**TODO LIST**

# The short-range effective field theory with van der Waals tail at next-to-leading order


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## Abstract

We construct the first subleading correction in an effective field theory with short-range interactions and a van der Waals tail. We analyze the of the coupling constants with the short-distance regulator necessary within this framework. We study the size of the corrections that such a next-to-leading order term gives and argue that a counting for higher order corrections should be done on the basis of a modified effective range expansion. Furthermore, we discuss constraints on the next-to-leading oder correction imposed by causality and consider some physically relevant two-body examples. Finally, we use this interaction to analyze subleading corrections in the three-body sector.



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## I. INTRODUCTION

The long-range part of the interaction between atoms is frequently the van der Waals interaction (vdW), *i.e.* $1/r^6$, where $r$ denotes the relative distance between two atoms. Frequently, this vdW part is combined with a more complicated short-distance form to construct models [[REF he4]] intended to describe observables of these systems to high accuracy.

An alternative approach to construct an Hamiltonian for atoms interacting at long distances through a vdW tail is to build an effective interaction. Such an interaction whose construction uses simple building blocks and is based on simple principles promises a

This approach is very similar in spirit to the quantum defect theory that has been applied to the vdW problem by Bo Gao to derive the two-body wave functions of two particles interacting through a vdW potential [1].

Recently, we evaluated the potential of such an effective theory approach using the $^4$He dimer and trimer system as our benchmark system [2]. We found that a regularized and renormalized interaction vdW interaction with one short-distance counterterm can describe these systems very well.[[expand]]k

In this manuscript, we will extend the work started in Ref. [2] and include the first subleading correction in $S$- and $P$-waves. We will focus on systems with a large scattering length in the S-wave and a large scattering volume in the P-wave and discuss the implications of Gao's work for these system. We will also address the constraints imposed by causality onto such an approach. Furthermore, we will construct the interaction that can be used in a momentum space formalism to calculate observables of two- but also higher-body systems. Since the vdW is singular, we will also explain how this interaction is regularized and renormalized. We will then again display how causality expresses itself in renormalized observables.

## II. QUANTUM DEFECT THEORY FOR THE VAN DER WAALS INTERACTION

### A. The van der Waals two-body wave functions

In Refs. [1], Gao derived exact solution for the two-body system interacting through a van der Waals interaction of the form

$$V(r) = -\frac{C_6}{r^6} \ . \tag{1}$$

Change this section to include an NLO discussion:

- What happens if we include K2 in the Gao stuff.
- What does Konigs work imply for K2 and thereby for the effective range. We can derive formulas that givegx explicit bounds close to the resonance. This would be a new result.
- What happens close to resonance. Discuss that linear terms in P-wave drops out. I think non-analytic pieces also drop out in the S-wave. Is this a general feature? What happens for example in the D-wave?

The van der Waals *strength* $C_6$ can be converted into a *characteristic* length scale $\beta_6 \equiv (mC_6)^{1/4}$, where $m$ is the mass of the interacting particles. Gao derived solutions to the attractive $1/r^6$ potential in Ref. [1]. The bound state wave function of the state with energy $E$ in partial wave $l$ is written as the linear combination of two solutions,$f_{El}(r)$ and $g_{El}(r$ of the van der Waals interaction

$$u_{El}(r) = A_{El}\left[f_{El}(r) - K_l g_{El}(r)\right] \ , \tag{2}$$

where $A_{El}$ is a normalization coefficient and $K_l$ denotes the so-called short-range K-matrix that fixes here an additional boundary condition on the wave function that is required due to the potentials's singularity at its origin. The precise forms of the functions $f_{El}(r)$ and $g_{El}(r)$ are given in Ref. [1]. For bound states, their asymptotic form is given by

$$\begin{aligned} f_{El}(r) &\to (2\pi\kappa)^{-1/2}(W_{f-}e^{\kappa r} + W_{f+}e^{-\kappa r}) \ , \\ g_{El}(r) &\to (2\pi\kappa)^{-1/2}(W_{g-}e^{\kappa r} + W_{g+}e^{\kappa r}) \ , \end{aligned} \tag{3}$$

where $\kappa$ represents the bound state momentum and the coefficients $W_{f\pm,g\pm}$ depend on the energy, $E$, and the angular momentum, $l$, of the of bound state [1].

Requiring Eq. (2) to give normalizable solution implies that the terms proportional to $e^{\kappa r}$ in Eq. (3) cancel and leads to

$$K_l(E) = \chi_l(\Delta) = W_{f-}/W_{g-} \ , \tag{4}$$

where $\Delta = 2\mu E\beta_6^2/16\hbar^2$.

The solid line in Fig. **??** shows the function $\chi_{l=0}(\Delta)$ for an arbitrary value $\beta_6$. The intersections between the dashed line and the solid line give the two-body binding energies in terms of the rescaled energy variable $\Delta$ once the boundary condition is chosen either by adjusting the energy ($\Delta$) - position of one the intersections or by adjusting a scattering observable.

Expressions for the asymptotic solutions at positive energies can be used to derive expressions for the two-body t-matrix and thereby for the effective range parameters. Gao obtains for the S-wave scattering length and effective range [3]

$$\begin{aligned} a_s &= \frac{2\pi}{[\Gamma(1/4)]^2}\frac{K_0(0)-1}{K_0(0)}\beta_6 \ , \\ r_s &\approx \frac{[\Gamma(1/4)]^2}{3\pi}\frac{K_0(0)^2+1}{[K_0(0)-1]^2}\beta_6 \ , \end{aligned} \tag{5}$$

where the $K_l(0)$ is evaluated at zero energy (threshold). The relation for $r_0$ is truncated under the assumption that the derivative of the short-range $K$-matrix is small. In effect, we can calculate the boundary condition, $K_0(0)$, from $a$, and then calculate $r_0$.

The scattering length is then dependent on the van der Waals length scale, $\beta_6$ and the short-range $K$-matrix, $K_l$, evaluated in the $s$-wave channel at zero energy.

### B. The modified effective range

We discussed above that the

## III. THE WIGNER BOUND AT UNITARITY

Elhatisari *et al.* [4] took the expansion of the short-range $K$ matrix

$$K^{(0)} = \tan\delta_\ell^{(\mathrm{short})}(k) = \sum_{n=0}^{\infty} K_{\ell,2n}k^{2n} \ , \tag{6}$$

and derived a causality bound on the second coefficient of the expansion, given by

$$K_{\ell,2} \leq b_\ell(r) \ . \tag{7}$$

This constraint on the subleading coefficient of the short-range K-matrix limits the values of the effective range. Below we will discuss the implications for S- and P-waves.

### A. $S$ Waves

Gao derived the scattering phaseshifts using the exact solutions of the wave functions of the two-body system interacting through a van der Waals interaction

$$\begin{aligned}
(\beta_6 k)\cot\delta = &\left[-\frac{(\beta_6 k)^2}{3} - \frac{1}{90}\pi\beta_6^6 k^6\left(K - \frac{181}{70\pi}\right) - \frac{11}{900}\beta_6^4 k^4\left(K - \frac{30\pi}{11}\right) + \frac{2\pi^2\beta_6^5 k^5(K-1)}{15\Gamma\left(\frac{1}{4}\right)^2} - K\right] \\
&\times\left\{\frac{1}{\Gamma\left(\frac{1}{4}\right)^2}\left[2\pi\left(-\frac{4}{15}\beta_6^4 k^4\log(\beta_6 k) + \frac{2}{15}\beta_6^4 k^4\left(\frac{22}{5} - \gamma + \log(2)\right) + 1\right)\right.\right. \\
&\times\left(-\frac{1}{90}\pi\beta_6^6 k^6\big(K + \frac{181(K+1)}{70\pi} - 1\big)\right. \\
&\left.\left.+\frac{11}{900}\beta_6^4 k^4\big(K + \frac{30}{11}\pi(K+1) - 1\big) + \frac{1}{3}\beta_6^2 k^2(K+1) + K - 1\right)\right] \\
&\left. - \frac{1}{15}\pi\beta_6^3 k^3\big(\frac{\beta_6^2 k^2}{3} + K\big)\right\}^{-1}
\end{aligned} \tag{8}$$

Using the expansion in Eq. (6) to first order and expanding Eq. (8) in powers of $k$ gives the effective range parameters and additional pieces that are non-analytic in the energy

$$k\cot\delta_S = -\frac{1}{a_0} + c_1 k + \frac{r_s}{2}k^2 + \dots \ . \tag{9}$$

For the $S$-wave scattering length, $a_0$, one finds [3]

$$a_0 = \frac{2\pi\beta_6(K_{0,0}-1)}{K_{0,0}\Gamma\left(\frac{1}{4}\right)^2} \ , \tag{10}$$

where it is uniquely determined by the leading order term of the short-range $K$-matrix expansion, $K_{0,0}$, and the van der Waals length, $\beta_6$.

The coefficient $c_1$ is zero

$$c_1 = 0 \ . \tag{11}$$

The $S$-wave effective range is then determined by $a_0$ and the coefficient of the second term of (6),

$$r_0 = \frac{a_0^2 \Gamma\left(\frac{1}{4}\right)^4 (\beta_6^2 + 3K_{1,2}) - 4\pi a_0 \Gamma\left(\frac{1}{4}\right)^2 (\beta_6^2 + 3K_{1,2}) + 4\pi^2 (2\beta_6^2 + 3K_{1,2})}{6\pi a_0^2 \beta_6 \Gamma\left(\frac{1}{4}\right)^2} \,. \tag{12}$$

In the unitary limit, $a_0 \to \infty$, leaving

$$r_0^{(\infty)} = \frac{\beta_6^2 \Gamma\left(\frac{1}{4}\right)^4 + 3K_{1,2}\Gamma\left(\frac{1}{4}\right)^4}{6\pi\beta_6\Gamma\left(\frac{1}{4}\right)^2} \tag{13}$$

The first contribution to this expansion that is non-analytic in the energy is $c_3$

$$c_3 = -\frac{K_{0,0}^2 \Gamma(\frac{1}{4})^4}{60\pi(K_{0,0}-1)^2}\beta_6^3 \,. \tag{14}$$

We note that it depends on $K_{0,0}$ but not on $K_{0,2}$. Using Eq. (10), and taking the limit $a_0 \to \infty$ gives

$$c_3^{(\infty)} = 0. \tag{15}$$

This result was used in Ref. [5] to apply the EFT with short-range interactions at next-to-next-to-leading order (N2LO)to the $^4$He trimer.

The first non-analytic contribution that doesn't vanish in the unitary limit is $c_5$

$$c_5 = \frac{\pi}{15}\beta_6^5 \,. \tag{16}$$

An N2LO calculation is therefore the most accurate calculation that can be carried out with the SREFT for vdW systems.

We now turn to the constraint placed on the effective range by the Wigner bound. In the zero-range limit, $K_{1,2}$ is negative because $\lim_{r\to 0} b_{\ell=1}(r) = 0$. This places an upper bound on the $S$-wave effective range

$$r_0^{(\infty)} \leq \frac{\beta_6 \Gamma\left(\frac{1}{4}\right)^2}{6\pi} \approx 0.697\beta_6 \,, \tag{17}$$

which essentially states that the effective range will be of order of the van der Waals length scale. [[LP: need to write a bit about what happens when we are not in the zero-range limit. Can we identify the breakdown scale for the $^4$He system from the convergence plots in our old paper? What is $b_0$ for that breakdown sacle. Is this consistent with the effective range in the $^4$ system?]]

*a.* **The $^4$He system-**

## B. $P$ Waves

Similar inferences can be made in the $P$-wave sector. The $P$-wave scattering volume, $a_1$, was predicted by Gao [3] to be

$$-\frac{\pi\beta_6^3(K_{1,0}+1)}{18K_{1,0}\Gamma\left(\frac{3}{4}\right)^2}\ , \tag{18}$$

where the scattering volume is again uniquely defined by the first term in the expansion (6) and the van der Waals length, $\beta_6$.

The $P$-wave effective range expansion for systems with a dominant, attractive $1/r^6$ potential at low energies contains nonanalytic terms (in $E$). The first of these nonanalytic terms is linear in $k$, and after swapping out the $K_{1,0}$ dependence with its relationship to $a_1$, we have

$$d_1 = \frac{\pi\beta^4}{35\mathrm{a1}^2}\ . \tag{19}$$

For our purposes, where we study systems near or at unitarity, this does not introduce any additional complexity because, as it is readily apparent, $\lim_{a_1\to\infty} d_1 = 0$.

The quadratic term in (6) for $\ell = 1$, the "effective momentum", can be written in terms of the short-range $K$ matrix and the scattering volume,

$$r_1 = -\frac{\pi^2\beta_6^8}{1225\mathrm{a1}^3} + \frac{\pi\left(5\beta_6^3K_{1,2}-2\beta_6^5\right)}{90\mathrm{a1}^2\Gamma\left(\frac{3}{4}\right)^2} + \frac{2K_{1,2}-\frac{2\beta_6^2}{5}}{\mathrm{a1}} - \frac{18\Gamma\left(\frac{3}{4}\right)^2\left(\beta_6^2-5K_{1,2}\right)}{5\pi\beta_6^3}\ . \tag{20}$$

In the unitary and zero-range limits, a constraint similar to the one derived for $r_0$ is placed on $r_1$,

$$r_1 \leq -\frac{36\Gamma\left(\frac{3}{4}\right)^2}{5(\pi\beta_6)} \approx -3.44\frac{1}{\beta_6}\ . \tag{21}$$

# IV. THE EFFECTIVE VDW INTERACTION AT NEXT-TO-LEADING ORDER

As a LO approximation of the $^4$He system, we take the $C_6$ coefficient from the LM2M2 potential [6], and account for the short-distance behavior with a single, two-body, momentum-space counterterm described below. We regulate (cut off) the potential distance $R$ with a regulator function $\rho(r;R)$

$$\rho(r;R) = \left[1-e^{-(10r/R)^2}\right]^8\ , \tag{22}$$

such that the full, coordinate-space potential is

$$V(r) \equiv \rho(r;R) V_6(r) \ . \tag{23}$$

The local regulator is evaluated at a shorter distance, $R/10$, than the nonlocal regulators described below. This ensures that cutoff effects are isolated to a single scale — that there are no interferences between the local and nonlocal regulators in the momentum-space potential. It is also worthwhile noting that other regulators can be used but that their specific form can influence the rate of convergence with respect to the number of grid points in numerical calculations.

We will solve for two- and three-body observables in momentum space. We therefore calculate the momentum space interaction through the Fourier transform of the regulated coordinate space version of the van der Waals interaction

$$\tilde{V}_{l,l'}(p,p') = \tilde{\rho}(p;R)\tilde{\rho}(p';R)\ \frac{2}{\pi}\int_0^\infty dr\, r^2 j_l(pr) V(r) j_{l'}(p'r) \ , \tag{24}$$

where

$$\tilde{\rho}(p;R) = e^{-(pR/2)^8} \ , \tag{25}$$

is the nonlocal regulator and $j_l(pr)$ are the spherical Bessel functions.

Once regulated at a short distance, $R$, physical observables are then dependent on the arbitrary choice of $R$ which is removed by introduction of the counterterm

$$\tilde{\chi}_{l,l'}(p,p';R) = g_l\ p^l (p')^{l'} \tilde{\rho}(p;R)\tilde{\rho}(p';R)\ \delta_{l,l'} \ . \tag{26}$$

For every value of $R$ the counterterm $g_l$ is readjusted such that a two-body observable is reproduced. We will refer to the functional dependence of $g_l$ as renormalization group flow. A more detailed discussion of the renormalization scheme can be found in Subsection **??**.

### A. $S$-wave renormalization

### B. $P$-wave renormalization

The unregularized form of the contact interaction is

$$V_{\text{contant,LO}} = g_0 \mathbf{p} \cdot \mathbf{p}` \ , \tag{27}$$

where

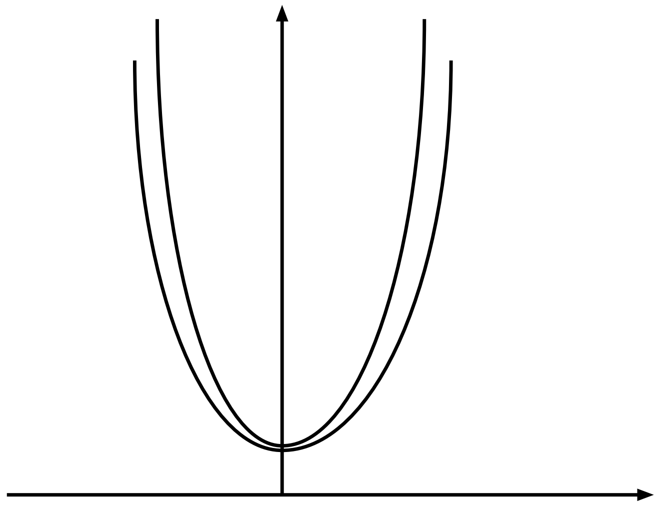

Figure 1. Coupling constant $g$ as a function of $g$

## V. RESULTS

### A. $S$-waves

### B. $P$-waves

## VI. SUMMARY

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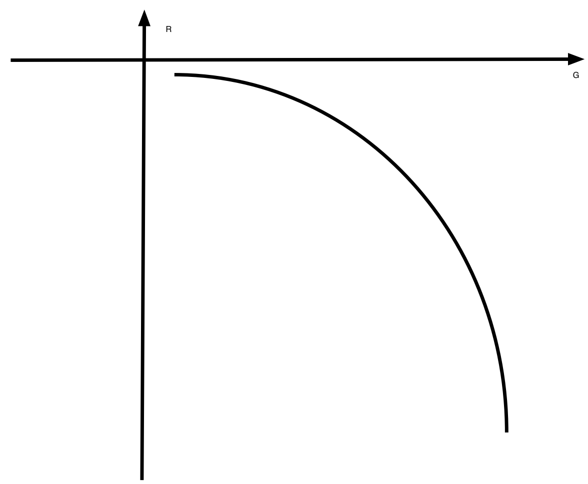


Figure 2. The $P$-wave effective range as a function of the coupling constant $g_0$

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