Effective Theories for van der Waals Systems

With Applications to the ^{4}He and ^{6}Li Few-Body Systems

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Outline

- Theory
  - SR-EFT
  - vdWEFT
- ^{4}He – A Comparison to the LM2M2 Potential
  - 2- and 3-body sectors
- 6Li – Seeking Improvement Over SR-EFT
  - 3-body recombination

Theory

Theory
SR-EFT

- Predominantly, the kinds of problems in AMO physics that I will discuss today have been studied with *ab initio* potentials.
- Recently, the EFT crowd has been successful analyzing these systems with SR-EFT (a.k.a. pionless EFT).
- SR-EFT accounts for the short-distance physics with contact interactions (LO, delta functions). It improves upon that description by including corrections coming from derivatives of those contact interactions (extra powers of momentum).
- SR-EFT is **short-ranged**. There is no long-range interaction.
- Applicable to systems with a large scattering length, $a_0 \gg R$.
- Large $a_0 \implies B_2 \approx 1/(ma_0^2)$ and (for bosons) the Efimov effect.

Theory
vdWEFT

- For cold, neutral atoms, the long-range potential goes like an attractive $1/r^6$ potential (induced polarization) with a characteristic length scale, β_6.
- If we explicitly include this interaction at LO *in addition* to the contact interactions, we can:
  - capture more low-energy physics
  - reap the benefits of vdW universality

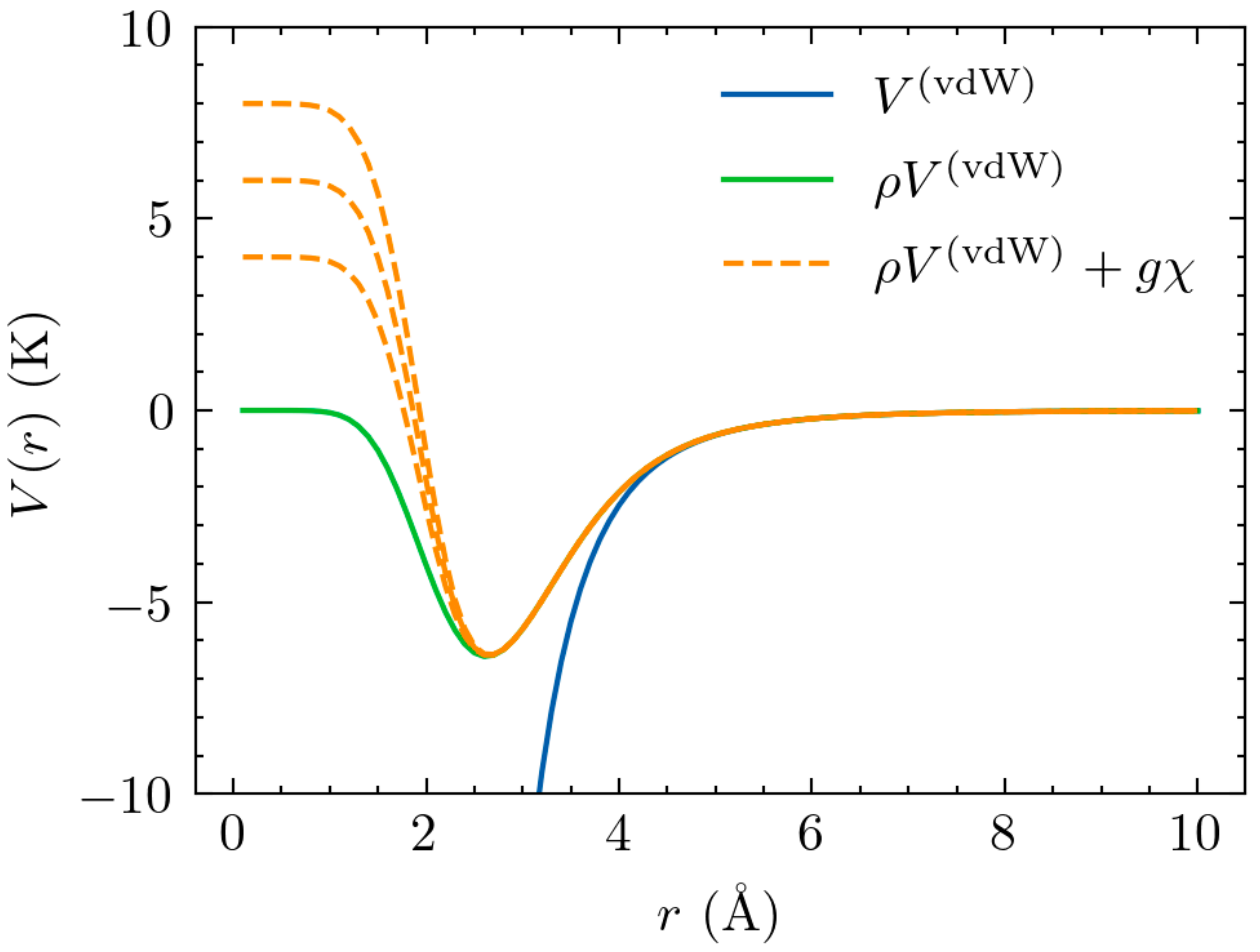
Theory
vdWEFT

The interaction is

$$V(r) = -\frac{C_6}{r^6} + g\delta(r)$$

- $C_6 > 0$ and g is a coupling constant that accounts for the short-distance physics
- The interaction diverges at the origin. so we regulate the vdW term.
- $\delta(r)$ functions are difficult to handle numerically, so we model the delta function with the same scale.

$$V(r) = \left[1 - e^{-(r/R)^2}\right]^6 \left(-\frac{C_6}{r^6}\right) + ge^{-(r/R)^6}$$



Theory

vdWEFT

But now we have introduced a scale, R, that we'd like to ignore. And every calculation using this potential will lead to observables that are dependent on R.

For every value of R we tune g to reproduce the same low-energy observable (e.g. B_2 or a_0). Now, we can study the limit

$$\lim_{R\to 0} \mathcal{O}(R) = \mathcal{O}_\infty (1 + c_1 \frac{R}{\beta_6} + \dots) \ ,$$

where $\mathcal{O}$ can be any other low-energy observable.

Theory

vdWEFT

The example I gave was a local interaction. We work in momentum space, so for the record, our interaction is

$$\tilde{V}_{\ell,\ell'}(p,p') = \tilde{V}^{(\mathrm{vdW})}_{\ell,\ell'}(p,p') + g\ \tilde{\chi}_{\ell,\ell'}(p,p')$$

where

$$\tilde{V}^{(\mathrm{vdW})}_{\ell,\ell'}(p,p') = \tilde{\rho}(p)\tilde{\rho}(p')\ \frac{2}{\pi}\int_0^\infty dr\, r^2 j_\ell(pr)\left[\rho(r)\left(\frac{-C_6}{r^6}\right)\right] j_{\ell'}(p'r)$$

and

$$\tilde{\chi}_{\ell,\ell'}(p,p') = g_\ell(R)\ p^\ell (p')^{\ell'} \tilde{\rho}(p)\tilde{\rho}(p')\ \delta_{\ell,\ell'}$$

Gao Phys. Rev. A 58, 1728 (1998)
Gao Phys. Rev. A 58, 4222 (1998)

Theory

vdW Universality | 2-Body (S-wave)

Bo Gao derived solutions to the Schrödinger equation for an attractive $1/r^6$ potential.

$$u_{E\ell}(r) = A_{E\ell}\left[f^0_{E\ell}(r) - K^0_\ell g^0_{E\ell}(r)\right]$$

He used these solutions in a QDT derivation of the low-energy, effective range expansion for small

$$\Delta \equiv \frac{\beta_6^2}{16}\frac{2\mu E}{\hbar^2} = \frac{(k\beta_6)^2}{16}$$

resulting in expressions for the S-wave parameters

$$a_0 = \frac{2\pi}{[\Gamma(1/4)]^2}\frac{K^0_{\ell=0}(0) - 1}{K^0_{\ell=0}(0)}\beta_6\ , \qquad r_0 \approx \frac{4}{3a_0^2}\left[\frac{2\pi\beta_6^3}{\Gamma\left(\frac{1}{4}\right)^2} - a_0\beta_6^2\right] + \frac{\beta_6\Gamma\left(\frac{1}{4}\right)^2}{3\pi}$$

With the vdW interaction, the effective range is set by the scattering length.

Gao Phys. Rev. A 58, 1728 (1998)
Gao Phys. Rev. A 58, 4222 (1998)

Theory

vdW Universality | 2-Body (P-wave)

Similarly, he found relations for the P-wave parameters

$$a_1 = -\frac{\pi}{18\left[\Gamma(3/4)\right]^2}\frac{K^0_{\ell=1}(0)+1}{K^0_{\ell=1}(0)}\beta_6^3\ ,$$

and

$$r_1 \approx -\frac{2\pi^2\beta_6^8}{1225a_1^3} - \frac{2\pi\beta_6^5}{45a_1^2\left[\Gamma(3/4)\right]^2} - \frac{4\beta_6^2}{5a_1} - \frac{36\left[\Gamma(3/4)\right]^2}{5\pi\beta_6}\ .$$

The phaseshifts for $\ell \geq 2$ are also fixed on β_6.

If we tune g to reproduce a large scattering length (or shallow bound state), we capture the effective range effects as well.

Naidon and Endo 2017 *Rep. Prog. Phys.* 80 056001

Theory

vdW Universality | 3-Body

In the 3-body sector, there has been empirical evidence for an approximate vdW universality.

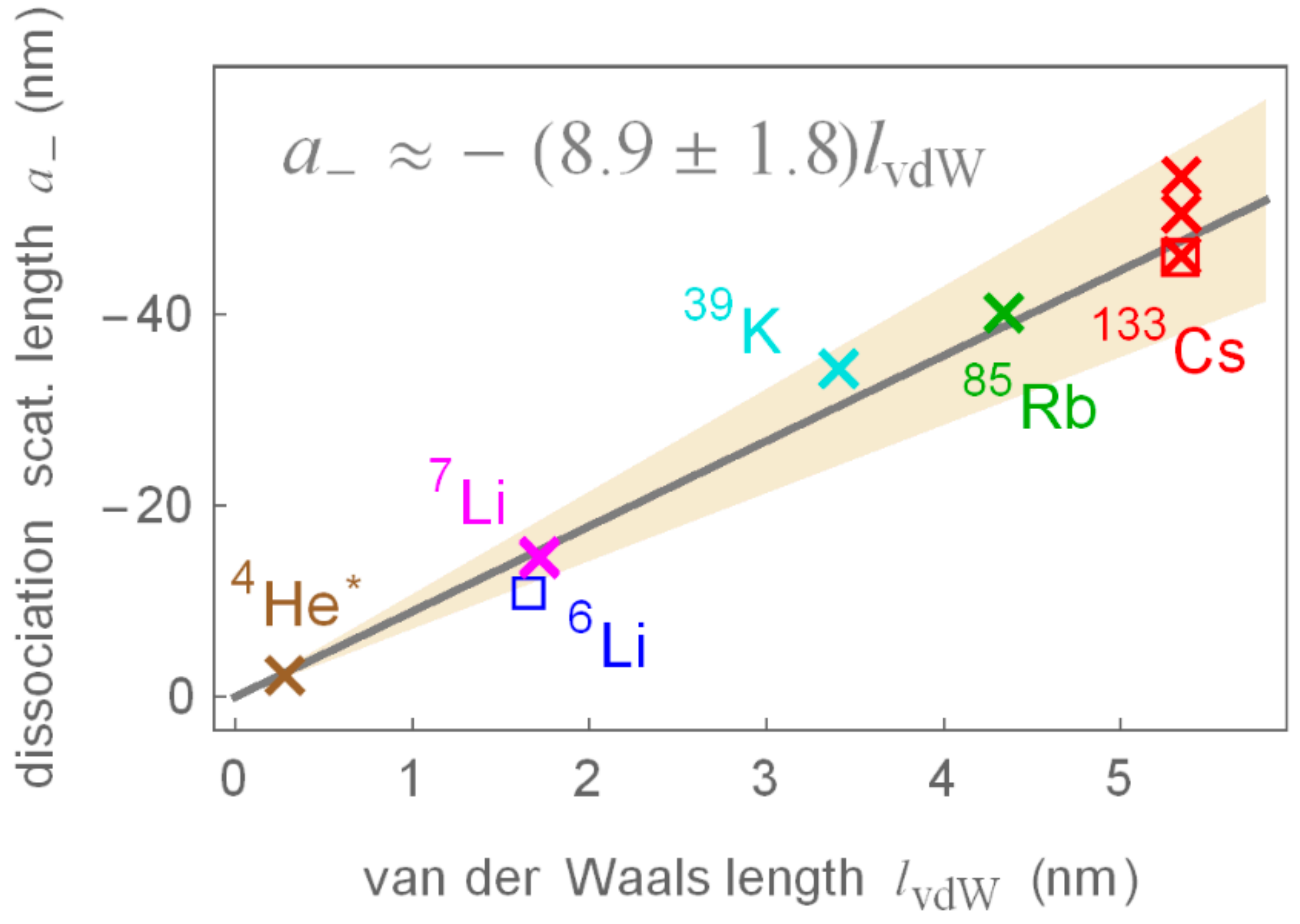
The 3-body parameters are correlated with the vdW length scale.

$$\kappa_*^{(0)} = 2(0.21 \pm 0.01)\ /\beta_6\ ,$$

and

$$a_-^{(0)} = -\,(1/2)(10.70 \pm 0.35)\beta_6\ .$$

Note: $l_{\mathrm{vdW}} = \dfrac{1}{2}\beta_6$



^4He

A Comparison to the LM2M2 Potential

^{4}He

Background

- The $^4He_2$ system exhibits a large scattering length and a strong vdW attraction making the 2- and 3-body systems both playgrounds for universal physics.

- The ^{4}He–^{4}He interaction has been extensively modeled by *ab initio* and semi-empirical potentials.

- The LM2M2 potential has terms that go like $1/r^n$ where $n =$ **6**, 8, and 10.

- We take C_6 from the LM2M2 potential, verify the renormalization (asymptotically R-independent) 2- and 3-body observables, and compare our results to the LM2M2 predictions.

n	β_n	$(m\beta_n^2)^{-1}$ [mK]
6	5.38	419.18
8	3.62	923.42
10	3.09	1272.3

^{4}He

Background

Ji and Phillips, *Few Body Syst.* 54 (2013) 2317-2355

Input		$B_t^{(1)}$ $[B_d]$	$B_t^{(0)}$ $[B_d]$	a_{ad} $[\gamma^{-1}]$	r_{ad} $[\gamma^{-1}]$
a_{ad}	LO	1.723	97.12	1.205	0.8352
a_{ad}	NLO	1.736	89.72	1.205	0.9049
a_{ad} , $B_t^{(1)}$	N^{2}LO	1.738	116.9	1.205	0.9132
$B_t^{(1)}$	LO	1.738	99.37	1.178	0.8752
$B_t^{(1)}$	NLO	1.738	89.77	1.201	0.9130
$B_t^{(1)}$, a_{ad}	N^{2}LO	1.738	115.9	1.205	0.9135
TTY [27, 28]		1.738	96.33	1.205	

The $^4He_2$ and $^4He_3$ systems have been well-characterized by predictions from universality:

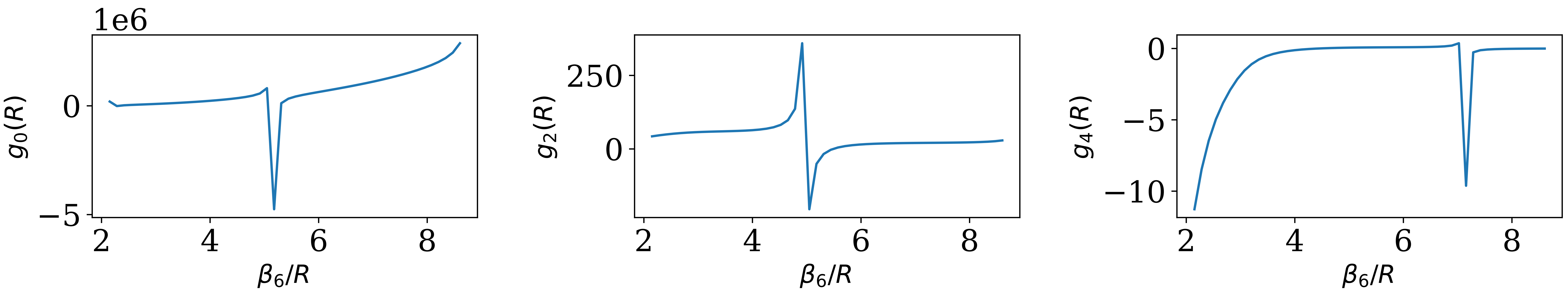
- $B_2 \approx 1/(ma_0^2)$
- The two 3-body states have been associated with Efimov states.

However, the order-by-order convergence of the 3-body ground state in SR-EFT does not appear to follow the behavior we expect.

Can this be improved by including some short-distance physics (long-range effects)?

^{4}He

RG Flows



We need a low-energy observable in each partial wave around which we can expand.

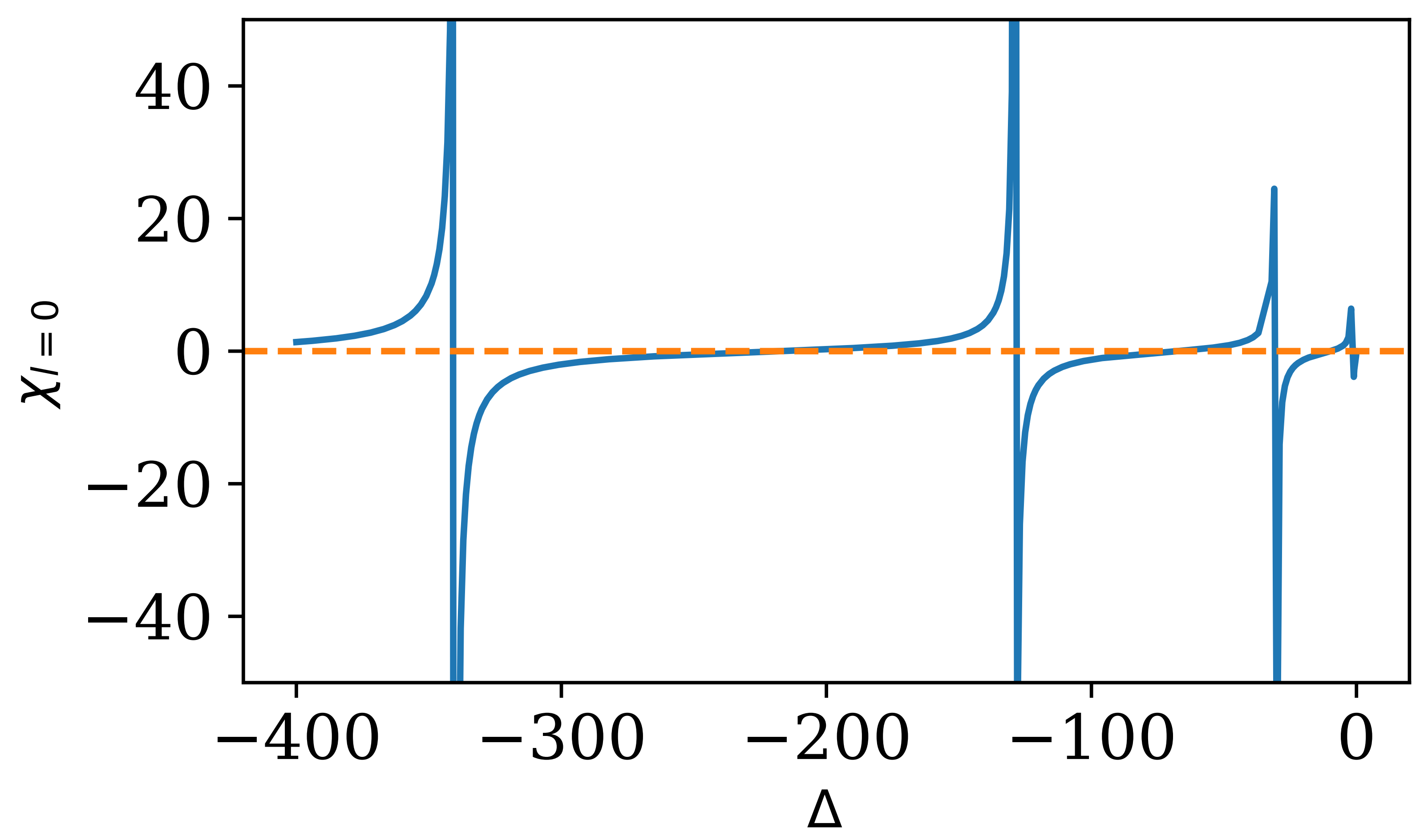
- S-wave: $B_2 = 1.31$ mK
- D-wave: LM2M2 predction for $\delta_{\ell=2}(\Delta = 0.01)$
- G-wave: LM2M2 prediction for $\delta_{\ell=4}(E \leq 15\mathrm{K})$

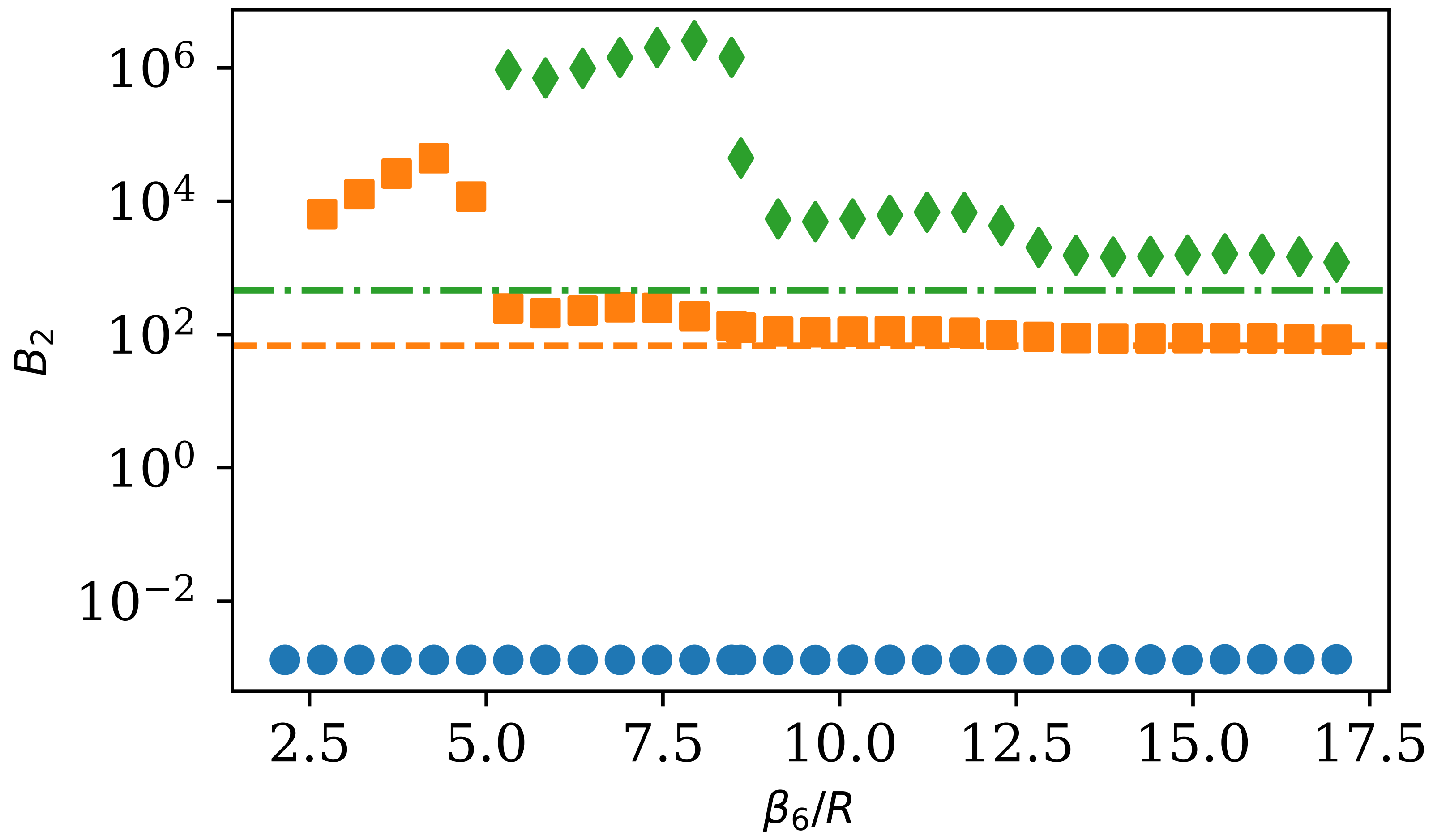
Each pole in the RG flow indicates the inclusion of a bound state.

Gao Phys. Rev. A 58, 1728 (1998)
Gao Phys. Rev. A 58, 4222 (1998)

^{4}He

2-Body Results





Generally, the argument against these bound states is that they are beyond the effective theory's energy regime.

Recall

$$u_{E\ell}(r) = A_{E\ell}\left[f^0_{E\ell}(r) - K^0_\ell g^0_{E\ell}(r)\right]$$

From the asymptotic behavior of the analytical solutions below threshold

$$f^0_{E\ell}(r) \rightarrow (2\pi\kappa)^{-1/2}\left(W_{f-}e^{\kappa r} + W_{f+}e^{-\kappa r}\right)$$

$$g^0_{E\ell}(r) \rightarrow (2\pi\kappa)^{-1/2}\left(W_{g-}e^{\kappa r} + W_{g+}e^{-\kappa r}\right)$$

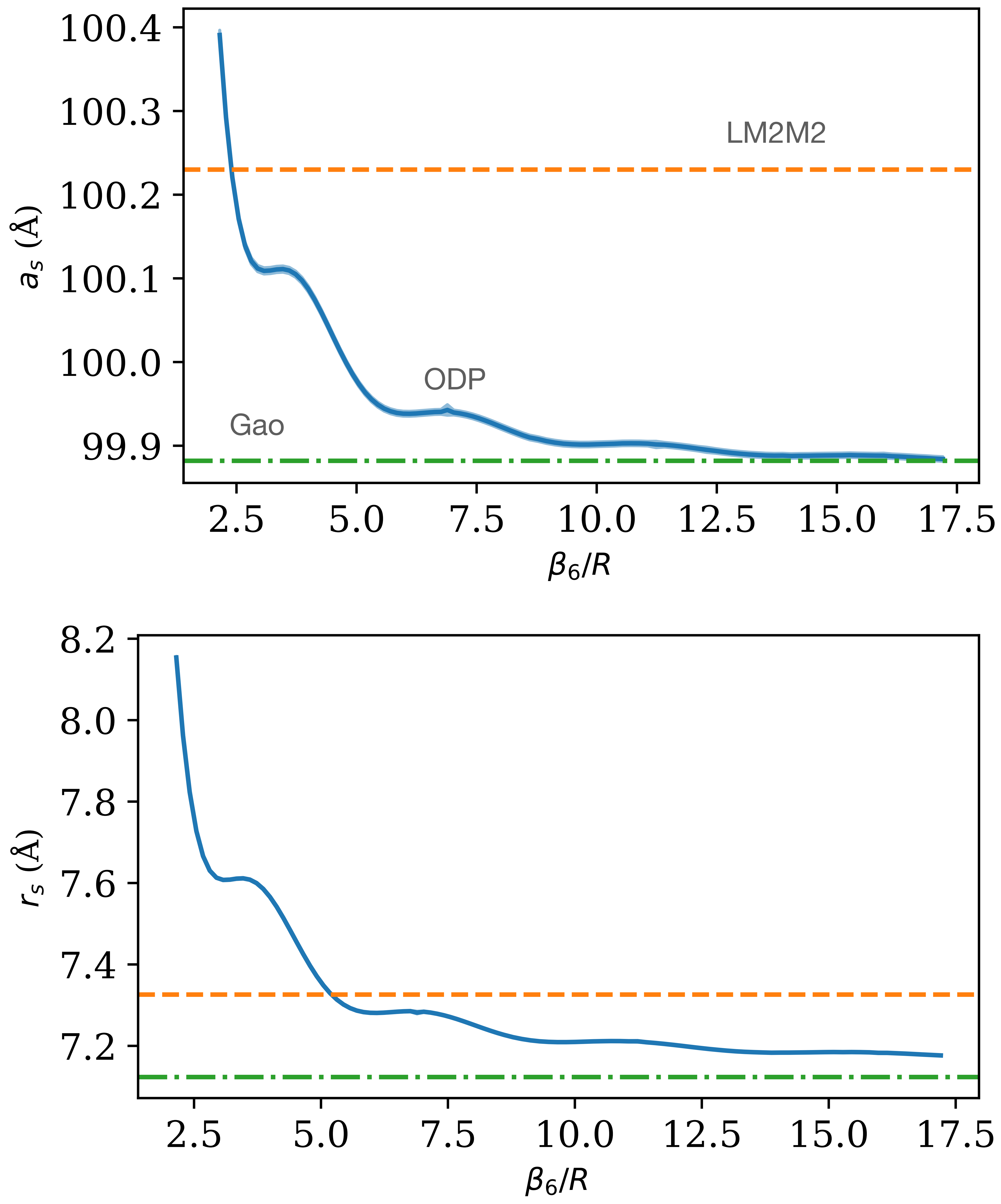
The $e^{\kappa r}$ terms have to cancel, leading to the ratio

$$\chi_\ell(\Delta) \equiv K^0_\ell(E) = W_{f-}/W_{g-}$$

^{4}He

2-Body Results

- $B_2 = 1.31\ \mathrm{mK}$ is fixed with $g(R)$.
- LM2M2: orange, dashed lines
- Gao: green, dashed-dotted lines
- Both converge toward the Gao prediction because our system is an ideal vdW system.
- a_0 is the result of (generic) universality
- r_0 is the result of vdW universality



^{4}He

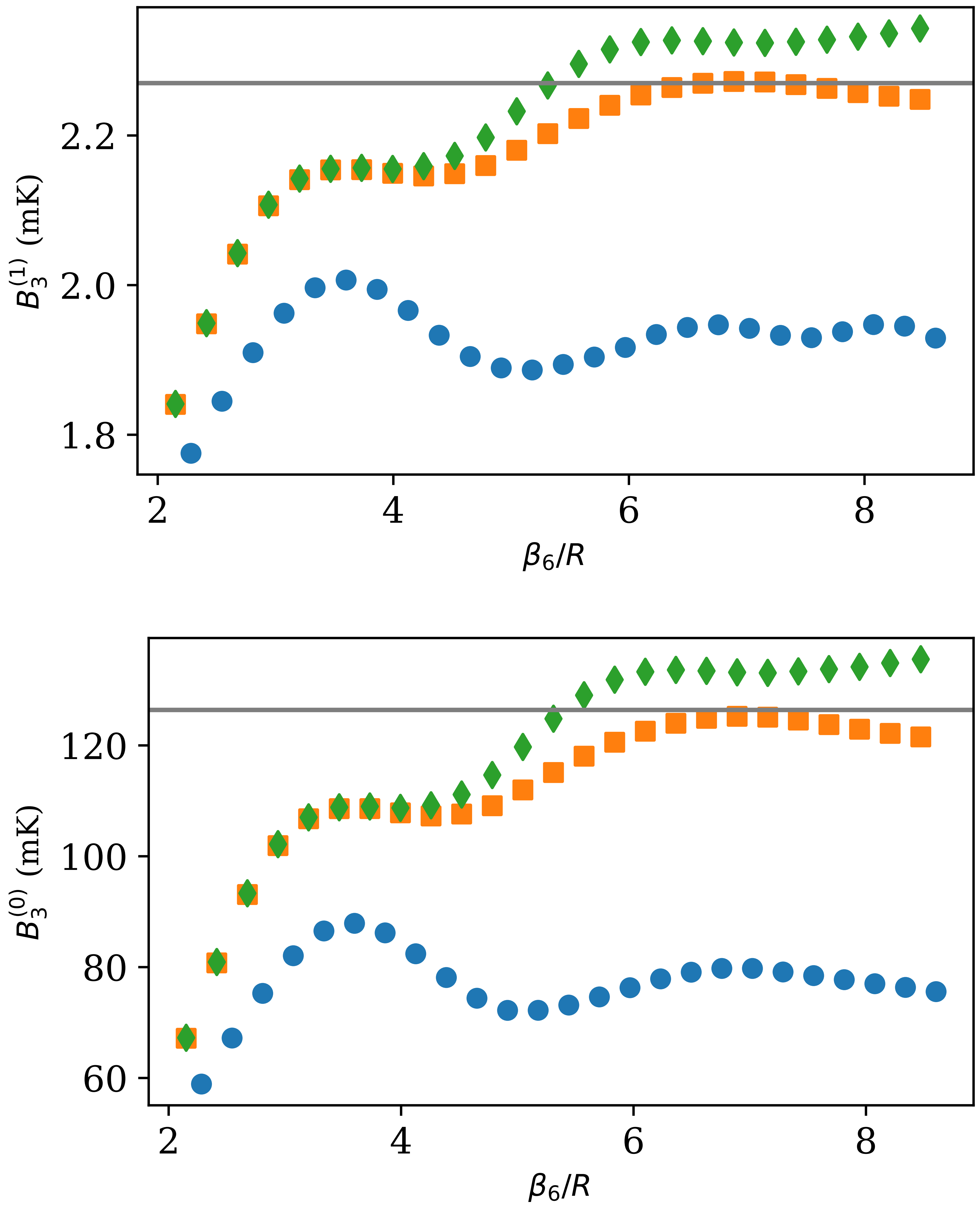
3-Body Results

- S (blue), SD (orange), and SDG (green) results are shown for the ground and excited trimer states. $(\ell, \lambda) \rightarrow J$

- The solid, grey line is the result of Roudnev and Cavagnero.

- There is significant (though apparently decreasingly so) contribution from higher partial waves.

- Calculations at arbitrarily small R are numerically difficult.

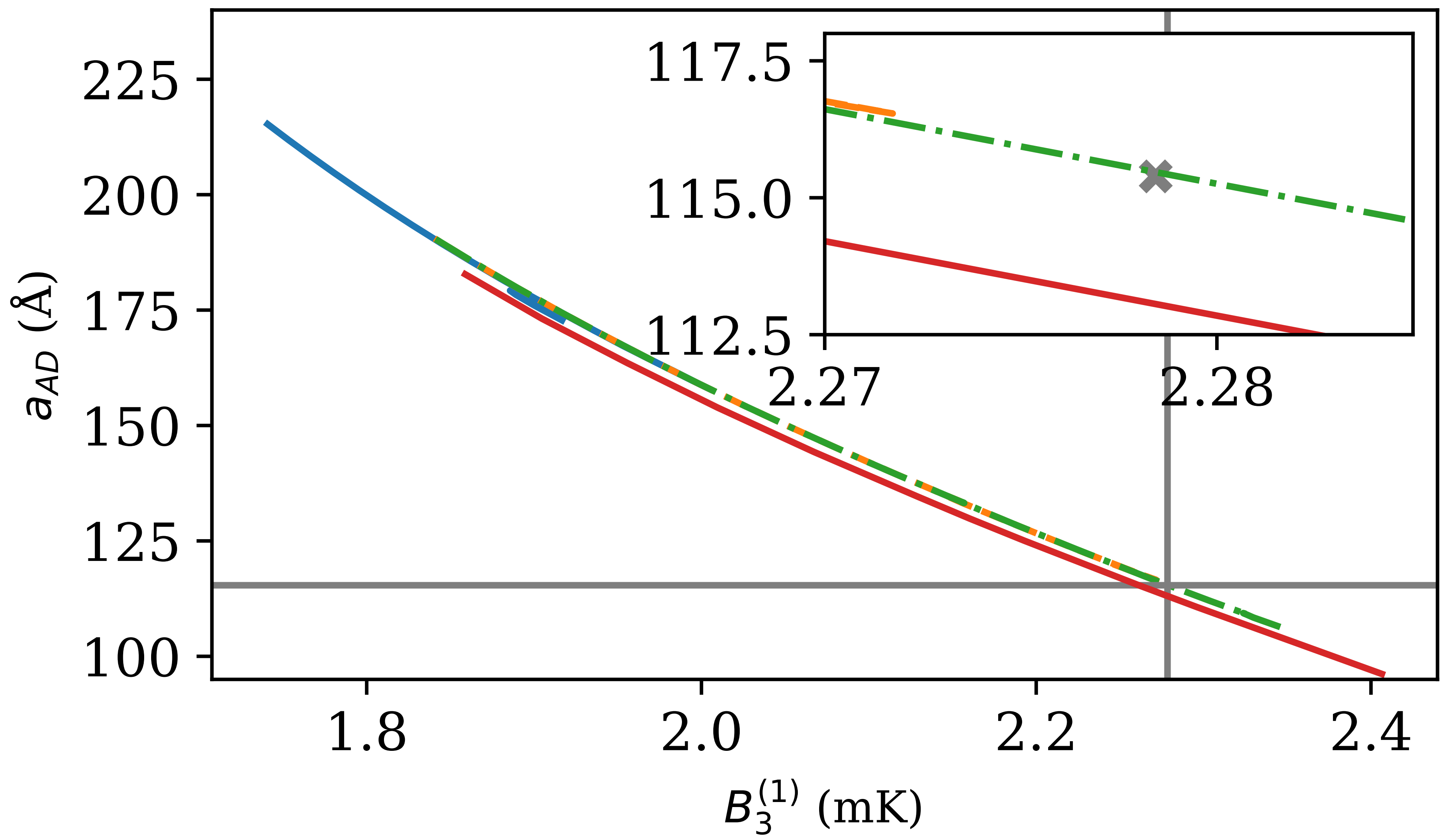


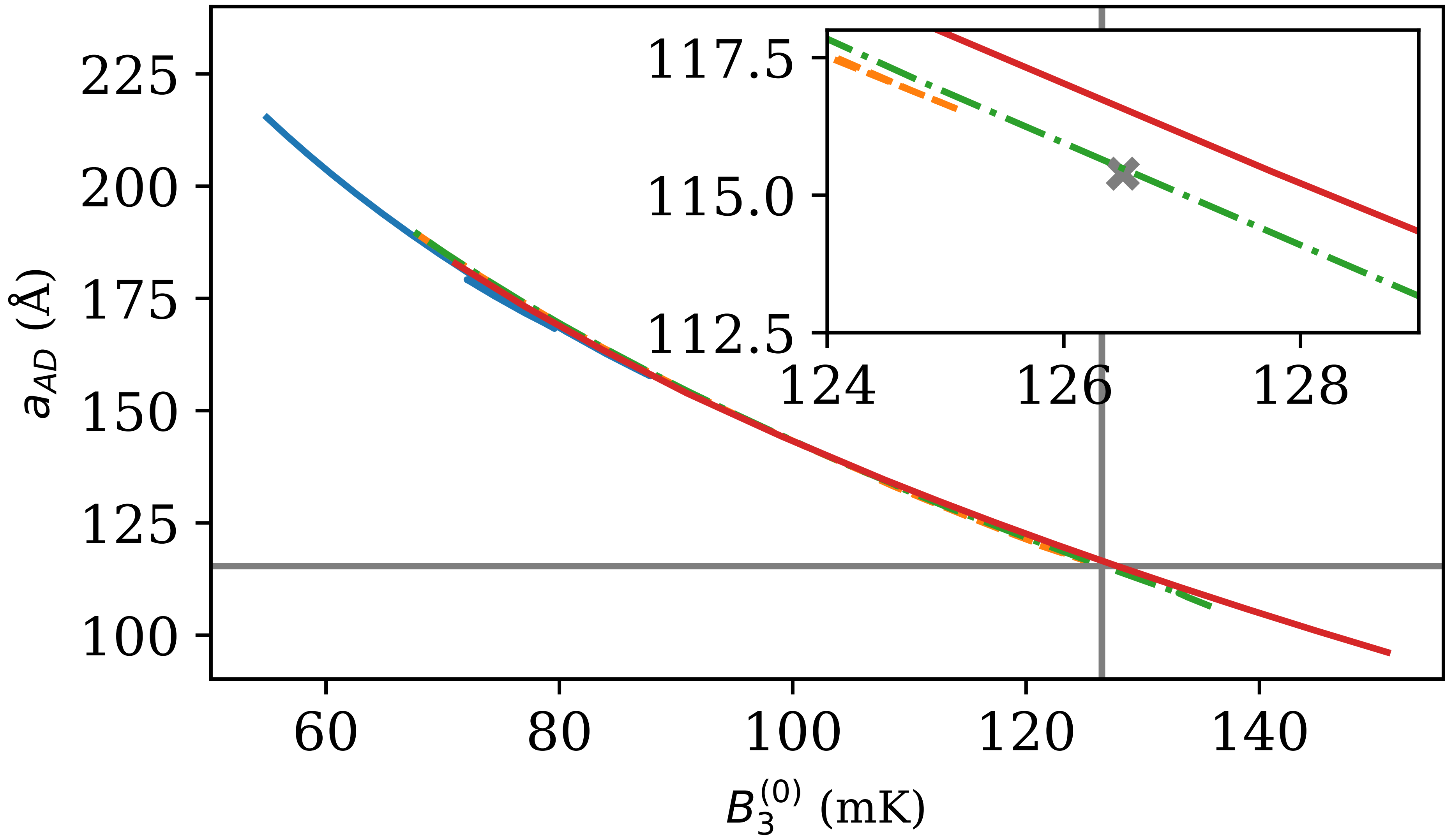
Roudnev and Cavagnero, Journal of Physics B: AMO Physics 45, 025101 (2011)

^{4}He

3-Body Results

- The Phillip's lines are shown for all partial-wave calculations: S (blue), SD (orange), and SDG (green).
- SR-EFT prediction is shown in red.
- Roudnev and Cavagnero is the grey x.
- From the insets, one can see the improvement that the vdW interaction brings.





^{4}He

Uncertainties

- Theory uncertainties need to be assessed with (minimally) an NLO calculation.
  - Our estimate takes the ground trimer state as the highest-energy prediction and compares it to the scale where we know non-vdW physics enters.
- Variations in $\mathcal{O}(R)$ above the breakdown scale ($\beta_6/R \approx 2, 3$), can be used to provide an uncertainty estimate.
  - This is **highly** regulator-dependent.

Theory

n	β_n	$(m\beta_n^2)^{-1}$ [mK]
6	5.38	419.18
8	3.62	923.42
10	3.09	1272.3

$$\sqrt{B_3^{(0)}/E_8} \approx 1/3$$

Regulator

$\mathcal{O}$	$\mathcal{O}((\beta_6/R)_{\max})$	$\delta\mathcal{O}$
a_s (Å)	99.9	0.1
r_s (Å)	7.2	0.1
$B_3^{(0)}$ (mK)	135	10
$B_3^{(1)}$ (mK)	2.3	0.1
a_{AD} (Å)	105	10
r_{AD} (Å)	85	10

^{6}Li

Seeking Improvement Over SR-EFT

^{6}Li

Motivation and Background

- 3-body recombination is the process of 3 free atoms interacting and resulting in a dimer and a spectator particle (now with newly available KE).

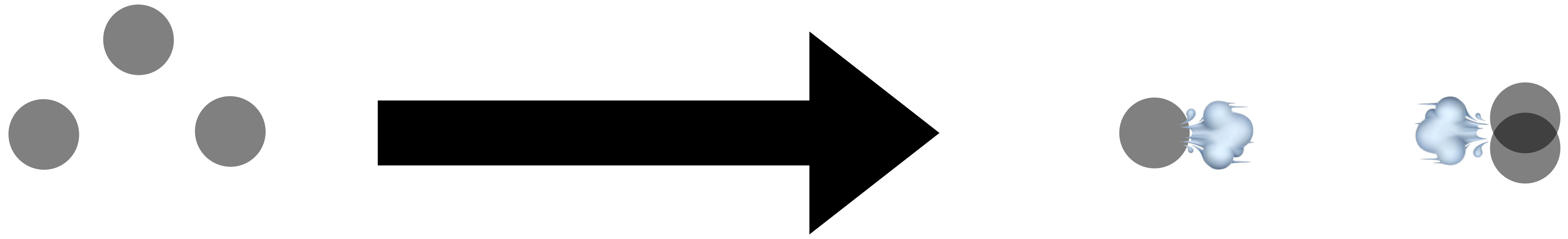
- In a trap of cold atoms, this drives the particles out.

- Measurements of the loss coefficient are directly proportional to the thermal average of the recombination rate.

- ^{6}Li is a fermion.

  - The dimer forms in a relative P-wave.

  - The experiments we compare to measure spin-polarized atoms (identical).



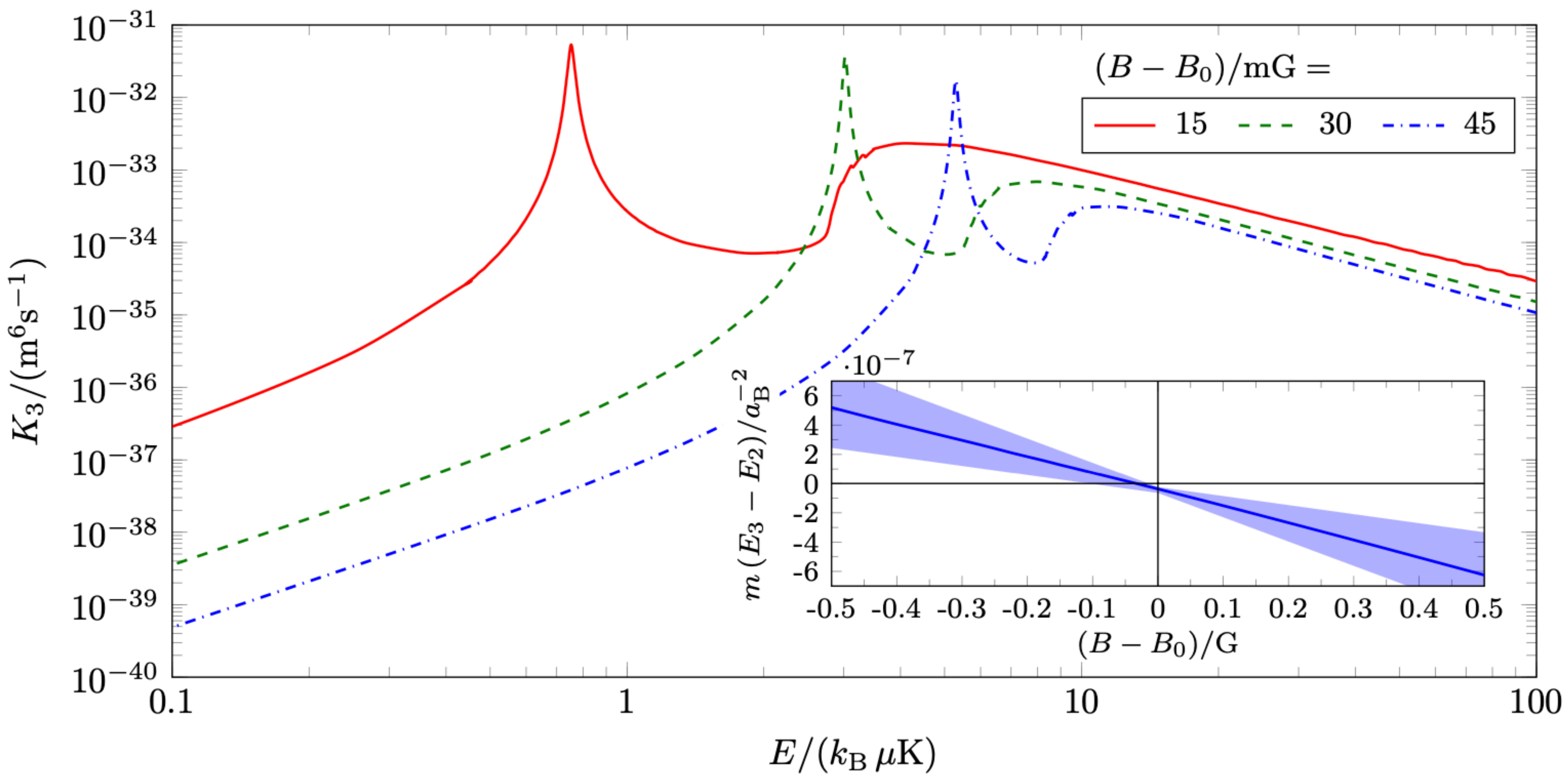
$$L_3(T) = \frac{1}{2}\langle K_3 \rangle (T)$$

- For (large) $a_1 > 0$, the dimer is shallow.

- For (large in magnitude), $a_1 < 0$, the dimer is deep (resonance is shallow).

^{6}Li

Motivation and Background



Schmidt, Platter, and Hammer Phys. Rev. A 101, 062702

Schmidt et al. predicted the recombination rate using SR-EFT.

They fit:

- r_1, the 3-body force (H), and the short-distance three-body parameter (F)
- H fixes the position the 3-body resonance.
- F quantifies the overlap between the deep dimer states and the continuum.

The peak is the 3-body resonance.

The “shoulder” is the effect of the 2-body resonance.

$$a_1(B) \approx \frac{a_{1,\mathrm{bg}}\Delta B}{B - B_0}$$

$$k_{\mathrm{res}}(B) = \sqrt{\frac{2}{a_1(B) r_1}}$$

^{6}Li
Theory

- We tune $g_{\rm LO}$ to reproduce a_1 (unique for each detuning, for $B = 15\ \mathrm{mG}$, $a_1 = -2.7e7\ \mathrm{\AA}^3$).
- The vdW interaction then gives r_1 and (maybe) the 3-body resonance…
- The interaction is similar to the S-wave case, except now the (LO) counterterm is

$$g_{\rm LO}\left(\frac{p}{\Lambda}\right)\left(\frac{p'}{\Lambda}\right)\tilde{\chi}(p)\,\tilde{\chi}(p')$$

^{6}Li

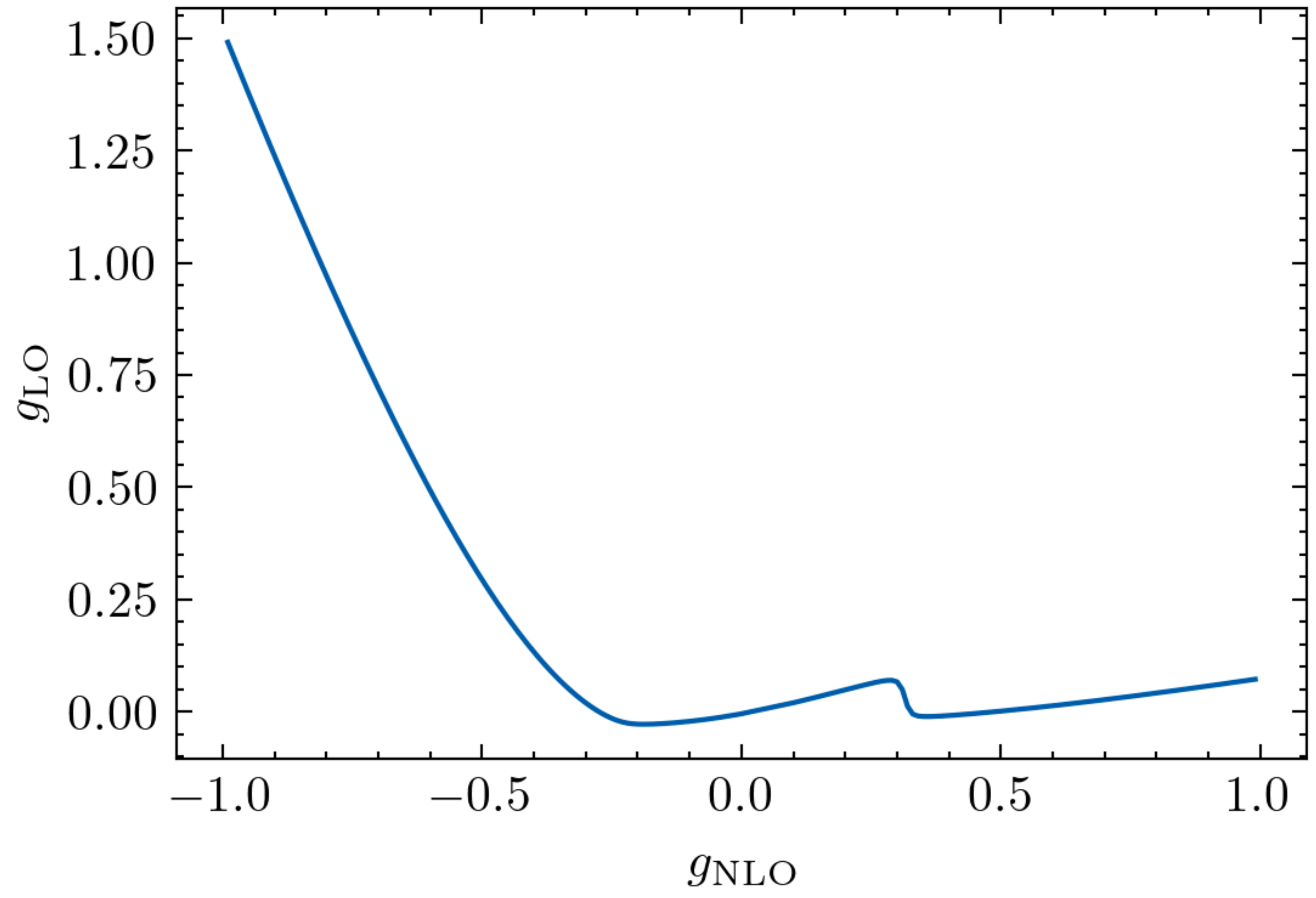
2-Body Results

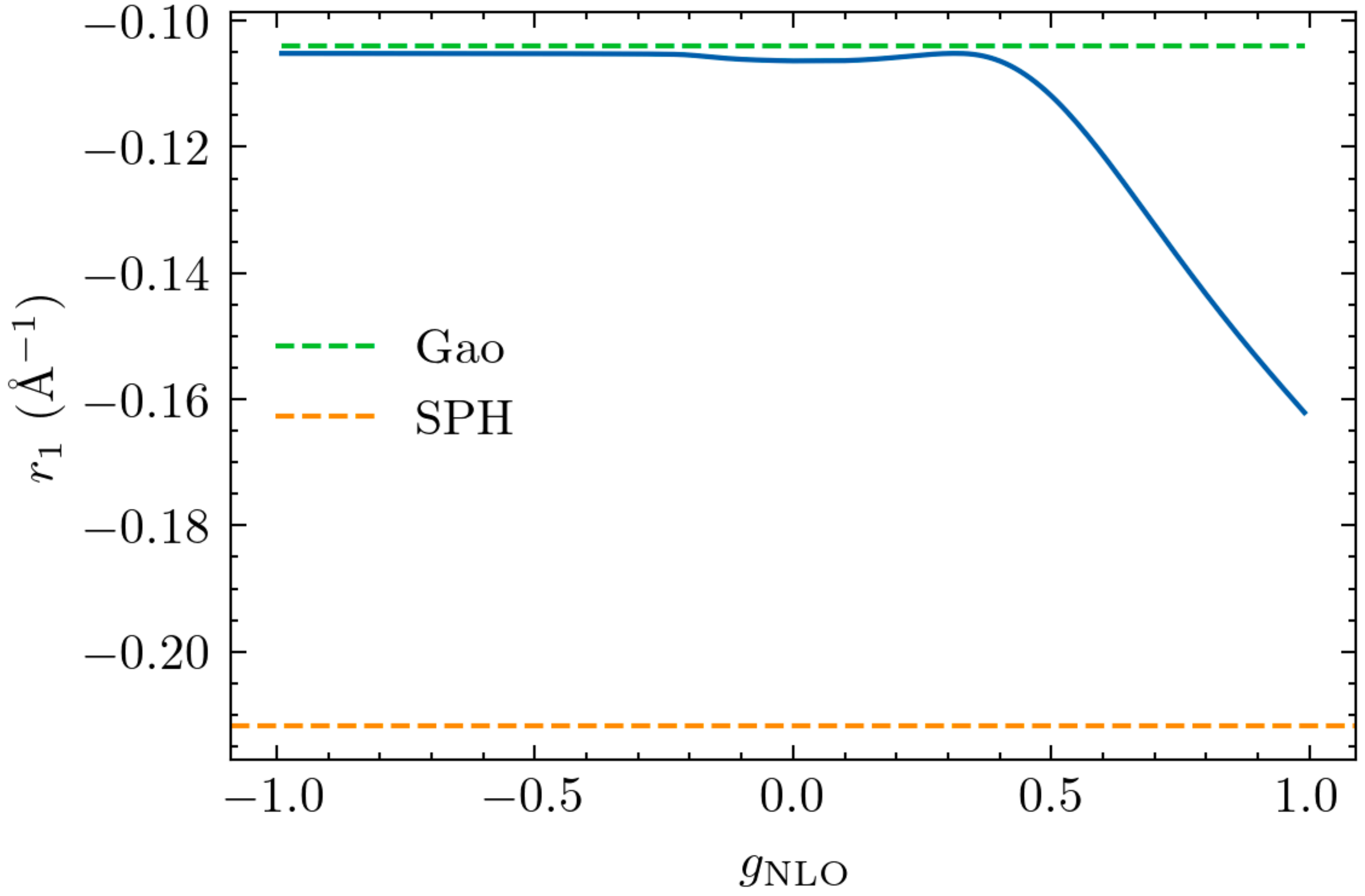
- The vdW r_1 is a factor of ≈2 smaller (in magnitude) than the r_1 found in the SPH fit.

- Proposed solution: Add an NLO counterterm.

$$g_{\rm NLO}\left(\frac{p}{\Lambda}\right)\left(\frac{p'}{\Lambda}\right)\left[\frac{(p/\Lambda)^2+(p'/\Lambda)^2}{2}\right]\tilde{\chi}(p)\,\tilde{\chi}(p')\ .$$

- The system appears to be very fine-tuned.

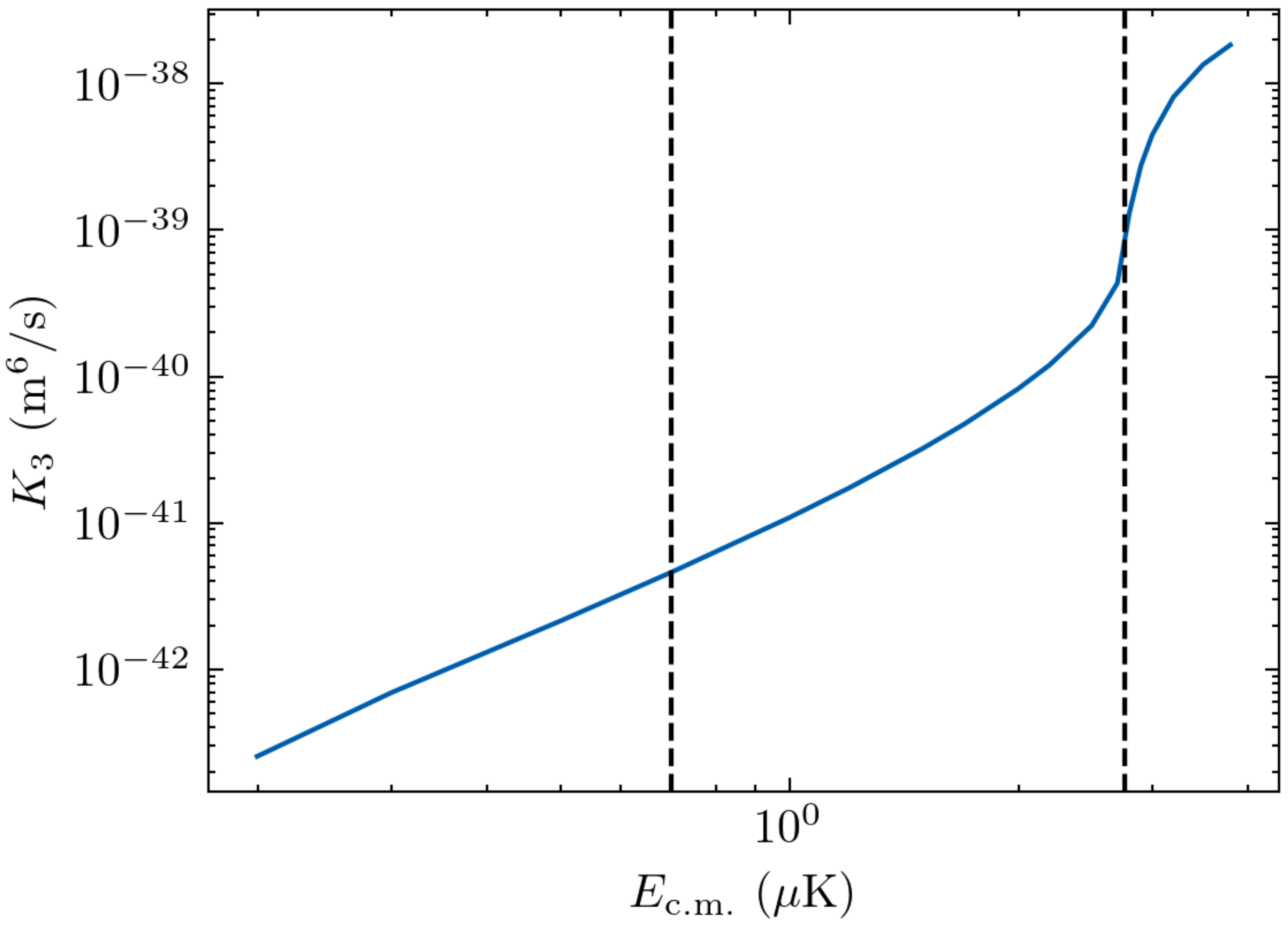




^{6}Li

3-Body Results

- The recombination rate, K_3, is shown for $R = 5.5\ \text{Å}$.
- We reproduce the SPH "shoulder" (by construction).
- The 3-body resonance at $E_{\text{c.m.}} = 0.7\ \mu\text{K}$ is missing.
    - This is the smallest R value we have tested.
    - $B_2 = 2.14\ \text{K}$



Closing Remarks

- Including more physics results in significant improvement.
  - The $^4He_2$ and $^4He_3$ systems are well-described by vdWEFT.
    - Improves the agreement with the Phillips line.
- $^6Li_2$ and $^6Li_3$ systems are fine-tuned; they may have some other significant effect that “obscures” the vdW attraction.
  - Is there some other piece of the interaction that contaminates the vdW attraction?
  - How much does the deep dimer spectrum matter?
  - Does P-wave vdW universality continue into the 3-body sector?