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Off-shell scattering due to a finite square well potential

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1. Abstract

Efimov physics is a description of three-body systems that has an infinite spectrum of bound states for diverging scattering length. The theory predicts universal behavior that depends only on the scattering length. Experiments, however, have shown discrepancies from the predictions. The scattering length as only parameter in the models appears to be insufficient to describe the whole process. The current models are based on a delta potential and therefore do not depend on the range of the potential. In this paper we use the finite square well potential to describe two-body scattering processes, both on-shell as off-shell. This model can be used to describe the Efimov physics with a finite range for the potentials.

The results have shown that the off-shell scattering amplitude shows significant changes in completely different ranges for the wave number of the incoming and outgoing wave. Some of the current models use a cut-off in the momentum space and make no distinction between the cut-off for the two different waves. We have concluded that this distinction is an important aspect to the scattering process and should there be made.

Contents

2. Introduction

2.1 Efimov physics

Three-body physics has been excessively studies in different fields of physics. In the field of nuclear physics a special state of three-particle systems was predicted in 1970 by Efimov [2]. According to the theory the three-body system has infinitely many bound states, if the two-body subsystems have an infinite scattering length. Such a bound state of three particles is called a trimer. A state is 22.7 times larger than the previous that and has an energy $22.7^2 = 515$ times smaller than the previous. This number follows from the mathematical equations and are independent of any parameters. The Efimov effect was thought to have a universal behavior, which means that only the scattering length of the two-body systems are of importance. Therefore the Efimov effect must play a role in three-body systems of any kind. It was not until 2006 that the Efimov states were experimentally observed, using caesium atoms [3].

Efimov states require an infinite scattering length of the two-body systems, which can only be accomplished in the case where the particles are cooled down to microscopic temperatures, where their kinetic energy approaches zero. This is the regime in which quantum mechanics dominates. It is therefore obvious that the physics of these states is hidden inside the Schrödinger equation. In figure **??** the properties of the Efimov states are depicted, where the energy of the bound Efimov states is plotted as a function of the inverse of the scattering length. The universal scaling factors 22.7 and $22.7^2 = 515$, the factor between the size and the energy of the consecutive, respectively, are shown in the plot. Trimers can exist in the green area and in the purple area there can only exist two-body systems, dimers, in combination with an unbound particle. The figure implies that the green area is not bounded, but this is not the case. There is a ground state that determines the minimal value of the scattering length at which a trimer can form. In the grey area above the particles have kinetic energy and are unbound. It is interesting to notice that for a positive scattering length the trimers can recombine into an atom and a dimer, both gaining a lot of kinetic energy, while for a negative scattering length no such process is possible. In this region there is no permitted state for a dimer, while a trimer is permitted. However, when the trimer "recombines", all three particles become unbound and the whole trimer falls apart. This situation can be compared to the practical example of Borromean rings, where by removing one of the three rings, all three rings become separated from each other.

When the Efimov states were first predicted, the related physics was thought to

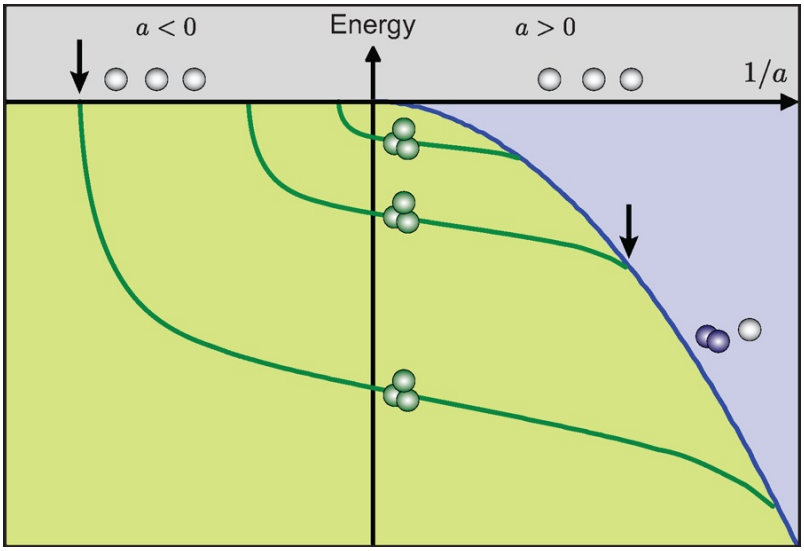


Figure 2.1: A plot of the energy of three of the infinite bound Efimov states as a function of the inverse of the scattering length. The universal scaling of the size of the states (factor 22.7) is indicated, as well as the universal scaling of the energy of the states (factor $22.^2 = 515$). Three-body bound states can exist on the curved lines in the green area. In the grey area to the right there are no permitted bound states.

behave universally. However, when it became possible to conduct experiments, it soon was shown that there were some discrepancies [3]. In the first models the only parameter was the scattering length and the scattering potentials were modelled as delta potential wells, but this proved to be insufficient. In this thesis we investigate the process of two-body scattering on a finite square well potential. After introducing a firm basis of scattering theory, we first look at the so-called "on-shell" scattering process, by which elastic scattering processes can be described and then we find a way to describe the "off-shell" scattering process, which describes inelastic scattering processes. The off-shell scattering process in two-body physics should first be understood in order to describe Efimov states. The outcome of the two-body scattering on a finite square well can be used to describe Efimov states, using a finite range of the potential. When a finite range model is implemented in the Efimov states it can be investigated whether this extra parameter is sufficient to match with the experimental values.

2.2 Feshbach resonance

In the previous section we stated that an infinite scattering length is necessary for trimers to exist. Thus we need a mechanism that enables us to tune the scattering length. Fortunately, such a mechanism is well known in the research field of cold atoms and is known as Feshbach resonance. When the particles are in a weakly bound state, they become resonant with other interaction channels, whereby the scattering length

diverges. In experiments this is done by applying a magnetic field to the system in such a way that the particles are weakly bound. The magnetic field should be adjusted to the energies due to Coulomb interaction, Zeeman splitting and hyperfine splitting. In this thesis, however, we assume we can simply adjust the depth of the potential well, since this technique is already mastered by experimenters.

In figure we see the scattering length, with background scattering, as function of the magnetic field. The scattering length diverges for $B = B_0$. The width of the resonance is Δ. We will choose the depth of the potential in this thesis, so that the scattering length matches the with diverging behavior.

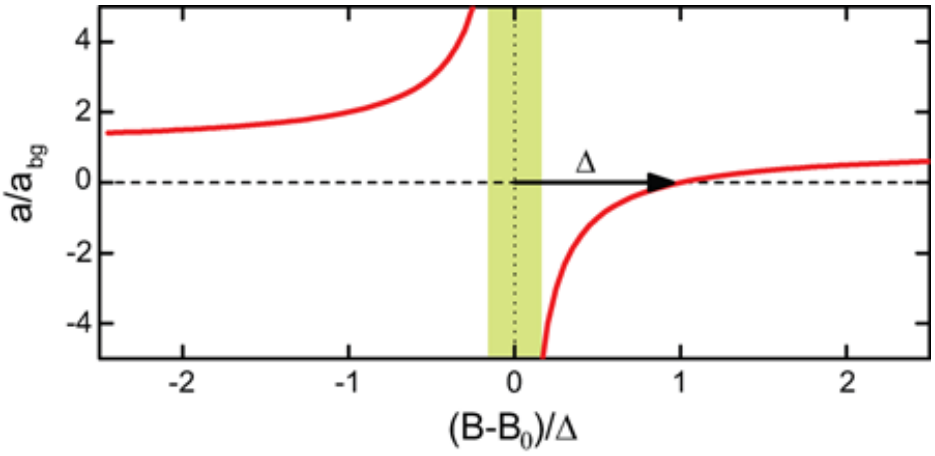


Figure 2.2: The scattering length is plotted as a function of the applied magnetic field. We aim at the green area, where the scattering length diverges. The width of the resonance is denoted by Δ. For a magnetic field far from resonance the scattering converges to the background scattering a_{bg}.

3. Scattering theory

In this chapter we introduce the theory that is used during the thesis. First we explain the theory of quantum scattering for two-body systems and the principle of Feshbach resonance and later we unite the two concepts. Let us first take a look at the theory of quantum scattering.

3.1 Lippmann-Schwinger equation

The time-independent Schrödinger equation can be written as

$$H|\psi\rangle = E|\psi\rangle, \tag{3.1}$$

in which H is the Hamiltonian operator and E is the energy of the system. Note that the circumflex on the operators is omitted, and will be in the remainder of this article, for convenience. The Hamiltonian consists of the the kinetic-energy operator H_0 and the potential operator V in such a way that

$$H = H_0 + V. \tag{3.2}$$

Let us now consider a particle residing in the presence of a potential well with a finite range. When the particle is far enough from the potential, the Schrödinger equation can be written as

$$H_0|\boldsymbol{k}\rangle = E|\boldsymbol{k}\rangle, \tag{3.3}$$

since the potential has a negligible contribution to the energy of the particle. Here the eigenvector $|\mathbf{k}\rangle$ denotes the state of a plane wave with wave number $\mathbf{k}$. According to Sakurai[1] the complete Schrödinger equation can be written as

$$|\psi\rangle = \frac{1}{E - H_0} V|\psi\rangle + |\boldsymbol{k}\rangle, \tag{3.4}$$

as the solution transforms into the equation 3.3 when the distance between the particle and the potential is large and V therefore vanishes. This expression gives rise to a singularity when $E = H_0$. We can solve the problem by making the energy E slightly complex and then we obtain the Lippmann-Schwinger equation in the form

$$|\psi^{(\pm)}\rangle = |\boldsymbol{k}\rangle + \frac{1}{E - H_0 \pm i\epsilon} V|\psi^{(\pm)}\rangle, \tag{3.5}$$

in which ϵ is an infinitesimal small number. Here $|\psi^{(+)}\rangle$ ($|\psi^{(-)}\rangle$) denotes state of the outgoing (incoming) wave function.

Using the projection of the state of the wave function on the position basis we obtain

$$|\psi^{(\pm)}\rangle = \langle \boldsymbol{x}|\boldsymbol{k}\rangle + \int d^3x' \langle \boldsymbol{x}| \frac{1}{E - H_0 \pm i\epsilon} |\boldsymbol{x'}\rangle \langle \boldsymbol{x'}|V|\psi^{(\pm)}\rangle, \tag{3.6}$$

in which $\mathbf{x}'$ is used as a dummy variable. The projection of the plane wave state $|\mathbf{k}\rangle$ on the position basis is expressed by

$$\langle \boldsymbol{x}|\boldsymbol{k}\rangle = \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{x}}}{(2\pi)^{3/2}}. \tag{3.7}$$

According to Sakurai[1] the matrix element from equation 3.6 is given by

$$G_\pm \equiv \frac{\hbar}{m} \langle \boldsymbol{x}| \frac{1}{E - H_0 \pm i\epsilon} |\boldsymbol{x'}\rangle = -\frac{1}{4\pi} \frac{e^{\pm ik|\boldsymbol{x}-\boldsymbol{x'}|}}{|\boldsymbol{x}-\boldsymbol{x'}|} \tag{3.8}$$

when the distance between the particle and the potential is large. $\hbar$ denotes the reduced Planck's constant and m denotes the mass of the two-body system. The result is obtained by applying complex integrals.

Since we assume that the potential is local, we claim that

$$\langle \boldsymbol{x'}|V|\boldsymbol{x''}\rangle = V(\boldsymbol{x'})\delta^3(\boldsymbol{x'} - \boldsymbol{x''}), \tag{3.9}$$

so that we can express the last term in equation 3.6 as

$$\langle \boldsymbol{x'}|V|\psi^{(\pm)}\rangle = \int d^3x'' \langle \boldsymbol{x'}|V|\boldsymbol{x''}\rangle \langle \boldsymbol{x''}|\psi^{(\pm)}\rangle = V(\boldsymbol{x'}) \langle \boldsymbol{x'}|\psi^{(\pm)}\rangle. \tag{3.10}$$

Now the total Lippmann-Schwinger equation becomes

$$\langle \boldsymbol{x}|\psi^{(\pm)}\rangle = \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{x}}}{(2\pi)^{3/2}} - \frac{m}{\hbar^2} \int d^3x \frac{e^{\pm ik|\boldsymbol{x}-\boldsymbol{x'}|}}{4\pi|\boldsymbol{x}-\boldsymbol{x'}|} V(\boldsymbol{x'}) \langle \boldsymbol{x'}|\psi^{(\pm)}\rangle. \tag{3.11}$$

The projection of the wave function state on the position basis for large distances between the particle and the potential can be expressed in terms of a plane wave and a spherical wave, multiplied by a scattering amplitude $f(\mathbf{k_0}, \mathbf{k})$ as follows

$$\langle \boldsymbol{x}|\psi^{(+)}\rangle = \langle \boldsymbol{x}|\boldsymbol{k}\rangle - \frac{1}{4\pi} \frac{m}{\hbar^2} \frac{e^{ikr}}{r} \int d^3x' e^{-i\boldsymbol{k'}\cdot\boldsymbol{x'}} V(\boldsymbol{x'}) \langle \boldsymbol{x'}|\psi^{(+)}\rangle = \frac{1}{(2\pi)^{3/2}} \left(e^{i\boldsymbol{k}\cdot\boldsymbol{x}} + \frac{e^{ikr}}{r} f(\boldsymbol{k_0}, \boldsymbol{k}) \right). \tag{3.12}$$

The scattering amplitude is given by

$$f(\boldsymbol{k'}, \boldsymbol{k}) = -\frac{1}{4\pi} \frac{m}{\hbar^2} (2\pi)^3 \int d^3x \frac{e^{-i\boldsymbol{k'}\cdot\boldsymbol{x'}}}{(2\pi)^{3/2}} V(\boldsymbol{x'}) \langle \boldsymbol{x}|\psi^{(+)}\rangle = -\frac{1}{4\pi} (2\pi)^3 \frac{m}{\hbar^2} \langle \boldsymbol{k'}|V|\psi^{(+)}\rangle. \tag{3.13}$$

It is clear that the scattering amplitude contains all the information of the potential and is therefore all we need to know.

3.2 Partial wave expansion

In Sakurai[1] an expansion has been derived for the scattering amplitude in terms of wave functions with different angular momenta. The scattering amplitude is given by

$$f(\boldsymbol{k'}, \boldsymbol{k}) = f(\theta, k) = \sum_{l=0}^{\infty} (2l+1) f_l(k) P_l(\cos\theta), \tag{3.14}$$

where θ is the angle between the wave vector of the incoming and outgoing wave. This approach is only viable in the case of a complete elastic collision, which is called "on-shell" scattering. Now the length of the wave number of the incoming and outgoing wave are equal, since the energies of both are equal in a complete elastic collision, and is denoted as k.

Equation 3.6 can be written in terms of this partial wave expansion. According to Sakurai[1] the equation becomes

$$\langle \boldsymbol{x} | \psi^{(+)} \rangle = \frac{1}{(2\pi)^{3/2}} \sum_{l=0}^{\infty} (2l+1) \frac{P_l(\cos\theta)}{2ik} \left((1 + 2ikf_l(k)) \frac{e^{ikr}}{r} - \frac{e^{-i(kr - l\pi)}}{r} \right). \tag{3.15}$$

Thus, the potential only contributes to the outgoing part of the wave function for each l. It is common to denote the amplitude of the outgoing part of the wave function for each l as

$$S_l(k) = 1 + 2ikf_l(k) \tag{3.16}$$

and to call its sum over all l the S-matrix.

Because of the conservation of probability the amplitude of the total wave function, and therefore the amplitude of the all partial waves, should be conserved. Therefore the relation

$$|S_l(k)| = 1 \tag{3.17}$$

must hold. This means that the presence of a potential can only manifest itself in a phase shift of the outgoing wave and S_l can be written as

$$S_l(k) = e^{2i\delta_l}, \tag{3.18}$$

in which the factor 2 is introduced for convenience and $2\delta_l(k)$ is the phase shift. A relation can be found between equation 3.16 and equation 3.17, i.e.

$$f_l(k) = \frac{S_l - 1}{2ik} \tag{3.19}$$

and rewriting this equation after substituting equation 3.18 we get

$$f_l(k) = \frac{1}{k \cot(\delta_l(k)) - ik}. \tag{3.20}$$

3.3 Ultra-cold limit

In the ultra-cold limit particles occupy the state with the lowest energy, i.e. the state with no angular momentum. Therefore we can simplify equation 3.14 by taking $l = 0$, so it takes the form

$$f(\theta, k) = f_0(k). \tag{3.21}$$

The scattering amplitude is thus independent of the angle between the outgoing and incoming waves in the ultra-cold limit. Now we know that only one term of the partial wave expansion contributes to the scattering amplitude, we know that the total scattering amplitude becomes

$$f(k) = \frac{1}{k \cot(\delta_0(k)) - ik}. \tag{3.22}$$

4. Scattering amplitude of a finite square well potential

Before we can calculate the scattering amplitude for the square well potential, we need to define the S-matrix that represents the transformation of the outgoing spherical wave. In the ultra-cold limit the S-matrix should only be dependent of the width of the potential, r_0, the depth of the potential, V_0, and the incoming wave number k. In this chapter we give analytic expressions, but also plots of the scattering amplitude and the wave function. We try to model the scattering of Rubidium-87 atoms and we will use its mass and its typical potential range, i.e. approximately 100 Bohr radii. Also, since the solution for this two-particle scattering process is supposed to be used to describe Efimov states, the scattering length of the system should approach infinity. We will find a condition for a large scattering length and substitute it in the S-matrix.

4.1 Weakly bound state

An expression for the scattering length can be derived by solving the Schrödinger equation for an extremely weakly bound state. The radial, time-independent Schrödinger equation is given by

$$-\frac{\hbar^2}{m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi\left(\boldsymbol{r}\right)}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi\left(\boldsymbol{r}\right)}{\partial\theta}\right)+\frac{1}{r^2\sin\theta^2}\frac{\partial^2\psi\left(\boldsymbol{r}\right)}{\partial\phi^2}+V\left(\boldsymbol{r}\right)\psi\left(\boldsymbol{r}\right)\right)=E\psi\left(\boldsymbol{r}\right), \tag{4.1}$$

where m is the total mass of the system, i.e. two times the mass of the atom. Using separation of variables we write the wave function as

$$\psi\left(\boldsymbol{r}\right)=R(r)Y_l^m(\theta,\phi), \tag{4.2}$$

where $R(r)$ is the radial part of the wave function and $Y_l^m(\theta,\phi)$ the angular part. Here l is the orbital quantum number and m is the magnetic quantum number, which we both choose to be zero, because we are working in the ultra-cold limit. The well-known angular solution for $l=0$ and $m=0$ is given by

$$Y_0^0=\sqrt{\frac{1}{4\pi}}. \tag{4.3}$$

For the radial part we write $u(r) = r\psi(r)$ and the Schrödinger equation becomes

$$-\frac{\hbar^2}{m}\frac{d^2u(r)}{dr^2} = (E - V(r))\,u(r). \tag{4.4}$$

The potential of the finite square well is given by

$$V(r) = \begin{cases} -V_0 & \text{if } r \leq r_0 \\ 0 & \text{if } r > r_0, \end{cases} \tag{4.5}$$

, where V_0 is a positive value. The potential is divided into two intervals, where the Schrödinger equation yields different solutions, so the wave function should be divided into two intervals as well. For a weakly bound state the energy E is negative and small. This means that the solution for $u(r)$ will be a sum of a sine function and a cosine function inside the potential and a decaying exponent outside the potential, i.e.

$$u(r) = \begin{cases} A_1\cos(\kappa_0 r) + B_1\sin(\kappa_0 r) & \text{if } r \leq r_0 \\ C_1 e^{\kappa r} + D_1 e^{-\kappa r} & \text{if } r > r_0, \end{cases} \tag{4.6}$$

where $\kappa_0 = \sqrt{\frac{m(E_{bound}+V_0)}{\hbar^2}}$ and $\kappa = \sqrt{\frac{mE}{\hbar^2}}$. E_{bound} is chosen to be infinitesimally small, since the wave function is extremely weakly bound. Since the radial solution is $R(r) = \frac{u(r)}{r}$, we know that $A_1 = 0$, because the cosine term would blow up to infinity. For the same reason we can eliminate the growing exponent, because it would blow up for $r \to \text{inf}$. Now $u(r)$ becomes

$$u(r) = \begin{cases} B_1\sin(\kappa_0 r) & \text{if } r \leq r_0 \\ D_1 e^{-\kappa r} & \text{if } r > r_0. \end{cases} \tag{4.7}$$

For the sake of continuity of the wave function and its first derivative, the solutions for both intervals should yield the same result. Therefore we can derive the relation

$$\frac{u'(r_0)}{u(r_0)} = \kappa_0\cot(\kappa_0 r0) = -\kappa. \tag{4.8}$$

Since the binding energy of the potential is expressed in terms of κ, this parameter should have some relation with the parameters that define the potential. This relation is derived further in the next section.

4.2 Scattering length

Let us now solve the Schrödinger equation for an unbound state with an infinitesimal amount of positive energy. The Schrödinger equation does not change for the interval inside the potential, but outside the potential it can be approximated by

$$\frac{d^2u}{dr^2} = 0, \tag{4.9}$$

since $E \to 0$. The solution is

$$u(r) = \begin{cases} A_2 \sin(k_0 r) + B_2 \cos(k_0 r) & \text{if } r \leq r_0 \\ C_2 r + D_2 & \text{if } r > r_0. \end{cases} \tag{4.10}$$

The solution outside the potential is a straight line, which can be understood by seeing it as a sine with an infinitesimal wave number. Again we claim that $B_2 = 0$, because the cosine term would blow up.

The solution inside the potential does not differ from the one that has been discussed in the prior section, because both the binding energy and the kinetic energy are infinitesimally small and contribute nothing to the wave number inside the potential well. This follows from

$$\begin{aligned} \kappa_0 = \sqrt{\frac{m}{\hbar^2}\left(E_{bound} + V_0\right)} = \sqrt{-\kappa^2 + \frac{mV_0}{\hbar^2}} \approx \sqrt{\frac{mV_0}{\hbar^2}}, \\ k_0 = \sqrt{\frac{m\left(E + V_0\right)}{\hbar^2}} = \sqrt{k^2 + \frac{mV_0}{\hbar^2}} \approx \sqrt{\frac{mV_0}{\hbar^2}}, \\ \kappa_0 \approx k_0. \end{aligned} \tag{4.11}$$

Now we define the value of r for which the wave function coincides with the x-axis for the first time outside the potential as the scattering length, a, hence from equation 4.10 it follows that

$$u(a) = C_2 a + D_2 = 0, \qquad a = -\frac{D_2}{C_2}. \tag{4.12}$$

The conditions for continuity of the wave function and its derivative, applied to equation 4.10 give

$$\sin(k_0 r_0) = C_2 r_0 + D_2, k_0 \cos(k_0 r_0) = C_2, k_0 \cot(k_0 r_0) = \frac{1}{r_0 + \frac{D_2}{C_2}} = \frac{1}{r_0 - a} = -\kappa, \tag{4.13}$$

were we have used the relation $k_0 \approx \kappa_0$ from equation 4.11. Inserting this relation in 4.8 we obtain

$$\sqrt{\kappa^2 + \frac{mV_0}{\hbar^2}} \cot(\sqrt{\kappa^2 + \frac{mV_0}{\hbar^2}} r_0) = -\kappa. \tag{4.14}$$

This is a transcendental equation and therefore cannot be solved algebraically for κ, but we can make an accurate approximation. Remember that we chose κ to be infinitesimally small, thus we can neglect the contribution of κ to the square roots in this equation. The scattering length can now be written as

$$a = r_0 + \frac{1}{\kappa}, \tag{4.15}$$

and by substituting equation 4.14

$$a = r0 - \frac{\tan(\sqrt{\frac{mV_0}{\hbar^2}} r_0)}{\frac{mV_0}{\hbar^2}}. \tag{4.16}$$

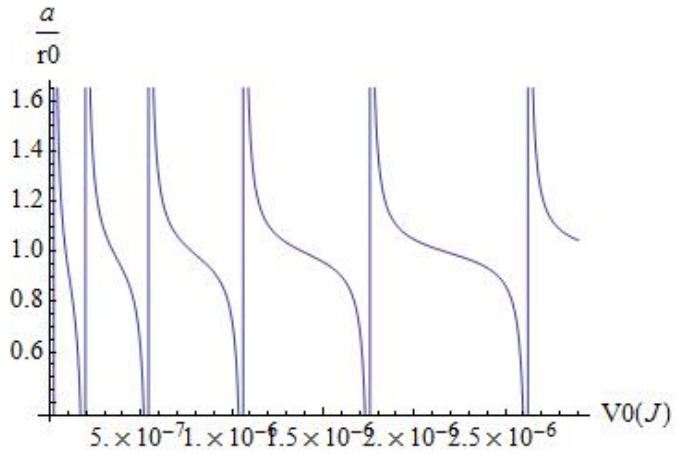


Figure 4.1: The scattering length of the potential as function of the potential depth, V_0. Each asymptote represents a bound state.

The scattering length is plotted in figure 4.1 as a function of the depth of the potential, V_0. Each vertical asymptote represents a bound state. Since we are interested in a potential with two bound states, we should fix V_0 at a value just after the second bound state. The potential depth becomes

$$V_0 = \frac{\hbar^2}{mr_0^2}(\frac{3\pi}{2})^2\xi, \tag{4.17}$$

where ξ is a slightly more than 1 and is further to be specified.

Now we have tuned all the parameters of the potential and we are ready to determine its phase shift.

4.3 Phase shift due to the finite square well potential

In the previous section we have solved the Schrödinger equation for an unbound state, by making use of the appromximation $E \approx 0$. In this section we find the exact solution for the Schrödinger equation, from which we can derive an expression for the phase shift due to the potential.

The time-independent Schrödinger equation for this problem is

$$\left(-\frac{\hbar^2}{mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + V(r)\right)R(r) = ER(r), \tag{4.18}$$

where the potential $V(r)$ is given by

$$V(r) = \begin{cases} -V_0 & \text{if } r \leq r_0 \\ 0 & \text{if } r > r_0, \end{cases} \tag{4.19}$$

where r_0 is the width of the potential. The Schrödinger equation should be solved in the two different intervals independently. It follows that the wave function becomes

$$u(r) = \begin{cases} A_1 \sin(k_0 r) + A_2 \cos(k_0 r) & \text{if } r \leq r_0 \\ B_1 e^{i\delta_0} \sin(kr) + B_2 e^{i\delta_0} \cos(kr) & \text{if } r > r_0, \end{cases} \tag{4.20}$$

with $R(r) = r\psi(r)$, k_0 the wave number of the particle inside the well, k the wave number outside the well and A_1,A_2,B_1 and B_2 are normalisation factors. It follows that $A_2 = 0$ from the boundary condition that $\psi = 0$ and therefore $R(r) = 0$ at $r = 0$. For the second interval there is no such condition we can use to cancel the sine or cosine term. However, we can rewrite the sum of the sine and cosine as a sine with a phase shift, as given by

$$u(r) = \begin{cases} A \sin(k_0 r) & \text{if } r \leq r_0 \\ B \sin(kr + \delta_0(k)) & \text{if } r > r_0, \end{cases} \tag{4.21}$$

Since the wave function and its derivative should be continuous at the point $r = r_0$ we have

$$\begin{aligned} \sin(k_0 r_0) &= e^{i\delta_0} \sin(kr_0 + \delta_0(k)), \\ k_0 \cos(k_0 r_0) &= k e^{i\delta_0} \cos(kr_0 + \delta_0(k)), \end{aligned} \tag{4.22}$$

which, by dividing each other, we can transform into

$$k_0 \cot(k_0 r_0) = k \cot(kr_0 + \delta_0(k)). \tag{4.23}$$

Solving the equation for the phase shift yields

$$\delta_0(k) = -kr_0 + \operatorname{arccot}\left(\frac{k_0}{k} \cot k_0 r_0\right). \tag{4.24}$$

In order to obtain an expression for the phase shift in terms of tuneable parameters, we combine equation **??** and the first expression of equation 4.11 to find

$$\kappa_0 = \sqrt{\frac{(\frac{3\pi\xi}{2})}{\tan(\frac{3\pi\xi}{2})^2} + (\frac{3\pi\xi}{2r_0})^2}, \tag{4.25}$$

which we can substitute in equation 4.24 via the last expression of equation 4.11 to obtain

$$\delta_0(k) = -kr_0 + \operatorname{arccot}\left(\frac{\sqrt{\frac{(\frac{3\pi\xi}{2})^2}{\tan(\frac{3\pi\xi}{2})^2} + (\frac{3\pi\xi}{2r_0})^2}}{k} \cot\left(\sqrt{\frac{(\frac{3\pi\xi}{2})^2}{\tan(\frac{3\pi\xi}{2})^2} + (\frac{3\pi\xi}{2r_0})^2} r_0\right)\right). \tag{4.26}$$

Now we have all the ingredients we need to calculate the on-shell scattering amplitude. However, we will first take a look at the normalisation of the exact solution we have found in this section, because we will need it for checking the validity of the on-shell scattering amplitude.

4.4 Normalisation of the wave function

When we will find an expression for the scattering amplitude, we will have to check its validity by comparing the wave function it gives with the exact solution of the Schrödinger equation. Therefore we have to normalise the solution of the Schrödinger equation first. Furthermore, normalisation is required to calculate the off-shell scattering amplitude.

It is usual to normalise both the radial and the angular parts of the wave function. However, we will add the normalisation factor of the angular part to the radial part, so that $Y_l^m(\theta, \phi) = 1$. Since we are considering an unbound state, the wave function cannot be normalised in the normal way by demanding $\int_v \psi^* \psi dV = 1$. In equation 3.5 we see that the state vectors are represented in the k-space, so we should normalise the wave function outside the potential by

$$\int_{k-space} \langle \psi_{k'} | \psi_k \rangle d^3k = 1. \tag{4.27}$$

Let us first calculate the inner product of the two wave functions with wave number k and k'. The inner product is given by

$$\langle \psi_{k'} | \psi_k \rangle = \int_V \psi^* \psi dV = B_{k'} B_k \int_V \frac{\sin(k'r + \delta_0') \sin(kr + \delta_0)}{r^2} dr. \tag{4.28}$$

We can write the sines as complex exponentials, which gives

$$\langle \psi_{k'} | \psi_k \rangle = \frac{4\pi B_{k'} B_k}{-4} \int_0^\infty \left(\left(e^{ik'r + \delta_0'} - e^{-(ik'r + \delta_0')} \right) \left(e^{ikr + \delta_0} - e^{-(ikr + \delta_0)} \right) \right) dr. \tag{4.29}$$

The integral of the exponentials can be simplified by using the formalism of the Dirac delta function. The Dirac delta function can be expressed by

$$\delta(x - a) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ip(x-a)} dp. \tag{4.30}$$

However, we use spherical coordinates and therefore we integrate from zero to ∞. This will give us

$$\frac{1}{2}\delta(x - a) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ip(x-a)} dp, \tag{4.31}$$

based on the symmetry of the Dirac delta function. Now the inner product can be written as

$$\pi B_{k'} B_k \int_0^\infty (e^{i(k'-k)r} + e^{i(k-k')}) dr = -2\pi^2 B_{k'} B_k (\delta(k -' k + \delta_0 - \delta_0')). \tag{4.32}$$

Please note that we have neglected the terms $e^{i(k+k'+\delta_0+\delta_0')}$, since they would require $k = -k'$ and therefore $k = k' = 0$, since k and k' are absolute values. This would give

rise to a non-physical situation. This can also be interpreted as integrating from ε to ∞, for which ε is an infinitesimal positive value. The delta functions do not depend explicitly on δ_0 and δ_0', since they are equal when k and k' are equal. Integrating equation 4.27 gives

$$8\pi^3 B_{k'} B_k \int_0^\infty \delta(k - k' + \delta_0 - \delta_0')k^2 dk = 1, \tag{4.33}$$

which only holds for $B_k = \frac{1}{(2\pi)^{3/2}k}$.

The wave function becomes

$$u(r) = \begin{cases} A\sin(k_0 r) & \text{if } r \leq r_0 \\ \frac{1}{(2\pi)^{3/2}} e^{i\delta_0} \sin(kr + \delta_0) & \text{if } r > r_0. \end{cases} \tag{4.34}$$

We can find the coefficient A by demanding using the boundary conditions again and demand that both parts of the wave function have the same value at the boundary of the potential. The expression for A is

$$A = \frac{1}{(2\pi)^{3/2}} \frac{\sin(kr_0 + \delta_0)}{\sin(k_0 r_0)} \tag{4.35}$$

and now the exact solution for the wave function is given by

$$u(r) = \begin{cases} \frac{1}{(2\pi)^{3/2}} \frac{\sin(kr_0+\delta_0)}{\sin(k_0 r_0)} \sin(k_0 r) & \text{if } r \leq r_0 \\ \frac{1}{(2\pi)^{3/2}} \sin(kr + \delta_0) & \text{if } r > r_0. \end{cases} \tag{4.36}$$

4.5 On-shell scattering amplitude

We now have all the ingredients to formulate an expression for the scattering amplitude of the potential. Substituting equation 4.26 in equation 3.22 from 3.3 gives

$$f = \frac{1}{k\cot\left(-kr_0 + \operatorname{arccot}\left(\frac{\sqrt{\frac{(\frac{3\pi\xi}{2})^2}{\tan(\frac{3\pi\xi}{2})^2} + (\frac{3\pi\xi}{2r_0})^2}}{k} \cot\left(\sqrt{\frac{(\frac{3\pi\xi}{2})^2}{\tan(\frac{3\pi\xi}{2})^2} + (\frac{3\pi\xi}{2r_0})^2} r_0\right)\right)\right) - ik}. \tag{4.37}$$

A better representation of the scattering amplitude is given graphically in figure 4.2. We have plotted the scattering amplitude for a rather arbitrary, but diverging value of the scattering length. The potential depth is set to $V_0 = 1.56371 * 10^-26$ and the resulting scattering length is $a = 450317 r_0$. The scattering amplitude decreases for an increasing wave number. This is exactly what we expect, because a wave with a high energy does not notice much difference between the regions inside and outside the potential. The wave number in this plot is expressed in $\frac{1}{r_0}$, where a wave number of a particle at a temperature of $10\mu K$ has a wave number of $k = \frac{0.313105}{r_0}$.

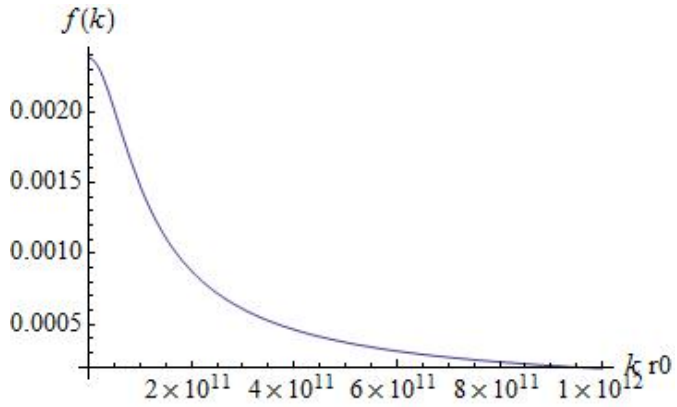


Figure 4.2: On-shell scattering amplitude as function of the incoming wave number, k. The scattering length is chosen to be $a = 450317r_0$.

An other characteristic of the scattering amplitude is its value for the limit $k \to 0$. The expression for the on-shell scattering amplitude from equation 3.22 contains the term $k \cot(k_0 r_0)$, which can be approximated from equation 4.23, since

$$k \cot(kr_0 + \delta_0) \approx k \cot(\delta_0). \tag{4.38}$$

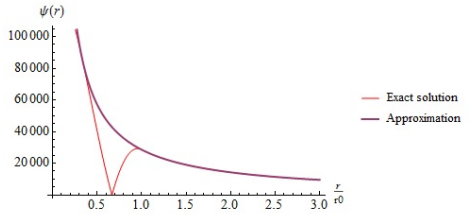
Using equations 4.8 and 4.15 the scattering amplitude becomes for $k \to 0$

$$f(k \to 0) = \frac{1}{-\kappa - ik} \approx \frac{1}{-\kappa} = r_0 - a \approx -a. \tag{4.39}$$

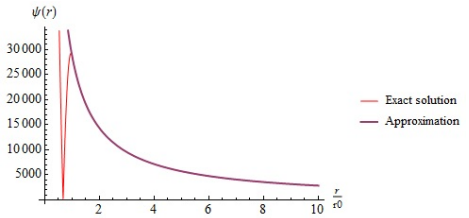
We are allowed to make an approximation in the last step, because we have adjusted the potential depth, so that $a >> r_0$. The conclusion is that the scattering amplitude should be equal to the scattering length in the limit $k \to 0$. In section 4.2 we found the value for the diverging scattering length. This is exactly the value the scattering amplitude approaches in the limit for low k.

A last test for the on-shell scattering amplitude would be to substitute the expression in equation 3.15 and compare it with the exact solution of the Schrödinger equation, which was derived in the previous section. We should note that equation 3.15 is an approximation that only works at large distances from the potential. We see exactly this behavior in figure 4.3, where the approximated wave function does not resemble the exact solution of the Schrödinger equation for small values of r. However, when directly outside the potential the two do coincide, thus the scattering amplitude works fine. The figure also shows the behavior of the wave function at large distances from the potential. In this region the wave function resembles a spherical wave with a phase shift, as expected.

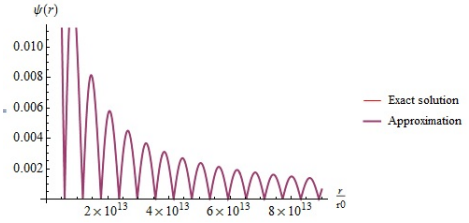
The on-shell scattering process of the finite square well potential can now be fully described using the on-shell scattering amplitude. The next task is to find an expression for the off-shell scattering amplitude, which is found in the next section.



(a) The absolute value of the wave function plotted near the potential for the approximation we have made using the scattering amplitude and the exact solution of the Schrödinger equation.



(b) The absolute value of the wave function plotted further away from the potential for the approximation we have made using the scattering amplitude and the exact solution of the Schrödinger equation.



(c) The absolute value of the wave function plotted at a great distance from the potential for the approximation we have made using the scattering amplitude and the exact solution of the Schrödinger equation.

Figure 4.3: The absolute value of the wave function as function of r is plotted for both the exact solution of the Schödinger equation and the expression from equation 3.15, in which we made use of the on-shell scattering amplitude. Three plots have been made at different distances from the potential. The used scattering length is $a = 450317 r_0$.

4.6 Off-shell scattering amplitude

In section 3.1 we have found an expression for the scattering amplitude, given by equation 3.13. Until now we have assumed that the incoming wave has the same wave number as the the outgoing wave. This scattering process is called on-shell scattering and only describes elastic scattering. However, in three-body systems inelastic scattering can occur between two particles, because energy is not conserved in the two-body sub-system. Inelastic scattering can be described by the so-called "off-shell" scattering amplitude. Efimov physics takes place in three body-system, so we want to derive an expression for the off-shell scattering amplitude.

The expression in equation 3.13 can be written as

$$f(\boldsymbol{k'}, \boldsymbol{k}) = \frac{-1}{4\pi}(2\pi^3)\frac{m}{\hbar^2}\langle \boldsymbol{k'}|V|\psi^{(+)}\rangle = -\frac{1}{4\pi}(2\pi)^3\frac{m}{\hbar}\int d^3x \int d^3x' \langle \boldsymbol{k'}|\boldsymbol{x'}\rangle\langle \boldsymbol{x'}|V|\boldsymbol{x}\rangle\langle \boldsymbol{x}|\psi^{(+)}\rangle. \tag{4.40}$$

Using the expressions from equations 3.9 and 3.7, we arrive at

$$f(\boldsymbol{k'}, \boldsymbol{k}) = -\frac{1}{4\pi}(2\pi)^3 \frac{m}{\hbar} \int_{\mathcal{V}} d^3x e^{-i\boldsymbol{k'}\cdot\boldsymbol{x}} V(\boldsymbol{x}) \langle \boldsymbol{x}|\psi^{(+)}\rangle, \tag{4.41}$$

which is nothing more than a Fourier transform over the range of the potential, $\mathcal{V}$. Writing out the inner product in the exponential empowers us to integrate over θ and gives us

$$\begin{aligned} f(\boldsymbol{k'}, \boldsymbol{k}) = \frac{1}{4\pi}(2\pi)^3 \frac{mV_0}{\hbar} \int_0^{2\pi} d\phi \int_0^{\pi} \sin(\theta) d\theta \int_0^{r_0} e^{-ik'r\cos(\theta)} \langle \boldsymbol{x}|\psi^{(+)}\rangle r^2 dr = \\ -\frac{1}{2}(2\pi)^3 \frac{mV_0}{\hbar k'} \int_0^{r_0} \sin(k'r) \langle \boldsymbol{x}|\psi^{(+)}\rangle r dr. \end{aligned} \tag{4.42}$$

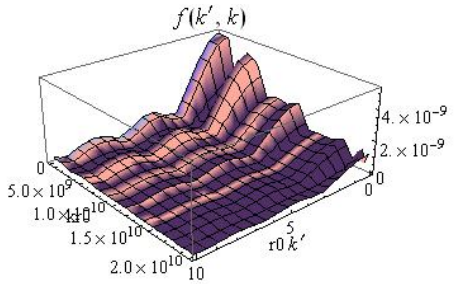
The expression we need for the wave function can be found in equation 4.36 and the integral results in

$$f(\boldsymbol{k'}, \boldsymbol{k}) = \frac{e^{-ikr_0} mV_0(-k_0 \sin(k'r_0) + k' \cos(k'r_0) \tan(k_0 r_0))}{(k_0 - k')kp(k_0 + k')\hbar^2(k_0 - ik1 \tan(k_0 r_0))}, \tag{4.43}$$

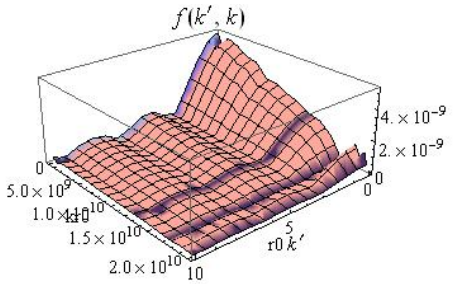
where we one should substitute the expression for k_0 from equation 4.11. We have omitted this substitution for the sake of keeping order in the expression. A three dimensional plot of the off-shell scattering amplitude is shown in figure 4.4. We see that the scattering amplitudes with a negative scattering length are more affected by a change in the scattering length, as they show more oscillations on the same interval. We also see that the scattering amplitude becomes more dependent on the wave number of the incoming wave, k, as the absolute value of the scattering length decreases. This can be explained by the fact that for a large scattering length the scattering process is dominated by effect from the Feshbach resonance. When the scattering length is decreased, these effects dominate less and the wave number of the incoming wave becomes of more importance. The most interesting conclusion, however, is that the scattering amplitude depends differently on the wave number of the incoming wave number than on the wave number of the outgoing wave function. Interesting changes in the scattering amplitude occur for values of the wave number of the incoming wave function of the order of 10^9 times smaller of the outgoing wave. This is especially interesting, because many models used today use a cut-off range in the momentum-space and the cut-off is normally considered to be equal for the incoming and the outgoing wave function. This figure shows that this is not the case. Future models can take this difference into account.

To see the consequences of the off-shell scattering, we have plotted the wave function as result of an on-shell scattering process and as result of an off-shell scattering process in the same graph in figure **??**, where we have chosen the wave number of the outgoing wave to be 1.2 times larger than the wave number of the incoming wave in the first plot and $k' = 1.05k$ in the second plot. We see, as one would expect, that the wave functions have a phase shift and amplitude shift compared to each other. We

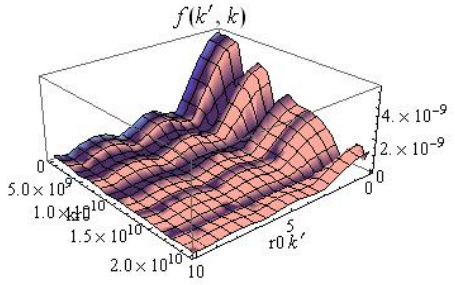
can check for validity of our off-shell scattering amplitude by letting k' approach k. We can conclude from figure **??** that the off-shell scattering amplitude indeed describes the correct on-shell scattering when $k' \to k$.



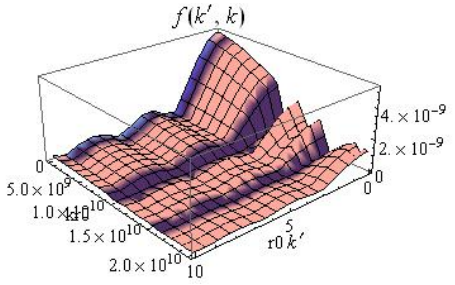
(a) The absolute value of the scattering amplitude as function of k and k' for a scattering length $a = -10000r0$.



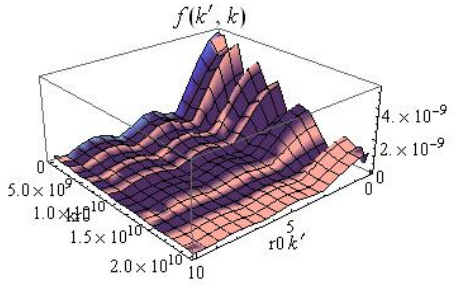
(b) The absolute value of the scattering amplitude as function of k and k' for a scattering length $a = 10000r0$.



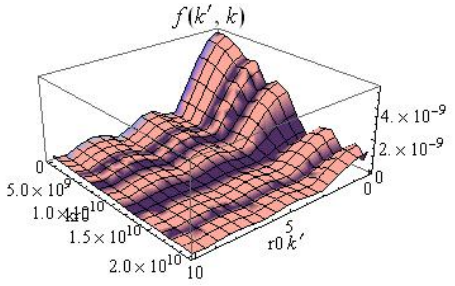
(c) The absolute value of the scattering amplitude as function of k and k' for a scattering length $a = -1000r0$.



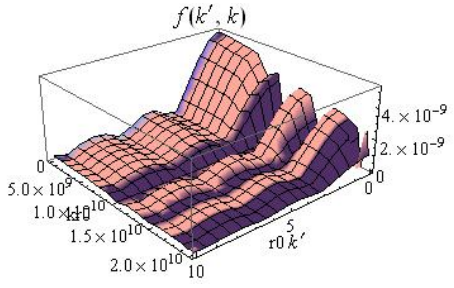
(d) The absolute value of the scattering amplitude as function of k and k' for a scattering length $a = 1000r0$.



(e) The absolute value of the scattering amplitude as function of k and k' for a scattering length $a = -100r0$.

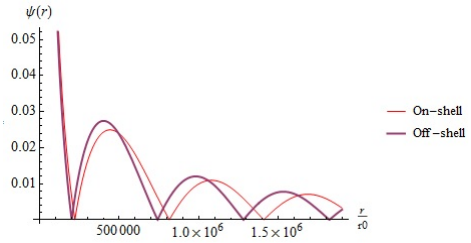


(f) The absolute value of the scattering amplitude as function of k and k' for a scattering length $a = 100r0$.

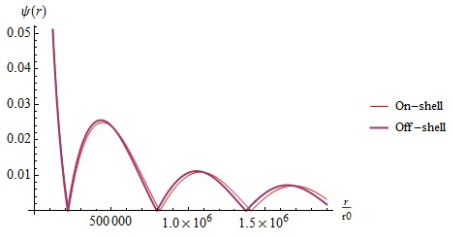


(g) The absolute value of the scattering amplitude as function of k and k' for a scattering length $a = 0$.

Figure 4.4: The absolute value of the scattering amplitude as function of k and k' for various scattering lengths. Scattering amplitudes with a negative scattering length are shown on the left and scattering amplitudes with positive scattering lengths are shown on the right.



(a) Comparison of the wavefunction due to an on-shell(red) and an off-shell(purple) scattering process for $k' = 1.2k$.



(b) Comparison of the wavefunction due to an on-shell(red) and an off-shell(purple) scattering process for $k' = 1.05k$.

Figure 4.5: Comparison of the wavefunction due to an on-shell(red) and an off-shell(purple) scattering process.

5. Conclusion and Outlook

Using a simplified version of Feshbach resonance we are able to describe the scattering processes on a finite square well potential in cold gases for diverging scattering length. The finite range of the scattering potential may give better predictions for the behavior of Efimov states.

The on-shell scattering amplitude, which contains all the information of the scattering process, is able to describe elastic scattering processes due to the potential. When the wave number of the incoming wave function approaches zero, the scattering amplitude is equal to the scattering length. A common approximation that is used for the scattering length, given in equation 4.15 fits the scattering length, that can be derived from the scattering amplitude, well. The exact solution of the Schrödinger equation is also in accordance with the wave function we obtain from the scattering amplitude.

We have found an expression for the off-shell scattering amplitude that is consistent with the on-shell amplitude when the wave number of the incoming and outgoing wave become equal. The dependence of the wave number of incoming and outgoing wave functions on the off-shell scattering amplitude shows some interesting behavior, i.e. the values for which the scattering amplitude shows significant changes differ with a factor 10^9 between the two wave numbers. Many models today use a cut-off for for the scattering amplitude in momentum space for both wave numbers. It is usual to make no distinction between the two, but we have concluded that this distinction should be made.

In Efimov physics the two-body interactions can be used to describe the three-body system. There are various models that try to justify the non-universal behavior of the Efimov states, such as describe by Rademaker [4]. The next step would be to implement the off-shell scattering amplitude in Rademaker's model to try to find predictions that match the observed non-universal behavior.

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