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Van der Waals Forces and Photon-Less Effective Field Theory

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Abstract In the ultra-cold regime Van der Waals forces between neutral atoms can be represented by short range effective interactions. We show that universal low energy scaling features of the underlying vdW long range force stemming from two photon exchange impose restrictions on an Effective Field Theory without explicit photons. The role of naively redundant operators, relevant to the definition of three body forces, is also analyzed.

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1 Introduction

From a fundamental QED point of view the underlying mechanism responsible for van der Waals (vdW) forces corresponds to two photon-exchange (see e.g. (1) and references therein). As compared to the short range and exponentially suppressed chemical bonding forces on sizes about a few Bohr radii, vdW forces are long range. For interatomic separations $a_B \ll r \ll \hbar c / \Delta E$, two photons are exchanged in a short time $\sim 2r/c$ while transitions with excitation energy ΔE take a much larger time $\sim 2\hbar / \Delta E$, yielding the potential

$$V(r) = -\frac{C_6}{r^6} - \frac{C_8}{r^8} - \frac{C_{10}}{r^{10}} - \dots \quad (1)$$

where C_n are the dispersion coefficients which are accurately known for many diatomic systems (see e.g. a compilation in (2)). The vdW length $R = (MC_6/\hbar^2)^{1/4}$ characterizes the size of the forces. For such potentials, low energy scattering with

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$kR \ll 1$ is dominated by S-waves which phase-shift, $\delta_0(k)$, fulfills the effective range expansion (ERE) (3)

$$k \cot \delta_0(k) = -\frac{1}{\alpha_0} + \frac{1}{2} r_0 k^2 + v_2 k^4 \log(k^2 R^2) + \dots \quad (2)$$

where α_0 is the scattering length, and r_0 is the effective range. Note that for this potential the long-range character starts at $\mathcal{O}(k^4)$ due to the logarithmic piece.

2 Low Energy Scaling of vdW Forces

Remarkably, the effective range was computed analytically (4; 5) when $C_{n \geq 8} = 0$ yielding

$$r_0/R = 1.395 - 1.333(R/\alpha_0) + 0.6373(R/\alpha_0)^2 \quad (3)$$

The scaling of the effective range r_0 in the vdW length and the quadratic $1/\alpha_0$ behaviour is just a particular case of a more general result (6) (see also (7) in these proceedings). In fact, the dominance of the leading long distance C_6 term tacitly assumed in Refs. (4; 5) was to be expected a priori by suitably re-writing higher order C_8, C_{10} contributions in vdW units $R^2 MV(r) = -(R/r)^6 [1 + g_1(R/r)^2 + g_2(R/r)^4 + \dots]$ where $g_1 \sim 10^{-2}$ and $g_2 \sim 10^{-4}$ for many homonuclear diatomic systems. Thus one expects that *even* for $kR \sim 1$ higher order corrections are negligible despite the strong divergence at short distance. These expectations are indeed met a posteriori on the light of about a hundred calculations based on phenomenological potentials (6). This result not only favours the view that these rather simple approaches based on the leading vdW forces are phenomenologically sound but also shows that a huge reduction of parameters takes place suggesting that atoms in the ultra-cold regime can indeed be handled without much explicit reference to the underlying electronic structure of atoms. The scaling universal relation, Eq. (3), allows for a quite general discussion on effective interactions in vdW units, as we advance here.

3 Effective Short Distance Potentials

In the ultra-cold regime, i.e. for extremely long de Broglie wavelengths much larger than the vdW scale, $\lambda = 1/k \gg R$, one expects the long range character to become largely irrelevant, keeping the first two terms in Eq. (2). Thus, one might want to represent the vdW potential by an effective potential with a finite range, r_c , featuring the truncated ERE, Eq. (2), and dismissing any explicit reference to the underlying photon exchange. However, even at very low energies, causality arguments provide the shortest possible value for r_c , which for vdW forces yields $r_c > 0.6R$ (2). Using for illustration a square well (SW) potential with range r_c and depth V_0 , $V_{\text{eff}}(r) = -V_0 \theta(r_c - r)$, one obtains

$$\alpha_0 = r_c - \tan \sqrt{MV_0} r_c / \sqrt{MV_0}, \quad r_0 = r_c [1 - 1/(\alpha_0 r_c M V_0) - r_c^2 / (3\alpha_0^2)]. \quad (4)$$

Reproducing Eq. (3) is not possible for a *common* potential. Indeed, the sign of the $1/\alpha_0^2$ term is just opposite, so that for small α_0 we cannot represent the interaction

by this short range potential. On the contrary, for large scattering lengths $\alpha_0 \gg R$ we obtain $r_c = 1.395R$ and $V_0 = \pi^2/(4r_c^2 M)$. In terms of volume integrals,

$$C_0 = \int d^3x V_{\text{eff}}(\mathbf{x}), \quad C_2 = -\frac{1}{6} \int d^3x r^2 V_{\text{eff}}(\mathbf{x}) \quad (5)$$

one gets $MC_0^{\text{SW}}/R = -14.41$ and $MC_2^{\text{SW}}/R^3 = 2.80$. If we use instead a delta-shell (DS) potential $V_{\text{eff}}(r) = -V_0 r_c \delta(r - r_c)$ we get for $\alpha_0 \gg R$ the results $MC_0^{\text{DS}}/R = -13.15$ and $MC_2^{\text{DS}}/R^3 = 2.40$, not far from the SW estimate. This suggests using a formulation based *directly* on the constants C_0 and C_2 . Note that while a C_4 exists for these short distance potentials, the original vdW potential yields a divergence, in harmony with the observation that the ERE for short range potentials differs at $\mathcal{O}(k^4)$ from the vdW expression, Eq. (3).

4 Effective Field Theory

The EFT approach has often been invoked to highlight universal features of ultracold few atoms systems (for reviews see e.g. (8; 9)). We re-analyze it on the light of the universal and extremely successful scaling relation, Eq. (3). For definiteness, we consider the Galilean invariant Lagrangian density (10) expanded in composite Bosonic spinless field operators with increasing energy dimensions and including multi-particle interactions,

$$\mathcal{L} = \psi^\dagger \left(i\partial_t + \frac{\nabla^2}{2m} \right) \psi - \frac{C_0}{2} (\psi^\dagger \psi)^2 - \frac{C_2}{2} [\nabla(\psi^\dagger \psi)]^2 - \frac{D_0}{6} (\psi^\dagger \psi)^3 + \dots \quad (6)$$

Here C_0, C_2 and D_0 are low energy constants which are fixed from few body dynamics. Using Feynman rules in the two-body sector one derives a scale dependent and momentum truncated self-adjoint pseudo-potential in the CM system (\mathbf{k} and \mathbf{k}' are relative momenta)

$$\langle \mathbf{k}' | V | \mathbf{k} \rangle = [C_0 + C_2(\mathbf{k}^2 + \mathbf{k}'^2) + \dots] \theta(\Lambda - k) \theta(\Lambda - k'). \quad (7)$$

The cut-off Λ is introduced here to handle the power divergent integrals arising in the scattering problem, which in terms of the Lippmann–Schwinger (LS) equation becomes

$$\langle \mathbf{k}' | T | \mathbf{k} \rangle = \langle \mathbf{k}' | V | \mathbf{k} \rangle + M \int \frac{d^3q}{(2\pi)^3} \frac{\langle \mathbf{k}' | V | \mathbf{q} \rangle \langle \mathbf{q} | T | \mathbf{k} \rangle}{p^2 - q^2 + i0^+}, \quad (8)$$

implementing unitarity for $p \leq \Lambda$. Using the potential of Eq. (7) the LS Eq. (8) reduces to a system of algebraic equations which solution is well known (see e.g. Ref. (11)) yielding

$$\begin{aligned} -\frac{1}{\alpha_0 \Lambda} &= \frac{4(-2c_2^2 + 90\pi^4 + 15(3c_0 + 2c_2)\pi^2)}{9\pi(c_2^2 - 10c_0\pi^2)}, \\ r_0 \Lambda &= \frac{16(c_2^2 + 12\pi^2 c_2 + 9\pi^4)}{\pi(c_2 + 6\pi^2)^2} - \frac{12c_2(c_2 + 12\pi^2)}{(c_2 + 6\pi^2)^2} \frac{1}{\alpha_0 \Lambda} + \frac{3c_2\pi(c_2 + 12\pi^2)}{(c_2 + 6\pi^2)^2} \frac{1}{\alpha_0^2 \Lambda^2}, \end{aligned} \quad (9)$$

Fig. 1 Cut-off dependence of the EFT coefficients MC_0/R when $C_2 = 0$ (dashed red) and MC_0/R^3 and MC_2/R^3 after Eqs. (9) (full blue) for the case $\alpha_0/R = 10$. R is the vdW scale defined as $R = (MC_6/\hbar^2)^{\frac{1}{4}}$

where $c_0 = M\Lambda C_0, c_2 = M\Lambda^3 C_2$. By eliminating C_0 in terms of α_0 we have written r_0 in a form similar to Eq. (3). This leads for any cut-off Λ to the mapping $(\alpha_0, r_0) \rightarrow (C_0, C_2)$. For $C_2 = 0$ one gets $r_0 = 4/\pi\Lambda$ which for $\alpha_0 \gg R$ yields $\Lambda R = 0.91$ and $MC_0/R = -21.6$ from matching the scattering length and the effective ranges $r_0^{\text{vdW}} = r_0^{\text{EFT}}$. The cut-off dependence for $C_2 \neq 0$ can be looked up at Fig. 1 in vdW units and for the specific case $\alpha_0/R = 10$ where a weakly bound state takes place. As we see there is a clear stability plateau in the region $\Lambda \sim \pi/(2R)$ illustrating the basic point of the EFT; low energy physics is cut-off independent within a given cut-off window which does not resolve length scales shorter than the vdW scale. Numerically we get $MC_0/R \sim -15$ and $MC_2/R^3 \sim 2$ for $\Lambda \sim \pi/(2R)$, in agreement with the previous SW and DS analysis. The values of Λ where the EFT low energy parameters diverge correspond to an upper bound above which C_0 and C_2 become complex, violating the self-adjointness of the potential (2) and the Lagrangian, $\mathcal{L}(x) \neq \mathcal{L}^\dagger(x)$. Thus, off-shell two-body unitarity and hence three-body unitarity are jeopardized for $\Lambda R \geq 4$, despite the phase shift being real and on-shell unitarity being fulfilled.

Direct inspection shows that a perfect matching between the vdW and the EFT effective ranges, Eq. (3) and Eq. (9) for *any* α_0 is not possible. So we try out including redundant operators which are usually discarded (10) but are needed to guarantee off-shell renormalizability of the LS equation (12). A Galilean invariant term of the form $\Delta\mathcal{L} = -\frac{1}{2}C'_2(\psi^\dagger\psi)[\psi^\dagger(i\partial_t + \nabla^2/2m)\psi]$ is formally redundant since it can be eliminated by a field transformation $\psi \rightarrow \psi + \frac{1}{4}C'_2\psi(\psi^\dagger\psi)$ which generates additional three body forces as well. The new term adds a correction $\Delta V = C'_2(2p^2 - \mathbf{k}^2 - \mathbf{k}'^2)/2$ to the potential, Eq. (7), vanishing on-shell. Solving the LS equation and eliminating C_0 in terms of α_0 yields

$$r_0\Lambda = \frac{16((c'_2 - 2c_2)^2 + 36\pi^4 + 6(8c_2 - c'_2)\pi^2)}{\pi(-2c_2 + c'_2 - 12\pi^2)^2} - \frac{12((c'_2 - 2c_2)^2 + 48c_2\pi^2)}{(-2c_2 + c'_2 - 12\pi^2)^2} \frac{1}{\Lambda\alpha_0} + \frac{3\pi((c'_2 - 2c_2)^2 + 48c_2\pi^2)}{(-2c_2 + c'_2 - 12\pi^2)^2} \frac{1}{\Lambda^2\alpha_0^2} \quad (10)$$

where $c'_2 = M\Lambda^3 C'_2$ appears through the combination $C'_2 - 2C_2$ which *cannot* be completely eliminated by making $C_2 \rightarrow C_2 + \frac{1}{2}C'_2$. Note the accidental correlation $-4/\pi$ between the second and the third coefficients holding regardless on the particular regularization method. Perfect matching can only be achieved with complex coefficients. Minimizing the difference between r_0^{EFT} and r_0^{vdW} provides a reasonable range $\Lambda R = 1.6 - 1.8 \sim \pi/2$. As we can see, universal two-body scaling features encoded in Eq. (3) and exhibiting the underlying vdW (two photon exchange) nature of interactions impose severe restrictions on the EFT solution with no explicit photonic degrees of freedom and distinguish between naively unitarily equivalent Hamiltonians mixing different particle number (see e.g. Ref.

(13)). Therefore, these limitations are expected to play a role in the EFT analysis of three-body forces.

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