UV extrapolations in finite oscillator bases

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in collaboration with S. K. Bogner, R. J. Furnstahl, S. N. More, and T. Papenbrock

Bound States and Resonances in Effective Field Theories and Lattice QCD calculations

Centro de Ciencias de Benasque Pedro Pascual. Benasque, Spain

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The Ohio State University

NUCLEI
Nuclear Computational Low-Energy Initiative

Truncated-basis calculations

$$\psi(r) = \sum_{n=0}^{n_{\max}} c_n u_n(b;r)$$

- **Expansions in oscillator eigenstates are convenient... but necessarily truncated!**

- Both IR and UV physics are cut off, balance determined by scale b

IR extrapolations

Low-energy spectrum of $\hat{p}^2$ indistinguishable from that in a box!
$\hookrightarrow$ **asymptotic wavefunctions + S-matrix govern extrapolations**

$$\Delta E(L) = \kappa_\infty \gamma_\infty^2 \mathrm{e}^{-2\kappa_\infty L} + \cdots$$

S. N. More et al., Phys. Rev. C **87**, 044326 (2013)
R. J. Furnstahl et al., Phys. Rev. C **89**, 044301 (2014)

Goal(s) now:

- Identify the relevant UV cutoff!
- Derive a physically motivated extrapolation formula!

UV cutoff from duality

Naïve choice would be $\Lambda_0 = \sqrt{2\mu E_{\rm max}} = \sqrt{2N+3}/b\ldots \qquad (N = 2n + \ell)$

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Configuration space

- effective hard-wall box
- consider smallest eigenvalue of $\hat{p}^2$

$$\hookrightarrow L = L_2 = \sqrt{2(N+3/2+\Delta)}\, b$$

with $\Delta = 2$

$$b = (\mu\hbar\Omega)^{-1/2}$$

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$$\hat{H}_{\mathrm{HO}} = \frac{\hat{p}^2}{2\mu} + \frac{\hat{r}^2}{2\mu\, b^2}$$

Momentum space

- same situation!
- consider smallest eigenvalue of $\hat{r}^2$

$$\hookrightarrow \Lambda = \Lambda_2 = \sqrt{2(N+3/2+\Delta)}/b$$

cf., *e.g.*, M. Caprio, NUCLEI2013 talk

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Subleading corrections

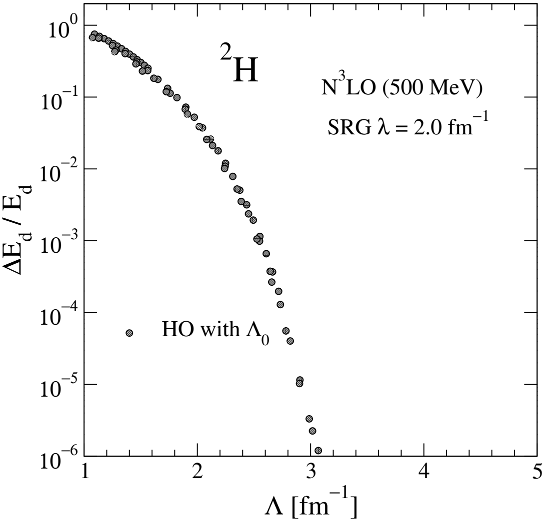
$$\Delta = \underbrace{\Delta_0}_{=2} + \frac{\Delta_1}{n} + \frac{\Delta_2}{n^2} + \cdots$$

x_ℓ = first positive root of $j_\ell(x)$

	$\ell = 0$	$\ell = 1$
Δ_1	$\frac{1}{48}(3 - 2\pi^2)$	$-\frac{7}{192}(3 - 2\pi^2)$
Δ_2	$-\frac{1}{48}(5 + 2x_1^2)$	$\frac{3}{64}(5 + 2x_1^2)$

Deuteron – Λ_0 vs. Λ_2

$$\Lambda_0 = \sqrt{2(N+3/2)}/b\ ,\ \Lambda_2 = \sqrt{2(N+3/2+2)}/b$$



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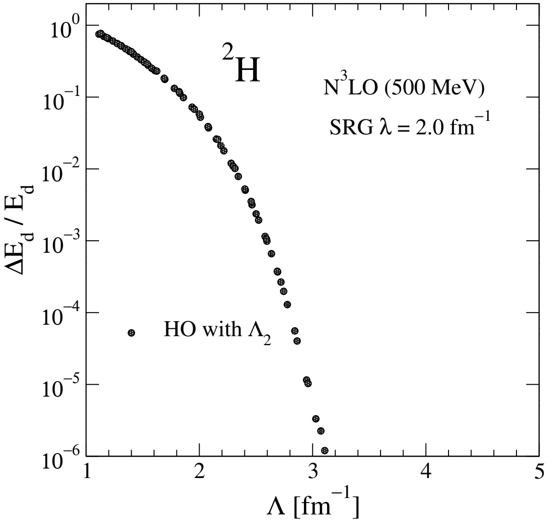

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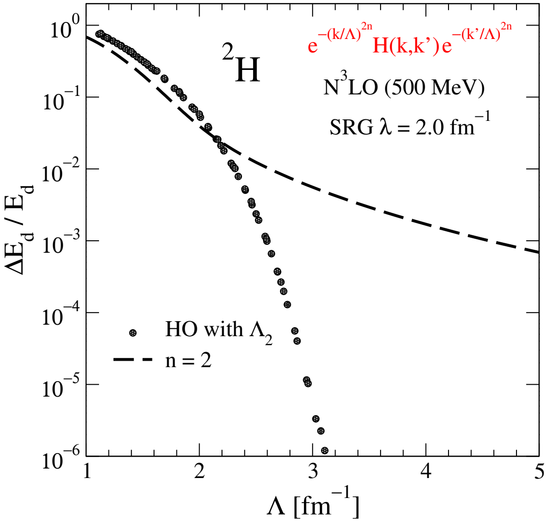

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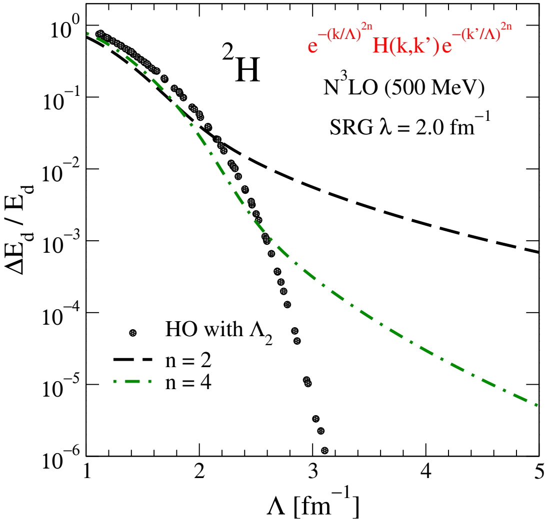

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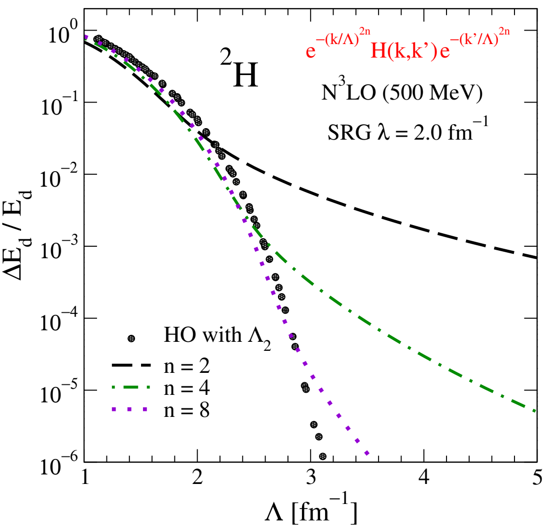

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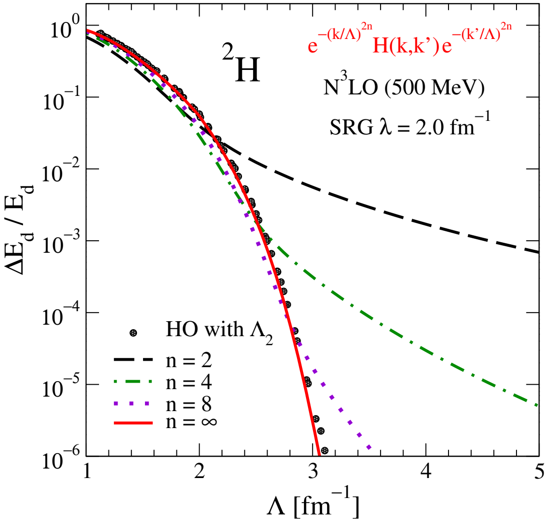


Regularized contact interaction

T. Papenbrock, S. Bogner, R. Furnstahl

Simple toy model: $V(k,k') \sim a\, f_\lambda(k') f_\lambda(k)$

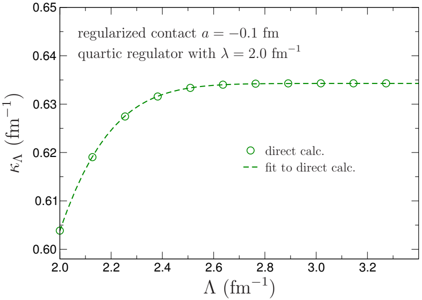
- $f_\lambda^{(4)}(k) = \mathrm{e}^{-\left(\frac{k}{\lambda}\right)^4}$

Exact cutoff dependence

$$-1 = 4\pi a \int_0^\Lambda \mathrm{d}k\, k^2 \frac{f_\lambda(k)^2}{\kappa_\Lambda^2 + k^2} \rightsquigarrow \kappa_\Lambda$$

- interaction motivated by non-rel. EFT
- regulator motivated by SRG evolution

$\rightsquigarrow$ fit $\kappa_\Lambda = \kappa_\infty - A \times \int_\Lambda^\infty \mathrm{d}k\, f_\lambda(k)^2$



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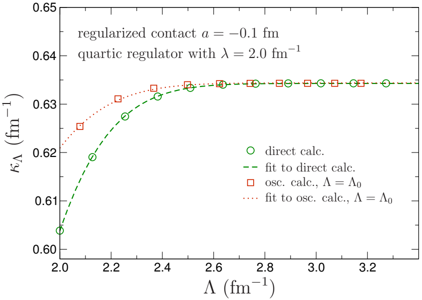

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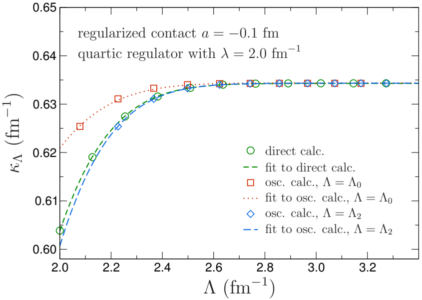

What now if the interaction is not separable?!

Separate and conquer

- take a given Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V} \ldots$
- ...and a (bound) state $|\psi\rangle$, $\boxed{\hat{H}\,|\psi\rangle = E\,|\psi\rangle}$
- set $\hat{V}_{\mathsf{sep}} = g|\eta\rangle\langle\eta|$ with $|\eta\rangle = \hat{V}\,|\psi\rangle$, $g^{-1} = \langle\psi|\hat{V}|\psi\rangle$

see, *e.g.*, Ernst, Shakin, Thaler (1973); Lovelace (1964)

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$\hookrightarrow$ **This reproduces the same state $|\psi\rangle$!**

$$\left(V_{\mathsf{sep}}\,|\psi\rangle = \frac{\hat{V}\,|\psi\rangle\,\langle\psi|\,\hat{V}}{\langle\psi|\hat{V}|\psi\rangle}\,|\psi\rangle = \hat{V}\,|\psi\rangle \quad \text{(quite simple\ldots)} \right)$$

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Just replace…

- $f_\lambda(k) \longrightarrow \eta(k)$
- $a \longrightarrow g$

…in previous relations!

Cutoff dependence

- $-1 = 4\pi g \times \int_0^\Lambda \mathrm{d}k\,k^2 \frac{\eta(k)^2}{\kappa_\Lambda^2 + k^2}$
- $\kappa_\Lambda = \kappa_\infty - A \times \int_\Lambda^\infty \mathrm{d}k\,\eta(k)^2$

This incorporates properties of the potential and the state!

Separable extrapolations

Just take $|\psi\rangle$ from the largest oscillator space!

$$|\eta\rangle = \hat{V}\,|\psi\rangle_{\mathsf{HO}}$$

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Fits

- $\kappa_{\Lambda,\mathsf{exp}} = \kappa_\infty - a \times \mathrm{e}^{-b\Lambda}$
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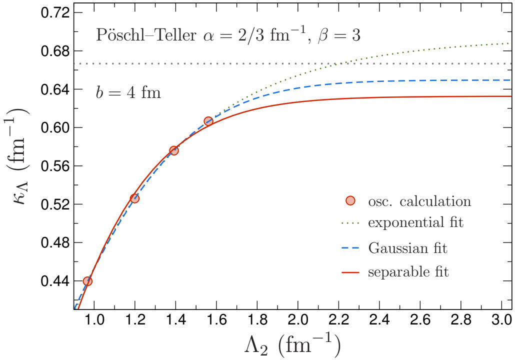

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n_{max}	8
$\kappa_{\infty,\text{exp}}$	0.6938
$\kappa_{\infty,\text{Gauss}}$	0.6495
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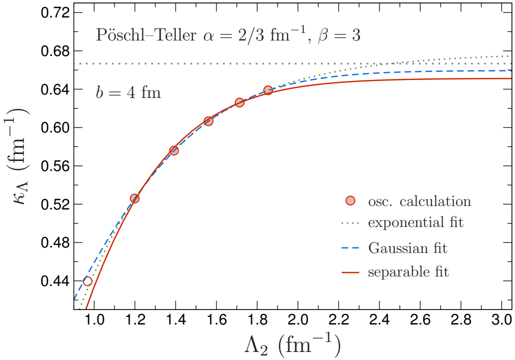

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n_{max}	8	12
$\kappa_{\infty,\text{exp}}$	0.6938	0.6778
$\kappa_{\infty,\text{Gauss}}$	0.6495	0.6594
$\kappa_{\infty,\text{sep}}$	0.6326	0.6513

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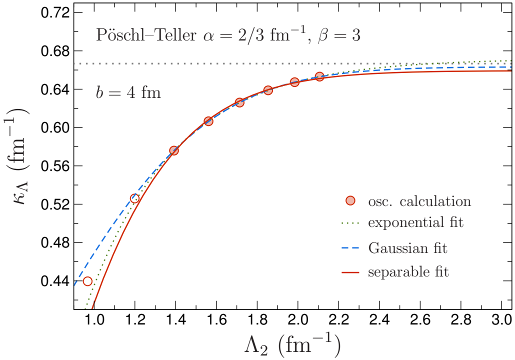

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n_{max}	8	12	16
$\kappa_{\infty,\text{exp}}$	0.6938	0.6778	0.6719
$\kappa_{\infty,\text{Gauss}}$	0.6495	0.6594	0.6633
$\kappa_{\infty,\text{sep}}$	0.6326	0.6513	0.6593

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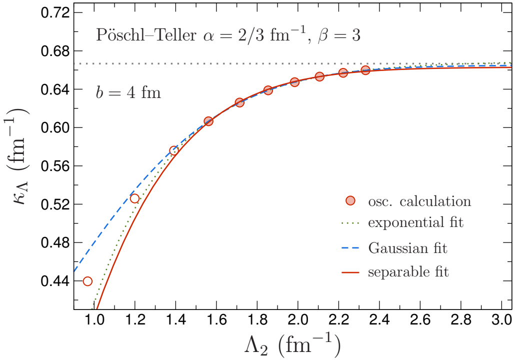

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n_{max}	8	12	16	20
$\kappa_{\infty,\mathsf{exp}}$	0.6938	0.6778	0.6719	0.6693
$\kappa_{\infty,\mathsf{Gauss}}$	0.6495	0.6594	0.6633	0.6649
$\kappa_{\infty,\mathsf{sep}}$	0.6326	0.6513	0.6593	0.6630

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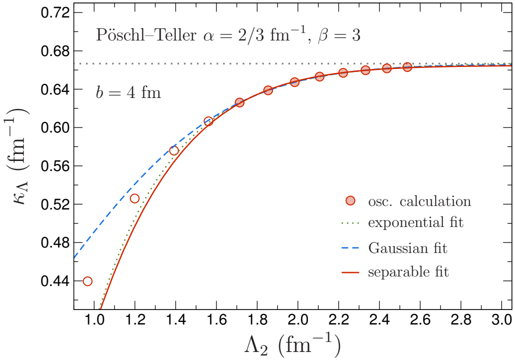

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n_{max}	8	12	16	20	24
$\kappa_{\infty,\mathsf{exp}}$	0.6938	0.6778	0.6719	0.6693	0.6680
$\kappa_{\infty,\mathsf{Gauss}}$	0.6495	0.6594	0.6633	0.6649	0.6657
$\kappa_{\infty,\mathsf{sep}}$	0.6326	0.6513	0.6593	0.6630	0.6648

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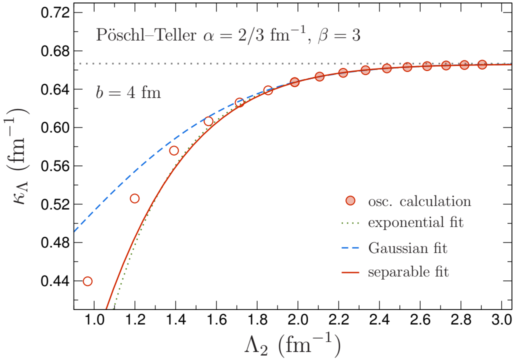

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n_{max}	8	12	16	20	24	32
$\kappa_{\infty,\text{exp}}$	0.6938	0.6778	0.6719	0.6693	0.6680	0.6671
$\kappa_{\infty,\text{Gauss}}$	0.6495	0.6594	0.6633	0.6649	0.6657	0.6663
$\kappa_{\infty,\text{sep}}$	0.6326	0.6513	0.6593	0.6630	0.6648	0.6661

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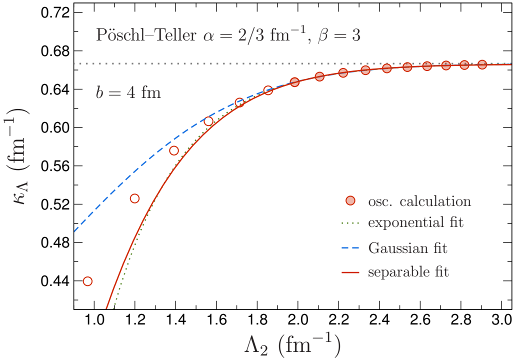

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only two parameters!

n_{max}	8	12	16	20	24	32
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Back to the deuteron

Finally, consider realistic nucleon–nucleon interactions!

$\hookrightarrow$ **Deuteron**

S–D coupled channels

$$\hat{V}_{SD} = \begin{pmatrix} \hat{V}_{00} & \hat{V}_{02} \\ \hat{V}_{20} & \hat{V}_{22} \end{pmatrix} \quad , \quad |\psi_d\rangle = \begin{pmatrix} |\psi_0\rangle \\ |\psi_2\rangle \end{pmatrix}$$

$$\hat{V}_{SD,\mathsf{sep}} = g \times \begin{pmatrix} |\eta_0\rangle \\ |\eta_2\rangle \end{pmatrix} \begin{pmatrix} \langle\eta_0| \\ \langle\eta_2| \end{pmatrix}^T \qquad \begin{aligned} |\eta_0\rangle &= \hat{V}_{00}\,|\psi_0\rangle + \hat{V}_{02}\,|\psi_2\rangle \\ |\eta_2\rangle &= \hat{V}_{20}\,|\psi_0\rangle + \hat{V}_{22}\,|\psi_2\rangle \end{aligned}$$

$$\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + g \times \begin{pmatrix} \langle\eta_0|\left(\hat{k}^2+\kappa^2\right)^{-1}|\eta_0\rangle & 0 \\ 0 & \langle\eta_2|\left(\hat{k}^2+\kappa^2\right)^{-1}|\eta_2\rangle \end{pmatrix}\right] \begin{pmatrix} |\eta_0\rangle \\ |\eta_2\rangle \end{pmatrix} = 0$$

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$$|\eta_0\rangle = \hat{V}_{00}\,|\psi_0\rangle + \hat{V}_{02}\,|\psi_2\rangle$$

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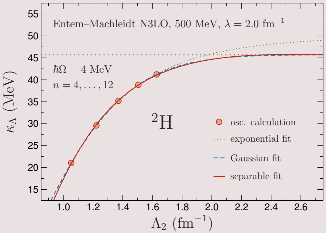
Quantization condition

$$-1 = 4\pi g \times \int_0^\Lambda \mathrm{d}k\,k^2\,\frac{\eta_0(k)^2+\eta_2(k)^2}{\kappa_\Lambda^2+k^2}$$

$\hookrightarrow$ **fit formulas, as before!**

Deuteron results

Entem–Machleidt



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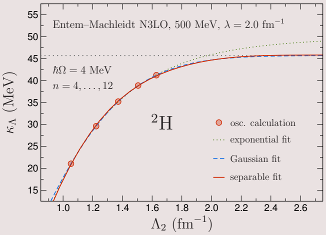

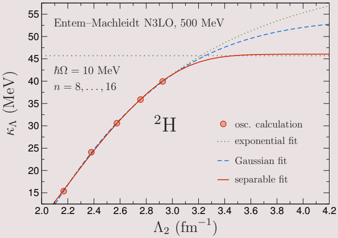

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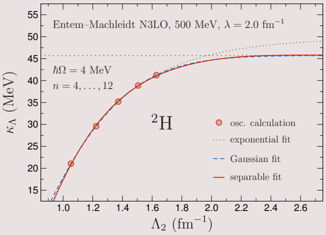
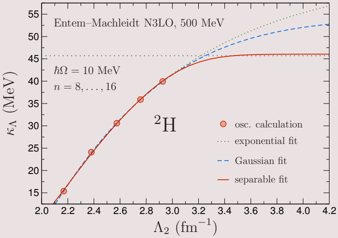
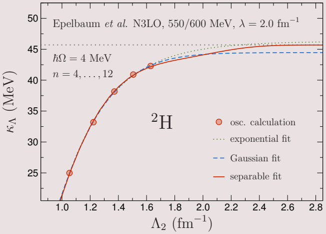




Epelbaum *et al.*



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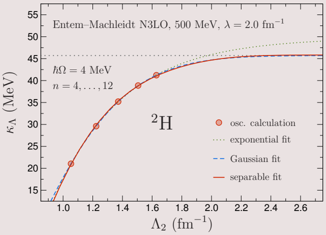
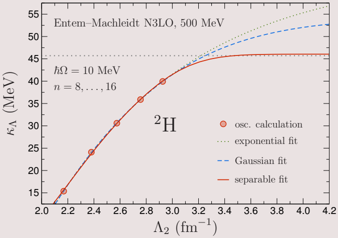
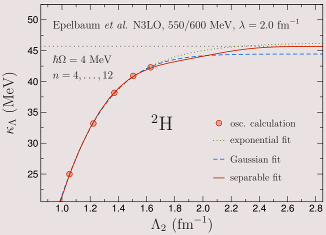
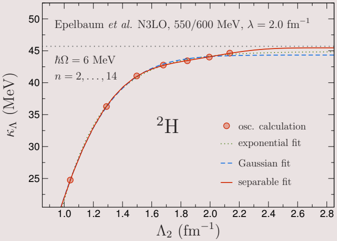
Entem–Machleidt





Epelbaum *et al.*





Quick summary

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Summary and outlook

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- duality of the oscillator Hamiltonian implies $\Lambda_{\mathrm{UV}} = \Lambda_2(N)$
- for separable interactions, the UV extrapolation is simple
- more generally, one can use separable approximations
- deuteron results look very promising!

Outlook / To Do

- scaling arguments suggests that by solving the two-body problem exactly one can extrapolate many-body results $\rightarrow$ check this!
- figure out how to do reliable combined IR and UV extrapolations

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Thanks for your attention!