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REGULARISATION, RENORMALISATION AND ANOMALIES IN QUANTUM MECHANICS

Henrik Ekström

Department of Astronomy and Theoretical Physics, Lund University

Bachelor thesis supervised by Johan Bijnens

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Abstract

This bachelor thesis studies three different singular potentials: the one dimensional δ-potential and its derivative, δ', as well as the two dimensional $\delta^{(2)}$-potential. The latter two potentials require regularisation and renormalisation and $\delta^{(2)}$ demonstrates anomalous symmetry breaking: the breaking of a symmetry (in this case scale invariance) through regularisation.

The δ-potential in one dimension does not *require* regularisation but it is done anyway, to show that it produces the same results. Bound states and scattering coefficients are calculated with boundary conditions and Fourier transforms and it is regularised using a finite well.

The δ' needs both regularisation and renormalisation. The potential is regularised by a finite well and barrier (called the 'threshold potential'), by two approaching δ-functions and by using Fourier transforms. The potential strength is renormalised in both cases to keep the energy levels, which are physical observables, finite and independent of any parameters connected to the regularisation.

The two dimesional $\delta^{(2)}$-function's bound states are regularised with Fourier transforms, while both bound states and scattering coefficients are regularised by a finite well.

Populärvetenskaplig sammanfattning

Kvantmekanik berör hur partiklar beter sig i olika potentialer. Några olika potentialer kommer att studeras i denna rapport, nämligen tre olika sorters δ-potentialer (i en och två dimensioner, samt derivatan av den endimensionella). Lösningar för dessa kommer kommas fram till från olika håll som, trevligt nog, alla ger samma resultat. En δ-potential kan tolkas som beskrivandes "punktinteraktioner", när (punktformiga) partiklar bara påverkas av varandra om de är i precis samma punkt. Det festliga med kvantmekanik är att saker händer på ett annorlunda sätt än man hade kunnat tro. Klassiskt påverkar en sådan potential inte systemet om inte partiklarna faktiskt kommer till exakt samma ställe, men kvantmekaniskt kommer δ-potentialen märkas av i en större utsträckning.

Väl givet en potential är det intressant att titta på två fall: spridning och bundna tillstånd. Spridning sker när en partikel har så hög energi att den kan trivas långt borta från potentialgropen, medan ett bundet tillstånd klassiskt inte kan lämna densamme alls. Kvantmekaniskt kan den dock det, lite grand, med bestämt beteende. Ibland ser energin ut att behöva vara oändlig, i vilket fall man får ta till vissa knep (renormering) för att få ut rimliga, fysikaliska, resultat vilket ibland går.

Renormering är en rimlig sak att göra då potentialen i sig inte kan mätas fysikaliskt. Klassiskt kan man mäta skillnader i potential och kvantmekaniskt kan man mäta energinivåer och spridningskoefficienter men man kan aldrig mäta potentialen själv. Därför kan det motiveras att om man justerar potentialen så att den ger rimliga resultat så kan man använda sig av de resultaten utan bekymmer. Hur magiskt det än verkar när oändligheter sväljs upp av diverse konstanter i systemet så är renormering något som används flitigt i framför allt kvantfältsteori. Detta arbete ser på fall där renormering dyker upp i kvantmekanik.

Contents

1 Introduction

The Schrödinger equation is the heart of quantum mechanics. Via separation of variables one can study the time independent Schödinger equation which, in units such that the mass $M = \frac{1}{2}$ and $\hbar = 1$, reads:

$$-\frac{d^2}{dx^2}\Psi(x) + V(x)\Psi(x) = E\Psi(x).$$

This will be studied for a variety of potentials: a few different potential wells, their corresponding δ-function potentials and the limit of the one going to the other.

What is interesting is that not all of these make sense immediately. Some require, or can make use of, regularisation: the introduction of some regulator to make the problem more well defined in troublesome areas. To produce physical results, some also require renormalisation: a redefinition of constants, defining them in a neat way to rid the problem of infinities. The main point is that physical results can appear from potentials that are singular. Since the potential itself is not physically measurable, it is reasonable to adjust or fine tune it until it yields reasonable results. Most often one can adjust a constant to approach either zero or infinity, by letting it depend on the regulator (for example a cut-off in the integrations or an adjustment in the potential itself). Once one has calculated bound state energies or scattering coefficients, the regulator is sent on its way to infinity or zero, depending on the case, and possibly some constant is sent along with it. An important aspect is that all physical results and observables should be independent of the regularisation method.

Sometimes a symmetry is lost in the regularisation and this way of loosing symmetries is called anomalous, or quantum mechanical, symmetry breaking. It is mostly seen in quantum field theory but it is also prevalent in some quantum mechanical problems. It is a third form of symmetry breaking (the first two being explicit and spontaneous symmetry breaking[1]), where the symmetry is lost in the quantisation of the problem or in the regularisation of it. The symmetry that is lost in our example is that of scale invariance: if bound states are found a scale is clearly present and it was introduced by the regulator.

Sections 2 and 3 show the bound states and scattering coefficients for the case of a single well and its limit to the one dimensional δ-potential. This is an example of regularisation (though it is technically not needed) and a simple singular potential defined by a limit. Section 4, the derivative of the δ-function, demands both regularisation and renormalisation: a constant is redefined to take care of a physical observable otherwise approaching infinity. Section 5 is an example of a potential (the two dimensional $\delta^{(2)}$) that requires regularisation, renormalisation and has anomalous symmetry breaking.

A statement on conventions: if a variable is imaginary it will be explicitly stated. When, for instance, $\sqrt{-E}$ appears, E is negative. Furthermore, all square roots are chosen positive.

2 Bound states for the single well

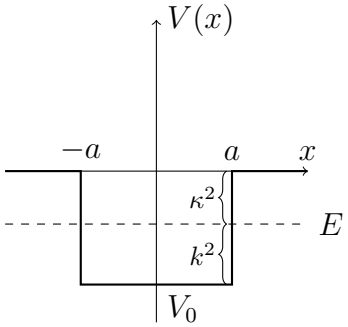
A good starting point is a finite potential well. The approach here is rather common and can be found in any textbook on the subject, e.g. [2]. The well will eventually be pinched to a δ-function and the results for the finite well will be needed so they are derived. Later sections will follow a similar approach and the method will become familiar.

2.1 The wave function and bound states for a single well

The well has depth $V_0 < 0$. We first consider bound states: $E < 0$.

$$V(x) = \begin{cases} 0, & |x| > a \\ V_0, & |x| \leq a \end{cases}$$

$$\begin{cases} \kappa^2 = |E| \\ k^2 = |V_0 - E| \end{cases}$$



The units are such that $M = 1/2$ (the mass), and $\hbar = 1$. In this problem one may invoke symmetry: with a symmetrical potential the solutions will be a linear combination of odd and even functions. Solving the Schrödinger equation for these symmetries gives

$$\begin{cases} \Psi_{even}(x) = Ae^{-\kappa|x|}, & |x| \geq a \\ \Psi_{even}(x) = B\cos kx, & |x| \leq a \\ \Psi_{odd}(x) = \mathrm{sgn}(x)Ce^{-\kappa|x|}, & |x| \geq a \\ \Psi_{odd}(x) = D\sin kx & |x| \leq a \end{cases}.$$

The constants can be determined from the boundary conditions that both $\Psi(x)$ and $\Psi'(x)$ should be continuous at $x = \pm a$, and the normalisation condition $\int_{-\infty}^{\infty} |\Psi(x)|^2 \, dx = 1$. In this case the constants will not provide any relevant information in themselves, so they are omitted. However, dividing the wave function with its derivative at $x = a$, and using $k^2 + \kappa^2 = |V_0| \Leftrightarrow \kappa = \sqrt{|V_0| - k^2}$, gives a condition for the energy levels:

$$\begin{cases} ka\tan ka = \sqrt{(a\sqrt{|V_0|})^2 - (ka)^2}, & \text{even} \\ \dfrac{-ka}{\tan ka} = \sqrt{(a\sqrt{|V_0|})^2 - (ka)^2}, & \text{odd} \end{cases}. \tag{2.1}$$

These conditions can be graphically presented as functions of ka. The right hand sides are viewed as a circle with radius $a\sqrt{|V_0|}$ and the bound states are the intersections this makes in the first quadrant with the left hand sides. One even state always exists and with increasing $a\sqrt{|V_0|}$ new states are added, alternating between odd and even.

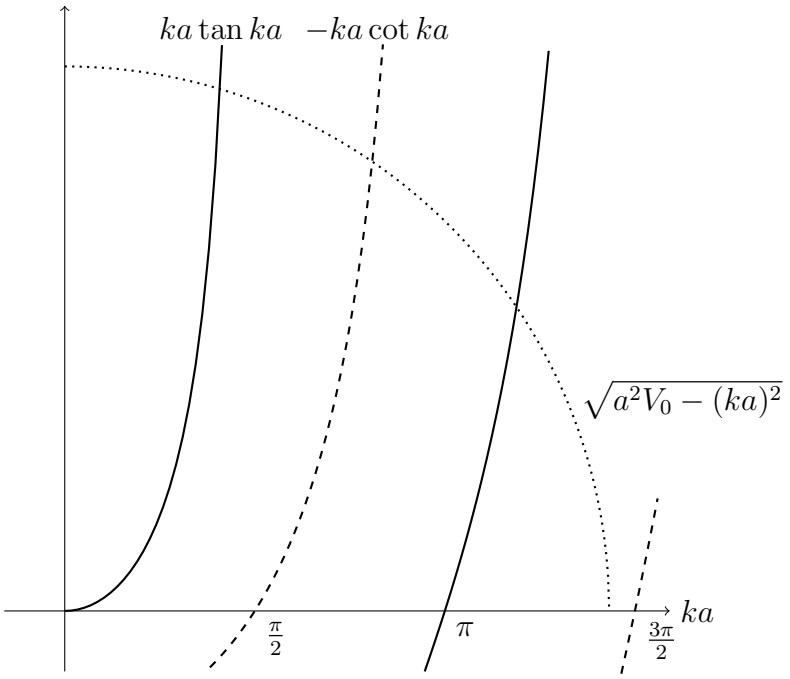


Figure 1: A graphical representation of equation (2.1). The thick lines are even wave functions, the dashed from odd wave functions and the intersections with the dotted circle are bound states. Note how at a small radius ($a\sqrt{|V_0|} < \pi/2$) only one (even) state is left.

2.2 The limit towards the δ-potential

One way of regularising the δ-potential is in terms of a finite well potential which is done in this section. One way of doing it is by changing the depth, $|V_0| \to \frac{1}{2a}$, and letting the width approach zero:

$$V(x) = b\delta(x) = \lim_{a\to 0} \begin{cases} \dfrac{b}{2a}, & |x| \le a \\ 0, & \text{elsewhere} \end{cases}. \tag{2.2}$$

This is a simple way of keeping the area constant (with a potential strength b). The method is used in [3], with agreeing results. There are multiple possible choises of regularisation, this particular one is chosen for its simplicity. Other methods should yield the same result.

From the geometrical interpretation, with the radius in figure 1 approaching zero, one would expect to find only one energy level, and indeed that is the case. The condition on the even function in (2.1) gives:

$$k\tan ka = \kappa \Leftrightarrow \sqrt{|V_0 - E|}\tan\left(\sqrt{|V_0 - E|}a\right) = \sqrt{|E|}.$$

Taylor expanding (and remembering that $|V_0 - E| = E - V_0$) gives

$$a(E - V_0) = \sqrt{|E|} \Rightarrow \lim_{a\to 0} a\left(E - \frac{b}{2a}\right) = \sqrt{-E} \Rightarrow -\frac{b}{2} = \sqrt{-E},$$

$$E = -\frac{b^2}{4} \tag{2.3}$$

and with $-b$ equalling a square root b must be negative. This is true since with a potitive b, $E > 0$ and no normalisable bound state can exist. We note that no odd state survives in the limit and that no renormalisation was necessary here, the limit was enough to reach the answer. Now that same answer would be pleasant to reach from the δ-function directly by other means.

2.3 The δ-potential via boundary conditions

The δ-potential will now be tackled with boundary conditions. The boundary conditions are not as simple as they were for the finite well, since when a potential has an infinite jump the derivative of the wave function is no longer continuous. One can get the conditions on the derivative by integrating the Schrödinger equation from $a - \varepsilon$ to $a + \varepsilon$, where a is the singularity and let $\varepsilon \to 0$. For a δ-potential with $a = 0$ the boundary conditions become[4]:

$$\begin{cases} \Psi'(0^+) - \Psi'(0^-) = b\Psi(0) \\ \Psi(0^+) = \Psi(0^-) \end{cases} \tag{2.4}$$

and, as before, that the wave function is normalisable and normalised, $\int |\Psi(x)|^2 dx = 1$.

We get a wave function of the form

$$\Psi(x) = \begin{cases} Ae^{\kappa x}, & x \leq 0 \\ Be^{-\kappa x}, & x \geq 0 \end{cases}$$

and the conditions become

$$\Psi(x) = \begin{cases} -B\kappa - A\kappa = bA \\ A = B \end{cases}.$$

Normalisation gives $A = \sqrt{\kappa}$ and we get

$$b = -2\kappa = -2\sqrt{-E}. \tag{2.5}$$

We now have the wave function, the bound state energy and a condition from (2.5) that b has to be negative for physical solutions:

$$\begin{cases} \Psi(x) = \sqrt{\kappa} e^{-\kappa|x|} \\ E = -\dfrac{b^2}{4} \\ b < 0 \end{cases} \tag{2.6}$$

This is in total agreement with the previous section.

2.4 The δ-potential via Fourier transforms

With one solution found twice, we now try another method: to solve the problem via Fourier transforms. One can, theoretically, solve any quantum mechanical problem in Fourier space as well as in position space, with the risk of encountering some difficulties in one representation or possibly both of them. This is, in principle, another method of regularisation where bounds are put on the integrals: they are integrated from $-\Lambda$ to Λ instead of from $-\infty$ to ∞. The cut-off Λ is then sent to infinity at the very end. However, with the δ-potential the regularisation is not needed.

In this thesis the following convention is used:

$$\widetilde{\Psi}(k) = \mathcal{F}\left[\Psi(x)\right] = \int \Psi(x) e^{-ikx} dx$$

$$\Psi(x) = \mathcal{F}^{-1}\left[\widetilde{\Psi}(k)\right] = \frac{1}{2\pi} \int \tilde{\Psi}(k) e^{ikx} dk$$

The method used seems rather convoluted: one Fourier transforms to momentum space the Schrödinger equation in the coordinate representation, $(S.E._{(x)})$, acting on the inversely Fourier transformed wave function from the momentum representation:

$$\mathcal{F}\left[\mathrm{S.E.}_{(x)}\left(\mathcal{F}^{-1}\left[\widetilde{\Psi}(k)\right]\right)\right]. \tag{2.7}$$

Equation (2.7) will be tackled from left to right. First, the Schrödinger equation is transformed to momentum space.

$$\int dx \left(-\frac{d^2}{dx^2}\Psi(x) + b\delta(x)\Psi(x)\right) e^{-ikx} = \int dx E\Psi(x) e^{-ikx}$$

Integration by parts is used twice on the first term (integrable wave functions obey $\lim_{x\to\pm\infty} \Psi(x) = 0$), and Fourier transforms are recognised, giving:

$$k^2\widetilde{\Psi}(k) + b\Psi(0) = E\widetilde{\Psi}(k) \tag{2.8}$$

Solving for $\widetilde{\Psi}(k)$, and having $\kappa^2 = -E$ (κ real) gives an expression for the transformed function,

$$\widetilde{\Psi}(k) = -\frac{b\Psi(0)}{k^2 + \kappa^2}.$$

Now the innermost transform in (2.7) is done using this expression and residue calculus.

$$\Psi(x) = \frac{1}{2\pi} \int \widetilde{\Psi}(k) e^{ikx} dk = -\frac{b\Psi(0)}{2\pi} \int \frac{e^{ikx}}{k^2 + \kappa^2} dk = Ae^{-\kappa|x|},$$

where A is a constant determined by the normalisation requirement so the wave function is:

$$\Psi(x) = \sqrt{\kappa} e^{-\kappa|x|}.$$

We note that it is the same as in the last section.

The connection between Fourier space and position space gives, doing the same transform at $x = 0$, a requirement on the energy level of the bound state:

$$\Psi(0) = \frac{1}{2\pi}\int \widetilde{\Psi}(k)e^{ikx}dk\bigg|_{x=0} = -\frac{1}{2\pi}\int \frac{b\Psi(0)}{k^2+\kappa^2}dk = -\frac{b\Psi(0)}{2\kappa}$$

$$b = -2\kappa \Leftrightarrow E = -\frac{b^2}{4}$$

There is only one bound state and the results are consistent with previous ones, (2.6). No regularisaion or renormalisation has been needed, and the energy is seen to be directly dependent on the potential strength which, in itself, is nothing strange.

The reason information can be extracted from the transforms is that if a bound state exist (which one assumes until contradictions occur), it must exist in all formalisms.

3 Scattering from a single well

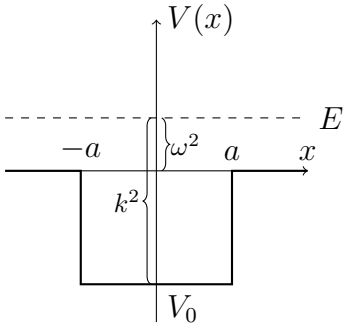
With a positive energy the wave function will scatter. This section will determine the reflection and transmission coefficients. This is an example of regularisation and a taken limit for another physical quantity.

3.1 Scattering from a finite well

With a wave function on the form

$$\Psi(x) = \begin{cases} e^{i\omega x} + re^{-i\omega x} & , \ x \leq -a \\ Ae^{ikx} + Be^{-ikx} & , \ |x| \leq a \\ te^{i\omega x} & , \ x \geq a \end{cases}$$

$$\begin{cases} \omega^2 = E \\ k^2 = E - V_0 \end{cases}$$



i.e. a plane wave, coming in from negative x, scattered at the well with reflection coefficient r and transmission coefficient t. Similar to previous sections, the demand for continuity in both the wave function and its derivative gives the following system of equations:

$$\begin{cases} e^{-i\omega a} + re^{i\omega a} = Ae^{-ika} + Be^{ika} \\ i\omega e^{-i\omega a} - ri\omega e^{i\omega a} = Aike^{-ika} - Bike^{ika} \\ te^{i\omega a} = Ae^{ika} + Be^{-ika} \\ ti\omega e^{i\omega a} = Aike^{ika} - Bike^{-ika} \end{cases}$$

which, through some algebra mainly consisting of taking the sum and difference of the first and last two equations, respectively, gives the coefficients:

$$\begin{cases} A = \dfrac{t}{2} e^{i\omega a - ika} \left(1 + \dfrac{\omega}{k}\right) \\ B = \dfrac{t}{2} e^{i\omega a + ika} \left(1 - \dfrac{\omega}{k}\right) \\ t = \dfrac{2e^{-2i\omega a}}{2\cos(2ka) - \left(\frac{\omega}{k} + \frac{k}{\omega}\right) i \sin(2ka)} \\ r = \dfrac{\left(\frac{\omega}{k} - \frac{k}{\omega}\right) e^{-2i\omega a} i \sin(ika)}{2\cos(2ka) - \left(\frac{\omega}{k} + \frac{k}{\omega}\right) i \sin(2ka)} \end{cases} \tag{3.9}$$

A and B here do not contribute with much information, but the transmission and reflection coefficients, t and r, give the probability of transmission and reflection as $|t|^2$ and $|r|^2$.

3.2 The limit to the δ-potential

With $V_0 = b/2a$ and the parenthesis terms put on a common denominator ($\omega^2 - k^2 = b/2a$), the scattering coefficients in equation (3.9) become

$$t = \frac{2e^{-2i\omega a}}{2\cos 2ka - \frac{2\omega^2 - b/(2a)}{k\omega} i \sin 2ka} \xrightarrow{a \to 0} \frac{1}{1 - \frac{b}{2i\omega}},$$

$$r = \frac{\frac{b/(2a)}{k\omega} e^{-2i\omega a} i \tan 2ka}{2 - \frac{2\omega^2 - b/(2a)}{k\omega} i \tan 2ka} \xrightarrow{a \to 0} \frac{1}{\frac{2i\omega}{b} - 1}.$$

Here $\omega a \to 0$ when $a \to 0$, as must be the case for a finite energy, but we also have $ka \to 0$ since $(ka)^2 = (\omega a)^2 - ba/2$.

The observables are thus independent of the regularisation parameter, as they should be.

3.3 The δ-potential via boundary conditions

The scattering too will be solved both from the boundary conditions and via Fourier space. With

$$\Psi(x) = \begin{cases} e^{i\omega x} + re^{-i\omega x}, & x \leq 0 \\ te^{i\omega x}, & x \geq 0 \end{cases}, \tag{3.10}$$

the boundary conditions for the δ-potential, (2.4), gives

$$\begin{cases} i\omega t - i\omega(1 - r) = bt \\ t = 1 + r \end{cases} \Leftrightarrow$$

$$\begin{cases} r = \dfrac{1}{\frac{2i\omega}{b} - 1} \\ t = \dfrac{1}{1 - \frac{b}{2i\omega}} \end{cases} \tag{3.11}$$

Once again, with different approaches the physical results match.

3.4 The δ-potential via Fourier transforms

Through Fourier space one can also get the coefficients, but it is less straightforward. The method is again on the form of (2.7), but this becomes slightly more complicated. One Fourier transforms the wave function, (3.10):

$$\widetilde{\Psi}(k) = \int_{-\infty}^{0} \left(e^{ix(\omega-k)} + re^{-ix(\omega+k)}\right)dx + \int_{0}^{\infty} (1+r)e^{ix(\omega-k)}dx =$$

$$= \int e^{ix(\omega-k)}dx + \underbrace{\int_{-\infty}^{0} re^{-ix(\omega+k)}dx + \int_{0}^{\infty} re^{ix(\omega-k)}dx}_{\equiv r\widetilde{\Xi}(k)}$$

$$\widetilde{\Psi}(k) = 2\pi\delta(\omega-k) + r\widetilde{\Xi}(k) \tag{3.12}$$

Here, $\widetilde{\Xi}(k)$ is not easily solvable. One could introduce a cut-off in the integrals, but here there exists a neater solution that uses the method of switching representations. The integral tells us that $\Xi(x) = e^{i\omega|x|}$, so finding $r\Xi(0)$ would give r directly.[1]

Equation (3.12) in the Fourier space Schrödinger equation, (2.8), gives:

$$k^2\left(2\pi\delta(\omega-k) + r\widetilde{\Xi}(k)\right) + b\Psi(0) = E\left(2\pi\delta(\omega-k) + r\widetilde{\Xi}(k)\right). \tag{3.13}$$

A δ-function outside of an integral is not particularly pleasant, so a closer look must be taken on what happens at $k = \omega$. Equation (3.13) is integrated around ω by some small parameter ε, later sent to 0. Let $\frac{d}{dk}G(k) \equiv k^2 r\widetilde{\Xi}(k)$ and $\frac{d}{dk}H(k) \equiv r\widetilde{\Xi}(k)$.

$$\int_{\omega-\varepsilon}^{\omega+\varepsilon} \left[k^2\left(2\pi\delta(\omega-k) + r\widetilde{\Xi}(k)\right) + b\Psi(0)\right]dk = \int_{\omega-\varepsilon}^{\omega+\varepsilon} E\left(2\pi\delta(\omega-k) + r\widetilde{\Xi}(k)\right)dk$$

$$\omega^2 2\pi + \left[G(k) + kb\Psi(0)\right]_{\omega-\varepsilon}^{\omega+\varepsilon} = E2\pi + \left[H(k)\right]_{\omega-\varepsilon}^{\omega+\varepsilon}$$

In the limit $\varepsilon \to 0$, the only thing remaining is the requirement

$$E = \omega^2$$

[1] Admittedly the boundary condition $t = 1 + r$ is used in the first line, but that same condition can be reached by other means as well. (3.12) is on the form of an incoming plane wave with an extra outgoing term, the coefficient of which can be argued to be $r + 1$ in the same way as the corresponding $(e^{2i\delta_m} - 1)$-coefficient in (6.38).

What remains in (3.13) is

$$r\widetilde{\Xi}(k) = -\frac{b\Psi(0)}{k^2-\omega^2}. \tag{3.14}$$

In order to find $\Xi(0)$, we make use of $\Psi(0)$. Using (3.12) and the inverse Fourier transform one gets

$$\Psi(0) = \frac{1}{2\pi}\int \widetilde{\Psi}(k)dk = 1 + \frac{1}{2\pi}\int r\widetilde{\Xi}(k)dk = 1 + r\Xi(0).$$

Now one connection between $\Xi(0)$ and $\Psi(0)$ has been found. Another is reached by integrating equation (3.14) in the same manner

$$r\Xi(0) = \int r\widetilde{\Xi}(k)dk = -b\Psi(0)\int \frac{dk}{k^2-\omega^2} = -b\Psi(0)\frac{i\pi}{\omega}.$$

These relations give

$$r\Xi(0) = \frac{-\frac{bi}{2\omega}}{1+\frac{bi}{2\omega}} = \frac{1}{\frac{2i\omega}{b}-1}. \tag{3.15}$$

Since we know $\Xi(0) = e^{i\omega|0|} = 1$, equation (3.15) must be r. With $t = 1 + r$, we again get:

$$\begin{cases} r = \dfrac{1}{\frac{2i\omega}{b}-1} \\ t = \dfrac{1}{1-\frac{b}{2i\omega}} \end{cases} \tag{3.16}$$

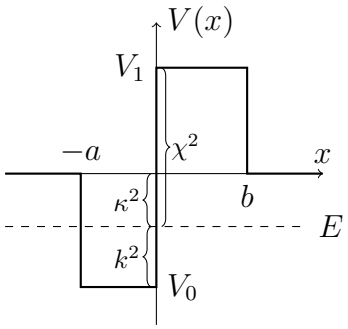
in agreement with before. One could solve for both $\widetilde{\Xi}(k)$ and $\widetilde{\Psi}(k)$, but the coefficients are discovered, which was the goal. No renormalisation was required in any method.

4 Bound states for the threshold potential

We now direct our attention to a potential that will be called the threshold potential. This is a means of regularisation of the soon to be pondered δ'-potential. For the sake of generality, both widths and strengths will be separate for the well and barrier, but towards the end of the section we will set $a = b$ and $V_1 = |V_0|$.

$$V(x) = \begin{cases} V_0 < 0, & -a \le x < 0 \\ V_1 > 0, & 0 < x \le b \\ 0, & \text{elsewhere} \end{cases}.$$

$$\begin{cases} \chi^2 = V_1 - E \\ \kappa^2 = -E \\ k^2 = E - V_0 \end{cases}.$$



4.1 The finite threshold potential

The wave function for the finite threshold potential becomes

$$\Psi(x) = \begin{cases} Ae^{\kappa x}, & x \leq -a \\ B\cos kx + C\sin kx, & -a \leq x \leq 0 \\ De^{\chi x} + Ee^{-\chi x}, & 0 \leq x \leq b \\ Fe^{-\kappa x}, & x \geq b \end{cases}$$

with boundary conditions from continuity:

$$\begin{cases} Ae^{-\kappa a} = B\cos ka - C\sin ka \\ A\kappa e^{-\kappa a} = Bk\sin ka + Ck\cos ka \\ B = D + E \\ Ck = \chi(D - E) \\ De^{\chi b} + Ee^{-\chi b} = Fe^{-\kappa b} \\ D\chi e^{\chi b} - E\chi e^{-\chi b} = -F\kappa e^{-\kappa b} \end{cases} \Leftrightarrow$$

$$\begin{cases} A = Fe^{\kappa(a-b)}\left\{\cos ka\left(\cosh\kappa b + \frac{\kappa}{\chi}\sinh\kappa b\right) + \sin ka\left(\frac{\kappa}{k}\cosh\kappa b + \frac{\chi}{k}\sinh\kappa b\right)\right\} \\ B = Fe^{-\kappa b}\left(\cosh\chi b + \frac{\kappa}{\chi}\sinh\chi b\right) \\ C = -Fe^{-\kappa b}\left(\frac{\kappa}{k}\cosh\chi b + \frac{\chi}{k}\sinh\chi b\right) \\ D = \frac{F}{2}e^{-b(\chi+\kappa)}\left(1 - \frac{\kappa}{\chi}\right) \\ E = \frac{F}{2}e^{b(\chi-\kappa)}\left(1 + \frac{\kappa}{\chi}\right) \\ A\kappa e^{-\kappa a} = Bk\sin ka + Ck\cos ka \end{cases}.$$

The last equation was not used to find the coefficients, but must also apply. With the coefficients inserted, it yields the following condition:

$$0 = \cos ka\left(2\cosh\chi b + \frac{\kappa^2 + \chi^2}{\kappa\chi}\sinh\chi b\right) +$$

$$\sin ka\left(\frac{\kappa^2 - k^2}{\kappa k}\cosh\chi b + \frac{\chi^2 - k^2}{\chi k}\sinh\chi b\right) \Leftrightarrow$$

$$\frac{\tan ka}{ka} = \frac{2(\chi a)(\kappa a) + [(\kappa a)^2 + (\chi a)^2]\tanh\chi b}{(\chi a)[(ka)^2 - (\kappa a)^2] + (\kappa a)[(ka)^2 - (\chi a)^2]\tanh\chi b} \tag{4.17}$$

This has to be fulfilled for bound states. From now on, for simplicity, $b = a$. With

$$\begin{cases} (ka)^2 = a^2(|V_0| - |E|) \\ (\kappa a)^2 = a^2|V_0| - (ka)^2 \\ (\chi a)^2 = a^2(|V_0| + V_1) - (ka)^2 \end{cases},$$

(4.17) is an equation dependent only on the potential strengths (which might as well be set to equal in magnitude), the width and the energy, which we know is confined to $V_0 < E < 0$.

Solutions to (4.17), and therefore bound states, must exist for $a = b, V_1 = -V_0$ but there is no guarantee for them to exist for any choice of a, b, V_0 and V_1. For $a \to 0$ one must be wary, as renormalisation is required.

4.2 The limit to δ'

Now the limit of the well becoming the δ' will be looked at. One way of writing $\delta'(x)$ is simply with the definition of the derivative:

$$c\delta'(x) = \lim_{a\to 0} \frac{c}{2a} \left(\delta(x-a) - \delta(x+a)\right), \tag{4.18}$$

and we remember how to make a basic square δ-function, (2.2). If that is between $-a$ and 0, it is of course $\delta(x + a/2)$. If the adjustments $b = a$, $V_1 = -V_0 = c/a$ are made[2] to the threshold potential one can get the limit wanted, in accordance with (4.18),

$$c\delta'(x) = \lim_{a\to 0} \begin{cases} -\dfrac{c}{a^2}, & -a < x < 0 \\ \dfrac{c}{a^2}, & 0 < x < a \\ 0, & \text{otherwise} \end{cases}.$$

With $-c/a^2 < E < 0$, one can define $\mathcal{E}$ to be the ratio of the energy and the well depth: $\mathcal{E} = -Ea^2/c$, $(0 < \mathcal{E} < 1)$. With this definition and the adjusted potential, equation (4.17) only depends on $\mathcal{E}$ and c:

$$\begin{cases} (ka)^2 = c(1 - \mathcal{E}) \\ (\kappa a)^2 = c\mathcal{E} \\ (\chi a)^2 = c(1 + \mathcal{E}) \end{cases},$$

Suddenly, there is an independence on the width as an $\mathcal{E}$ that solves (4.17) will stay the same when a is changed. Therefore the energy, which goes as $E = -\mathcal{E}c/a^2$, must shoot off to negative infinity if c is constant. If $c \to 0$ there does seem to be one state left, with $\mathcal{E} \to 0$. That could mean that if $c \to 0$ in an appropriate way, there is a single bound state with finite energy. Redefining c appropriately is called renormalising the problem. Exactly how $c \to 0$ could be seen from (4.17), but the limit would have to be taken carefully and no

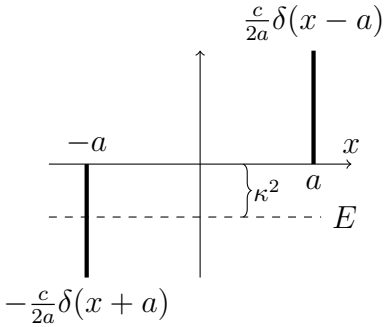
[2] the sign of c is taken to be positive to keep in line with previous equations, but a negative c would not alter any results.

neat, analytical way of doing so has been found. Instead, the renormalisation will be found with other limits. As with the δ-potential, it will be done by using boundary conditions and Fourier space.

4.3 The δ'-potential via 2 δ-functions

We now regularise the δ'-potential with two δ-functions in accordance with (4.18). One gets the wave function:

$$\Psi(x) = \begin{cases} Ae^{\kappa x}, & x \leq -a \\ Be^{\kappa x} + Ce^{-\kappa x}, & |x| \leq a \\ De^{-\kappa x}, & x \geq a \end{cases}.$$



The boundary conditions are the same as before, (2.4), but with the strength $\pm c/2a$ for each δ-potential, and they give

$$\begin{cases} Ae^{-\kappa a} = Be^{-\kappa a} + Ce^{\kappa a} \\ \kappa\left(Be^{-\kappa a} - Ce^{\kappa a} - Ae^{-\kappa a}\right) = -\dfrac{c}{2a}Ae^{-\kappa a} \\ Be^{\kappa a} + Ce^{-\kappa a} = De^{-\kappa a} \\ \kappa\left(-De^{-\kappa a} - Be^{\kappa a} + Ce^{-\kappa a}\right) = \dfrac{c}{2a}De^{-\kappa a} \end{cases} \Leftrightarrow \begin{cases} A = C\dfrac{4\kappa a}{c} \\ Be^{-2\kappa a} = C\left(\dfrac{4\kappa a}{c} - 1\right) \\ C = -Be^{2\kappa a}\left(\dfrac{4\kappa a}{c} + 1\right) \\ D = -Be^{2\kappa a}\dfrac{4\kappa a}{c} \end{cases}.$$

Which coefficients depend on which is of course arbitrary, but irrespecticve of the approach the system gives a relation that has to be fulfilled for κa.

$$e^{-4\kappa a} = -\left(\frac{4\kappa a}{c} - 1\right)\left(\frac{4\kappa a}{c} + 1\right) \Leftrightarrow \tag{4.19}$$

$$c^2 = \frac{16(\kappa a)^2}{1 - e^{-4\kappa a}} \tag{4.20}$$

If c is constant and $a \to 0$, the energy would have to $\to \infty$ to maintain (4.20). This can be mended by renormalisation so the energy remains constant and $c \to 0$. Taylor expanding (4.20) for small κa (as they again must be if the energy is to remain finite when $a \to 0$) gives an expression for c:

$$c = 4\sqrt{\kappa a}. \tag{4.21}$$

With this renormalisation, (4.19) can be solved with a finite energy even when $a \to 0$.

4.4 The δ'-potential via Fourier transforms

The derivative of the δ-function is also defined through integration by parts.

$$\int \delta'(x)f(x)dx = [\delta(x)f(x)] - \int \delta(x)f'(x)dx = -f'(0)$$

The second method, via Fourier space, starts with transforming the Schrödinger equation, now

$$-\frac{d^2}{dx^2}\Psi(x) + c\delta'(x)\Psi(x) = E\Psi(x),$$

to Fourier space. Only the potential term will be done explicitly now, as the rest is the same as before.

$$c\int \delta'(x)\Psi(x)e^{-ikx}dx =$$

$$= c[\delta(x)\Psi(x)e^{-ikx}] - c\int \delta(x)\Psi'(x)e^{-ikx}dx - (-ik)c\int \delta(x)\Psi(x)e^{-ikx}dx$$

$$= -c\Psi'(0) + cik\Psi(0)$$

giving us, with $E = -\kappa^2$:

$$k^2\widetilde{\Psi}(k) - c\Psi'(0) + cik\Psi(0) = E\widetilde{\Psi}(k) \Leftrightarrow$$

$$\widetilde{\Psi}(k) = \frac{c}{k^2+\kappa^2}\left(\Psi'(0) - ik\Psi(0)\right) \tag{4.22}$$

As with the δ-potential, equation (4.22) is used for the innermost Fourier transform. In the last line, the integral will diverge, so a cut-off (a regulator) Λ is introduced.

$$\Psi(0) = \frac{1}{2\pi}\int \tilde{\Psi}(k)dk = \frac{c\Psi'(0)}{2\pi}\int \frac{dk}{k^2+\kappa^2} - \frac{ic\Psi(0)}{2\pi}\int \frac{kdk}{k^2+\kappa^2} = \frac{c}{2\kappa}\Psi'(0) \tag{4.23}$$

$$\Psi'(0) = \frac{1}{2\pi}\int (-ik)\widetilde{\Psi}(k)dk = \frac{-ic\Psi'(0)}{2\pi}\int \frac{kdk}{k^2+\kappa^2} - \frac{c\Psi(0)}{2\pi}\int \frac{k^2dk}{k^2+\kappa^2} =$$

$$= \lim_{\Lambda\to\infty}\frac{c\Psi(0)}{2\pi}\left(2\Lambda - \left[\arctan\frac{k}{\kappa}\right]_{-\Lambda}^{\Lambda}\right) = \lim_{\Lambda\to\infty}\frac{c\Psi(0)}{\pi}\Lambda \tag{4.24}$$

Combining equations (4.23) and (4.24) we get, keeping in mind that Λ will be sent to infinity at some point and only keeping the leading term:

$$c = \sqrt{\frac{2\pi\kappa}{\Lambda}}. \tag{4.25}$$

Again the renormalised c allows a finite energy. This renormalisation and (4.19) differ slightly, but both approach zero similarly and that the factors are different is no problem; if one were to calculate observables they would agree regardless of the regularisation method and renormalisation used.

5 Bound states for the two dimensional well

The potential of interest in two dimensions, the two dimensional $\delta^{(2)}$-potential, exhibits scale invariance: there is no length scale in the system and its energy levels, were they naïvely derived, would be a continuum stretching down to negative infinity (with no ground state, which is unphysical). When renormalisation rescales the results to be physical (a finite amount of bounded energy levels) a scale is present (the energy levels can be used as one). In this section the scale is introduced first in the well width and later in the momentum integral cut-off.

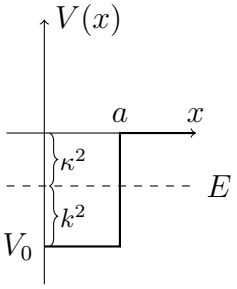
The Fourier transform is most comfortably done in Cartesian coordinates (x, y), but these are not particularly agreeable when the potential is the two dimensional square well. The infinite square well (a problem where the potential is infinite outside of the well) can be solved in Cartesian coordinates as the boundary condition for that is $\Psi(x, y) = 0$ on the well's edge, but when the wave function is allowed to spread further the boundary conditions are more complicated. The finite square well in two dimensions is not a simple problem. We therefore choose to use the finite circular well for which polar coordinates, (r, φ), are more appropriate.

5.1 Bound states for the finite, circular, two dimensional well

The problem is like previous sections approached from a finite regularisation of $\delta^{(2)}$. The method here bears much resemblance to the one dimensional well, with Bessel functions instead of exponential functions.

$$V(r) = \begin{cases} V_0, & r \leq a \\ 0, & \text{otherwise} \end{cases}$$

$$\begin{cases} \kappa^2 = -E \\ k^2 = E - V_0 \end{cases}$$



In two dimensions, the Schrödinger equation,

$$-\nabla_{2D}^2 \Psi(r, \varphi) + V(x)\Psi(r, \varphi) = E\Psi(r, \varphi), \tag{5.26}$$

with

$$\nabla_{2D}^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2},$$

prompts us to use separation of variables. Let

$$\Psi_m(r, \varphi) \propto R_m(r)\Phi_m(\varphi) \tag{5.27}$$

and insert it into (5.26), multiplying by r^2 and dividing with $R_m(r)\Phi_m(\varphi)$:

$$-r^2 \frac{R_m''(r)}{R_m(r)} - r\frac{R_m'(r)}{R_m(r)} + r^2\left(V(x) - E\right) = \frac{\Phi_m''(\varphi)}{\Phi_m(\varphi)} = -m^2. \tag{5.28}$$

Here primes represent derivatives. We have used a harmonic oscillator as our solution in the angular part, ensuring $m \in \mathbb{Z}$,

$$\Phi_m(\varphi) = e^{im\varphi}.$$

The radial part inside the well turns into

$$R''_{in}(r) + \frac{1}{r}R'_{in}(r) + \left(k^2 - \frac{m^2}{r^2}\right) R_{in}(r) = 0,$$

$k^2 = E - V_0$. This is turned into the Bessel equation by letting $R_{in}(r) \to R_{in}(kr)$. For convenience, the function will still be called R_{in}, but the kr-dependence will be held explicit.

$$R''_{in}(kr) + \frac{1}{kr}R'_{in}(kr) + \left(1 - \frac{m^2}{(kr)^2}\right) R_{in}(kr) = 0$$

The only Bessel functions finite at the origin are those of the first kind, J_m. Outside the well, the equation will be similar but without V_0: instead of k^2 there will be $-\kappa^2 = E$. This sign difference turns the equation into

$$R''_{out}(\kappa r) + \frac{1}{\kappa r}R'_{out}(\kappa r) - \left(1 + \frac{m^2}{(\kappa r)^2}\right) R_{out}(\kappa r) = 0,$$

the modified Bessel equation. The only modified Bessel functions finite at $x \to \infty$ are those of the second kind, K_m. We have

$$R_m(r) = \begin{cases} J_m(kr), & x \leq a \\ K_m(\kappa r), & x \geq a \end{cases}$$

and the complete wave function is then given by

$$\sum_{m=-\infty}^{\infty} A_m R_m(r)\Phi_m(\varphi) \tag{5.29}$$

with a free (and uninteresting) coefficient.

We require continuity, both in the wave function and its derivative. The radial function must be continuous at a and, similar to the one dimensional well, $kR'_{in,m}(ka)/R_{in,m}(ka) = \kappa R'_{out,m}(\kappa a)/R_{out,m}(\kappa a)$ gives

$$ka\frac{J'_m(ka)}{J_m(ka)} = \kappa a\frac{K'_m(\kappa a)}{K_m(\kappa a)} \tag{5.30}$$

and limits the number of bound states. There always exist at least one bound state for $m = 0$, but the potential strength, b, determines how many more there are. For a certain b, $m = 0$ always has the most bound states, with larger m having fewer.

A plot of the functions (as functions of b and varying the energy in $V_0 < E < 0$) reveal that the right hand side looks roughly like a negative square root (of $-b$) with a factor in front mildly varying with E and m, while the left hand side looks like a tan-function, horisontally stretched (i.e., its singularities occurring more rarely as $-b$ increases), stretching more with an increase in energy, E, and order, m. $m = 0$ always has one bound state. For each m, every intersection to the right of b at $E = V_0$ will pass b with the increase of E.

5.2 The limit to the $\delta^{(2)}$-potential

Now the well will be pinched to a $\delta^{(2)}$-potential. The integral over it gives the coefficient, knowing the volume of the $\delta^{(2)}$ should be equal to 1:

$$b \stackrel{!}{=} \int d^2 r b\delta^{(2)} = \int_0^{2\pi} d\varphi \int_0^a dr\ rV_{lim} = \lim_{a\to 0} 2\pi \frac{a^2}{2} V_0,$$

$$b\delta^{(2)} = \lim_{a\to 0} \begin{cases} \dfrac{b}{\pi a^2}, & r \le a \\ 0, & \text{otherwise} \end{cases}$$

The energies for bound states lie in $\frac{b}{\pi a^2} < E < 0$, so one may again define, as done in [3], the fraction $\mathcal{E} \equiv \frac{E\pi a^2}{b}$, $0 < \mathcal{E} < 1$ (positive, since neither E nor b is). Then equation (5.30) does not depend on the width of the potential well. The arguments become

$$\begin{cases} (ka)^2 = \dfrac{b}{\pi}(\mathcal{E} - 1) \\ (\kappa a)^2 = -\dfrac{\mathcal{E} b}{\pi} \end{cases}$$

and the bound states energy ratios, $\mathcal{E}$, that solve (5.30) are the same ones as they would be for the finite well, but as $a \to 0$, the energies will all be (negative and) infinite, since $E = \frac{\mathcal{E} b}{\pi a^2}$. Again, there does seem to be a chance of a finite energy if $b \to 0$. If this is the case the ground state must be for $m = 0$.

If a bound state with finite energy exists, κa is known to approach zero. It is now assumed that ka approaches zero as well, though how quickly it does so remains to be found. The following approximate forms for small arguments are used, Eqs. (9.4.1) and (9.6.8) in[5]. The derivatives are with respect to z, i.e. ka and κa, respectively, as the inner derivatives are taken care of in (5.30).

$$\begin{aligned} J_0(z) &= 1 + \mathcal{O}(z^2), & J_0'(z) &= -\frac{1}{2} z + \mathcal{O}(z^3) \\ K_0(z) &= -\ln(z) - \gamma + \mathcal{O}(z^2 \ln(z)), & K_0'(z) &\approx -\frac{1}{z} + \mathcal{O}(z) \end{aligned} \tag{5.31}$$

where γ is the Euler Mascheroni constant. They, inserted in (5.30), give

$$ka \frac{-\frac{ka}{2}}{1} = \kappa a \frac{-\frac{1}{\kappa a}}{-\ln \kappa a - \gamma} \Leftrightarrow -\frac{(ka)^2}{2} = \frac{1}{\ln \kappa a + \gamma} \Leftrightarrow \frac{b}{2\pi} + (\kappa a)^2 = \frac{1}{\ln \kappa a + \gamma}$$

Seeing as a will be sent to zero the $(\kappa a)^2$ term will be neglected.

$$b = \frac{2\pi}{\ln \kappa a + \gamma} \tag{5.32}$$

Like before the potential strength gets renormalised to enable a finite energy. This result will be used in the scattering case later. The denominator can be rewritten as $\ln(\kappa a e^{\gamma})$, which makes this renormalisation simpler to compare with the one soon to be defined with the Fourier transform method, (5.33).

5.3 The $\delta^{(2)}$-potential via Fourier transforms

To clarify, k is now the wave vector and not a square root of some energy. The $\delta^{(2)}$-potential can be renormalised with Fourier transforms, as could the δ'. The Schrödinger equation is transformed, with $\int b\delta^{(2)}\Psi(\vec{x})d\vec{x} = \widetilde{\Psi}(\vec{0})$:

$$\vec{k}^2\widetilde{\Psi}(\vec{k}) + b\Psi(\vec{0}) = E\widetilde{\Psi}(\vec{k}) = -\kappa\widetilde{\Psi}(\vec{k}) \Leftrightarrow$$

$$\widetilde{\Psi}(\vec{k}) = -\frac{b\Psi(\vec{0})}{\kappa + k^2}.$$

The same trick as before yields

$$\Psi(\vec{0}) = -\frac{1}{(2\pi)^2}\int d^2k \frac{b\Psi(\vec{0})}{\kappa + k^2} e^{i\vec{k}\cdot\vec{0}} = -\lim_{\Lambda\to\infty} \frac{b\Psi(\vec{0})}{4\pi} \ln\frac{\Lambda^2}{\kappa^2} \Leftrightarrow$$

$$b = -\frac{4\pi}{\ln \Lambda^2/\kappa^2} = \frac{2\pi}{\ln \kappa/\Lambda} \tag{5.33}$$

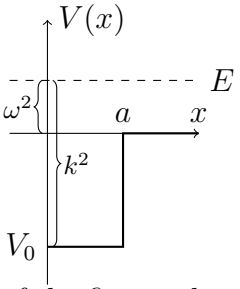
The result of this regularisation matches that of the last section (the argument of ln varies, but the limits are different accordingly: $\Lambda \to \infty, a \to 0$ and the constant with γ is again acceptable).

6 Scattering from a two dimensional well

6.1 Scattering from the finite two dimensional well

The solving of the equation is the same as in the previous section, but with different wave numbers.

$$\begin{cases} \omega^2 = E \\ k^2 = E - V_0 \end{cases}$$



The solution consists of ordinary Bessel functions of the first and second kind, respectively.

The second kind are written as $N_m(z)$ in this thesis (as they are often called the 'Neumann functions'), but the notation $Y_m(z)$ is also common. $N_m(z)$ diverges at the origin, but $J_m(z)$ does not diverge at infinity. One could go on with the exterior radial part being linear combination of Bessel functions of the first and second kinds, but when the area of interest is at $r \to \infty$ it is more fitting and mathematically convenient to use the Hankel functions. The latter are linear combinations of the former or, if one prefers, vice versa.

$$H_m^{(1)}(x) = J_m(x) + iN_m(x), \quad H_m^{(2)}(x) = J_m(x) - iN_m(x) \tag{6.34}$$

$H_m^{(1)}(\kappa r)$ $\left(H_m^{(2)}(\kappa r)\right)$ represents a cylindrical wave travelling out from (in towards) the origin.

The angular part will once again be $\Phi_m(\varphi) = e^{im\varphi}$ and the radial function will have the form

$$R_m(r) = \begin{cases} A_m J_m(kr), & x \leq a \\ B_m H_m^{(1)}(\omega r) + C_m H_m^{(2)}(\omega r), & x \geq a \end{cases}. \tag{6.35}$$

The corresponding equation that must be fulfilled for continuity is

$$ka\frac{J_m'(ka)}{J_m(ka)} = \omega a \frac{B_m H_m'^{(1)}(\omega a) + C_m H_m'^{(2)}(\omega a)}{B_m H_m^{(1)}(\omega a) + C_m H_m^{(2)}(\omega a)} \Leftrightarrow$$

$$\frac{B_m}{C_m} = -\frac{\omega a H_m'^{(2)}(\omega a) - ka\frac{J_m'(ka)}{J_m(ka)} H_m^{(2)}(\omega a)}{\omega a H_m'^{(1)}(\omega a) - ka\frac{J_m'(ka)}{J_m(ka)} H_m^{(1)}(\omega a)} = e^{2i\delta_m} \tag{6.36}$$

where the last equality includes the as of yet undefined scattering phase shift, δ_m, and will be derived shortly.

Now a demand has come from near the origin and it is time for the wider perspective. The wave function can, far away from the well ($r \to \infty$), be split into the incoming part, chosen to be a plane wave in the positive x-direction, and the outgoing part, spherical waves from the scatterer. The plane wave can be expanded in Bessel (and therefore Hankel) functions, using equation (8.511.4) in[6],

$$e^{i\omega x} = e^{i\omega r\cos\varphi} = \sum_{m=-\infty}^{\infty} e^{im\varphi} i^m J_m(\omega r) = \sum_{m=-\infty}^{\infty} e^{im\varphi} i^m \frac{1}{2}\left(H_m^{(1)}(\omega r) + H_m^{(2)}(\omega r)\right).$$

A free particle will also have the plane wave as a solution and the only difference between that solution and this one at $r \to \infty$ can be a phase, δ_m[7]. The convention here is to have the same phase for the incoming waves (from the plane wave expansion) and the free particle; the incoming cylindrical waves are reasonably not affected by the presence of a potential at the origin. With this convention, the phase change will only affect the outgoing cylindrical waves and the phase is for historical reasons called $2\delta_m$. This turns the plane wave part into

$$e^{i\omega x} + \sum_{m=-\infty}^{\infty} e^{im\varphi} i^m \frac{1}{2}\left(e^{i2\delta_m} - 1\right) H_m^{(1)}(\omega r). \tag{6.37}$$

There exists a long range expression for the Hankel functions[5]:

$$H_m^{(1,2)}(\omega r) \xrightarrow{r\to\infty} \sqrt{\frac{2}{\pi\omega r}} e^{\pm i\left(\omega r - \frac{m\pi}{2} - \frac{\pi}{4}\right)}$$

with which (6.37) can be written

$$e^{i\omega x} + \sum_{m=-\infty}^{\infty} \frac{1}{\sqrt{2\pi\omega r}} e^{im\varphi} i^m \left(e^{i2\delta_m} - 1\right) e^{i\left(\omega r - \frac{m\pi}{2} - \frac{\pi}{4}\right)} \Leftrightarrow$$

$$e^{i\omega x} + \underbrace{\sum_{m=-\infty}^{\infty} \frac{1}{\sqrt{2\pi\omega}} e^{i\left(m\varphi - \frac{\pi}{4}\right)} \left(e^{i2\delta_m} - 1\right)}_{\equiv f(\varphi)} \frac{e^{i\omega r}}{\sqrt{r}} \tag{6.38}$$

Where $f(\varphi)$, is the scattering amplitude. Expanding both (6.38) and (6.35) for $r \to \infty$ and recognising coefficients of $e^{\pm i\omega r}$, one finds

$$B_m = \frac{1}{2} e^{m\pi/2} e^{i2\delta_m}, \quad C_m = \frac{1}{2} e^{m\pi/2}. \tag{6.39}$$

This means that $e^{i2\delta_m}$ is given by (6.36) and therefore the entire scattering amplitude, $f(\varphi)$, is known.

6.2 Scattering in the limit to the $\delta^{(2)}$-potential

In the limit of $a \to 0$ the potential strength will have to be renormalised as it was for the bound state (it is the same well) and the scattering amplitude can be found. The scattering phase,

$$e^{2i\delta_m} = -\frac{\omega a H_m'^{(2)}(\omega a) - ka \frac{J_m'(ka)}{J_m(ka)} H_m^{(2)}(\omega a)}{\omega a H_m'^{(1)}(\omega a) - ka \frac{J_m'(ka)}{J_m(ka)} H_m^{(1)}(\omega a)}, \tag{6.40}$$

will be rewritten using limiting forms of the Bessel functions for $a \to 0$. The ones used for $m \neq 0$ are equations (9.1.7) and (9.1.9) in[5].

$$\begin{aligned} J_m(z) &\approx \left(\frac{z}{2}\right)^m \frac{1}{\Gamma(m+1)}, \qquad J_m'(z) \approx J_m(z)\frac{2m}{z} \\ N_m(z) &\approx -\frac{\Gamma(m)}{\pi}\left(\frac{z}{2}\right)^{-m}, \quad N_m'(z) \approx -N_m(z)\frac{2m}{z} \end{aligned} \tag{6.41}$$

Equation (6.40) becomes, for $m \neq 0$, using (6.34) and with the short hand notation $J = J_m(\omega a), N = N_m(\omega a)$:

$$e^{2i\delta_m}\big|_{m\neq 0} = -\frac{\omega a \frac{J'-iN'}{N} - ka \frac{J_m'(ka)}{J_m(ka)} \frac{J-iN}{N}}{\omega a \frac{J'+iN'}{N} - ka \frac{J_m'(ka)}{J_m(ka)} \frac{J+iN}{N}}$$

which can be dramatically simplified inserting

$$\frac{J}{N} = -\left(\frac{z}{2}\right)^{2m} \frac{\pi}{\Gamma(m+1)\Gamma(m)} \equiv c_1 z^{2m}$$

and the relations (6.41), making it turn into

$$-\frac{\omega a\left(2mc_1 z^{2m} - ic_1(-2m)\right) - (2m)(c_1 z^{2m} - i)}{\omega a\left(2mc_1 z^{2m} + ic_1(-2m)\right) - (2m)(c_1 z^{2m} + i)} \Leftrightarrow$$

$$\frac{-\left(i\omega a c_1 2m + 2mi\right) - (\omega a)^{2m}\left(\omega a c_1 2m - c_1 2m\right)}{-\left(i\omega a c_1 2m + 2mi\right) + (\omega a)^{2m}\left(\omega a c_1 2m - c_1 2m\right)} \xrightarrow{a\to 0} = 1.$$

No partial waves with $m \neq 0$ are scattered!

The $m = 0$ case need a bit more care. In addition to the limiting forms of J_0 in (5.31) we will now need 9.1.13 in [5],

$$N_m(z) \approx \frac{2}{\pi}\ln z + \frac{2\gamma}{\pi} + \mathcal{O}(z^2\ln(z)), \quad N_m'(z) \approx \frac{2}{\pi z} + \mathcal{O}(z),$$

as well. Equation (6.40) turns into

$$e^{2i\delta_m} = -\frac{\omega a\left(-\frac{\omega a}{2} - i\frac{2}{\pi\omega a}\right) - \left(-\frac{(ka)^2}{2}\right)\left(1 - i\frac{2}{\pi}(\ln(\omega a) + \gamma)\right) + \mathcal{O}\left((\omega a)^2\ln(\omega a)\right)}{\omega a\left(-\frac{\omega a}{2} + i\frac{2}{\pi\omega a}\right) - \left(-\frac{(ka)^2}{2}\right)\left(1 + i\frac{2}{\pi}(\ln(\omega a) + \gamma)\right) + \mathcal{O}\left((\omega a)^2\ln(\omega a)\right)}.$$

Using the renormalisation (5.32) and $(ka)^2 = (\omega a)^2 - b/\pi$ we get that $-\frac{(ka)^2}{2} = 1/(\ln\kappa a + \gamma)$ if we only keep terms up to $\mathcal{O}(\omega a)$. Multiplying by $\ln\omega a + \gamma$ and discarding terms of order ωa we get

$$-\frac{(\ln\kappa a + \gamma)\frac{-2i}{\pi} - \left(1 - i\frac{2}{\pi}(\ln(\kappa a) + \gamma)\right) + \mathcal{O}(\omega a)}{(\ln\kappa a + \gamma)\frac{2i}{\pi} - \left(1 + i\frac{2}{\pi}(\ln(\kappa a) + \gamma)\right) + \mathcal{O}(\omega a)} = \frac{\frac{2i}{\pi}\ln\frac{\omega}{\kappa} - 1 + \mathcal{O}(\omega a)}{\frac{2i}{\pi}\ln\frac{\omega}{\kappa} + 1 + \mathcal{O}(\omega a)}$$

The scattering phase became dependent on a only with terms that easily vanish as $a \to 0$. With the phase unity in all other channels than $m = 0$, the scattering amplitude simply becomes

$$f(\varphi) = \frac{1}{\sqrt{2\pi k}} e^{-i\pi/4}\left(e^{2i\delta_0} - 1\right) = \frac{1}{\sqrt{2\pi k}} \frac{2i\pi}{\frac{2}{\pi}\ln\frac{\omega}{\kappa} - i} \tag{6.42}$$

One can see the broken scale invariance explicitly in the ω dependence which could not have been there if the scale invariance were maintained. The result agrees with that retained via Fourier transforms, which is done in [1, 8]. The latter reference uses the method of defining a running coupling constant instead of assuming the observables constant and redefining the potential strength to make that possible.

7 Conclusions

The main conclusion of this thesis is that singular potentials can yield reasonable results for physical quantities by means of regularisation and renormalisation, but that some times a symmetry or invariance is broken anomalously in the process. This is all done with rather simple quantum mechanics and no ventures into quantum field theory, a complex and delicate field that is the main utiliser of these methods. All renormalisations use the technique of forcing physical observables to remain constant (and not veer towards infinity) when the limit is taken of the cut-off in question.

Section 2 solved the finite potential well the classical way (using symmetries and continuity demands) and derived the equation (2.1), solutions of which corresponds to bound states. It then took the limit from a finite well to a δ-potential, calculating the single bound state energy that remains, (2.3). This is a regularisation method for the δ-potential. The δ-potential was then itself solved using boundary conditions from an integration of the Schrödinger equation around $x = 0$ and through the method of Fourier transforms, producing results in agreement with the already calculated one. The corresponding was done regarding scattering for the same potential in section 3, arriving at the finite well scattering coefficients, t and r, (3.9) and the δ-potential coefficients (3.11).

Bound states for a potential well directly followed by a potential barrier (called the threshold potential) was discussed in section 4, with the bound states satisfying (4.17). The limit to the derivative of the δ-function, δ', was shown how it should be taken, but was deemed unfavourable in comparison with another solution. That other solution was the limit of two approaching δ-functions, (4.18), and the potential strength needed to be renormalised to (4.20). A Fourier space method followed, with matching results. Scattering was not studied for δ'.

The two dimensional potential well, section 5, has a wave function on the form (5.29) and the bound states energies satisfy (5.30). For the $\delta^{(2)}$-potential the potential strength must be renormalised like (5.32), which breaks the inherent scale invariance of the potential anomalously. The scattering states for that same well are for $r \to \infty$ on the form (6.38) with $e^{i2\delta_m}$ given by (6.36).

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