The singular inverse square potential, limit cycles and self-adjoint extensions

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(Dated: April 1, 2022)

Abstract

We study the radial Schroedinger equation for a particle of mass m in the field of a singular attractive \(\alpha/r^2\) potential with \(2m\alpha > 1/4\). This potential is relevant to the fabrication of nanoscale atom optical devices, is said to be the potential describing the dipole-bound anions of polar molecules, and is the effective potential underlying the universal behavior of three-body systems in nuclear physics and atomic physics, including aspects of Bose-Einstein condensates, first described by Efimov. New results in three-body physical systems motivate the present investigation. Using the regularization method of Beane et al., we show that the corresponding “renormalization group flow” equation can be solved analytically. We find that it exhibits a limit cycle behavior and has infinitely many branches. We show that a physical meaning for self-adjoint extensions of the Hamiltonian arises naturally in this framework.

PACS numbers: 34.20.-b, 03.65.Ca, 03.65.Ge, 11.10.Hi,
In this note, we study the regularization and renormalization of the singular attractive $\alpha/r^2$ potential, a problem motivated, in part, by recent results in three-body physics. Specifically, there has been renewed interest in the non-relativistic three-body system with short-range interactions. The current investigations are stimulated by the promise that effective field theories (EFT's) offer a systematic and model-independent treatment of atomic, nuclear and hadronic physics at low energies. That is, a low-energy system with a clear-cut separation of distance scales can be described by an EFT involving explicitly only the long-wavelength degrees of freedom. The short-range dynamics can be treated as a set of local operators which correspond to delta-function interactions in coordinate space. The details of the short distance physics cannot be of importance to the low energy aspects of the system; if they are, it is an indication of a need for renormalization of the EFT.

Such a renormalization of an EFT of a three-body system with delta-function two-body interactions [1] has lead to the rediscovery of the one-parameter contact three-body interaction shown to restore the lower bound of this three-body Hamiltonian [2]. (Here we mention that the unboundedness of the Hamiltonian from below is interpreted in EFT’s as the onset of short-distance physics whose effect must be included in local counterterms [3]; hence the three-body counterterm in the EFT equations for 3-body systems, both bound and scattering states [4].) The three-body counterterm exhibits a convergence of the renormalization group flow to one-dimensional limit cycles. This was earlier proved in Ref. [2], a mathematical analysis of the Efimov effect which occurs in bound 3-body systems when more than one of the two-body subsystems has a zero energy resonance [5]. The presumed novelty of a renormalization group flow with a limit cycle has inspired additional recent work [6].

As the applications of EFT's continue [4, 7], it will be important to understand how to explicitly renormalize higher orders in an EFT. For example, a renormalized equation for two-nucleon systems with explicit pion-exchange would be of great potential value. Pion exchange gives rise to a singular $1/r^3$ potential and the questions arise: Can the resummation of pion graphs be renormalized by a single local operator? Would this operator exhibit a limit cycle as does the three-body contact operator in the pion-less three-nucleon EFT? Could one calculate the evolution of such an operator analytically? A positive answer to the last question would help future numerical work with EFT's. Already, the short distance physics of the $^3S_1$ coupled channels of the single pion exchange potential has been renormalized by a short range four-nucleon counterterm using the method introduced in ref.[3], but the
treatment was numerical and these questions were not addressed in that investigation.

Such questions, coupled with the interesting limit cycle behavior found in the three-body system, have prompted investigations of the renormalization group behavior of the short range counterterms which serve to regularize given long range potentials (including singular potentials) in the two-body Schroedinger equation. Since these long range potentials are often singular at the origin, it has been argued that the short range interaction should not be represented by a 3-dimensional delta-function at the origin. Birse et al. choose a delta-shell potential and Beane et al. suggest that a simple attractive square well represents a “smeared out” delta-function potential. In either case, it is said, the details of the short distance regularization should not matter; the low energy aspects of the system should be invariant in the same way under suitable changes of the short range potential.

For completeness, we list other regularization and renormalization schemes which do not follow from the separation of scales of an ETF, but also have been applied to the inverse square potential description of physical systems. The problem of a neutral atom interacting with a charged wire, relevant to the development of nanoscale atom optical devices, has been treated with the method of self-adjoint extensions. A short distance cutoff scheme which renormalizes the strength of the $1/r^2$ potential, yields a critical dipole moment that has been confronted with the experimental capture of electrons by dipole molecules and formation of anions as an example of quantum mechanical symmetry breaking. These alternative regularizations are not the subject of our present investigation.

In this note, we follow the regularization method of Beane et al. to obtain analytically the renormalization group behavior of the coupling constant of the short range attractive square well they use to regularize the long range inverse square potential. The $1/r^2$ potential is on the boundary between singular and regular potentials and thus does or does not require a self-adjoint extension, depending on the strength of the interaction. More interesting from the EFT point of view is the Efimov observation that the low energy behavior of three-body systems is determined by a long range three-body effective interaction of the form $1/R^2$ where $R$ is built from the relative distances between the particles. Thus, the two-body inverse square potential is the analogue to the interaction in a three-body system in the limit of zero energy resonance (and infinite two-body scattering lengths).

A further advantage of our analytic approach to the “EFT style” renormalization of the inverse square potential is that we can then more readily make contact with the mathe-
matically rigorous and well studied approach to regularization via self-adjoint extensions.

The theory of self-adjoint extensions of Hamiltonians underlies the first discussions of limit cycle behavior in three-body systems [2]. The self-adjoint extensions of the inverse square potential are well known [15] and can be compared with the results of our study, which we now begin.

The starting point of our study is the $s$–wave reduced radial Schroedinger equation for one particle of mass $m$ in the external potential $V(r)$:

$$ \left( \frac{d^2}{dr^2} - 2mV(r) + k^2 \right) \psi = 0 $$ (1)

where $V(r)$ is given by [3]:

$$ V(r) = -\frac{\alpha s \theta(R-r)}{R^2} - \frac{\alpha \theta(r-R)}{r^2} \quad (\alpha_s, \alpha > 0). $$ (2)

That is, the long range attractive $\alpha/r^2$ second term in eq. (2) is cutoff at a short distance radius $R$ by an attractive square well. As in [3], we first solve eq. (1) for the zero energy solution ($k = 0$) $\psi_o$. It is given by:

$$ \psi_o(r) = A \frac{r^{1/2}}{r_o^{1/2}} \cos \left( \nu \ln \frac{r}{r_o} + \phi_o \right) \quad r > R $$ (3)

$$ \psi_o(r) = A \cos(\nu \ln \frac{R}{r_o} + \phi_o) \left( \frac{R^{1/2}}{r_o^{1/2}} \right) \sin K_o r \quad r < R $$ (4)

where $\nu = (2m\alpha - 1/4)^{1/2}$, $\phi_o$ is the zero energy phase [3], $K_o^2 = (2m\alpha_s)/R^2$ and $r_o$ is an arbitrary scale.

The usual matching condition of the wave function and its derivative at $r = R$ then yields:

$$ (2m\alpha_s)^{1/2} \cot \{ (2m\alpha_s)^{1/2} \} = \frac{1}{2} - \nu \tan \left( \nu \ln \left( \frac{R}{r_o} \right) + \phi_o \right) $$ (5)

Following [3] we now consider eq. (5) to be a transcendental equation defining the value of the short range coupling constant $\alpha_s$. This equation is of the form $\beta \cot \beta = 1/\omega$ and can be solved exactly in closed form using a method based upon the solution to the Riemann problem in complex variable analysis [16].

The solution to eq. (5) then turns out to be [17]:

$$ \beta_o = \pm \left( \frac{\omega - 1}{\omega} \right)^{1/2} \exp \left( \frac{1}{\pi} \int_0^1 \arg \Lambda_o(t) \frac{dt}{t} \right), \quad \omega > 0 $$ (6)

$$ \beta_n = \pm n\pi \exp \left( \frac{1}{\pi} \int_0^1 \arg \Omega_n(t) \frac{dt}{t} \right), \quad -\infty < \omega < +\infty, \quad n = 1, 2, ... $$ (7)
where:

\[ \beta = (2m\alpha_s)^{1/2} \quad (8) \]

\[ \frac{1}{\omega} = \frac{1}{2} - \nu \tan \left( \nu \ln \left( \frac{R}{r_o} \right) + \phi_o \right) \quad (9) \]

\[ \Lambda_o(t) = \lambda(t) + \frac{1}{2} \omega t \pi \quad (10) \]

\[ \lambda(t) = 1 + \frac{1}{2} \omega t \ln \frac{1-t}{1+t} \quad (11) \]

\[ \Omega_n(t) = \Lambda_o(t)^2 + n^2 \pi^2 \omega^2 t^2 \quad (12) \]

Formula (9) does not restrict \( \omega \) to be positive, so that all the solutions that we consider follow from the positive branch of (7). If we interpret eq. (5) to be an equation for the running coupling constant \( \beta = (2m\alpha_s)^{1/2} \), this amounts to requiring that \( \beta \) must be defined for all values of \( R/r_o \) except for those points where \( \omega \) (or its inverse) vanish. This is potentially important when comparing our analytic solution with numerical solutions to eq. (5). Indeed, numerical investigations in general will mix solutions that only exist in a limited range of \( R/r_o \)-values, with solutions which we consider to be the only physically relevant solutions. From now on, we shall therefore use \( \beta \) to mean only a solution of eq. (7), and suppress the subscript \( n \) when it is not needed for the discussion. We then find from eq. (7) that eq. (5) has infinitely many roots, in agreement with \[6\]. We have plotted \( \beta \) in eq. (5) as a function of \( \ln x \) (\( x = R/r_o \)) for fixed \( \phi_o = 1.0 \), and \( n = 1 \) in figures 1 and 2. The strength of the long range potential \( \alpha/r^2 \) increases with succeeding figures; \( \nu = 0.5 \) in fig. 1, \( \nu = 3.0 \) in fig. 2. The running coupling \( \beta \) exhibits a limit cycle behavior for all values of \( \nu > 0 \); the period becomes smaller as the strength of the attractive \( \alpha/r^2 \) potential increases, according to the argument \( (\nu \ln x + \phi_o) \) of the tangent function in the source term of eq. (5). The behavior described by \( \beta \), for large enough \( \nu \), is of a “sawtooth” type, with a periodic sharp increase of the value of the coupling constant with decreasing values of \( \ln x \). This “increase” is actually a genuine discontinuity of \( \beta \) at the zeros of \( 1/\omega \) and must be a multiple of \( \pi \). Indeed, a discontinuity can only occur at a zero of \( \cot \beta \) in order that \( \beta \cot \beta \) be continuous at all points where \( 1/\omega \) is a continuous function. Once \( \beta \) has reached the smallest positive zero \( (\beta = \pi/2) \), for some \( x \)-value, it increases by \( \pi \) as \( x \) is further decreased. Altering the zero energy phase shift \( \phi_o \) from 0 through 2 (and keeping \( n=1 \) and \( \nu = 3 \)) does not qualitatively change the appearance of the pattern of Fig. 2: the discontinuity moves to lower \( x \), but the magnitude of the discontinuity remains the same multiple of \( \pi \). This feature can be traced to the periodicity of the right hand side of eq. (5)
with respect to $\phi_0$. The branches which correspond to roots with $n > 1$ are qualitatively similar to Fig 2., but the slow fall-off with decreasing $x$ seen in Fig. 2 increases and the “saw-tooth” appearance becomes more of a rounded off square wave. This feature of the solutions is illustrated by Fig. 3 which plots $\beta$ for the same strength and initial phase $\nu = 3$, $\phi_0 = 1$ as Fig. 2, but $n$ has increased to 16. The magnitude of the discontinuity of this $\beta_{16}$ remains $\pi$, however.

Finally we plot as Fig. 4 the analytical solution of eq. (5) for the values $\nu = 2.0$, $\phi_0 = 0.0$ to compare with the numerical solutions of eq. (5), with the same input, displayed in Figure 1 of Ref. [3]. The latter numerical solution is in excellent agreement with the analytical solution presented here, if one allows a solution to go from a higher branch ($n = 2$) to the next lower branch ($n = 1$) as it crosses a zero of $1/\omega$. However, as discussed above and shown on Fig.4, $\beta_1$ itself must ultimately increase by $\pi$ after reaching its lowest value $\pi/2$, thus exhibiting a limit cycle behavior of the solution. It is evident that the limit cycle behavior of the solutions of equation (5) is a consequence of the requirement that a solution $\beta_n$ be defined for all values of $R/r_o$ for which omega or its inverse is nonzero. This requirement includes solutions for $R \to 0$ and therefore corresponds to our understanding of the emulation proposed in ref [3] of the contact term which encapsulates the short range dynamics of an EFT. From Figures 1-3, it is clear that the limit cycle behavior of a given branch continues to the left as $R \to 0$ and $\ln x$ becomes arbitrarily small. Consider, however, the behavior for small $R$ of a numerical solution of ref. [3], shown in Figure 4 which segues smoothly between different branches of the analytic solutions of equation (5) as it crosses a zero of $1/\omega$. For some value of negative $\ln x$, as $R$ becomes arbitrarily small, the numerical solution must pass to the $\beta_0$ solution. But, as we have noted, this solution exists for only a limited range of $R/r_o$ values. Thus, the two numerical solutions of Fig. 4 would appear to not be defined for arbitrarily small $R/r_o$. One could, however, choose another numerical solution corresponding to a higher value of $n$ which does not pass to $\beta_0$ on the way from large to arbitrarily small $R/r_o$ and avoid this problem. This exercise need not be performed, however, with our requirement of a well defined solution for all values of $R/r_o$ for which omega or its inverse is nonzero.

A motivation for both the study of Ref. [3] and the present discussion is the expectation that the two-body inverse square potential is the analogue to the interaction in a three-body system in the limit of zero energy resonances. Indeed, the approximate solution of eq. (5)
FIG. 1: The running coupling constant $\beta$ as a function of $\ln x = \ln \frac{\alpha}{r_0}$ for $\phi_o = 1.0$, $\nu = 0.5$, $n = 1$

FIG. 2: The running coupling constant $\beta$ as a function of $\ln x$ for $\phi_o = 1.0$, $\nu = 3.0$, $n = 1$

displayed in eq. 8 of [3] is quite similar to the equation which describes the running of the three-body counterterm of the pion-less three-nucleon EFT’s of Refs. [1, 4]. Both equations have poles and the three-body counterterm seems to reach arbitrarily high values. We, to the contrary, find no poles in the analytic solutions of eq. (5). Furthermore, no evidence of multiple branches was found in the renormalized pion-less three-nucleon problem. The renormalization of short distance physics in these two problems needs more understanding in light of the results of Efimov [14].

Now we turn to the bound state aspects of the related two problems (three-body system with contact potentials and the $1/r^2$ singular potential) and again find discrepancies. First we show that the regularization method that was used to solve the Schroedinger equation (1) with potential (2) amounts to specifying a particular self-adjoint extension in Case’s solution of the bound state (B.S.) spectrum of the attractive singular $1/r^2$ potential [15, 18]. In order to do this, we note that the B.S. wavefunction that solves eqs. (1)-(2) is given by:
FIG. 3: $\beta$ as a function of $\ln x$ for $\phi_o = 1.0$, $\nu = 3.0$, $n = 16$

FIG. 4: $\beta$ as a function of $\ln x$ for $\phi_o = 0.0$, $\nu = 2.0$. The three branches, from bottom to top, correspond to $n=1$ (dash-dotted curve), $n=2$ (dotted curve) and $n=3$ (solid curve). As explained in the text, the discontinuity in $\beta$ is always $\pi$ for each curve. The two thicker curves are two numerical solutions for the same parameters taken from ref. [3], as discussed in the text.

$$\psi = Cr^{1/2}K_\nu(kr) \quad r > R$$
$$\psi = C' \sin(Kr) \quad r < R$$ (13) (14)

where:

$$K^2 = \frac{2m\alpha_s}{R^2} - k^2$$ (15)

and $C$ and $C'$ are constants.

For $kR << 1$, the matching condition now gives (one still has $KR = (2m\alpha_s)^{1/2}$ in that limit):

$$k = \frac{1}{2r_o} \exp \phi_o + \arg \Gamma(1 + i\nu) - \frac{(n + 1/2)\pi}{\nu} \quad n = 0, \pm 1, \pm 2, ....$$ (16)
where we have used eq. (5) together with the small-r behavior of $\psi(r)$ 

$$\psi(r) \simeq r^{1/2} \sin \left( \nu \log \frac{kr}{2} - \arg \Gamma(1 + i\nu) \right).$$  \hspace{1cm} (17)

The spectrum given in eq. (16) is essentially the spectrum given by Case [18], where Case’s arbitrary phase (which fixes the self-adjoint extension) $B$ is now given by:

$$B = \phi_o + \arg \Gamma(1 + i\nu)$$  \hspace{1cm} (18)

It is important to note that the binding energy $E_B = (k^2)/2m$, after this regularization, no longer depends on the cut-off radius $R$ (for $kR \ll 1$) but instead on the arbitrary scale $r_o$. Thus, fixing the zero energy phase of the wavefunction $\phi_o$ removes the cut-off dependence of the B.S. spectrum for $kR \ll 1$. Our result explicitly shows that the physical interpretation of the phase characterizing the self-adjoint extension of the Hamiltonian indeed can be found from a renormalization of the short-range coupling constant in the regularization method described in Ref. [3]. By the same token, it illustrates why a cut-off method with a constant strength fails [15] to provide a physical meaning for this arbitrary phase.

Note, however, that the ground state of the $1/r^2$ potential remains at negative infinity, and no renormalization of the bound state spectrum has been achieved. Contrast this result of the EFT style renormalization of Ref. [3] with the restoration of the lower bound of the pion-less three-body problem obtained in Refs. [1, 2]. A clue to this discrepancy may lie in the distinction between the contact interaction used in Ref. 2 and the “EFT” type regularization of the conventional 3-dimensional delta function. That is, the attractive square well in eq. (2) does not provide a unique way of regularizing (“smearing out”) a 3-dimensional delta function, and its limit when $R \to 0$ is not the contact interaction discussed in Ref. 2 and 14. In that respect, it would be quite interesting to reexamine the solution of the Schroedinger equation with a singular $\alpha/r^2$ potential in conjunction with local realizations of the contact interaction of Ref. 14 implemented by Kruppa, Varga and Revai [21]. Such a study might throw additional light on the corresponding renormalization group flow properties in the 3-body problem.
Acknowledgments

The work of M.B. was supported by the National Fund for Scientific Research, Belgium and that of S.A.C. by NSF grant PHY-0070938. We thank Silas Beane for providing us with details of the numerical calculations of Ref. 3 and Mary Alberg for a communication about our plots of the analytical solutions.

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