This file contains more exercises on quantum mechanics ... hope I can help you with learning quantum mechanics …

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Exercise 1

Given a particle of mass m in a one-dimensional potential $V(x)$ with the wavefunction:

$$\psi(x) = C \cdot x \cdot e^{-\frac{1}{2}ax^2}, a > 0$$

Normalize $\psi(x)$ to determine the constant C.

Calculate the expectation value of the position operator $\langle \hat{x} \rangle$.

Calculate the expectation value $\langle \hat{x}^2 \rangle$.

Exercise 2

Given a particle of mass m in a one-dimensional potential $V(x)$ with the wavefunction:

$$\psi(x) = C \cdot x \cdot e^{-\frac{1}{2}ax^2}, a > 0$$

Calculate the expectation value of the momentum operator $\langle \hat{p} \rangle$.

Calculate the expectation value of $\langle \hat{p}^2 \rangle$.

Note: the momentum operator $\hat{p}$:

$$\hat{p} = -i\hbar \frac{d}{dx}$$

Exercise 3

Given the wave function:

$$\psi(x) = C \cdot x \cdot e^{-\frac{1}{2}ax^2}, a > 0$$

Calculate the expectation value of the Hamiltonian $\langle \hat{H} \rangle$:

$$\langle \hat{H} \rangle = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

Assume that the potential vanishes, $V(x) = 0$.

[Exercise 4]

We assume $\psi(x)$ to be an energy eigenstate. From the potential $V(x)$ we only know that $V(0)$is zero.

$$\psi(x) = C \cdot x \cdot e^{-\frac{1}{2}ax^2}, a > 0$$

Using the Hamiltonian, find the potential $V(x)$.

Calculate the Energy E.

[Exercise 5]

The wave function $\psi(x) = C \cdot x \cdot e^{-\frac{1}{2}ax^2}, a > 0$ cannot be a ground state wave function of the harmonic oscillator (why?).

We use the momentum operator

$$\hat{p} = -i\hbar \frac{d}{dx}$$

and the position operator $\hat{x} \coloneqq x$ and define the lowering operator:

$$\hat{a}^- = \frac{i}{\sqrt{2\hbar\omega}}\left(\hat{P} - i\omega\hat{X}\right)$$

Apply the lowering operator to $\psi(x)$.

Verify that the result is a ground state.

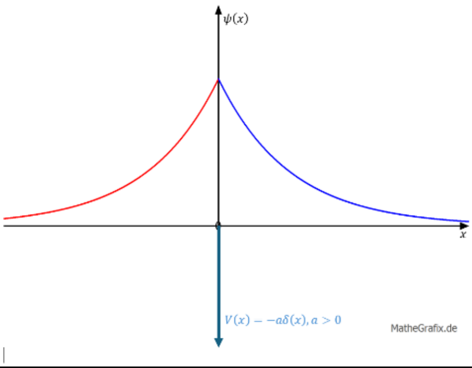
[Exercise 6]

Given a particle of mass m moving in a 1D δ-potential

$V(x) = -a\delta(x), a > 0.$

This kind of potential allows one bound state.

Calculate the energy of the bound state.



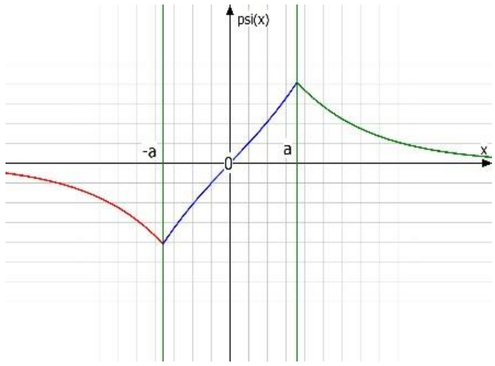
Exercise 7

Given a particle of mass m moving in a one-dimensional region with two δ-potentials

$$V(x) = -V_0\big(\delta(x+a) + \delta(x-a)\big), a > 0$$

Shown is the odd bound wave function.

Calculate the minimum energy for V_0 to guarantee an odd bound solution.



Exercise 1

Given a particle of mass m in a one-dimensional potential $V(x)$ with the wavefunction:

$$\psi(x) = C \cdot x \cdot e^{-\frac{1}{2}ax^2}, a > 0$$

Normalize $\psi(x)$ to determine the constant C.

Calculate the expectation value of the position operator $\langle \hat{x} \rangle$.

Calculate the expectation value of the square of the position operator $\langle \hat{x}^2 \rangle$.

a) Normalizing a wave function:

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1$$

In our case the wave function is real, $\psi^*(x) = \psi(x)$.

We calculate:

$$\int_{-\infty}^{\infty} C \cdot x \cdot e^{-\frac{1}{2}ax^2} \cdot C \cdot x \cdot e^{-\frac{1}{2}ax^2} dx = C^2 \int_{-\infty}^{\infty} x^2 \cdot e^{-ax^2} dx =;$$

A look at Wikipedia (*https://en.wikipedia.org/wiki/List_of_integrals_of_exponential_functions*) shows:

$$\int_{-\infty}^{\infty} x^2 \cdot e^{-ax^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{a^3}}$$

We get:

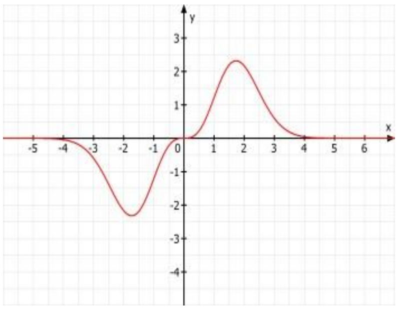
$$C^2 \cdot \frac{1}{2}\sqrt{\frac{\pi}{a^3}} = 1 \rightarrow C^2 = \sqrt{\frac{4 \cdot a^3}{\pi}} \rightarrow C = \left(\frac{4 \cdot a^3}{\pi}\right)^{\frac{1}{4}}$$

Note: $a > 0$ so C is strictly positive.

b) The expectation value of the position operator $\langle \hat{x} \rangle$:

$$\langle \hat{x} \rangle = \int_{-\infty}^{\infty} \psi^*(x) \cdot x \cdot \psi(x)dx$$

$$\int_{-\infty}^{\infty} C \cdot x \cdot e^{-\frac{1}{2}ax^2} \cdot x \cdot C \cdot x \cdot e^{-\frac{1}{2}ax^2} dx = C^2 \int_{-\infty}^{\infty} x^3 \cdot e^{-ax^2} dx =;$$



The function is antisymmetric so any integral symmetric to 0 is zero:

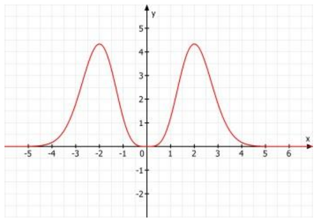
$$\langle \hat{x} \rangle = 0$$

c) The expectation value of the squared position operator $\langle \hat{x}^2 \rangle$:

$$\langle \hat{x}^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x) \cdot x^2 \cdot \psi(x) dx$$

$$\int_{-\infty}^{\infty} C \cdot x \cdot e^{-\frac{1}{2}ax^2} \cdot x^2 \cdot C \cdot x \cdot e^{-\frac{1}{2}ax^2} dx = C^2 \int_{-\infty}^{\infty} x^4 \cdot e^{-ax^2} dx =;$$

We look at the shape of the function. This is a symmetric function; the integral will give a (real) value. Going with the integration borders to $\pm\infty$ we get the necessary condition that the function must go to zero for $x \to \pm\infty$. This normally is guaranteed by multiplying by an exponential e^{-x^2}.



We use Wikipedia:

$$\int_0^{\infty} x^n \cdot e^{-ax^2} dx = \frac{\Gamma\left(\frac{n+1}{2}\right)}{2\left(a^{\frac{n+1}{2}}\right)}$$

We have $n = 4$:

$$\int_0^{\infty} x^4 \cdot e^{-ax^2} dx = \frac{\Gamma\left(\frac{5}{2}\right)}{2\left(a^{\frac{5}{2}}\right)}$$

We use Wikipedia (Gamma function - Wikipedia):

$$\Gamma\left(\frac{5}{2}\right) = \frac{3}{4}\sqrt{\pi}$$

$$\int_0^{\infty} x^4 \cdot e^{-ax^2} dx = \frac{3}{8}\sqrt{\pi} \cdot a^{-\frac{5}{2}} \rightarrow \int_{-\infty}^{\infty} x^4 \cdot e^{-ax^2} dx = \frac{3}{4}\sqrt{\pi} \cdot a^{-\frac{5}{2}}$$

We collect the results:

$$C^2 \int_{-\infty}^{\infty} x^4 \cdot e^{-ax^2} dx = C^2 \cdot \frac{3}{4}\sqrt{\pi} \cdot a^{-\frac{5}{2}}$$

We use:

$$C = \left(\frac{4 \cdot a^3}{\pi}\right)^{\frac{1}{4}}$$

We get:

$$\langle \hat{x}^2 \rangle = C^2 \int_{-\infty}^{\infty} x^4 \cdot e^{-ax^2} dx = \sqrt{\frac{4 \cdot a^3}{\pi}} \cdot \frac{3}{4}\sqrt{\pi} \cdot a^{-\frac{5}{2}} = \sqrt{4 \cdot a^3} \cdot \frac{3}{4} a^{-\frac{5}{2}} = 2 \cdot a^{\frac{3}{2}} \cdot \frac{3}{4} a^{-\frac{5}{2}} = \frac{3}{2a}$$

Exercise 2

Given a particle of mass m in a one-dimensional potential $V(x)$ with the wavefunction:

$$\psi(x) = C \cdot x \cdot e^{-\frac{1}{2}ax^2}, a > 0$$

Calculate the expectation value of the momentum operator $\langle \hat{p} \rangle$.

Calculate the expectation value of $\langle \hat{p}^2 \rangle$.

Note: the momentum operator $\hat{p}$:

$$\hat{p} = -i\hbar \frac{d}{dx}$$

a) Calculate the expectation value of the momentum operator $\langle \hat{p} \rangle$.

The momentum operator $\hat{p}$ applied to the wave function:

$$\hat{p}\psi(x) = -i\hbar \frac{d\psi(x)}{dx} = -i\hbar C \cdot \frac{d}{dx}\left(x \cdot e^{-\frac{1}{2}ax^2}\right) =$$

$$-i\hbar C \left(e^{-\frac{1}{2}ax^2} - ax^2 e^{-\frac{1}{2}ax^2}\right) = -i\hbar C \cdot e^{-\frac{1}{2}ax^2}(1 - ax^2)$$

We have two approaches to the solution.

The high-level approach:

$$\langle \hat{p} \rangle = m \frac{d\langle \hat{x} \rangle}{dx} = 0$$

The expectation value of momentum vanishes if we have a closed system with internal forces only.

The low-level approach:

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \psi^*(x) \cdot \hat{p} \cdot \psi(x) dx$$

We will do this carefully. We need:

$$\psi^*(x), \hat{p}, \psi(x)$$

$$\psi^*(x) = \psi(x) = C \cdot x \cdot e^{-\frac{1}{2}ax^2}, \qquad \hat{p}\psi(x) = -i\hbar C e^{-\frac{1}{2}ax^2}(1 - ax^2)$$

We calculate the argument of the integral:

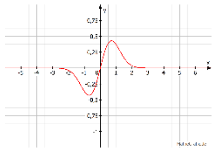
$$\psi^*(x) \cdot \hat{p}(\psi(x)) =$$

$$C \cdot x \cdot e^{-\frac{1}{2}ax^2} \cdot \left(-i\hbar C e^{-\frac{1}{2}ax^2}(1 - ax^2)\right) = C \cdot x \cdot (-i)\hbar C(1 - ax^2) \cdot e^{-ax^2} =$$

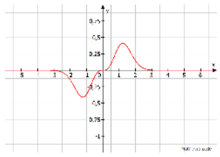
$$-i\hbar C^2\big(x(1-ax^2)\big)\cdot e^{-ax^2} = -i\hbar C^2(x-ax^3)\cdot e^{-ax^2} =$$

$$i\hbar C^2 ax^3\cdot e^{-ax^2} - i\hbar C^2 x\cdot e^{-ax^2}$$

We get the Integrals:



$$-i\hbar C^2\int_{-\infty}^{\infty} x\cdot e^{-ax^2}dx$$



$$i\hbar C^2 a\int_{-\infty}^{\infty} x^3\cdot e^{-ax^2}dx$$

Both integrals are antisymmetric, the value of each integral is zero.

b) Calculate the expectation value of $\langle\hat{p}^2\rangle$.

Note: It is easier if you try to express results in terms of $\psi(x)$ because you can use some results of exercise one. If you resolve anything down to the exponentials, you must go through Wikipedia and the integrals again.

The square of the momentum operator:

$$\hat{p}^2 = \left(-i\hbar\frac{d}{dx}\right)\left(-i\hbar\frac{d}{dx}\right) = -\hbar^2\frac{d^2}{dx^2}$$

The expectation value of the square of the momentum operator:

$$\langle\hat{p}^2\rangle = \int_{-\infty}^{\infty}\psi^*(x)\cdot\hat{p}^2\cdot\psi(x)dx = -\hbar^2\int_{-\infty}^{\infty}\psi^*(x)\cdot\frac{d^2}{dx^2}\psi(x)dx =;$$

We need the first and second derivative of $\psi(x)$.

$\frac{d}{dx}\big(\psi(x)\big)$ we take from part a):

$$\frac{d}{dx}\big(\psi(x)\big) = Ce^{-\frac{1}{2}ax^2}(1-ax^2) = Ce^{-\frac{1}{2}ax^2} - Cax^2e^{-\frac{1}{2}ax^2}$$

We note:

$$\psi^*(x) = \psi(x) = C\cdot x\cdot e^{-\frac{1}{2}ax^2}$$

We rewrite in terms of $\psi(x)$:

$$\frac{d}{dx}\big(\psi(x)\big) = \psi(x)\left(\frac{1}{x} - ax\right)$$

Second derivative:

$$\frac{d^2}{dx^2}\psi(x) = \frac{d}{dx}\left(\psi(x)\left(\frac{1}{x} - ax\right)\right) = \psi(x)\left(\frac{1}{x} - ax\right)\left(\frac{1}{x} - ax\right) + \psi(x)\left(-\frac{1}{x^2} - a\right) =$$

$$\psi(x)\left(\frac{1}{x^2} - 2a + a^2x^2\right) + \psi(x)\left(-\frac{1}{x^2} - a\right) = \psi(x)(-3a + a^2x^2)$$

We calculate the Integral:

$$\langle\hat{p}^2\rangle = \int_{-\infty}^{\infty}\psi^*(x)\cdot\hat{p}^2\cdot\psi(x)dx = -\hbar^2\int_{-\infty}^{\infty}\psi^*(x)\cdot\frac{d^2}{dx^2}\psi(x)dx =$$

$$-\hbar^2\int_{-\infty}^{\infty}\psi^*(x)\cdot\psi(x)(-3a + a^2x^2)dx =$$

$$3a\hbar^2\int_{-\infty}^{\infty}\psi^*(x)\cdot\psi(x)dx - \hbar^2a^2\int_{-\infty}^{\infty}\psi^*(x)\cdot\psi(x)\cdot x^2dx$$

The first integral is the normalizing condition.

$$3a\hbar^2\int_{-\infty}^{\infty}\psi^*(x)\cdot\psi(x)dx = 3a\hbar^2$$

The second integral is the expectation value of $\langle\hat{x}^2\rangle$:

$$\hbar^2a^2\int_{-\infty}^{\infty}\psi^*(x)\cdot\psi(x)\cdot x^2dx = \frac{3\hbar^2a^2}{2a} = \frac{3}{2}\hbar^2a$$

We get:

$$3a\hbar^2\int_{-\infty}^{\infty}\psi^*(x)\cdot\psi(x)dx - \hbar^2a^2\int_{-\infty}^{\infty}\psi^*(x)\cdot\psi(x)\cdot x^2dx = \frac{3}{2}\hbar^2a$$

$$\langle\hat{p}^2\rangle = \frac{3}{2}\hbar^2a$$

Exercise 3

Given the normalized wave function:

$$\psi(x) = C \cdot x \cdot e^{-\frac{1}{2}ax^2}, a > 0$$

Calculate the expectation value of the Hamiltonian $\langle \hat{H} \rangle$.

Assume that the potential vanishes, $V(x) = 0$.

The Hamiltonian with potential zero:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

The expectation value of the Hamiltonian with our specific wave function:

$$\int_{-\infty}^{\infty} \psi^*(x) \cdot \hat{H}(\psi(x))dx = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \psi^*(x) \cdot \frac{d^2}{dx^2}(\psi(x))dx =;$$

The second derivative of $\psi(x)$ we get from exercise two:

$$\frac{d^2}{dx^2}\psi(x) = \psi(x)(-3a + a^2x^2)$$

We continue with the expectation value:

$$-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \psi^*(x) \cdot \frac{d^2}{dx^2}(\psi(x))dx = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \psi^*(x) \cdot \psi(x)(-3a + a^2x^2)dx =$$

$$= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \psi^*(x) \cdot \psi(x)(-3a + a^2x^2)dx =$$

$$\frac{3}{2}a\frac{\hbar^2}{m}\int_{-\infty}^{\infty} \psi^*(x) \cdot \psi(x)dx - a^2\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \psi^*(x) \cdot \psi(x) \cdot x^2 dx$$

Note: The first integral is the normalized wavefunction giving 1. The second integral is the expectation value of the squared position operator $\langle \hat{x}^2 \rangle$ *(see exercise 1c)* $\frac{3}{2a}$.

We get:

$$\frac{3}{2}a\frac{\hbar^2}{m}\int_{-\infty}^{\infty} \psi^*(x) \cdot \psi(x)dx - a^2\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \psi^*(x) \cdot \psi(x) \cdot x^2 dx = \frac{3}{2}a\frac{\hbar^2}{m} - a^2\frac{\hbar^2}{2m}\frac{3}{2a} =$$

$$\frac{3}{2}\frac{a\hbar^2}{m} - \frac{3}{4}\frac{a\hbar^2}{m} = \frac{3}{4}\frac{a\hbar^2}{m}$$

$$\langle \hat{H} \rangle = \frac{3}{4}\frac{a\hbar^2}{m}$$

Exercise 4

We assume $\psi(x)$ to be an energy eigenstate. From the potential $V(x)$ we only know that $V(0)$ is zero.

$$\psi(x) = C \cdot x \cdot e^{-\frac{1}{2}ax^2}, a > 0$$

a) Calculate the Energy eigenvalue E.

b) Using the Hamiltonian, find the potential $V(x)$.

a) Calculate the Energy eigenvalue E.

The Hamiltonian $\hat{H}$:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) = E$$

From exercise 3 we get the second derivative of $\psi(x)$:

$$\frac{d^2}{dx^2}\psi(x) = \psi(x)(-3a + a^2x^2)$$

We solve the equation:

$$-\frac{\hbar^2}{2m}\psi(x)(-3a + a^2x^2) + V(x)\psi(x) = E\psi(x)$$

We use $x = 0$ and $V(0) = 0$:

$$\frac{3a\hbar^2}{2m}\psi(0) = E\psi(0)$$

$\psi(0 + \varepsilon)$ is a number, we get in the limes $\varepsilon \to 0$:

$$\frac{3a\hbar^2}{2m} = E$$

b) Using the Hamiltonian, find the potential $V(x)$.

For finding the potential $V(x)$ we use the energy eigenvalue we got from part a):

$$-\frac{\hbar^2}{2m}\psi(x)(-3a + a^2x^2) + V(x)\psi(x) = \frac{3a\hbar^2}{2m}\psi(x)$$

Now we divide by $\psi(x)$. This is mathematically not correct because there might be values of x where $\psi(x)$ is zero … but we are physicists … we get:

$$-\frac{\hbar^2}{2m}(-3a + a^2x^2) + V(x) = \frac{3a\hbar^2}{2m}$$

We solve the equation for the variable $V(x)$:

$$V(x) = \frac{3a\hbar^2}{2m} + \frac{\hbar^2}{2m}(-3a + a^2x^2) = \frac{3a\hbar^2}{2m} - \frac{3a\hbar^2}{2m} + x^2\frac{a^2\hbar^2}{2m} = x^2\frac{a^2\hbar^2}{2m}$$

Note: this is a quadratic potential fitting for the harmonic oscillator.

Note: Dividing the equation by $\psi(x)$ is unproblematic as long as $\psi(x)$ is zero only at discrete points.

Exercise 5

The wave function $\psi(x) = C \cdot x \cdot e^{-\frac{1}{2}ax^2}, a > 0$ cannot be a ground state wave function of the harmonic oscillator (why?).

We use the momentum operator $\hat{p} = -i\hbar\frac{d}{dx}$, the position operator $\hat{x} = x$ and define the lowering operator $\hat{a}^-$:

$$\hat{a}^- = (\hat{p} - ia\hbar\hat{x})$$

a) Apply the lowering operator to $\psi(x)$.

b) Verify that the result is a ground state.

$\psi(x) = C \cdot x \cdot e^{-\frac{1}{2}ax^2}, a > 0$ cannot be a ground state wave function because the "x" in it causes a node, a zero crossing. Ground state functions are node-free.

a) Apply the lowering operator to $\psi(x)$.

$$\hat{a}^- \left(\psi(x)\right) = (\hat{p} - ia\hbar\hat{x})\left(\psi(x)\right) = \left(i\hbar\frac{d}{dx} - ia\hbar\hat{x}\right)\left(\psi(x)\right) =;$$

We use the first derivative of $\psi(x)$ from exercise 2 and rewrite in terms of $\psi(x)$:

$$\frac{d}{dx}\psi(x) = Ce^{-\frac{1}{2}ax^2} - ax\psi(x) = \psi(x)\left(\frac{1}{x} - ax\right)$$

We get:

$$\hat{a}^- \left(\psi(x)\right) = \left(-i\hbar\frac{d}{dx} - ia\hbar\hat{x}\right)\left(\psi(x)\right) = -i\hbar\psi(x)\left(\frac{1}{x} - ax\right) - ia\hbar x\psi(x) = -\frac{i\hbar\psi(x)}{x}$$

We expand $\psi(x)$:

$$\hat{a}^- \left(\psi(x)\right) = -\frac{i\hbar}{x}C \cdot x \cdot e^{-\frac{1}{2}ax^2} = -i\hbar Ce^{-\frac{1}{2}ax^2}$$

This is a new, node-free wave function – the hopefully ground state wave function.

b) Verify that the result is a ground state.

We apply the lowering operator again. The result must be zero because the lowering operator applied to the ground state annihilates the ground state.

We name the ground state $\psi_0(x)$:

$$\psi_0(x) = -i\hbar Ce^{-\frac{1}{2}ax^2}$$

We need the derivative of the ground state:

$$\frac{d}{dx}\psi_0(x) = -ax\psi_0(x)$$

We apply the lowering operator to the ground state:

$$\left(-i\hbar\frac{d}{dx} - ia\hbar\hat{x}\right)\left(\psi_0(x)\right) = -i\hbar\frac{d}{dx}\psi_0(x) - ia\hbar x\psi_0(x) =$$

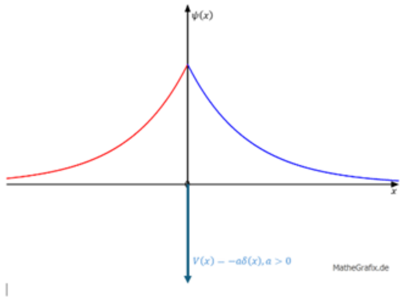
$$i\hbar ax\psi_0(x) - ia\hbar x\psi_0(x) = 0$$

Exercise 6

Given a particle of mass m moving in a one-dimensional δ potential $V(x) = -a\delta(x), a > 0$.

This kind of potential allows one bound state.

Calculate the energy of the bound state.



Note: units are $length = m$ for meter, $mass = kg$ for kilogram, $time = s$ for seconds.

Step 1: dimensional access.

The potential has the unit:	$[V] = energy = Joule = \frac{kg \cdot m^2}{s^2}$
The δ-function has the unit:	$[\delta] = \frac{1}{m}$
Planck's constant has the unit:	$[\hbar] = Joule \cdot seconds$

This leads to the unit of a:

$$[a] = Joule \cdot m = \frac{kg \cdot m^3}{s^2}$$

With these units we can express the energy for the bound state we are looking for as:

$$E = -c\frac{ma^2}{\hbar^2}$$

Note: "$c > 0$" is a number, a placeholder for a factor to be determined in the end (step 6). The minus sign is needed because the energy of bound states must be negative.

We check the units

$$\left[\frac{m \cdot a^2}{\hbar^2}\right] = kg \cdot \frac{kg^2 \cdot m^6}{s^4} \cdot \frac{s^4}{kg^2 \cdot m^4 \cdot s^2} = \frac{kg \cdot m^2}{s^2} = [E]$$

Note: a is not the acceleration but a number that determines the strength of the potential V.

Step 2: We solve the Schrödinger equation:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) = E$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = \big(E - V(x)\big)\psi(x)$$

This is a differential equation.

We distinguish between $x \neq 0$, the region outside the δ-function and $x = 0$, the "region" with the δ function. Outside the potential $V(x)$ is zero.

Outside:

$$\frac{d^2}{dx^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x)$$

For easier writing we use:

$$-\frac{2mE}{\hbar^2}\psi(x) \coloneqq k^2\psi(x)$$

The energy E for bound states must be negative, so k^2 has correctly a positive value.

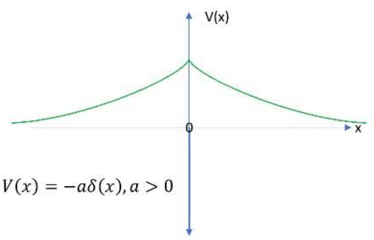
The differential equation

$$\frac{d^2}{dx^2}\psi(x) = k^2\psi(x)$$

has the solution $\psi(x) = e^{kx}, e^{-kx}$ and any linear combination of these two.

Step 3: We determine the two branches.

A look at the graphic shows that on the left side the only possible solution is Ae^{kx} because we need the function to become zero for large negative values of x.



The solution on the right side is Be^{-kx}.

Both branches meet at $x = 0$ and we get $A = B$.

Note: $\psi(0) = A$.

Step 4: We investigate the discontinuity caused by the $\boldsymbol{\delta}$-function.

We use $\varepsilon > 0$ and integrate the Hamiltonian. This time the potential $V(x)$ does not vanish:

$$V(x) = -a\delta(x), a > 0$$

We integrate:

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{d^2}{dx^2}\psi(x)dx - a\int_{-\varepsilon}^{\varepsilon}\delta(x)\psi(x)dx = \int_{-\varepsilon}^{\varepsilon}E\psi(x)dx$$

We handle the parts.

$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{d^2}{dx^2}\psi(x)dx = -\frac{\hbar^2}{2m}\left[\frac{d}{dx}\psi(x)\right]_{-\varepsilon}^{\varepsilon}$ Note: $\left[\frac{d}{dx}\psi(x)\right]_{-\varepsilon}^{\varepsilon} = \frac{d}{dx}\psi(\varepsilon) - \frac{d}{dx}\psi(-\varepsilon)$. We write this as $\Delta\frac{d}{dx}\psi(\varepsilon)$. In the limit $\varepsilon \to 0$ this becomes: $\Delta\left(\frac{d}{dx}\psi(0)\right)$ Note: This is a discontinuity.	$-a\int_{-\varepsilon}^{\varepsilon}\delta(x)\psi(x)dx = -a\psi(0)$	$\int_{-\varepsilon}^{\varepsilon}E\psi(x)dx = 0$

Result:

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{d^2}{dx^2}\psi(x)dx - a\int_{-\varepsilon}^{\varepsilon}\delta(x)\psi(x)dx = \int_{-\varepsilon}^{\varepsilon}E\psi(x)dx \to -\frac{\hbar^2}{2m}\Delta\left(\frac{d}{dx}\psi(0)\right) - a\psi(0) = 0$$

$$\to \Delta\left(\frac{d}{dx}\psi(0)\right) = -\frac{2ma}{\hbar^2}\psi(0)$$

We use $\psi(0) = A$ and get:

$$\Delta\left(\frac{d}{dx}\psi(0)\right) = -\frac{2ma}{\hbar^2}A$$

The discontinuity caused by the δ-function is proportional to the strength of the wave function. The kink in the gradient becomes larger the larger the value A. For $A \to 0$ we get no kink.

Step 5: We determine the value of k.

k contains the value for the energy E. For bound states E cannot take any value but only discrete ones. We use the discontinuity of $\frac{d}{dx}\psi(x)$ at $x = 0$.

$\frac{d}{dx}\psi(\varepsilon) = Ake^{k\varepsilon}$	$\frac{d}{dx}\psi(-\varepsilon) = -Ake^{-k\varepsilon}$

We calculate the limit:

$$\lim_{\varepsilon\to 0}\left(\frac{d}{dx}\psi(\varepsilon) - \frac{d}{dx}\psi(-\varepsilon)\right) = \lim_{\varepsilon\to 0}\left(-Ake^{k\varepsilon} - \left(Ake^{-k\varepsilon}\right)\right) = -2Ak \coloneqq \Delta\left(\frac{d}{dx}\psi(0)\right)$$

From step 4 we have:

$$\Delta\left(\frac{d}{dx}\psi(0)\right) = -\frac{2ma}{\hbar^2}A$$

We get:

$$-2Ak = -2\frac{ma}{\hbar^2}A \rightarrow k = \frac{ma}{\hbar^2}$$

Step 6: We calculate E:

From step 2 we have:

$$k^2 = -\frac{2mE}{\hbar^2}$$

From step 5 we have:

$$k = \frac{ma}{\hbar^2} \rightarrow k^2 = \frac{m^2a^2}{\hbar^4}$$

We combine and calculate E:

$$\frac{m^2a^2}{\hbar^4} = -\frac{2mE}{\hbar^2} \;\rightarrow\; E = -\frac{1}{2}\frac{ma^2}{\hbar^2}$$

The energy of the bound state:

$$E = -\frac{1}{2}\frac{m}{\hbar^2}a^2$$

Answer: the energy is proportional to the square of the strength a of the δ-potential.

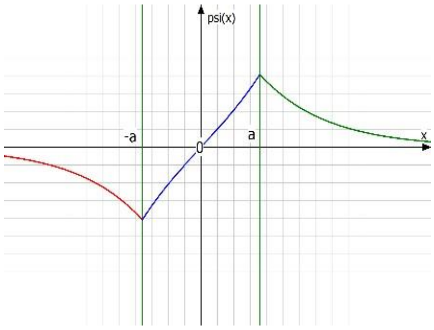
Exercise 7

Given a particle of mass m moving in a one-dimensional region with two δ-potentials:

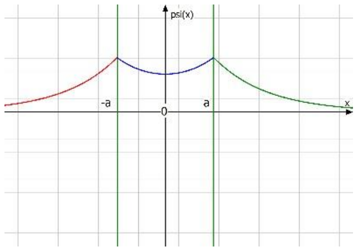
$V(x) = -V_0\big(\delta(x+a) + \delta(x-a)\big), a > 0$

Shown is the odd bound wave function.

Calculate the minimum energy for V_0 to guarantee an odd bound solution.



Note: there is always an even solution. The odd solution needs a minimum Energy for the potential to exist.



Step 1: We solve the Schrödinger equation.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = \Big(E + V_0\big(\delta(x+a) + \delta(x-a)\big)\Big)\psi(x)$$

We distinguish between $x \neq -a, a$, the region outside the δ-functions and $x = -a, a$, the "regions" with the δ-function. Outside the potential is zero.

Outside:

$$\frac{d^2}{dx^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x)$$

For easier writing we use:

$$k^2 = -\frac{2mE}{\hbar^2}$$

Note: the energy E for bound states must be negative, so k^2 correctly has a positive value.

The differential equation

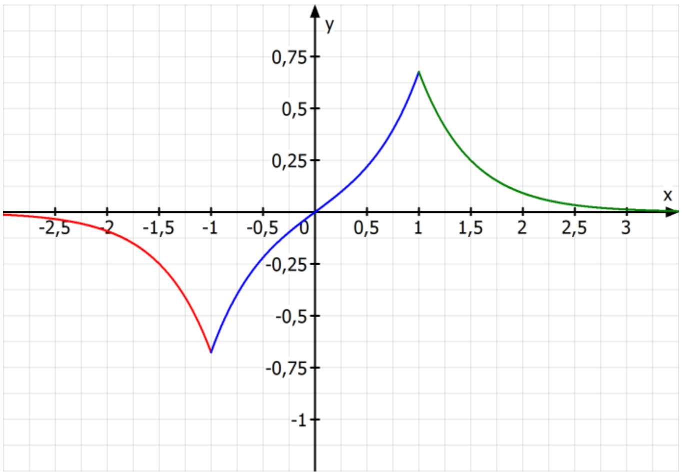
$$\frac{d^2}{dx^2}\psi(x) = k^2\psi(x)$$

has the solution $\psi(x) = e^{kx}, e^{-kx}$ and any linear combination of these two.

Step 2: We determine the three (two) branches.

A look at the graphic shows that on the left side $-\infty < x < -a$ the only possible solution is:

$$\psi_l(x) = -Ae^{kx}$$



Note: This picture produced with parameters $A = 5, k = 2, a = \pm 1$

The wave function is antisymmetric, on the right side we have:

$$\psi_r(x) = Ae^{-kx}$$

The solution in between has a zero at $x = 0$ and is antisymmetric too:

$$\psi_m(x) = B\left(e^{kx} - e^{-kx}\right)$$

We concentrate on the right side. The left side then is the antisymmetric equivalent. The crucial point on the right side is $x = a$. Both branches meet at $x = a$.

Right branch:

$$\psi_r(a) = Ae^{-ka}$$

Middle branch:

$$\psi_m(a) = B\left(e^{ka} - e^{-ka}\right)$$

Note: Think of $a \pm \varepsilon$ …

Both branches meet at $x = a$:

$$Ae^{-ka} = B\left(e^{ka} - e^{-ka}\right) \rightarrow B = A\frac{e^{-ka}}{e^{ka} - e^{-ka}} \rightarrow B = A\frac{1}{e^{2ka} - 1}$$

We rename:

$$u := \frac{1}{e^{2ka} - 1}$$

We get:

$$\psi_m(a) = Au\left(e^{ka} - e^{-ka}\right)$$

Step 3: We investigate the discontinuity at $\boldsymbol{x = a}$ caused by the $\boldsymbol{\delta}$-function.

We take $\varepsilon > 0$ and integrate the Hamiltonian close to $x = a$. The potential $V(x)$ does not vanish:

$$-\frac{\hbar^2}{2m}\int_{a-\varepsilon}^{a+\varepsilon}\frac{d^2}{dx^2}\psi(x)dx - V_0\int_{a-\varepsilon}^{a+\varepsilon}\delta(x-a)\psi(x)dx = \int_{a-\varepsilon}^{a+\varepsilon}E\psi(x)dx$$

We handle the parts.

$-\frac{\hbar^2}{2m}\int_{a-\varepsilon}^{a+\varepsilon}\frac{d^2}{dx^2}\psi(x)dx = -\frac{\hbar^2}{2m}\left[\frac{d}{dx}\psi(x)\right]_{a-\varepsilon}^{a+\varepsilon} = -\frac{\hbar^2}{2m}\left(\frac{d}{dx}\psi(a+\varepsilon) - \frac{d}{dx}\psi(a-\varepsilon)\right)$ We write this as: $= -\frac{\hbar^2}{2m}\Delta\frac{d}{dx}\psi(a)$
$-V_0\int_{a-\varepsilon}^{a+\varepsilon}\delta(x-a)\psi(x)dx = -V_0\psi(a)$
$\int_{a-\varepsilon}^{a+\varepsilon}E\psi(x)dx = 0$

Result:

$$-\frac{\hbar^2}{2m}\Delta\frac{d}{dx}\psi_r(a) = V_0\psi_r(a)$$

$$\Delta\frac{d}{dx}\psi(a) = -\frac{2mV_0}{\hbar^2}\psi_r(a) = -\frac{2mV_0}{\hbar^2}Ae^{-ka}$$

Step 4: We determine the potential needed for the first excited state.

Note: this will become a bit lengthy …

We use the discontinuity of $\Delta\frac{d}{dx}\psi(x)$.

$\psi_m(x) = Au\left(e^{kx} - e^{-kx}\right)$	$\psi_r(x) = Ae^{-kx}$

We differentiate:

$\frac{d}{dx}\psi_m(x) = \frac{d}{dx}Au\left(e^{kx} - e^{-kx}\right) =$ $Au\left(ke^{kx} + ke^{-kx}\right)$	$\frac{d}{dx}\psi_r(x) = \frac{d}{dx}Ae^{-kx} =$ $-kAe^{-kx}$
$\frac{d}{dx}\psi_m(a-\varepsilon) = Au\left(ke^{k(a-\varepsilon)} + ke^{-k(a-\varepsilon)}\right)$	$\frac{d}{dx}\psi_r(a+\varepsilon) = -kAe^{-k(a+\varepsilon)}$

We calculate the limit $\varepsilon \to 0$:

$$\lim_{\varepsilon \to 0} \frac{d}{dx}\psi_r(a+\varepsilon) - \frac{d}{dx}\psi_m(a-\varepsilon) = -kAe^{-ka} - Au\left(ke^{ka} + ke^{-ka}\right) =$$

$$-Auke^{ka} - kAe^{-ka} - Auke^{-ka} = -Auke^{ka} - Ake^{-ka}(1+u) =$$

$$-Auke^{ka} - Auke^{-ka}\left(\frac{1}{u} + 1\right) =$$

$$-Auk\left(e^{ka} + e^{-ka}\left(\frac{1}{u} + 1\right)\right)$$

We replace u by its original expression:

$$u \coloneqq \frac{1}{e^{2ka} - 1}$$

We calculate:

$$-\frac{Ak}{e^{2ka} - 1}\left(e^{ka} + e^{-ka}\left(e^{2ka} - 1 + 1\right)\right) = -\frac{Ak}{e^{2ka} - 1}\left(e^{ka} + e^{ka}\right) = -\frac{2Ake^{ka}}{e^{2ka} - 1} = \frac{2Ak}{e^{ka} - e^{-ka}}$$

Result:

$$\Delta \frac{d}{dx}\psi(a) = \frac{2Ak}{e^{ka} - e^{-ka}}$$

From step 3 we have:

$$\Delta \frac{d}{dx}\psi(a) = -\frac{2mV_0}{\hbar^2}Ae^{-ka}$$

We get:

$$-\frac{2Ak}{e^{ka} - e^{-ka}} = -\frac{2mV_0}{\hbar^2}Ae^{-ka}$$

$$\frac{k}{e^{ka} - e^{-ka}} = \frac{mV_0}{\hbar^2}e^{-ka}$$

We search for the energy so we solve with respect to k:

$$k = \frac{mV_0}{\hbar^2}e^{-ka}\left(e^{ka} - e^{-ka}\right) = \frac{mV_0}{\hbar^2}\left(1 - e^{-2ka}\right)$$

$$\frac{k\hbar^2}{mV_0} = \left(1 - e^{-2ka}\right) \to \frac{k\hbar^2}{mV_0} - 1 = -e^{-2ka}$$

Note: $|a| \neq 0$

This is a transcendental equation. We solve it graphically.

We substitute $2ka \coloneqq z.$

We use:

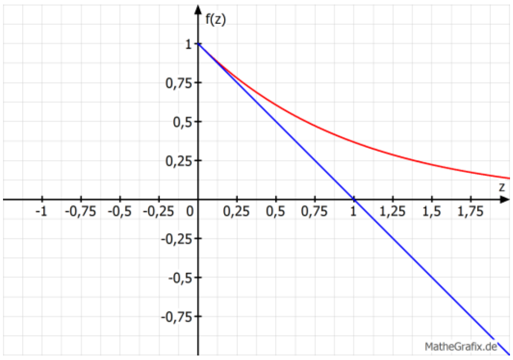
$$\frac{k\hbar^2}{mV_0} \coloneqq cz$$

We get an expression for c:

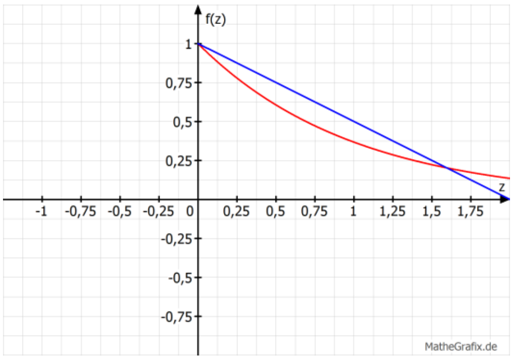
$$c = \frac{\hbar^2}{2amV_0}$$

The new transcendental equation:

$$e^{-z} = 1 - cz$$



$c = 1$



$c = \frac{1}{2}$

This equation always has a solution for $z = 0$. It has a further solution (intersection) if the gradient of the linear function is smaller than the gradient of the exponential function at $x = 0$.

The slope of the linear function: $f(z) = 1 - cz \rightarrow f'(z) = -c$

The slope of the exponential function: $g(z) = e^{-z} \rightarrow g'(z) = -e^{-z}$

Evaluated at $z = 0$: $f'(0) = -c, g'(0) = -1$

The condition for intersection: $-c > -1 \rightarrow c < 1$

From our substitution we get:

$$\frac{k\hbar^2}{mV_0} = 2cka \rightarrow c = \frac{\hbar^2}{2amV_0}$$

We get an odd bound state if:

$$\frac{\hbar^2}{2amV_0} < 1 \quad \rightarrow \quad \frac{\hbar^2}{2am} < V_0$$