UV extrapolations in finite oscillator bases

Sebastian König

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

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SK, Bogner, Furnstahl, More, Papenbrock, PRC **90** 064007, 1409.5997 [nucl-th]

and work in progress

Truncation artifacts

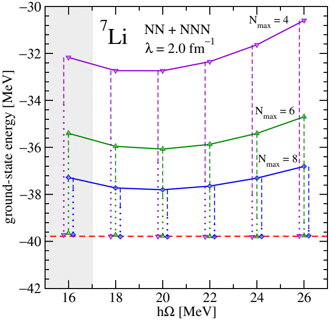
$$u(r) = \sum_{n=0}^{n_{\max}} c_n u_n(b; r)$$

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

- Both IR and UV physics are cut off, balance determined by scale b
- Oscillator length $b \sim \sqrt{1/(m\Omega)}$, $\Omega =$ frequency

UV error dominates

- small $\Omega \leftrightarrow$ large b



Jurgenson *et al.*
Phys. Rev. C **87** 054312 (2013)

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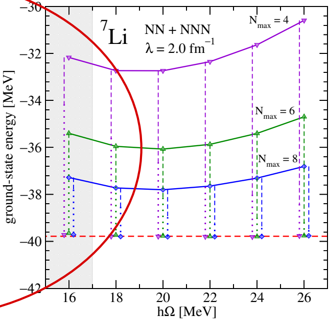

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There's no universal universality. . .

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UV cutoff from oscillator duality

Naïve estimate for UV cutoff

Consider largest included energy level. . .

$\hookrightarrow \Lambda_0 = \sqrt{2\mu E_{\mathrm{max}}} = \sqrt{2N+3}/b \qquad (N = 2n + \ell)$

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HO Hamiltonian

$$\hat{H}_{\mathrm{HO}} = \frac{\hat{p}^2}{2\mu} + \frac{\hat{r}^2}{2\mu\, b^4}$$

Duality!

R-space

Q-space

original images by D. Bellot
via Wikimedia Commons

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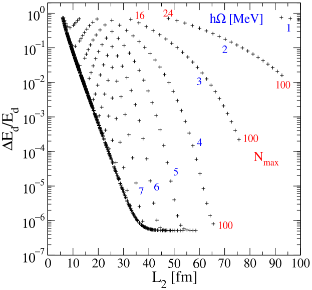
original images by D. Bellot via Wikimedia Commons

- $\hat{p}^2$ and $\hat{r}^2$ have same spectrum
- ...and wavefunctions
- same analysis in momentum space!
- UV physics $\leftrightarrow$ short distance scales

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

$\sim 1/\sqrt{\text{smallest eigenvalue of } \hat{r}^2}$

Deuteron calculations



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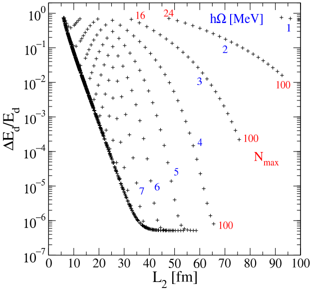

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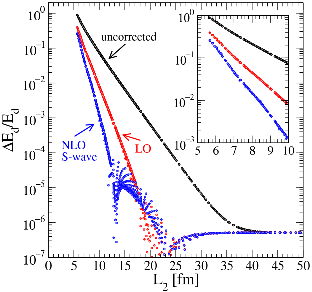

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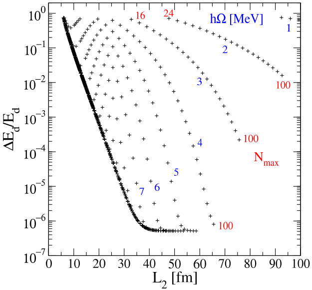

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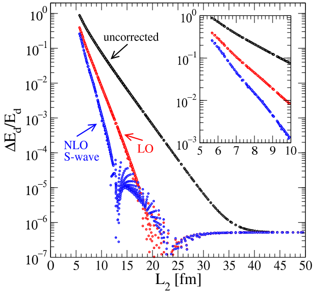

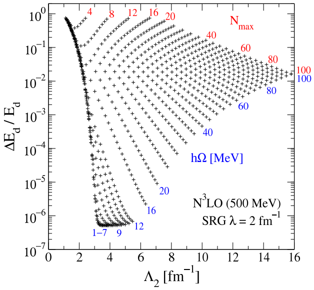

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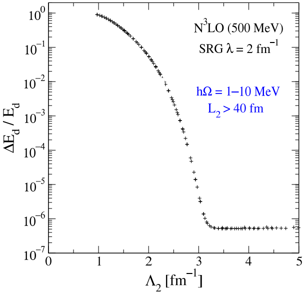
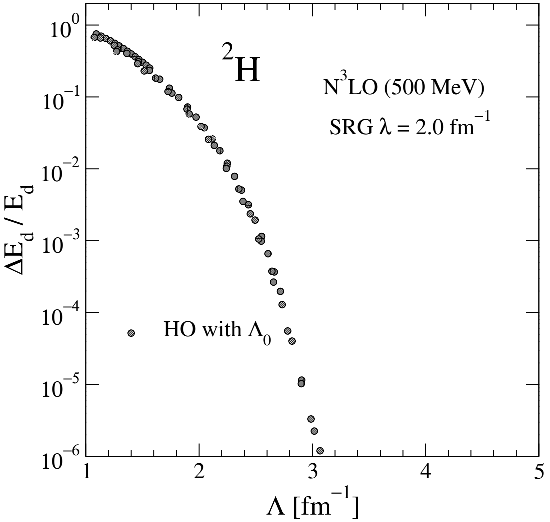


Deuteron – Λ_0 vs. Λ_2

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



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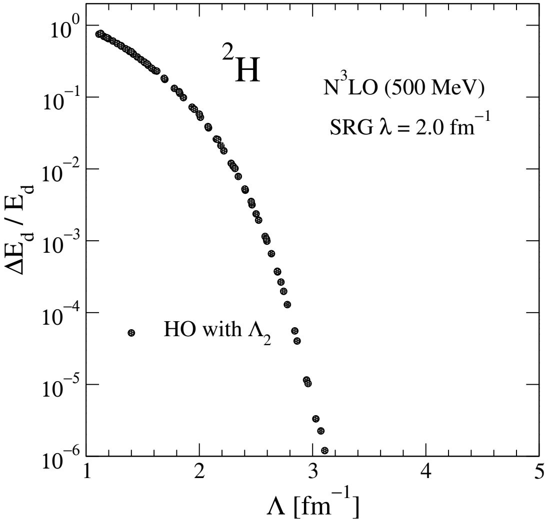

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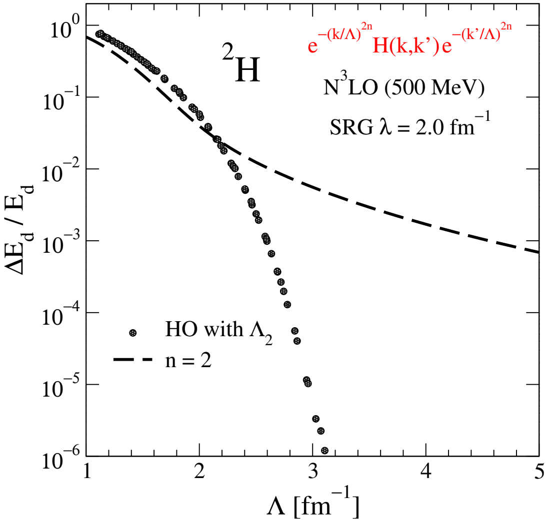

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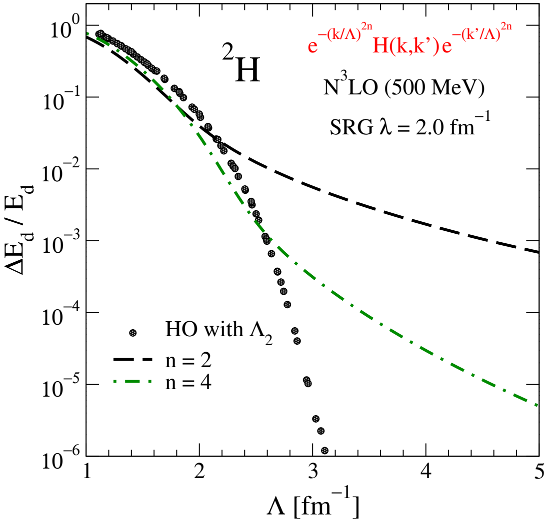

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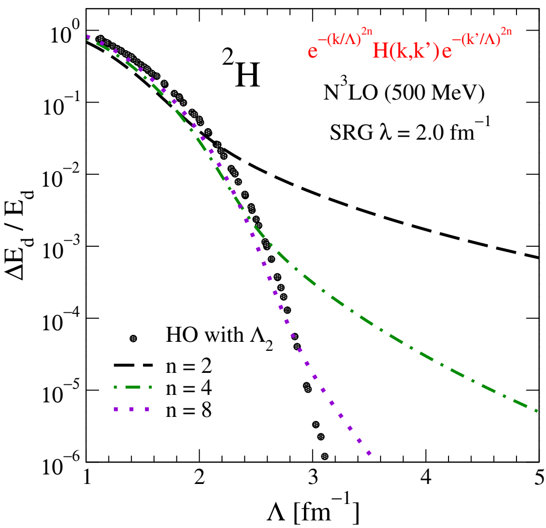

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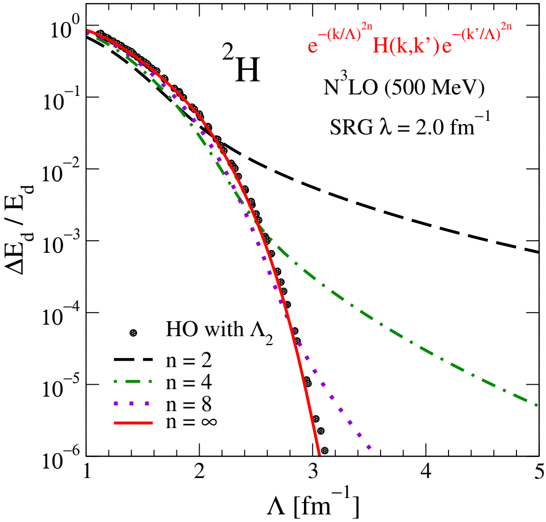

Separable two-body extrapolations

Regularized contact interaction

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

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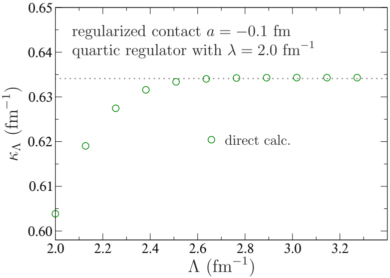

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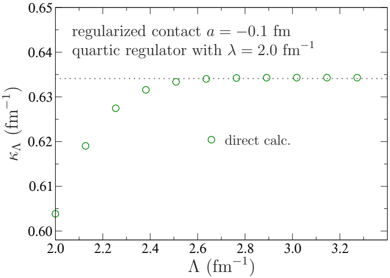
$$\kappa_\Lambda = \kappa_\infty - A \times \int_\Lambda^\infty \mathrm{d}k\, f_\lambda(k)^2$$



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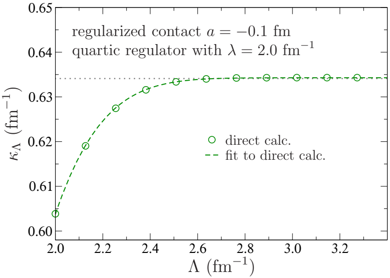

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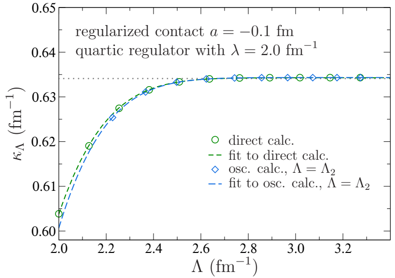

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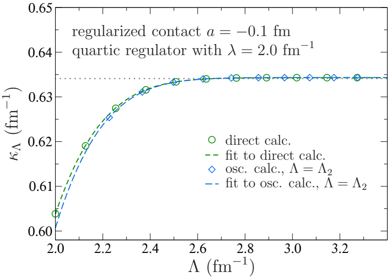

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What now if the interaction is not separable?!

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 $\hat{V}_{\text{sep}} = g|\eta\rangle\langle\eta|$ with $|\eta\rangle = \hat{V}|\psi\rangle$, $g^{-1} = \langle\psi|\hat{V}|\psi\rangle$

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

↪ This reproduces the same state $|\psi\rangle$!

$$\left(\hat{V}_{\text{sep}}|\psi\rangle = \frac{\hat{V}|\psi\rangle\langle\psi|\hat{V}}{\langle\psi|\hat{V}|\psi\rangle}|\psi\rangle = \hat{V}|\psi\rangle \quad \text{(quite simple…)}\right)$$

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!

But typically we don't know the exact state!

Separable extrapolations

But typically we don't know the exact state!

Final step

Just take $|\psi\rangle$ from the most-converged oscillator calculation!

$$\eta(k) = \langle k | V_{\text{full}} | \psi_{\text{osc}} \rangle$$

- use information about full potential!
- performance can be tested with analytically solvable models
- compare to phenomenological fits
- $\hookrightarrow$ can perform just as well...

Fits

- $\kappa_{\Lambda,\text{exp}} = \kappa_\infty - a \times \mathrm{e}^{-b\Lambda}$
- $\kappa_{\Lambda,\text{Gauss}} = \kappa_\infty - a \times \mathrm{e}^{-b\Lambda^2}$
- $\kappa_{\Lambda,\text{sep}} = \kappa_\infty - a \int_\Lambda^\infty \mathrm{d}k \, \eta(k)^2$

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- **…with only two fit parameters!**

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- $\kappa_{\Lambda,\text{Gauss}} = \kappa_\infty - a \times e^{-b\Lambda^2}$
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only two parameters!

Back to the deuteron

Finally, consider realistic nucleon–nucleon interactions!

$\hookrightarrow$ **Deuteron**

S–D coupled channels

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

$$\hat{V}_{SD,\text{sep}} = g \times \begin{pmatrix} |\eta_0\rangle \\ |\eta_2\rangle \end{pmatrix} \begin{pmatrix} \langle\eta_0| \\ \langle\eta_2| \end{pmatrix}^T$$

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

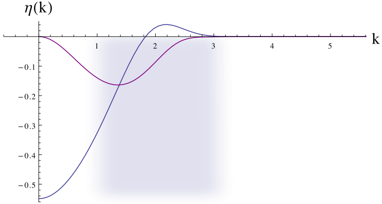
$$|\eta_2\rangle = \hat{V}_{20}|\psi_0\rangle + \hat{V}_{22}|\psi_2\rangle$$

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

Quantization condition

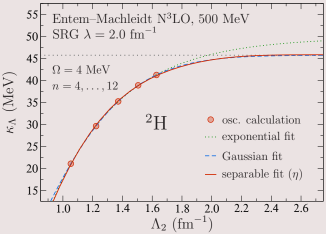
$$-1 = 4\pi g \times \int_0^\Lambda \mathrm{d}k\, k^2\, \frac{\eta_0(k)^2 + \eta_2(k)^2}{\kappa_\Lambda^2 + k^2}$$

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



Deuteron results

Entem–Machleidt



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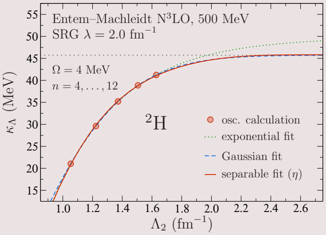

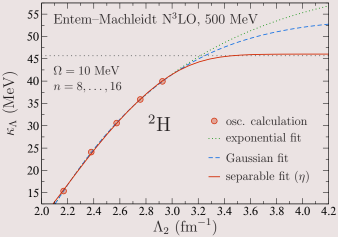

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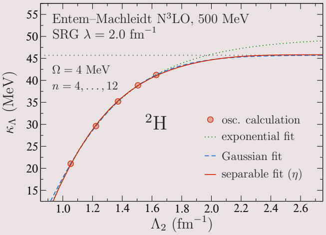
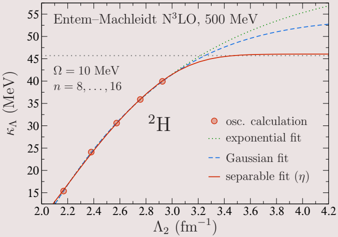
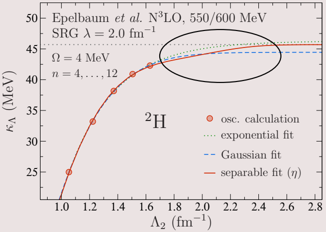




Epelbaum *et al.*



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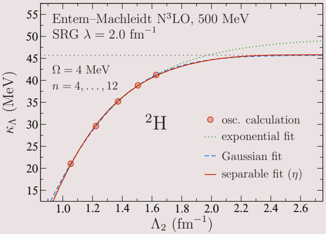

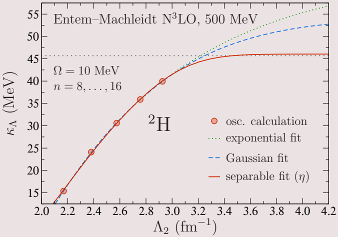

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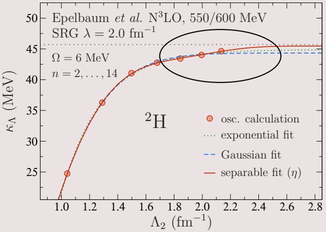

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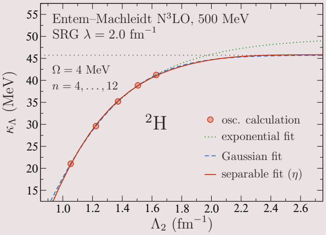

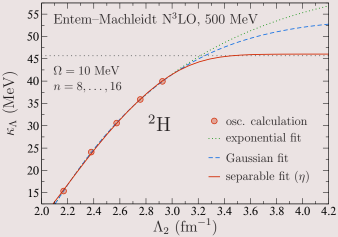

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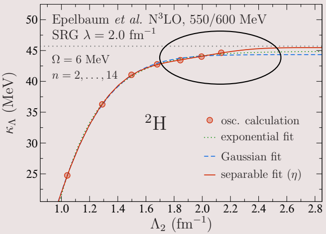
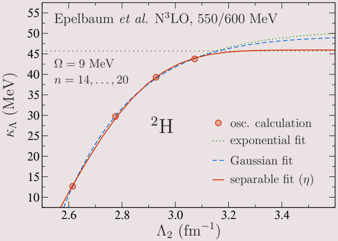




Interlude: Gaussian dependence

Gaussian dependence

Observation

Fits of the form

$$E_\Lambda = E_\infty + A_0\, e^{-4(\Lambda/\lambda)^2}\ , \quad \lambda = \text{SRG evolution scale}$$

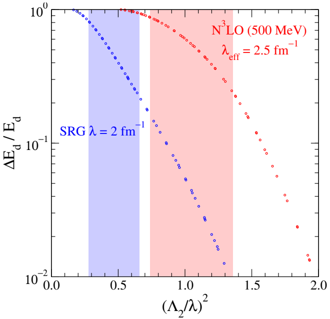
work very well!

- it can be shown that $\Delta E = \Delta E(\Lambda^2)$
- define $g(\Lambda^2) \equiv \log \Delta E_\Lambda(\Lambda^2)$
- expand about $\Lambda^2 = \Lambda_*^2$:

  $g(\Lambda^2) = g_0 + g_1(\Lambda^2 - \Lambda_*^2) + \frac{1}{2} g_2 (\Lambda^2 - \Lambda_*^2)^2 + \cdots$
- if g_1 dominates:

  $\Delta E_\Lambda = [e^{(g_0 - g_1 \Lambda_*^2)}]\, e^{g_1 \Lambda^2} = \text{(const.)} \times e^{-b_1 \Lambda^2}$

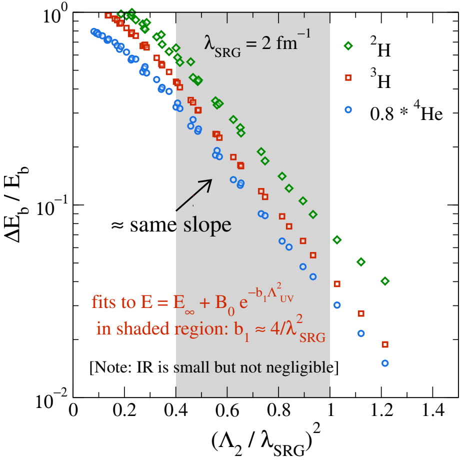
$$g_2 \sim -\frac{1}{\Delta E_\Lambda^2}\left(\frac{d\Delta E_\Lambda}{d\Lambda^2}\right)^2 + \frac{1}{\Delta E_\Lambda}\frac{d^2 \Delta E_\Lambda}{d(\Lambda^2)^2}$$



straight line segments ↔ Gaussian fit works well

Gaussian universality

- slope and region of validity are roughly independent of A
- $\rightsquigarrow$ **evidence for UV universality!**



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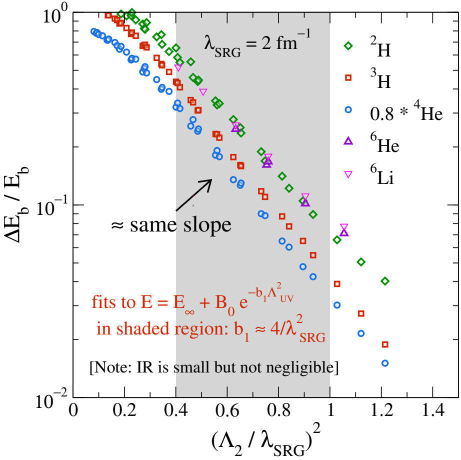

Moving on: Three particles

More general perspective

Schrödinger equation: $H|\psi\rangle = (H_0 + V)|\psi\rangle = -E_B|\psi\rangle$

Green's function: $G_0(z) = (z - H_0)^{-1}$

$$\hookrightarrow \quad |\psi\rangle = \quad G_0(-E_B)V|\psi\rangle$$

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Quantization condition

$$\rightsquigarrow 1 = \frac{\langle\psi|V \;\; G_0(-E_B) \;\; V|\psi\rangle}{\langle\psi|V|\psi\rangle}$$

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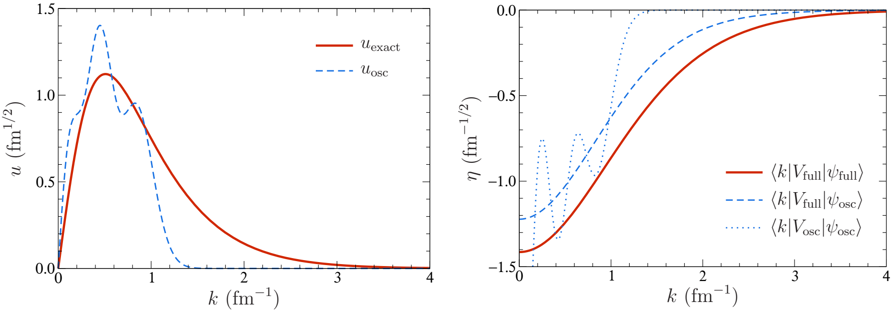
Nothing here is explicitly two-body!

Why does it work?

Why does it work?

- we use the oscillator wavefunction, which is truncated at Λ_2
- **but we know the full potential!** $\to \eta(k) = \langle k|V_{\mathsf{full}}|\psi_{\mathsf{osc}}\rangle$



$\rightsquigarrow$ **Restoration of high-momentum tail!**

How well does it work?

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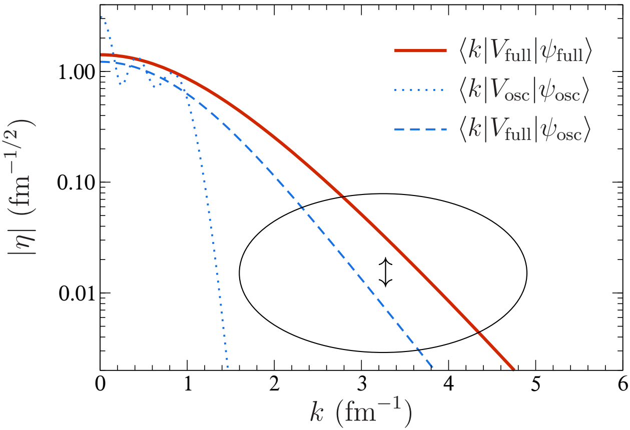

- significant part of tail restored in $\langle k|V_{\sf full}|\psi_{\sf osc}\rangle\ldots$
- **. . . but not quite all of it!** (slope is different at large momenta)

We can in fact do better yet!

Define

$$\mathcal{P}_\Lambda = \int_0^\Lambda \frac{\mathrm{d}^3p}{(2\pi)^3}|\mathbf{p}\rangle\langle\mathbf{p}| \quad , \quad \mathcal{Q}_\Lambda = \int_\Lambda^\infty \frac{\mathrm{d}^3p}{(2\pi)^3}|\mathbf{p}\rangle\langle\mathbf{p}| \quad , \quad \mathcal{P}_\Lambda + \mathcal{Q}_\Lambda = \mathbf{1}$$

to project onto low- and high-momentum subspaces.

$$\begin{pmatrix} \mathcal{P}_\Lambda H \mathcal{P}_\Lambda & \mathcal{P}_\Lambda H \mathcal{Q}_\Lambda \\ \mathcal{Q}_\Lambda H \mathcal{P}_\Lambda & \mathcal{Q}_\Lambda H \mathcal{Q}_\Lambda \end{pmatrix} \begin{pmatrix} \mathcal{P}_\Lambda|\psi\rangle \\ \mathcal{Q}_\Lambda|\psi\rangle \end{pmatrix} = -E_B \begin{pmatrix} \mathcal{P}_\Lambda|\psi\rangle \\ \mathcal{Q}_\Lambda|\psi\rangle \end{pmatrix}$$

Master formula

$$\mathcal{Q}_\Lambda|\psi\rangle = \left(-E_B - \mathcal{Q}_\Lambda H \mathcal{Q}_\Lambda\right)^{-1} \mathcal{Q}_\Lambda V \, \mathcal{P}_\Lambda|\psi\rangle \quad , \quad \boxed{\mathcal{P}_\Lambda|\psi\rangle \approx Z|\psi_\Lambda\rangle}$$

$\hookrightarrow$ **express UV tail in terms of low-momentum part!**

Bogner and Roscher, PRC **86** 064304 (2012)

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↪ **express UV tail in terms of low-momentum part!**

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Oscillator input

$$\Lambda \to \Lambda_2(n_{\max}, \Omega) \quad , \quad \mathcal{P}_\Lambda|\psi\rangle \to Z|\psi_{\text{osc}}\rangle$$

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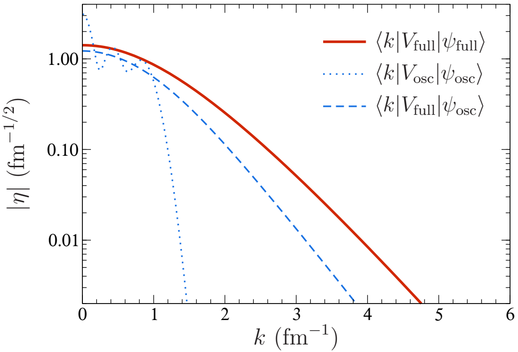

$$\langle k|V_{\text{full}}|\psi_{\text{full}}\rangle = \langle k|V_{\text{full}}(\mathcal{P}_\Lambda + \mathcal{Q}_\Lambda)|\psi_{\text{full}}\rangle \approx Z \times \langle k|V_{\text{full}}|\psi_{\text{osc}}\rangle + \text{corr.}$$

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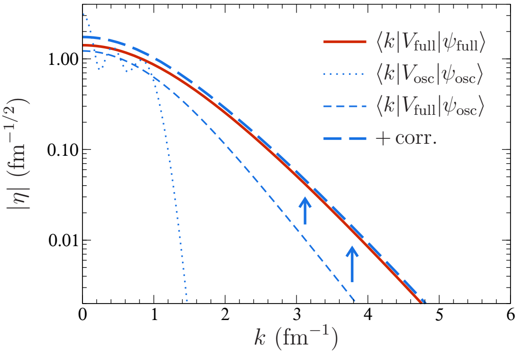

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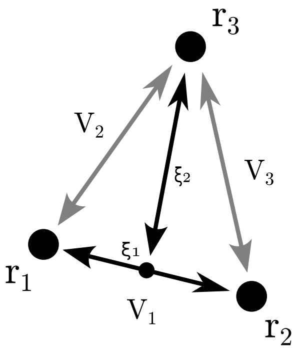
Three-body toy model



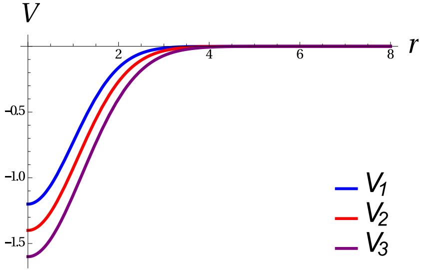
Jacobi coordinates

$$\boldsymbol{\xi}_0 = \frac{1}{\sqrt{3}}(\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3)$$

$$\boldsymbol{\xi}_1 = \frac{1}{\sqrt{2}}(\mathbf{r}_1 - \mathbf{r}_2)$$

$$\boldsymbol{\xi}_2 = \sqrt{\frac{2}{3}}\left[\frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2) - \mathbf{r}_3\right]$$

- factor out center-of-mass motion
- assume local pairwise interactions



Three-body quantization condition

$$\rightsquigarrow 1 = \frac{\overbrace{\langle\psi|V}^{\langle\eta|}\ G_0(-E_B)\ \overbrace{V|\psi\rangle}^{|\eta\rangle}}{\underbrace{\langle\psi|V|\psi\rangle}_{g_0}}$$

$$\hookrightarrow 1 = g_0 \times \int \mathrm{d}^3\wp_1 \int \mathrm{d}^3\wp_2 \, \frac{\eta(\wp_1,\wp_2)^2}{-E_B - \frac{1}{2}\frac{\wp_1^2}{2\mu} - \frac{1}{2}\frac{\wp_2^2}{2\mu}}$$

$$\eta(\wp_1,\wp_2) = \langle\wp_1,\wp_2|V|\psi\rangle$$

Jacobi momenta: $\wp_{1,2} \leftrightarrow \boldsymbol{\xi}_{1,2}$

How to cut off these integrals?

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Truncated three-body oscillator basis

$$\psi_{\lambda\mu}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2) = \sum_{(n_1,l_1),(n_2,l_2)} c_{n_1 l_1, n_2 l_2} \langle \boldsymbol{\xi}_1, \boldsymbol{\xi}_2 | n_1 n_2, (l_1 l_2)\lambda, \mu\rangle$$

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$(n_{\max}, l_{\max})$-truncation

- $n_{1,2} \leq n_{\max}$, $l_{1,2} \leq l_{\max}$
- $\rightsquigarrow$ **rectangular cutoff:** $\wp_{1,2} \leq \Lambda$

$N_{\max}$-truncation

- $N = 2n_1 + l_1 + 2n_2 + l_2 \leq N_{\max}$
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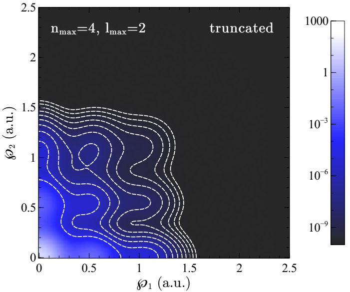

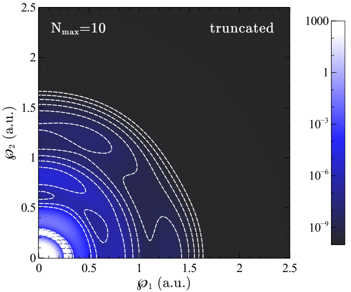

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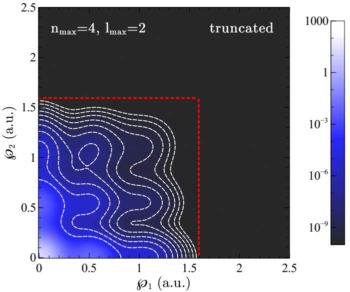
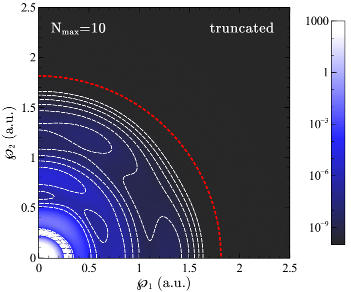


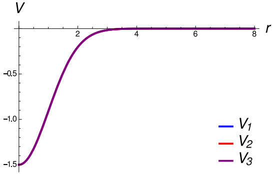


Cutoff dependence and fitting

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

General effective cutoff

$\Lambda_{\text{eff}} \sim$ (smallest eigenvalue of $\hat{r}^2)^{-1/2}$



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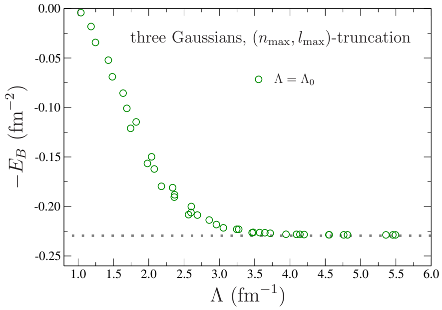

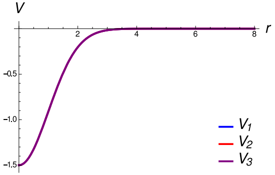

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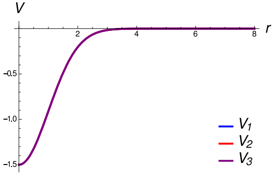

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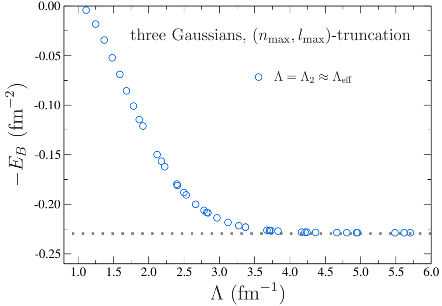

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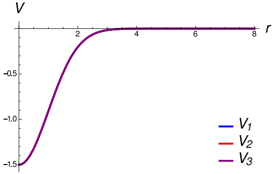

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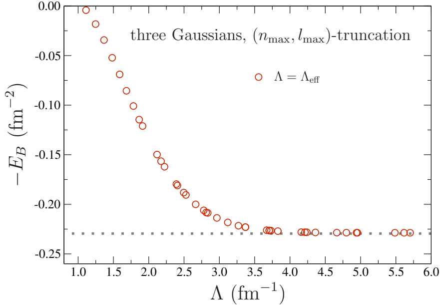

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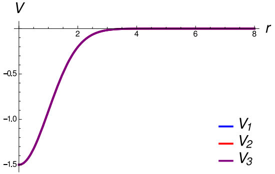

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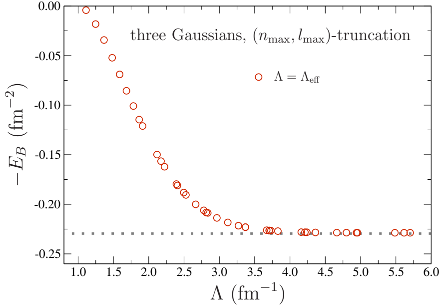

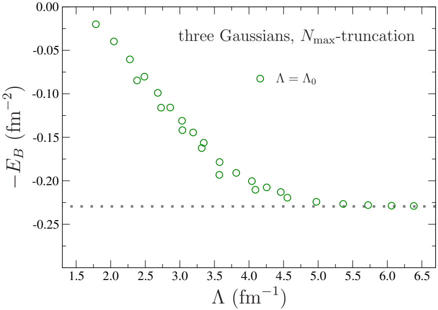

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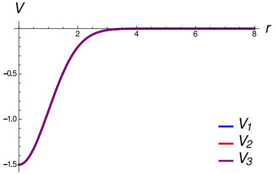

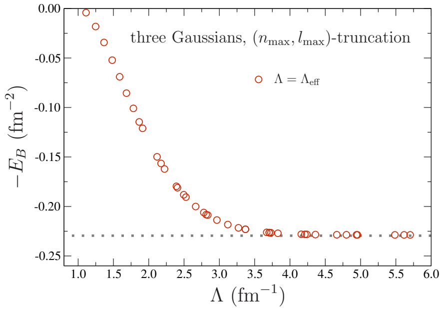

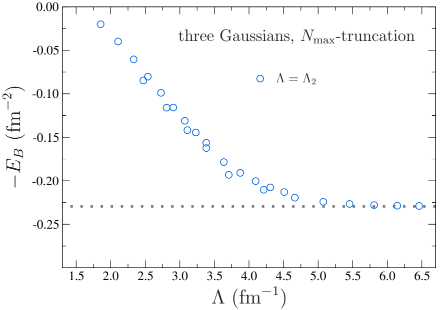

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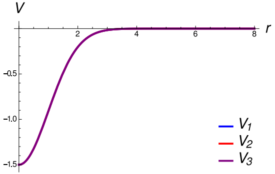

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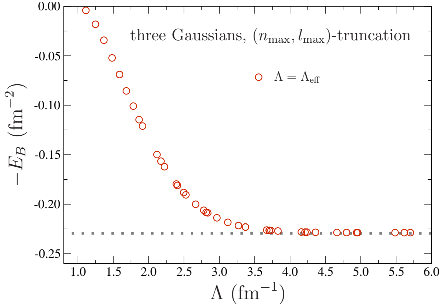

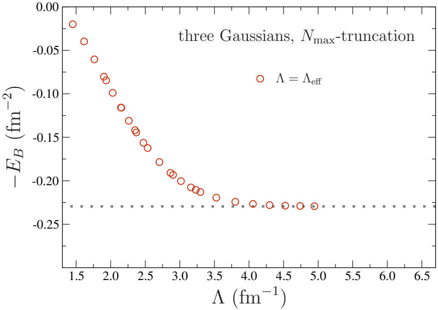

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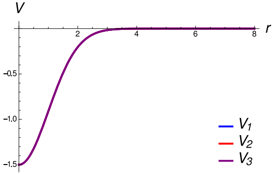

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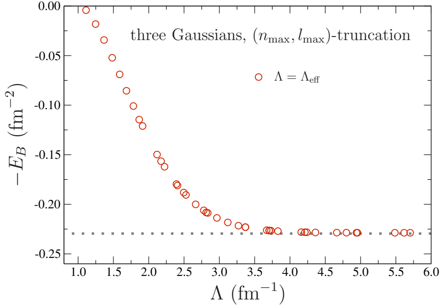
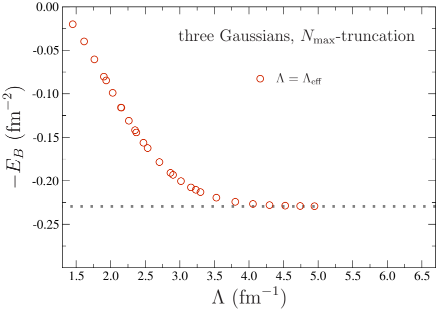
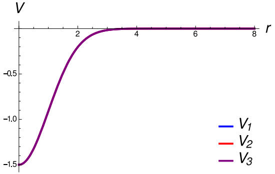




- smooth cutoff dependence for both truncation schemes ✓

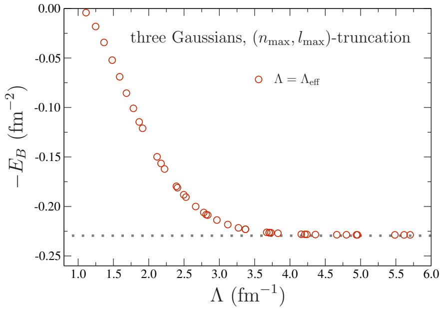
Cutoff dependence and fitting

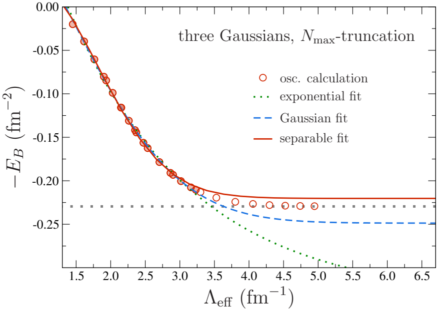
$$\Lambda_0 = \sqrt{2(N+3/2)}/b\,,\ \Lambda_2 = \sqrt{2(N+3/2+2)}/b$$



General effective cutoff

$\Lambda_{\rm eff} \sim$ (smallest eigenvalue of $\hat{r}^2)^{-1/2}$





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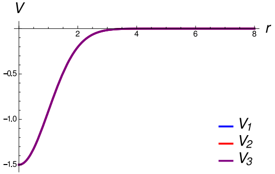

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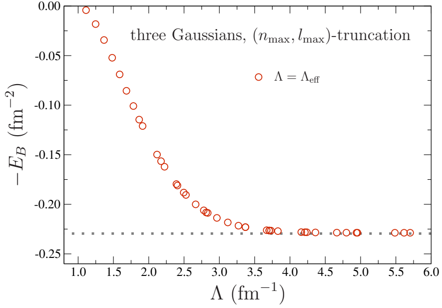

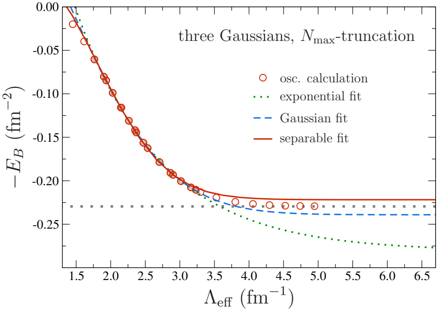

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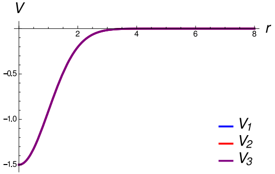

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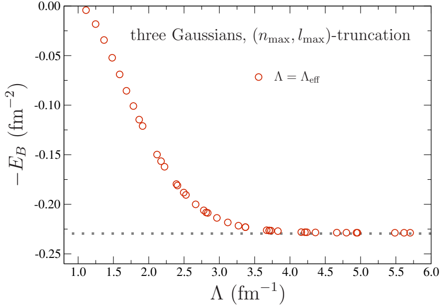

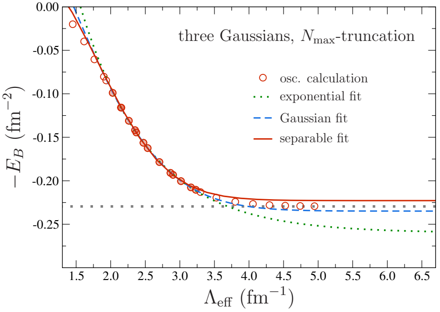

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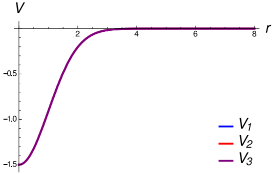

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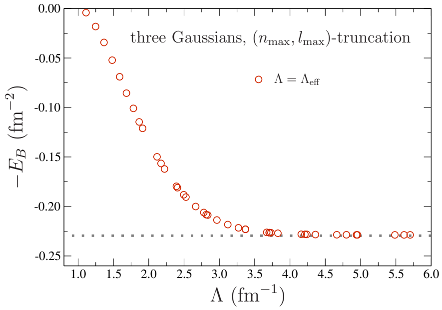

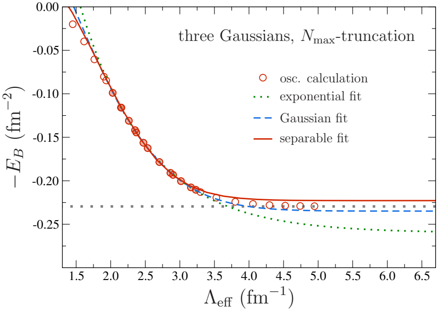

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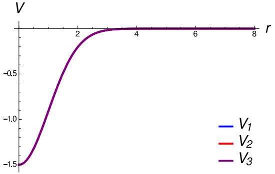

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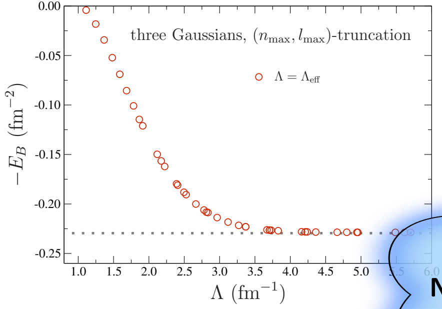

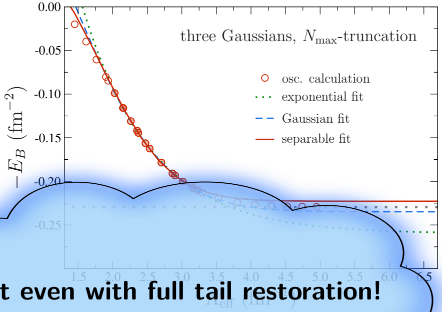

Not even with full tail restoration!

- smooth cutoff dependence for both truncation schemes ✓
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Summary and outlook

Summary

- oscillator basis truncation corresponds to sharp UV cutoff
- for separable interactions, the UV extrapolation is simple
- more generally, one can use separable approximations
- deuteron results are quite impressive!
- extension to three particles looks promising
- evidence for UV universality with SRG-evolved interactions

Outlook / To Do

- analyze three-body system in more detail
- extend to large scale many-body calculations
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Thanks for your attention!