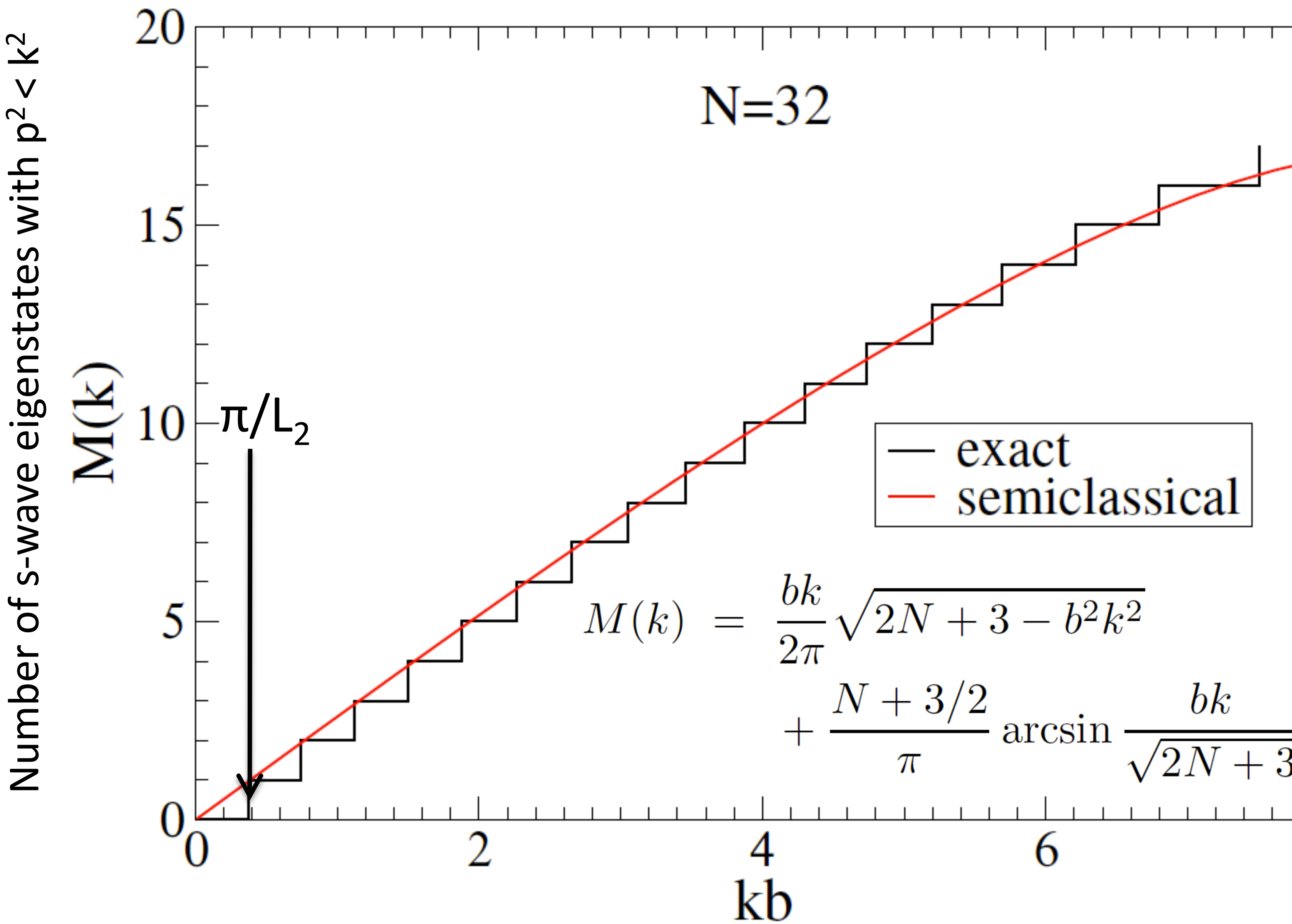
Very precise answer [More, Ekström, Furnstahl, Hagen, TP (2013)] based on length scale

$$L_2 = \sqrt{2(N+3/2+2)}b$$

1. At low energies, the HO basis looks like a "box" of radius L_2.
2. π/L_2 is the infrared cutoff.
3. Knowledge can be used for theoretically founded extrapolations in HO basis, computations of phase shifts in HO basis …

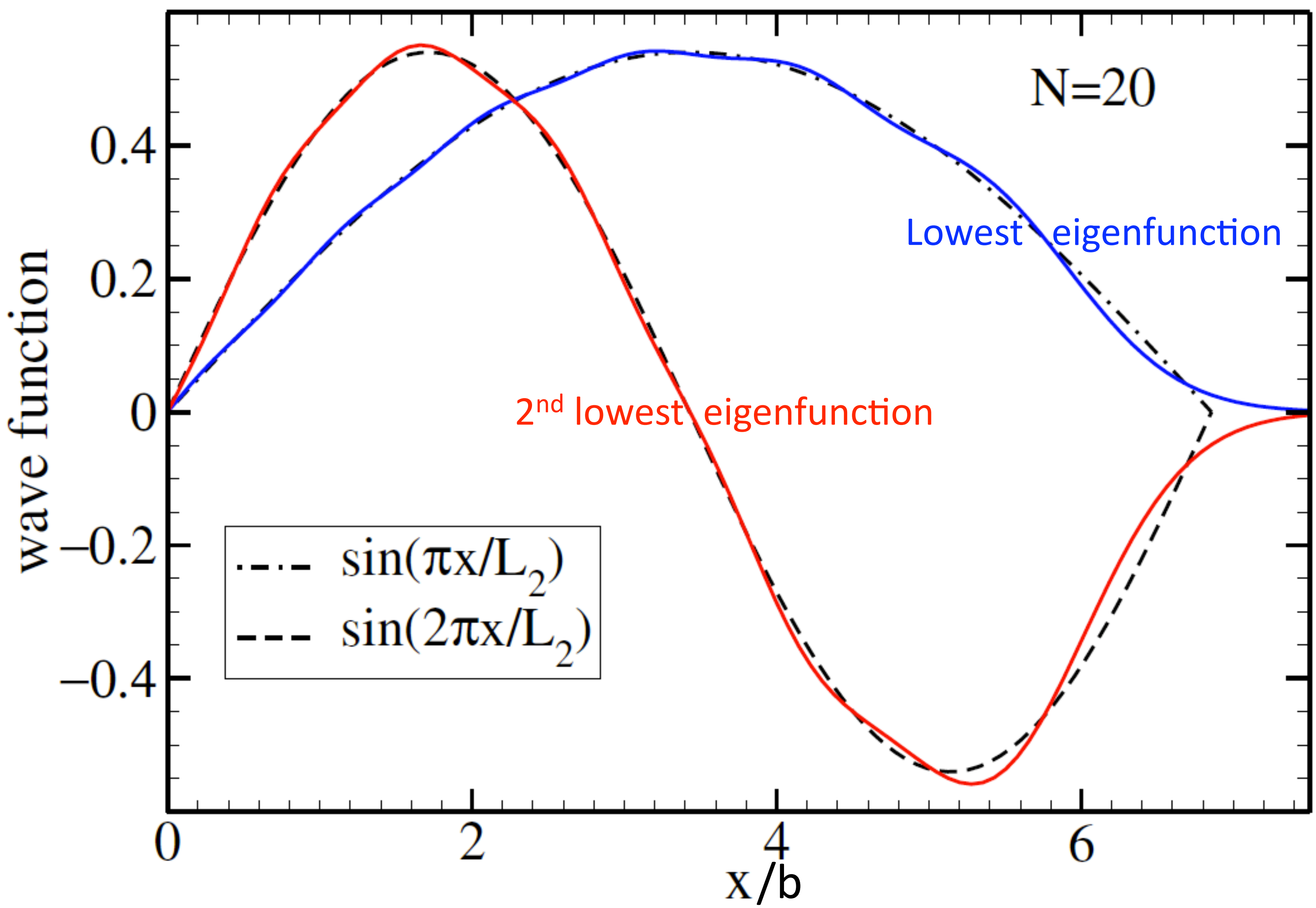
1/b can serve as an IR regulator [Stetcu, Barrett, van Kolck, Phys. Lett. B 653, 358 (2007); Stetcu, Rotureau, Barrett, van Kolck, J. of Phys. G 37, 064033 (2010); Coon, Avetian, Kruse, Kolck, Maris, Vary, Phys. Rev. C 86, 054002 (2012)]

Spectrum of the operator p^2 in the HO basis



- At low momentum, number of states increases linearly with increasing momentum
- Spectrum looks like that of the momentum operator in a box

Eigenfunctions of p^2 with lowest eigenvalues in oscillator basis



Eigenfunctions look like those from a box of size L_2.

Squared infrared cutoff is the lowest eigenvalue of p^2

The lowest eigenvalue κ_{min} can be computed analytically for N>>1. **Result: π/L_2**

Note: N>>1 does not imply impractically large model spaces

N	$\kappa_{\rm min}$	π/L_2	π/L_0
0	1.2247	1.1874	1.8138
2	0.9586	0.9472	1.1874
4	0.8163	0.8112	0.9472
6	0.7236	0.7207	0.8112
8	0.6568	0.6551	0.7207
10	0.6058	0.6046	0.6551
12	0.5651	0.5642	0.6046
14	0.5316	0.5310	0.5642
16	0.5035	0.5031	0.5310
18	0.4795	0.4791	0.5031
20	0.4585	0.4582	0.4791

$$L_i \equiv \sqrt{2(N+3/2+i)}b$$

1% deviation at N>2

0.1% deviation at N>14

π/L_2 is very precise value of the IR cutoff

IR corrections to bound-state energies

Simple view: A node in the wave function

$$u_E(r) \xrightarrow{r \gg R} A_E(e^{-k_E r} + \alpha_E e^{+k_E r})$$

at $r=L_2$ requires $\alpha_E = -\exp(-2k_E L_2)$. This yields a (kinetic) energy correction

$$E_L = E_\infty + a_0 e^{-2k_\infty L}$$

Model-independent approach based on linear energy method [D. Djajaputra & B. R. Cooper, Eur. J. Phys. 21, 261 (2000)] yields energy correction

$$\Delta E_L \approx -u_\infty(L) \left(\left. \frac{du_E(L)}{dE} \right|_{E_\infty} \right)^{-1}$$

Final results [Furnstahl, Hagen, TP, Phys. Rev. C 86, 031301 (2012); More, Ekström, Furnstahl, Hagen, TP, Phys. Rev. C 87, 044326 (2013)]

ANC^2 Binding momentum

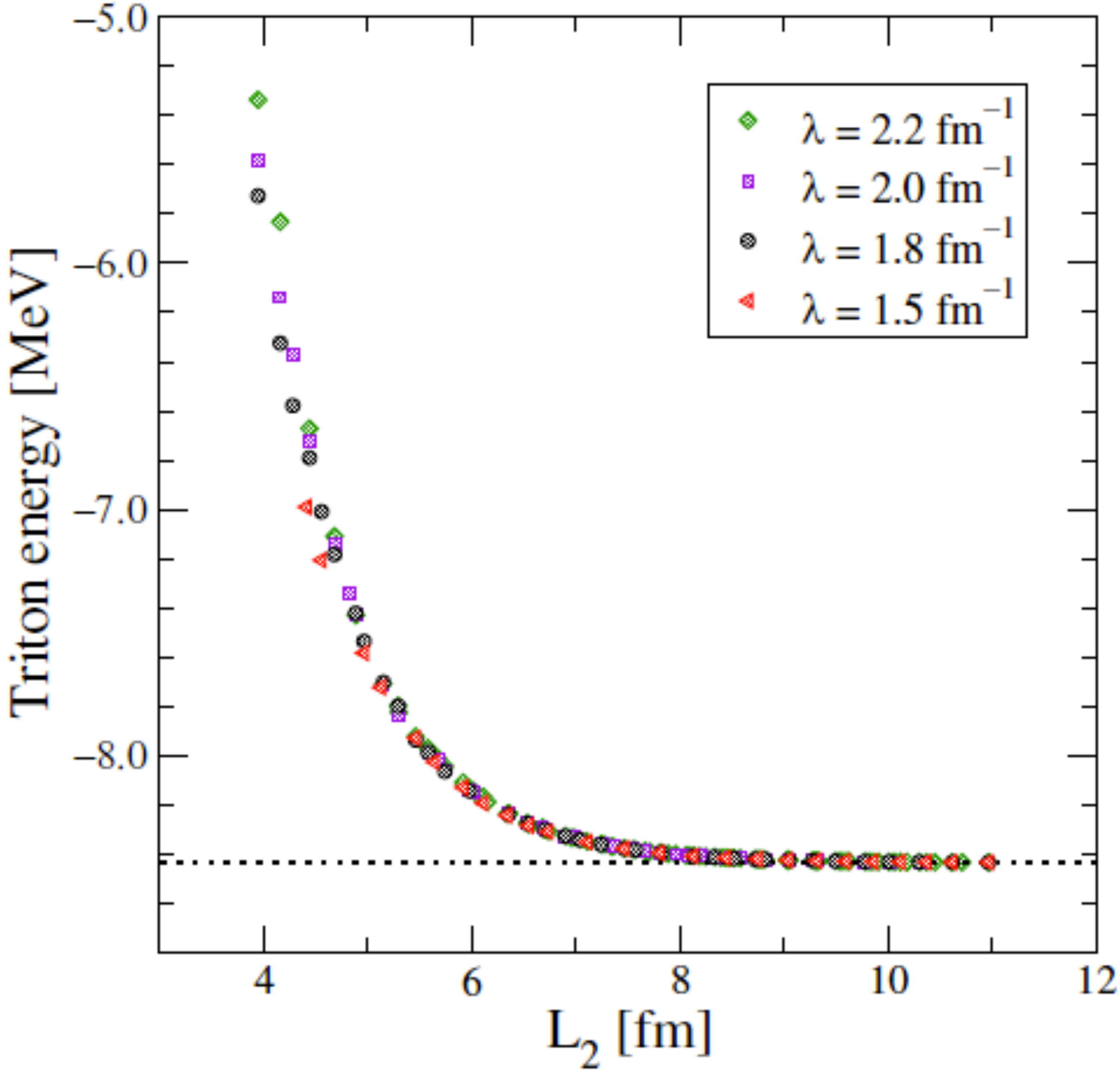
$$\Delta E_L = \frac{\hbar^2 k_\infty \gamma_\infty^2}{\mu} e^{-2k_\infty L} + \mathcal{O}(e^{-4k_\infty L})$$

only observables enter

$$\langle r^2 \rangle_L \approx \langle r^2 \rangle_\infty [1 - (c_0 \beta^3 + c_1 \beta) e^{-\beta}] \qquad (\text{with } \beta \equiv 2k_\infty L)$$

Energy extrapolation explains findings by Coon et al, Phys. Rev. C 86, 054002 (2012)

Triton binding energy from SRG interactions: only observables enter into the IR extrapolation



Phase shifts computed directly in the HO basis

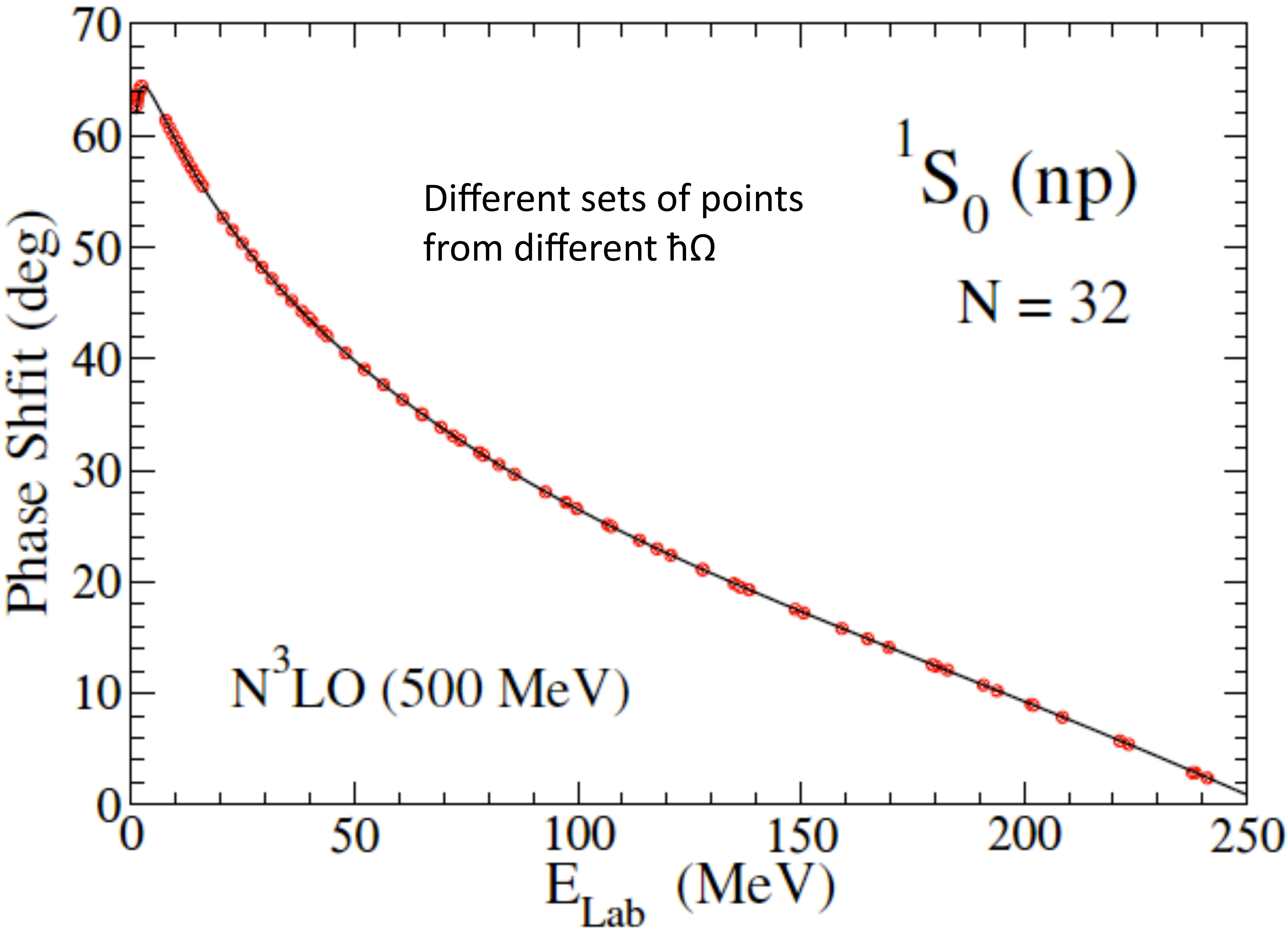
1. Compute states with positive energies E_i and momentum p_i in HO basis at fixed N
2. The i^{th} state determines the box size $L_i = L(p_i)$ at that energy via $j_l(p_i L_i/\hbar) = 0$
3. Compute phase shift from usual formula: $\tan\delta_l(k_i) = \frac{j_l(k_i L(\hbar k_i))}{\eta_l(k_i L(\hbar k_i))}$
4. Repeat for several ħΩ

Harmonic oscillator representation of scattering equations: Bang, Mazur, Shirokov, Smirnov, Zaytsev, Ann. Phys. (NY) 280, 299 (2000).

Alternative approaches based on [Busch *et al* 1998] employ a harmonic potential and use ħΩ→0 for finite-range interactions.

Luu, Savage, Schwenk, Vary, Phys. Rev. C 82, 034003 (2010).
Stetcu, Rotureau, Barrett, van Kolck, J. Phys. G 37, 064033 (2010).

Phase shifts



How well can one distinguish L_2 in practice?

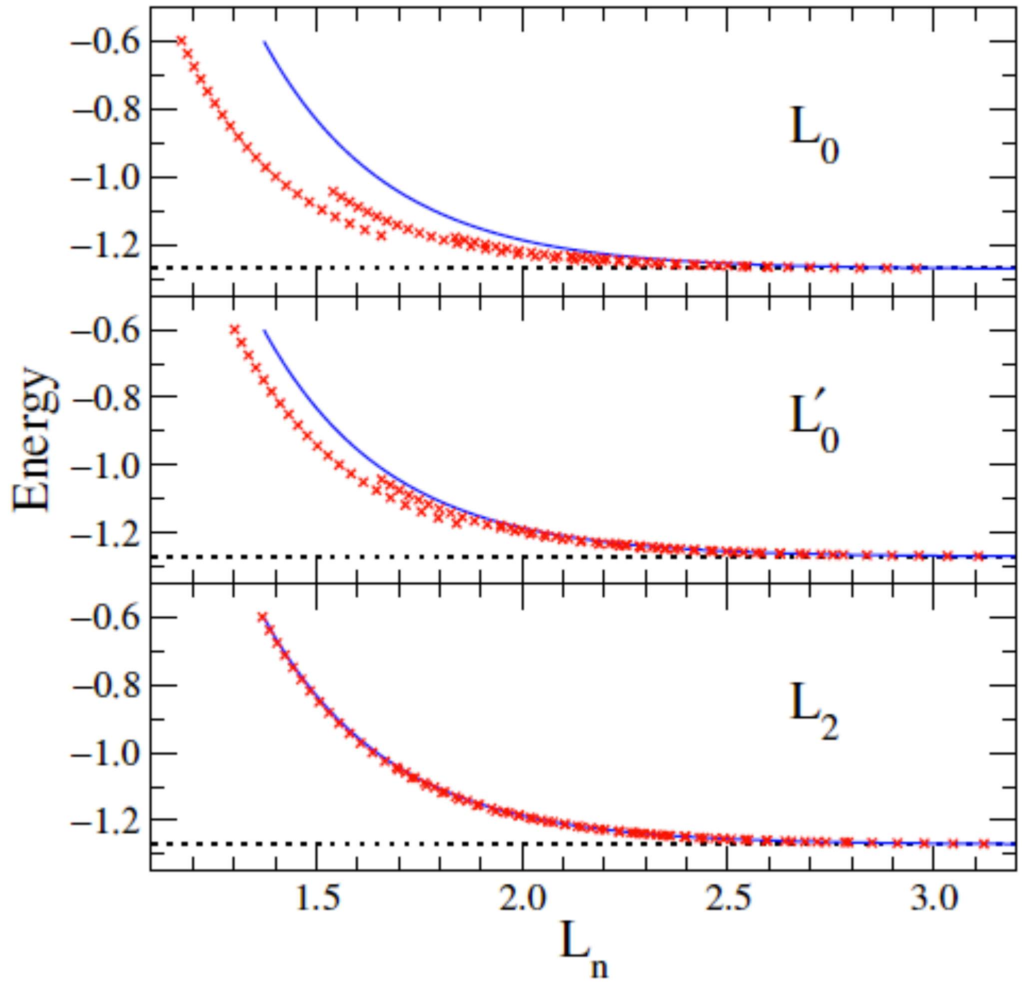
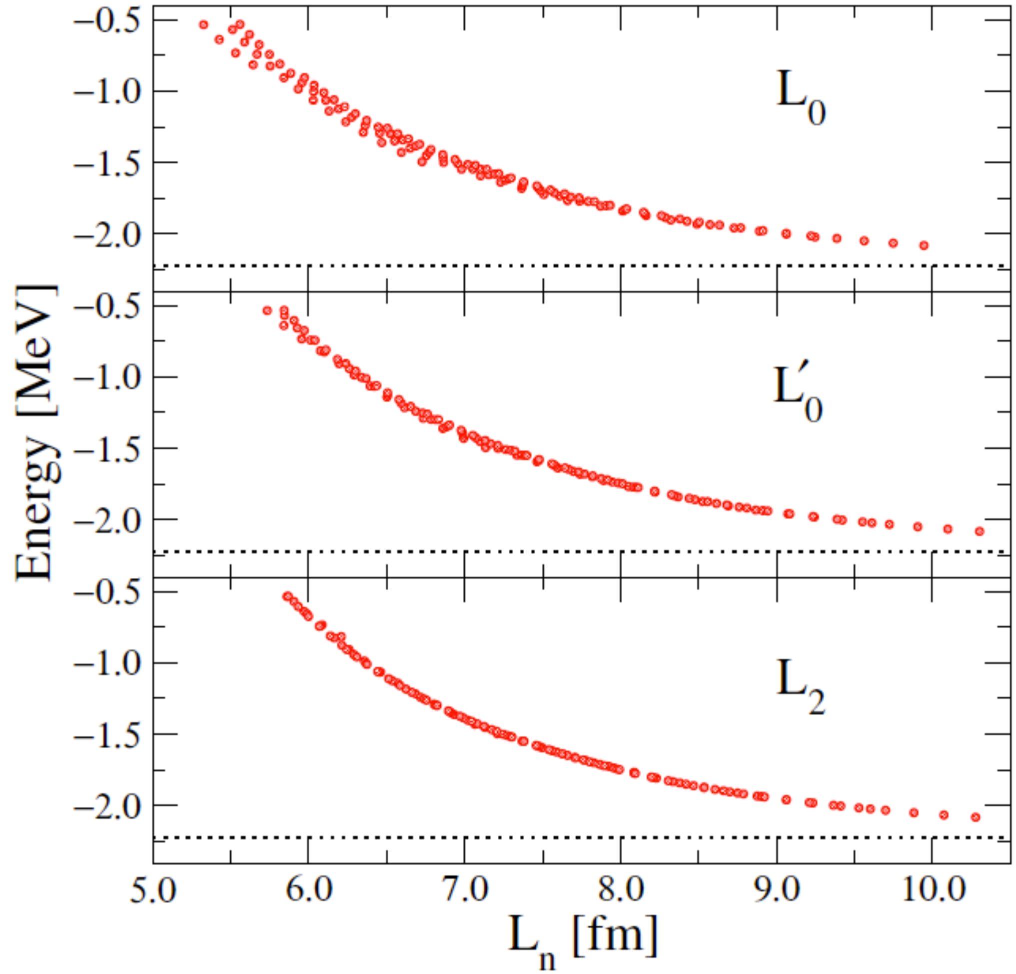
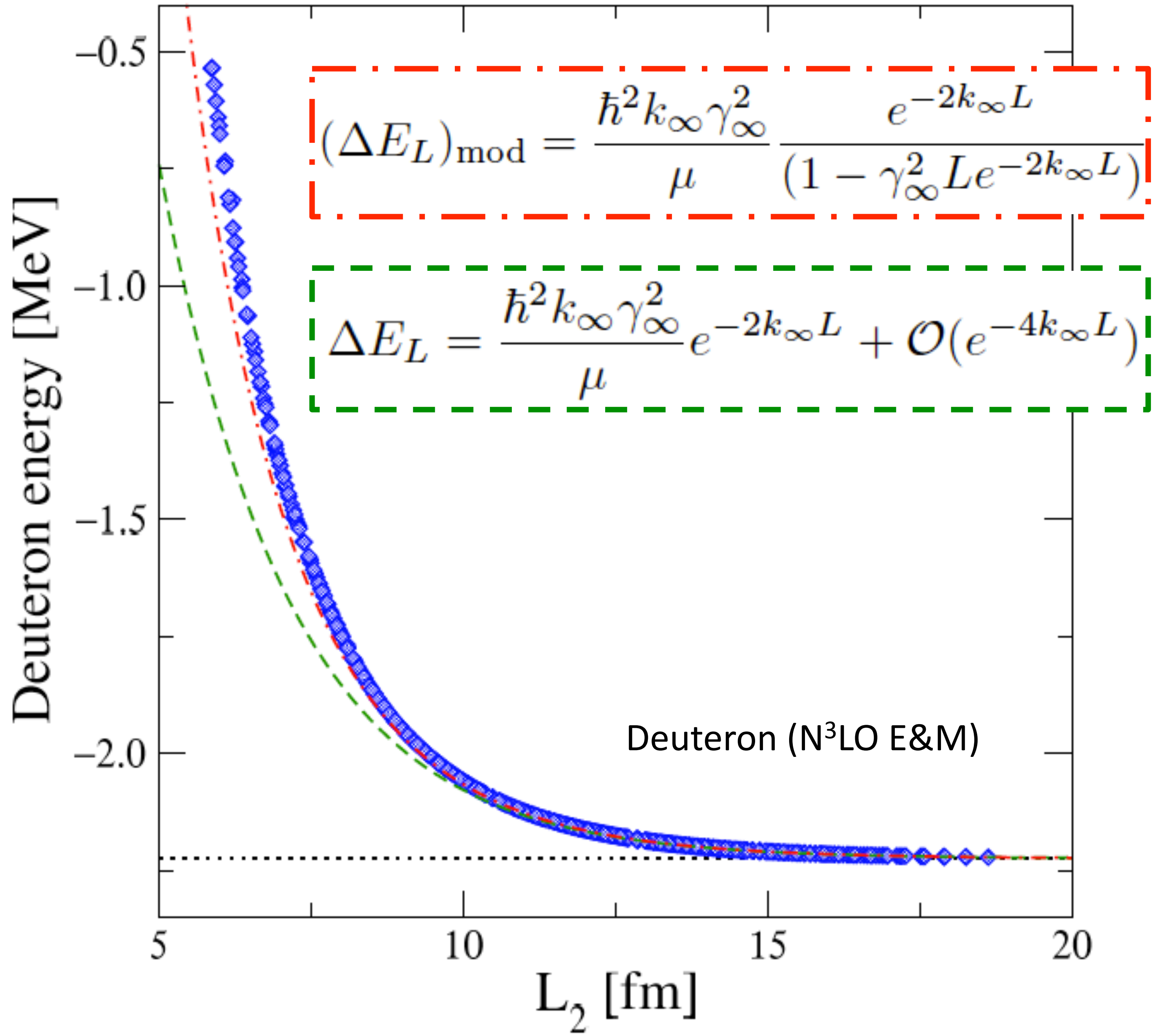


FIG. 2: (color online) Ground-state energies versus L_0 (top), L_0' (middle), and L_2 (bottom) for a Gaussian potential well Eq. (5) with $V_0 = 5$ and $R = 1$. The crosses are the energies from HO basis truncation. The energies obtained by numerically solving the Schrödinger equation with a Dirichlet boundary condition at L lie on the solid line. The horizontal dotted lines mark the exact energy $E_\infty = -1.27$.



Deuteron (N^3LO E&M)

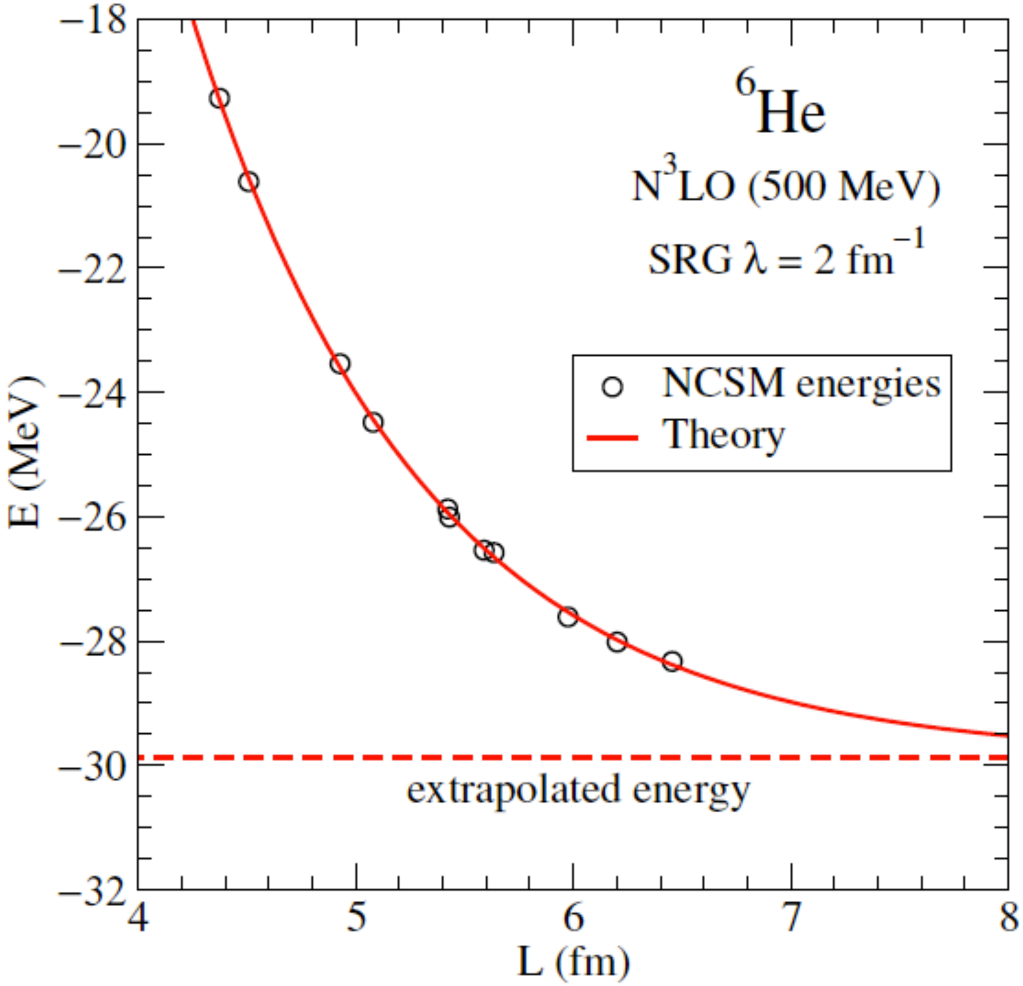
Corrections for shallow bound states



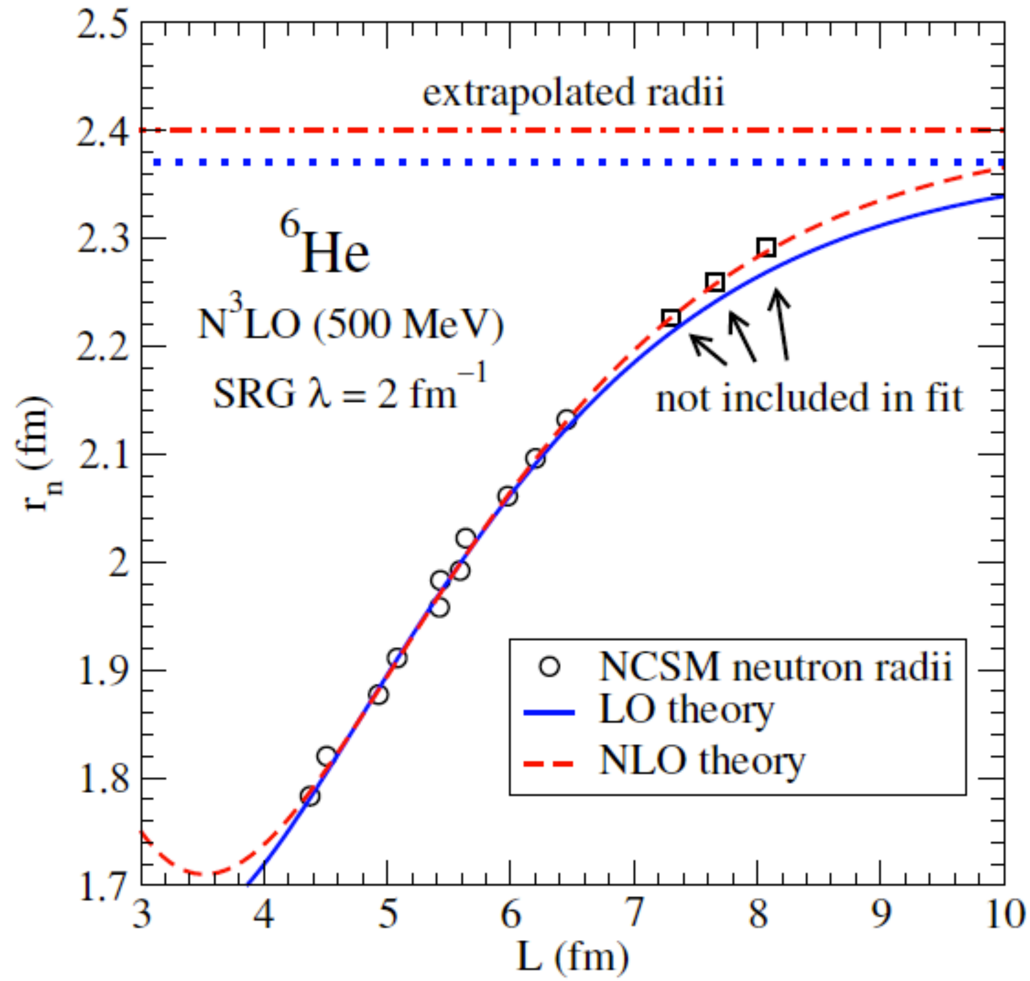
Corrections due to finite Hilbert spaces

- UV practically converged (because $\lambda < \Lambda_{UV}$)
- IR convergence is slower due to exponential decay of wave function
- Dirichlet boundary condition at x=L in position space, k_∞ from energy fit

$$E_L = E_\infty + a_0 e^{-2k_\infty L}$$



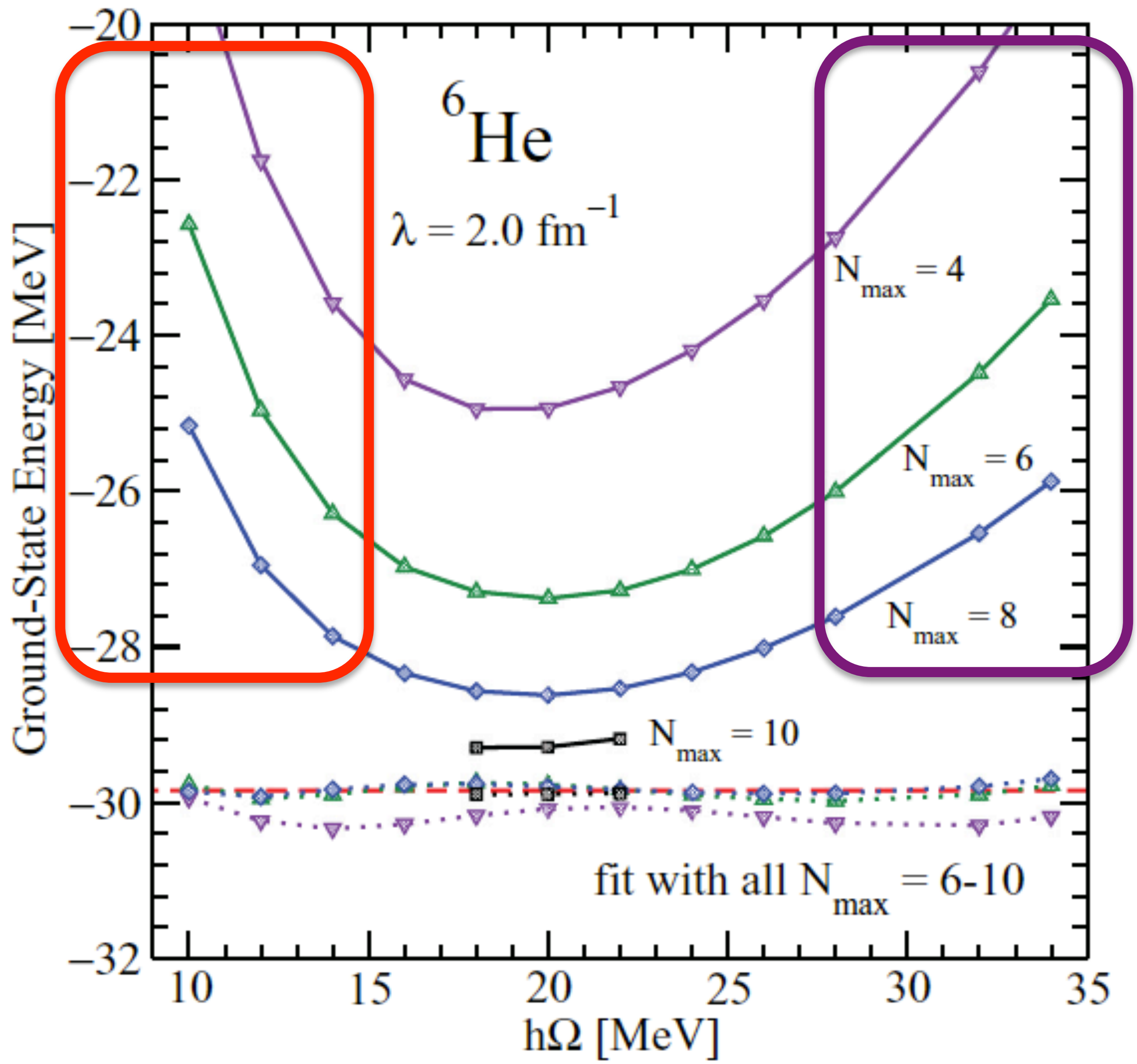
$$\langle r^2 \rangle_L \approx \langle r^2 \rangle_\infty [1 - (c_0\beta^3 + c_1\beta)e^{-\beta}]$$
$$\beta \equiv 2k_\infty L$$



Empirical approach: combined UV and IR fits for SRG interactions

$$E(\Lambda_{\rm UV}, L) \approx E_\infty + A_0 e^{-2\Lambda_{\rm UV}^2/A_1^2} + A_2 e^{-2k_\infty L}$$

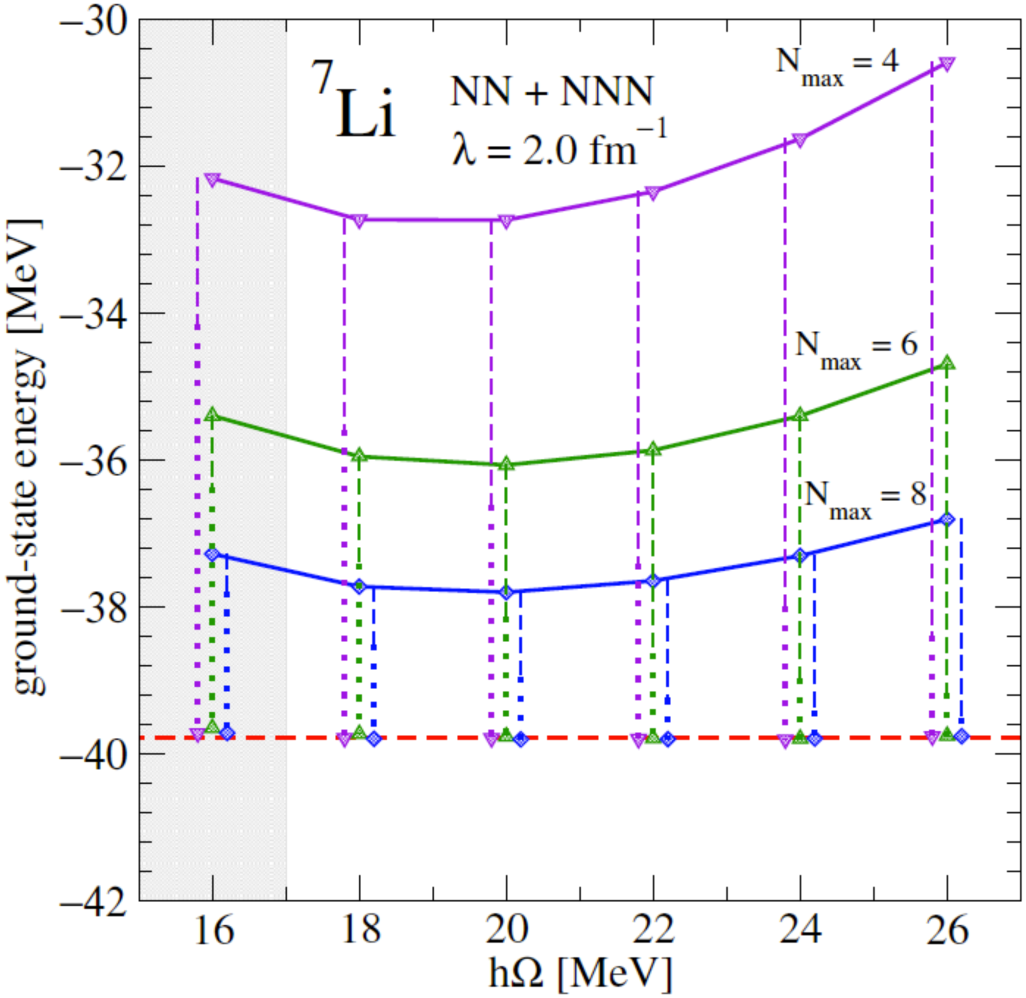
At lower ħΩ:
- IR converged
- extrapolate UV

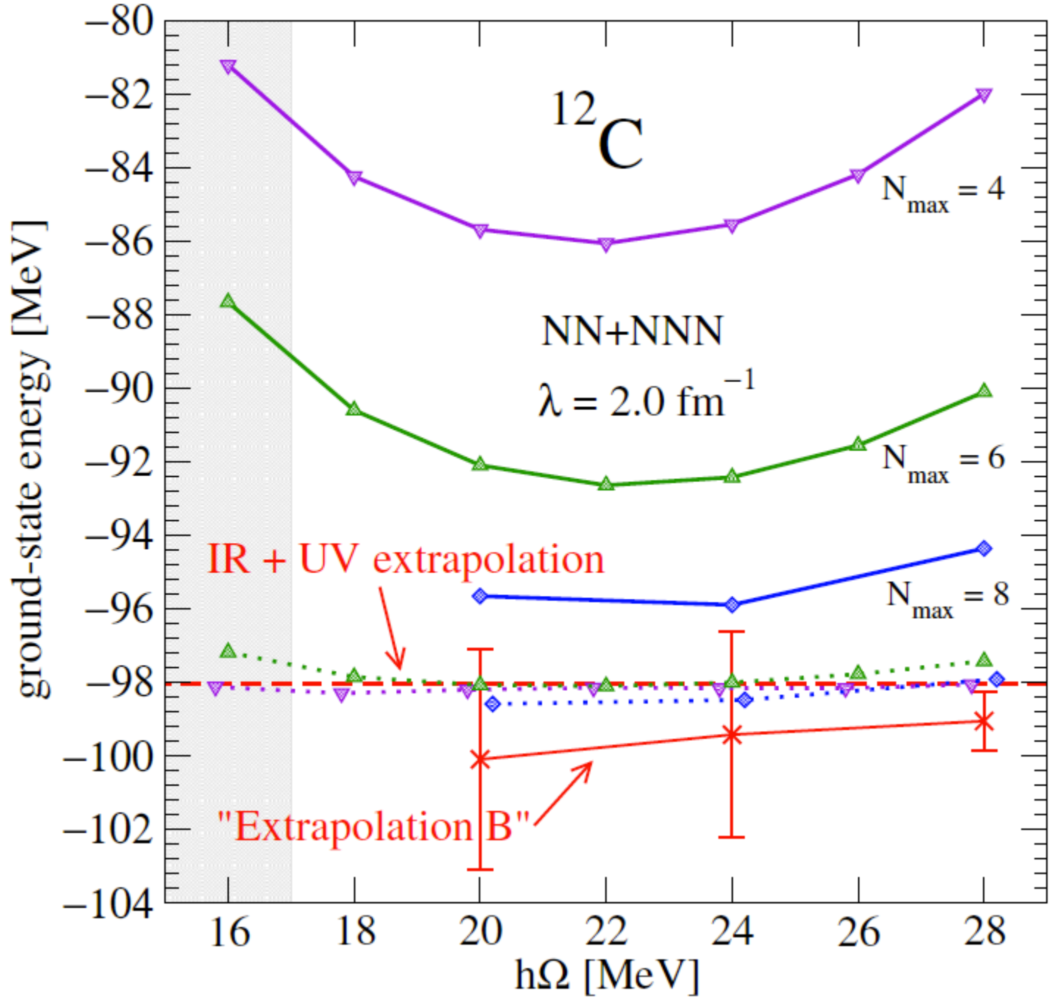


At higher ħΩ:
- UV converged
- extrapolate IR

Empirical approach: combined UV and IR fits for SRG interactions

$$E(\Lambda_{\rm UV}, L) \approx E_\infty + A_0 e^{-2\Lambda_{\rm UV}^2/A_1^2} + A_2 e^{-2k_\infty L}$$





Error analysis of combined extrapolation lacking. Goodness-of-fit can be estimated.

"Extrapolation B" from [Maris, Vary, Shirokov, Phys. Rev. C 79, 014308 (2009)]

Figures from [Jurgenson, Maris, Furnstahl, Navratil, Ormand, Vary Phys. Rev. C 87, 054312]

Recipe

1. Perform calculations at sufficiently large values of $\hbar\Omega$ (these have small or no UV corrections)
2. Plot results (energies, radii) vs. L_2 (UV converged results are expected to fall onto a single line)
3. Perform fit to extrapolation formulas and read off asymptotic value
4. General: Compute IR and UV cutoffs from diagonalization of p^2

Summary

- Understanding of IR properties of HO basis
- At low momenta, HO basis behaves as a box of size L_2
- π/L_2 is the IR cutoff
- Computation of phase shifts directly from the positive energy states in HO basis
- Energy extrapolation law expressed solely in terms of observables
- Corrections for shallow bound states worked out

Outlook: IR properties in *any localized* basis

- Diagonalize operator p^2 in a given model space → IR and UV cutoffs, and L for this model space.
- Be in the UV-converged regime.
- Plot energies and radii as a function of L, and extrapolate.

Happy birthday,
James!