Infrared properties of the harmonic oscillator basis

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R. J. Furnstahl, G. Hagen, TP, Phys. Rev. C 86, 031301(R) (2012); arXiv:1207.6100
Sushant N. More, A. Ekström, R. J. Furnstahl, G. Hagen, TP, arXiv:1302.3815

More Progress in Ab Initio Techniques in Nuclear Physics

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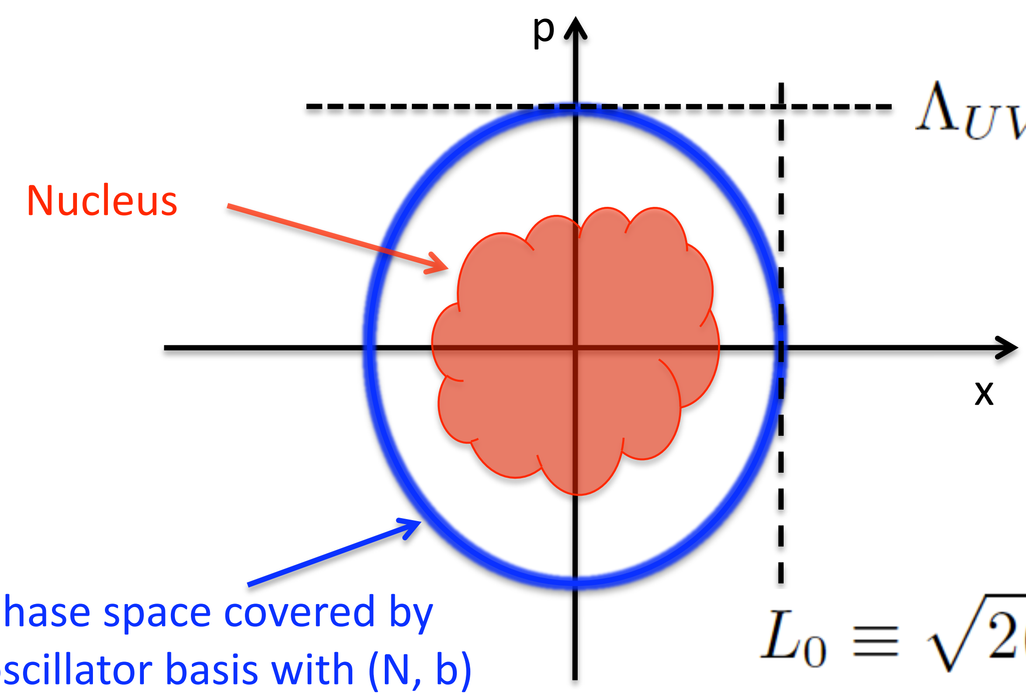
Convergence in finite oscillator spaces

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



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

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

Nucleus needs to "fit" into basis:
- Nuclear radius $R < L$
- cutoff of interaction $\Lambda < \Lambda_{UV}$

"What is the infrared cutoff in the HO basis?"

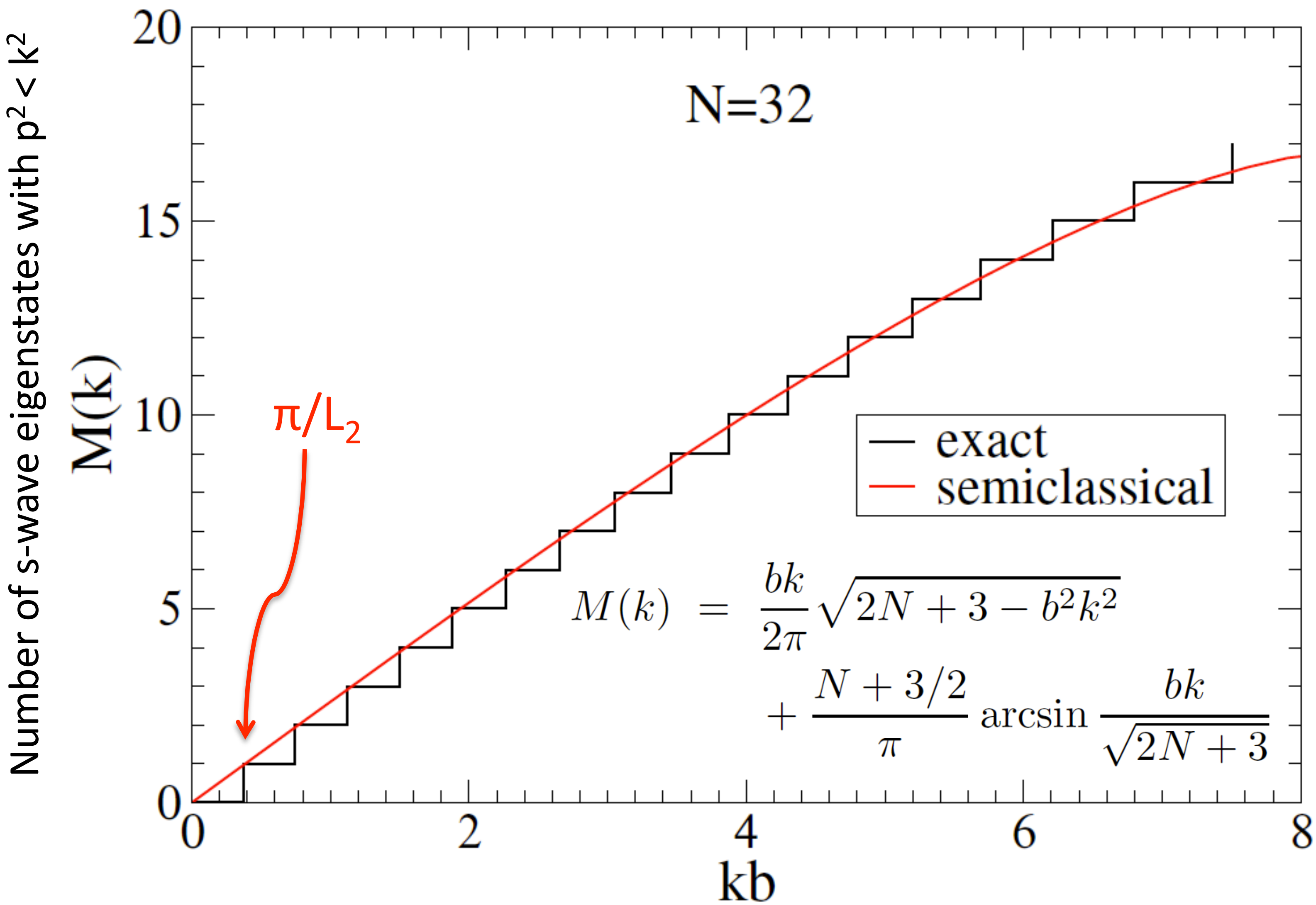
[U. van Kolck at INT workshop in spring 2009]

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 …

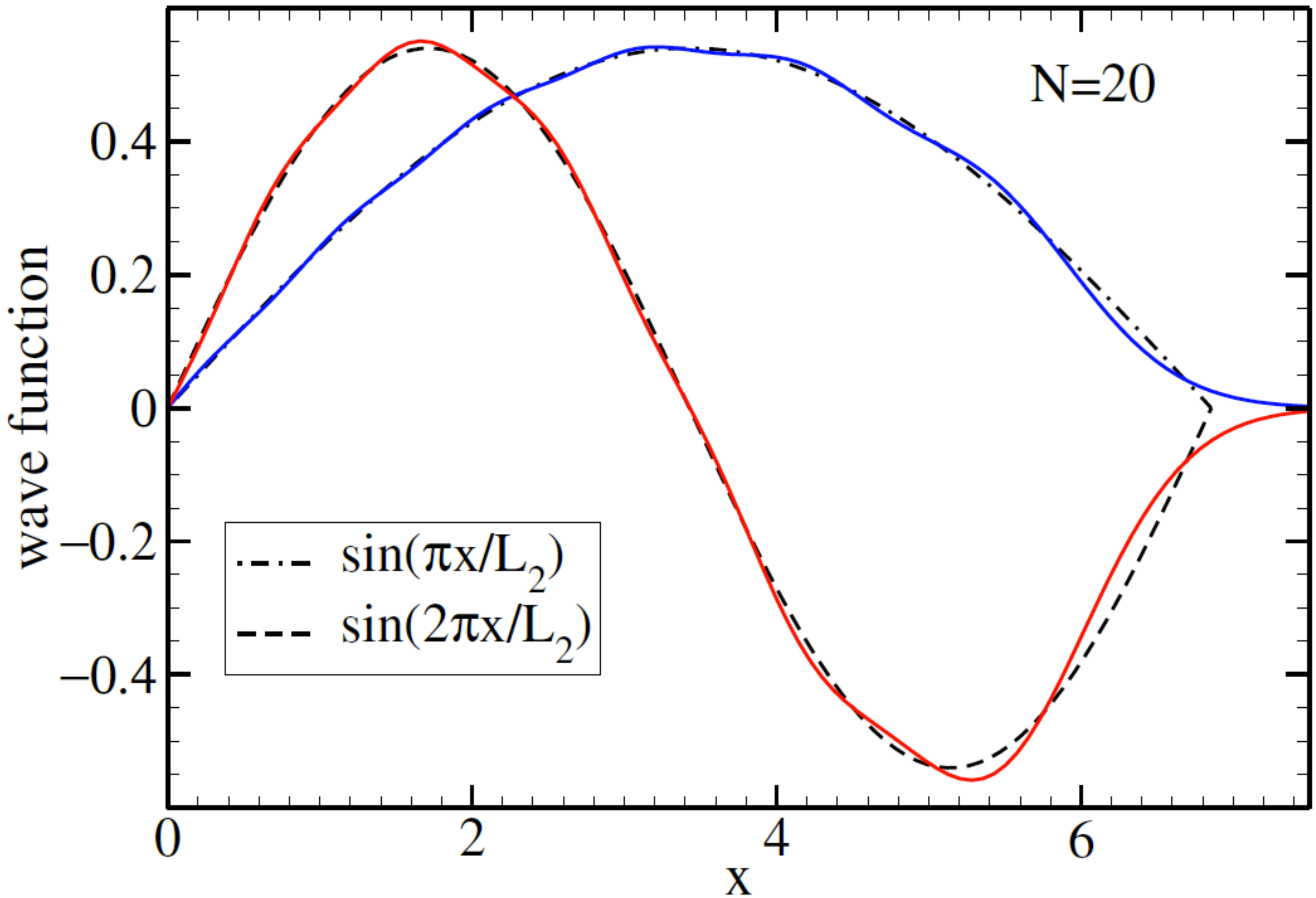
Spectrum of the operator p^2



$$M(k) = \frac{bk}{2\pi}\sqrt{2N+3-b^2k^2} + \frac{N+3/2}{\pi}\arcsin\frac{bk}{\sqrt{2N+3}}$$

- 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 looks 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**

"N>>1" does not imply impractically large model spaces

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

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

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 α_E=exp(-2$k_E L_2$). This yields a (kinetic) energy correction

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

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

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

Final results: ANC^2 Binding momentum

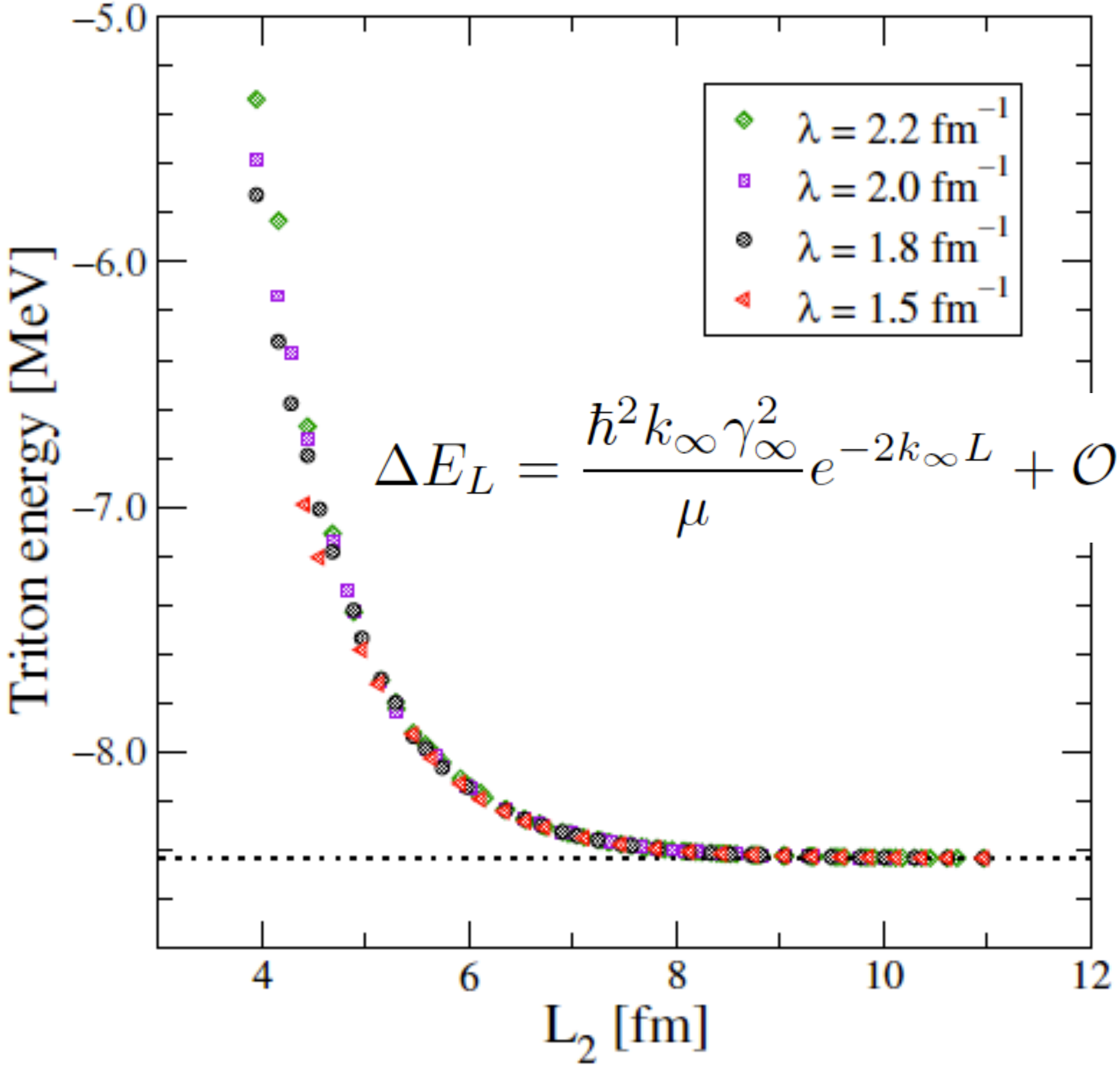
$$\Delta E_L = \frac{\hbar^2 k_\infty \gamma_\infty^2}{\mu} e^{-2k_\infty L} + \mathcal{O}(e^{-4k_\infty L})$$

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)

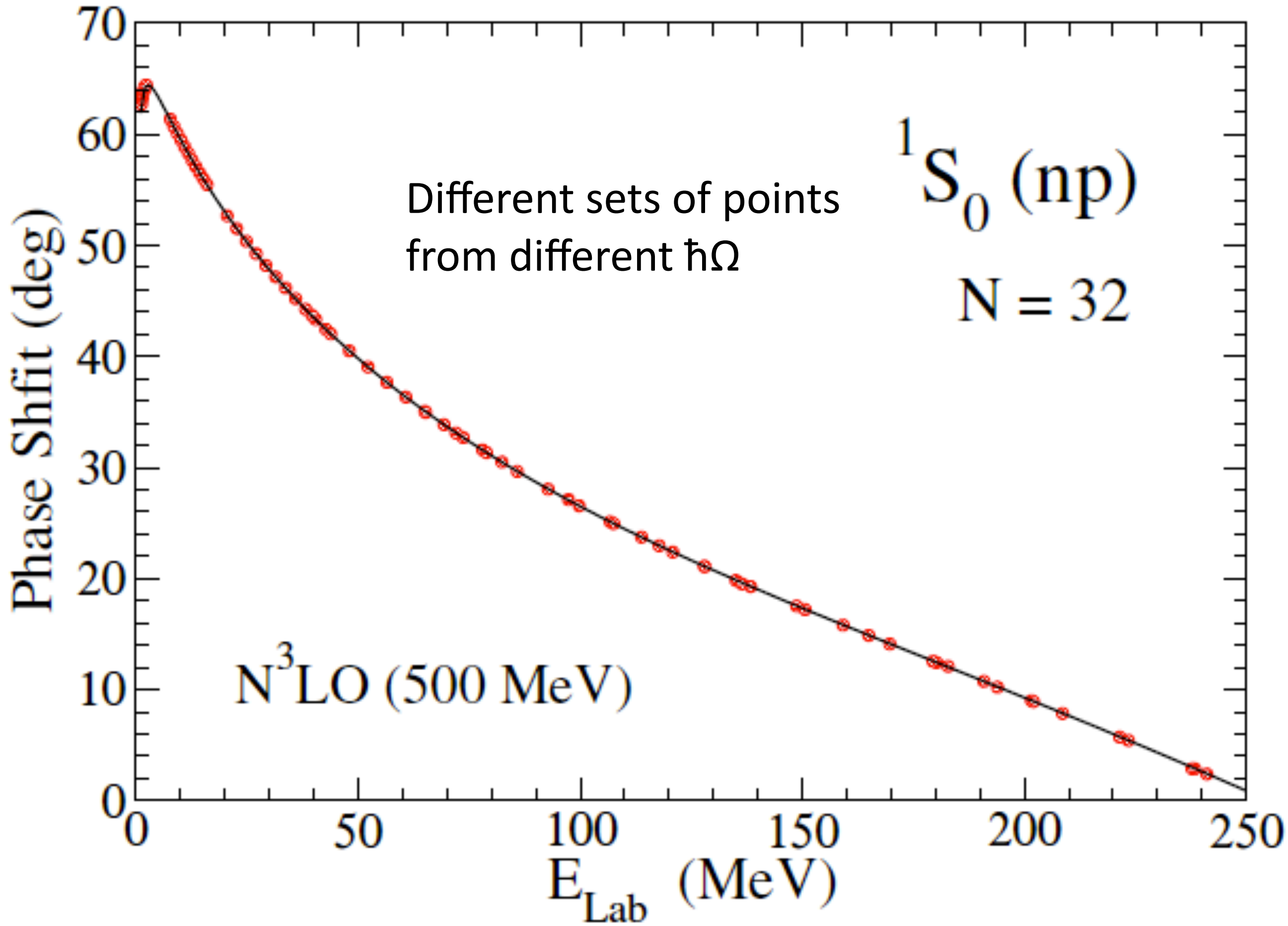
Triton binding energy from SRG interactions: only observables enter into the IR extrapolation



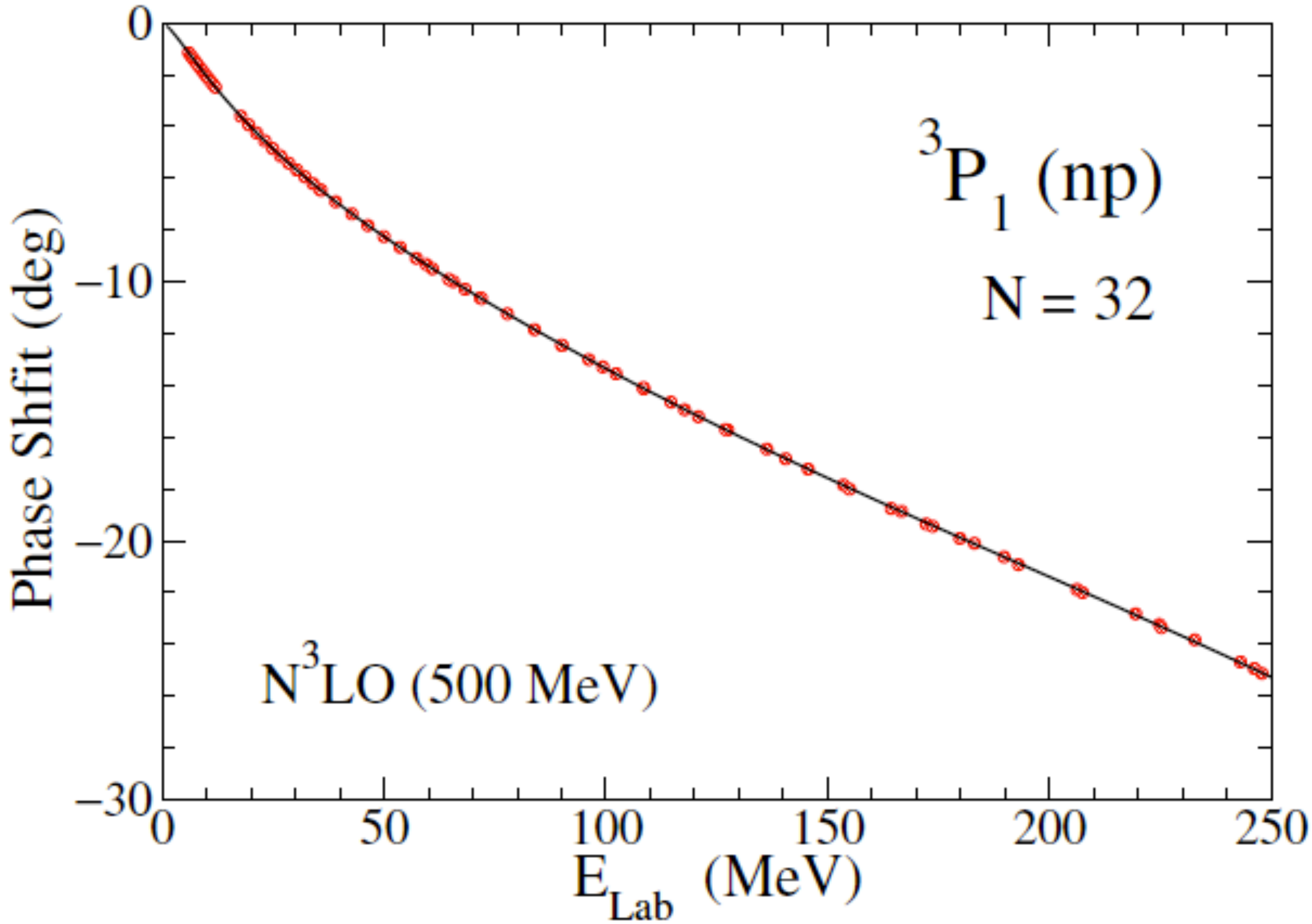
$$\Delta E_L = \frac{\hbar^2 k_\infty \gamma_\infty^2}{\mu} e^{-2k_\infty L} + \mathcal{O}(e^{-4k_\infty L})$$

Phase shifts

1. Compute states in channel l with positive energies E_i and momentum p_i in HO basis at fixed N
2. In a box, 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



Phase shifts



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

T. Luu, M. J. Savage, A. Schwenk, and J. P. Vary, Phys. Rev. C 82, 034003 (2010).

I. Stetcu, J. Rotureau, B. R. Barrett, and U. van Kolck, J. Phys. G 37, 064033 (2010).

How well can one distinguish L_2 in practice?

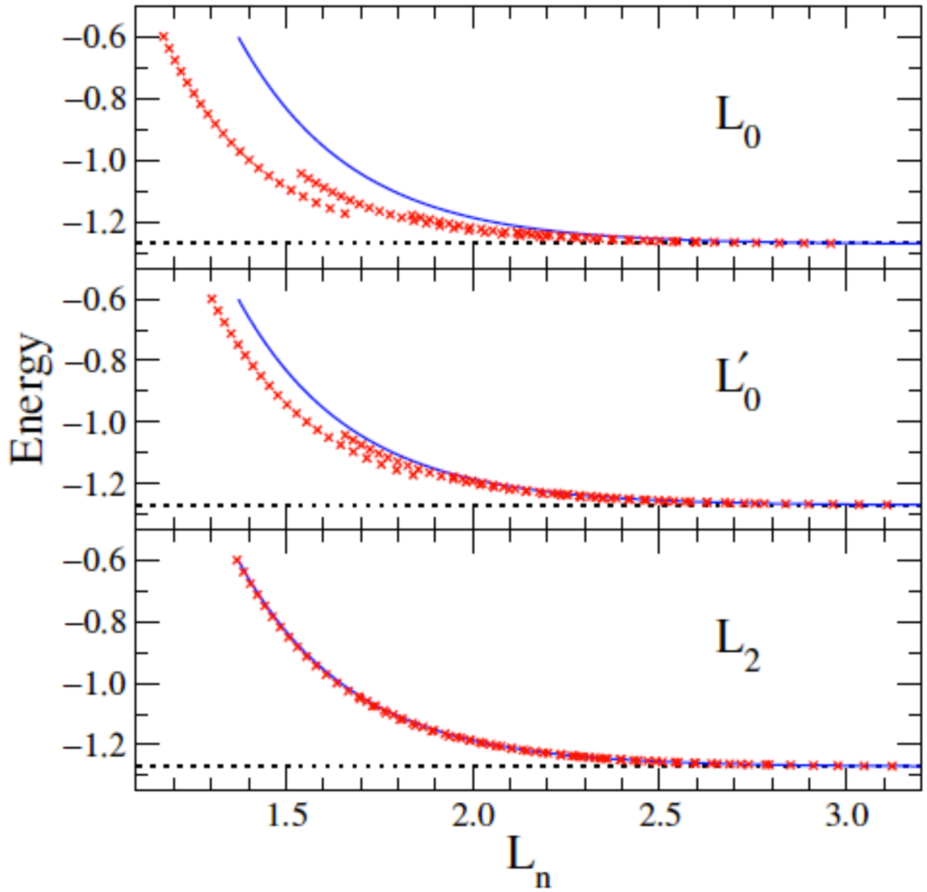
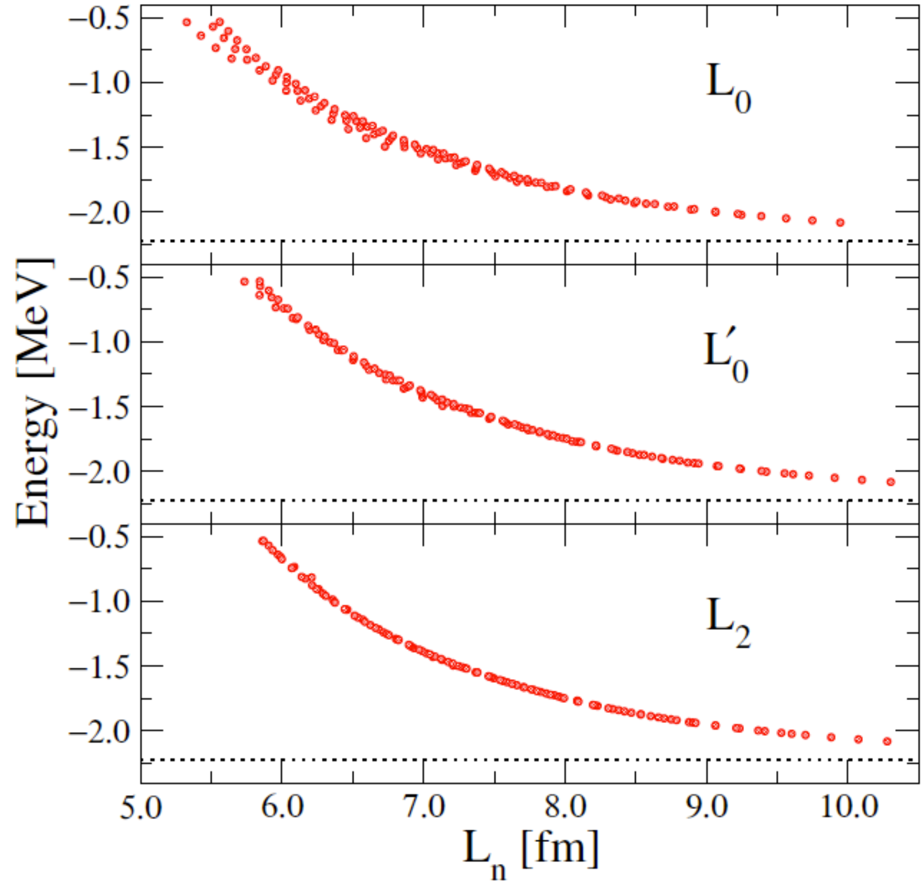
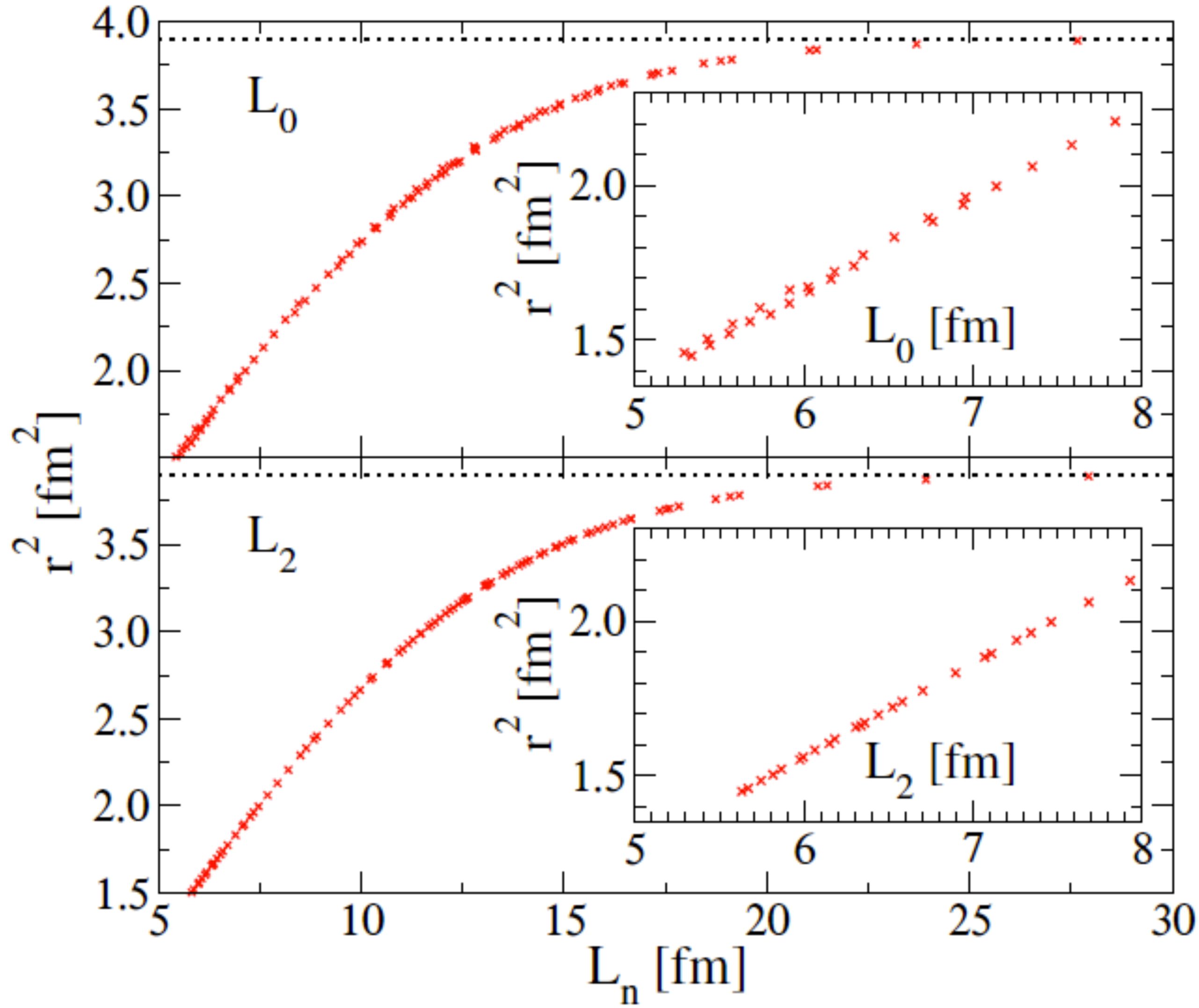


FIG. 2: (color online) Ground-state energies versus L_0 (top), L_0' (middle), and L_2 (bottom) for a Gaussian potential well Eq. (5) with $V_0 = 5$ and $R = 1$. The crosses are the energies from HO basis truncation. The energies obtained by numerically solving the Schrödinger equation with a Dirichlet 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)

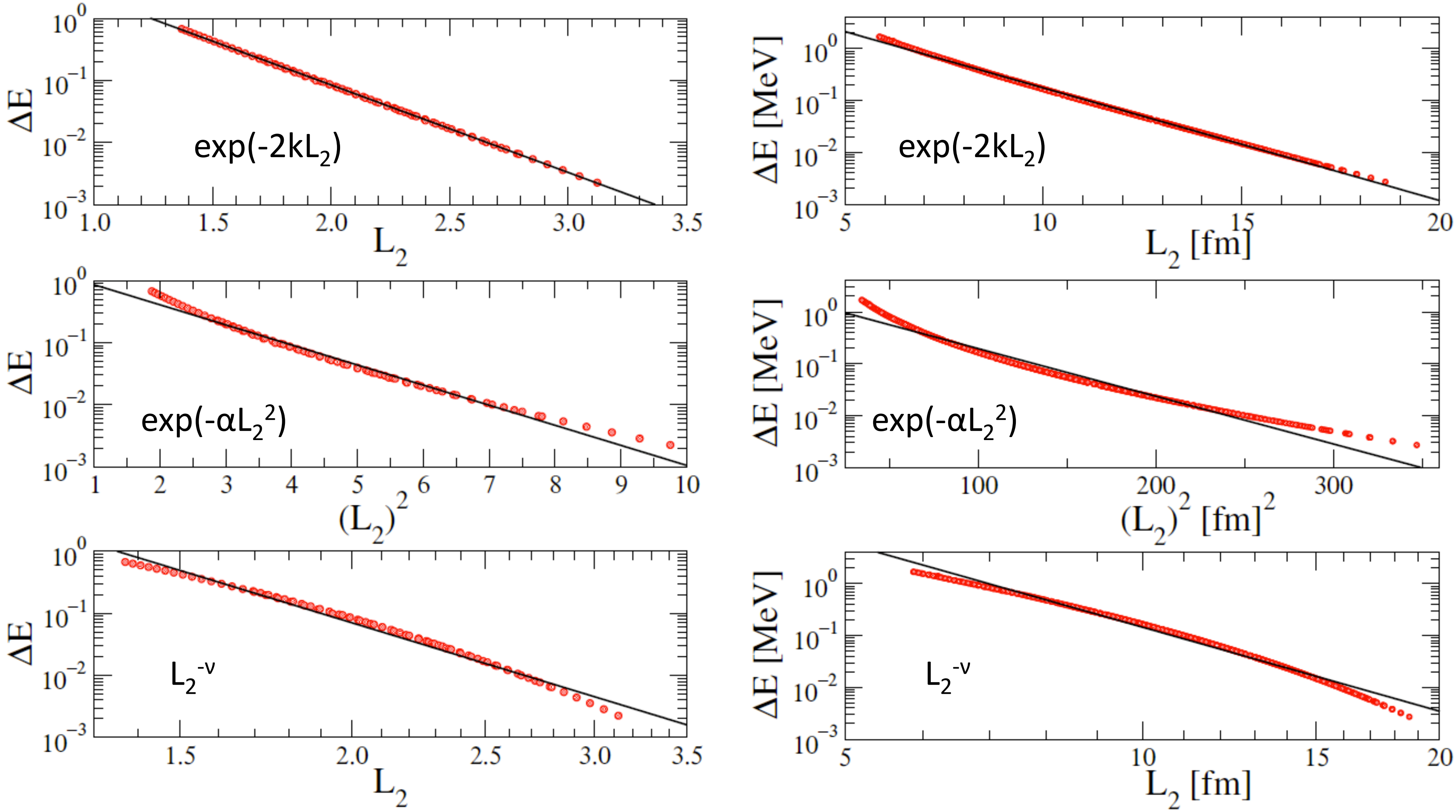
How well can one distinguish L_2 in practice?



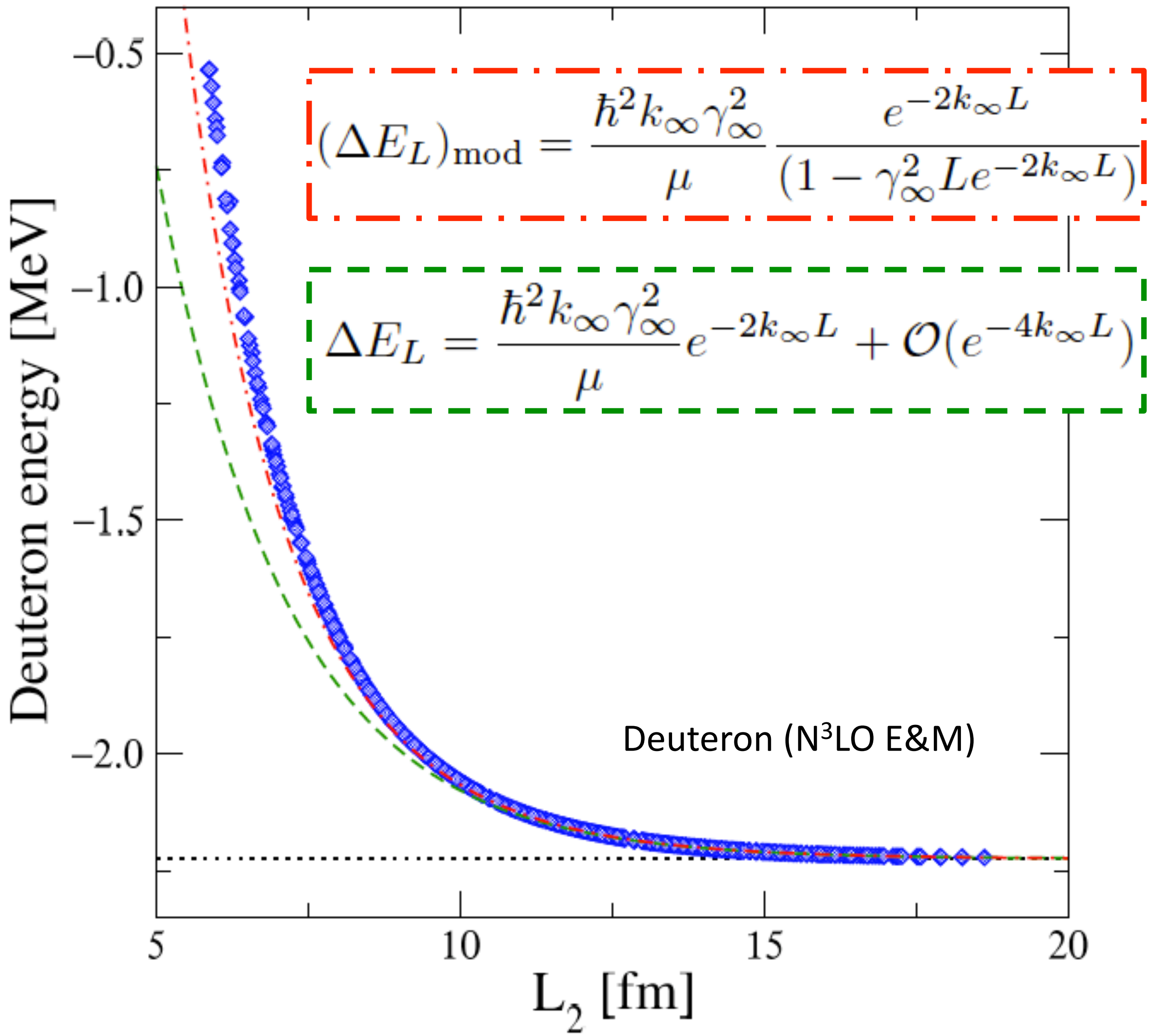
Deuteron (N^3LO E&M)

How well can one distinguish the exponential law in practice?

Gaussian well — Deuteron (N^3LO E&M)



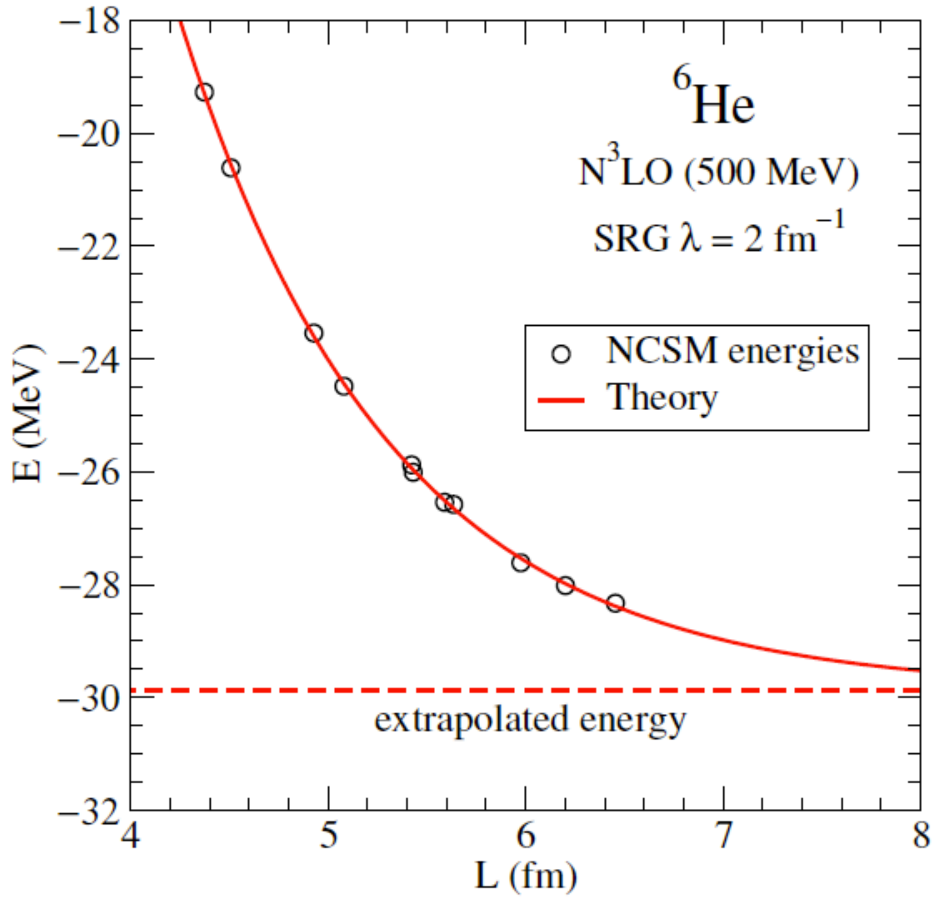
Corrections for shallow bound states



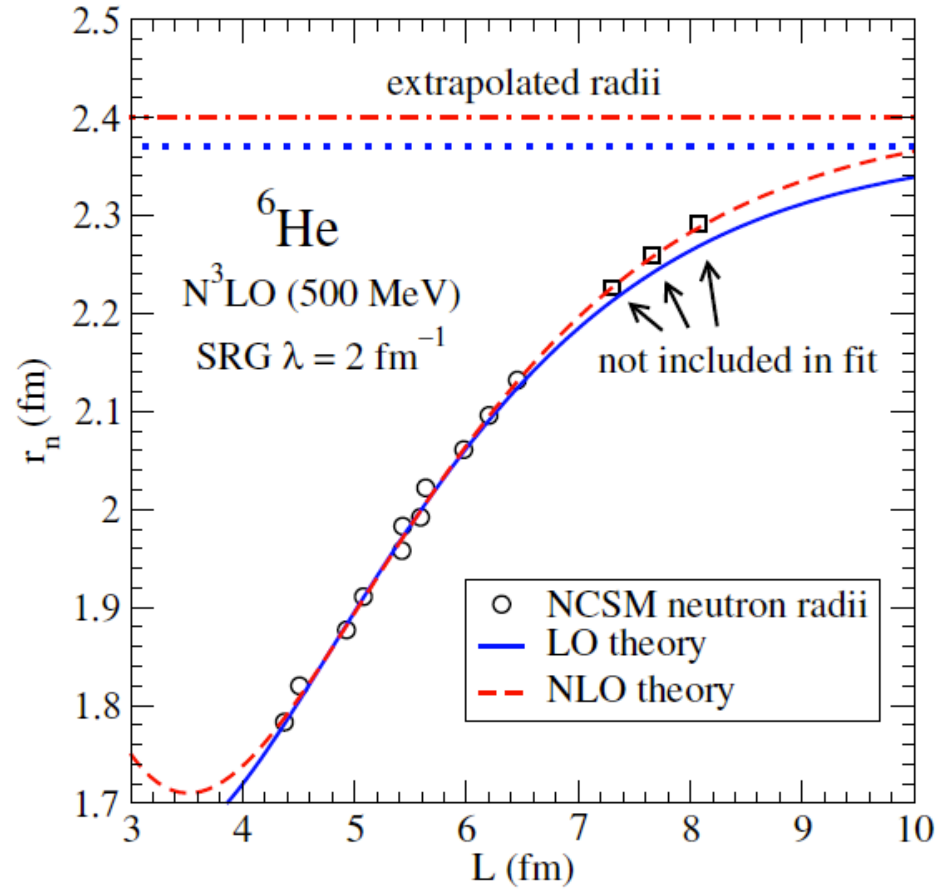
Corrections due to finite Hilbert spaces

- 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

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



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

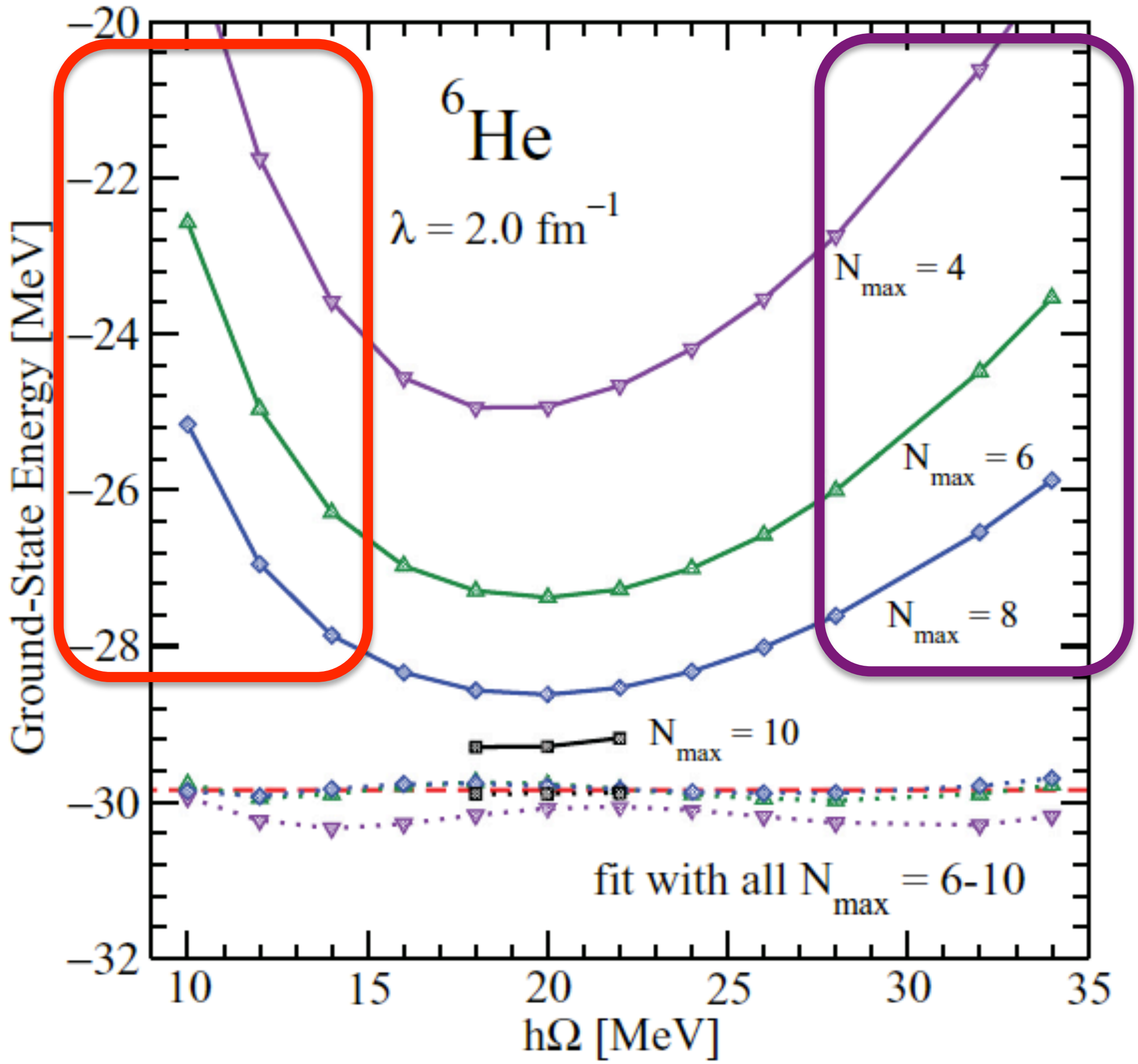


Empirical approach: combined UV and IR fits for SRG interactions

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

IR converged

extrapolate UV



UV converged

extrapolate IR

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

Summary

- Much improved 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 → L for this model space
- Be in the UV-converged regime
- Plot energies and radii as a function of L, and extrapolate