1 Problems: Why Quantum Mechanics?

1.1. Hamilton's equations:

Write down Hamilton's equations for a particle in a harmonic potential,

$$V = \frac{1}{2}m\omega^2 x^2 \,. \tag{1}$$

and show that its solutions are as stated.

Solution:

The Hamiltonian and its derivatives with respect to x and p are

$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2 \,, \quad \frac{\partial H}{\partial x} = m\omega^2 x \,, \quad \frac{\partial H}{\partial p} = \frac{p}{m} \,. \tag{2}$$

Hamilton's equations are thus

$$\dot{x}(t) = \frac{p(t)}{m} \,, \quad \dot{p}(t) = -m\omega^2 x(t) \,, \tag{3}$$

which you can solve in a variety of ways, e.g. by taking the time-derivative of the first and then inserting the second, to get

$$\ddot{x}(t) = -\omega^2 x(t) \,, \tag{4}$$

and observing that this is solved by

$$x(t) = C\sin(t\omega + \phi) \,. \tag{5}$$

The constant C is fixed by inserting both $x(t)$ and $p(t)$ into the Hamiltonian, and noting that the result should be E.

1.2. Quantisation condition:

Consider the simple harmonic oscillator. Fill in the missing steps in the computation that takes you from the ad-hoc quantisation condition

$$\int_{\text{orbit}} p\mathrm{d}x = nh \,, \quad n \in \mathbb{Z} \,, \tag{6}$$

to the conclusion that $E = \nu h n$ with $n \in \mathbb{Z}$.

Solution:

Inserting the solution

$$\begin{aligned} x(t) &= \sqrt{\frac{2E}{m\omega^2}}\sin(\omega t + \phi) \,, \\ p(t) &= \sqrt{2mE}\cos(\omega t + \phi) \,, \end{aligned} \tag{7}$$

into the integral gives

$$\int_{\text{orbit}} p\mathrm{d}x = 2E \int_{\text{orbit}} \cos(\omega t + \phi)\mathrm{d}\left(\frac{1}{\omega}\sin(\omega t + \phi)\right) \,. \tag{8}$$

By applying the chain rule we can rewrite the complicated differential $\mathrm{d}(\ldots)$ in terms of $\mathrm{d}t$. Moreover, one orbit is given by taking t from 0 to $2\pi/\omega$. Together, this gives

$$= 2E \int_0^{2\pi/\omega} \cos^2(\omega t + \phi)\mathrm{d}t = \frac{2\pi E}{\omega} \,. \tag{9}$$

2 Problems: The Double Slit Experiment

2.1. Approximations:

We have discussed several approximations to arrive at the wave interference pattern

$$I(x) = 4C^2 \cos^2\left(\frac{k}{2}(r_1 - r_2)\right) \,. \tag{10}$$

There is one hidden assumption which we have not mentioned explicitly, which is related to the normalisation constant C. Can you spot it? What would the effect be of relaxing this assumption?

Solution:

Strictly speaking, the intensity of the wave drops as a function of the distance from the source, unless you are in one dimension. In two dimensions, you would have $C \sim 1/r$. This means that as you get further away from the axis, and the distance to the slit gets larger, the intensity drops.

2.2. Finite-width single slit:

Another approximation we have made is that the slits are infinitesimally thin, which of course in the real world would not allow for electrons to pass through. We can do better than that.

PROBLEMS CLASS 1

Consider first a single slit of width b as in the figure below, centered on the x-axis.

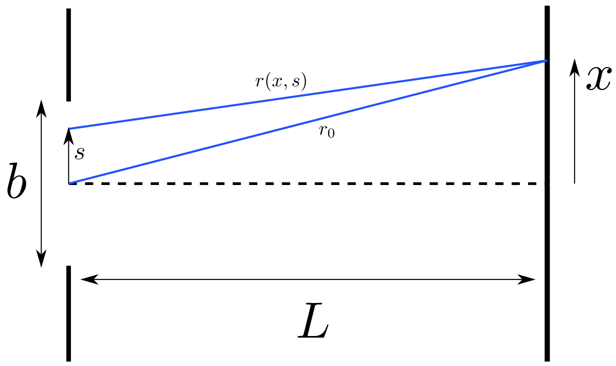


Figure 1: Finite-width single slit experiment, with a slit of width b.

You can view this as a superposition of a continuum of sources, so that the wave is given by

$$\psi(x,t) = C \int_{s=-b/2}^{b/2} e^{ikr(x,s)-i\omega t}\mathrm{d}s \,. \tag{11}$$

Express $r(x,s)$ as the sum of r_0 plus a correction, then perform this integral. Show that the intensity $|\psi(x,t)|^2$ takes the form

$$|\psi(x,t)|^2 = \tilde{C}^2 \frac{\sin^2\beta}{\beta^2} \,, \quad \beta = \frac{bkx}{2L} \,. \tag{12}$$

Give a qualitative plot of $|\psi(x,t)|^2$ versus x.

Solution:

Start by writing

$$r_0^2 = L^2 + x^2\,, \quad r^2(x,s) = L^2 + (x-s)^2\,. \tag{13}$$

Expanding to first order in x/L gives

$$r_0(x) = L + \mathcal{O}((x/L)^2)\,, \quad r(x,s) = L\sqrt{(s/L)^2+1} - \frac{L}{\sqrt{(s/L)^2+1}}(x/L) + \mathcal{O}((x/L)^2)\,. \tag{14}$$

Now also expand $r(x,s)$ to first order in s/L to get

$$r(x,s) = L - L(s/L)(x/L) + \mathcal{O}((x/L)^2, (s/L)^2)\,. \tag{15}$$

A Taylor series expansion to lowest order in s/L and x/L thus yields

$$r(x,s) = r_0 - \frac{sx}{L} + \mathcal{O}((x/L)^2, (s/L)^2)\,. \tag{16}$$

This means that the amplitude at the screen is

$$\begin{aligned}\psi(x) &\approx C\int_{-b/2}^{b/2} e^{ikr(x,s)-i\omega t}\mathrm{d}s = Ce^{ikr_0-i\omega t}\int_{-b/2}^{b/2} e^{-iksx/L}\mathrm{d}s \\ &= Ce^{ikr_0-i\omega t}\frac{iL}{kx}e^{-iksx/L}\Big|_{s=-b/2}^{b/2} = Ce^{ikr_0-i\omega t}\frac{2L}{kx}\sin\left(\frac{kbx}{2L}\right)\,.\end{aligned} \tag{17}$$

The intensity is the norm-squared, so

$$|\psi(x)|^2 = |C|^2 b^2 \frac{\sin^2\beta}{\beta^2}\,, \quad \beta = \frac{kbx}{2L}\,. \tag{18}$$

A plot for $kb/2L = 1$ is given below.

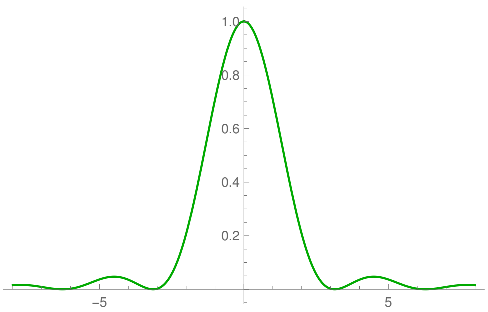


Figure 2: Interference pattern for a single slit, with the size of the slit b set by $kb/2L = 1$ (with arbitrary normalisation for C).

2.3. Finite-width double slit:

Now consider a situation with finite-width slits, as in the figure below. Instead of integrating the contributions from $-b/2$ to $b/2$, we should now integrate (11) over $(a-b)/2$ to $(a+b)/2$, and then add the contribution from the second slit.

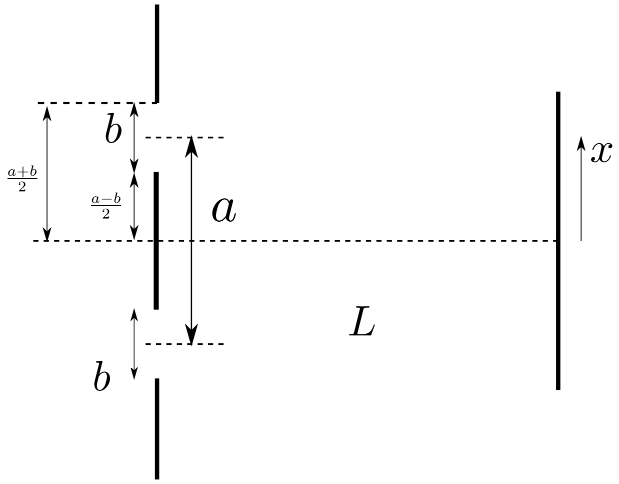


Figure 3: Finite-width double slit experiment, with slits of width b with their midpoints separated by a distance a.

Perform these integrals. Show that the result can be written in the form of the product of two factors, one which is the interference pattern of infinitesimally thin double slits separated by a distance a, and one the interference pattern of a single slit of finite width b.

Solution:

Instead of doing the integral over $-b/2 < s < b/2$, we now have two integrals, one ranging over $(a-b)/2 < s < (a+b)/2$ and the other ranging over $-(a+b)/2 < s < -(a-b)/2$. The integrand is the same. Working out the 4 exponential terms, you get, up to the factors irrelevant for $|\psi|^2$,

$$\psi(x) \propto \left(\frac{2L}{kx}\sin\beta\right)\cos\alpha\,, \tag{19}$$

where the first factor is the single-slit result and the second factor the double-slit. We can write the intensity as

$$|\psi(x)|^2 \propto \frac{\sin^2\beta}{\beta^2}\cos^2(\alpha)\,, \quad \beta = \frac{kbx}{2L}\,, \quad \alpha = \frac{kax}{2L}\,. \tag{20}$$

Plots for separation a equal to 5 times the slit size b are given below.

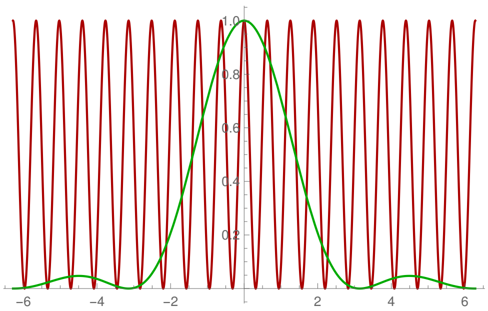


Figure 4: Interference pattern for a single slit superposed with the interference pattern of a double-slit screen with infinitesimally small slits. The single slit parameter is set to $kb/2L = 1$ and the double-slit separation parameter is $ka/2L = 5$.

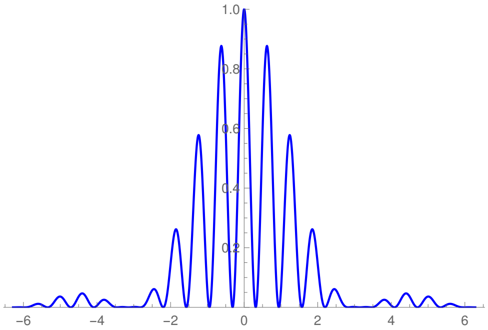


Figure 5: Interference pattern for a finite-size double slit, parameters as above.

3 Problems: Wave function and Probabilities

3.1. Practice with wave functions: **PROBLEMS CLASS 1**

The wave function of a particle at time $t = 0$ is

$$\psi(x) = \begin{cases} C\,\dfrac{x}{a} & 0 \le x \le a \\ C\,\dfrac{b-x}{b-a} & a < x \le b \\ 0 & \text{otherwise} \end{cases} \tag{21}$$

for constants $0 < a < b$.

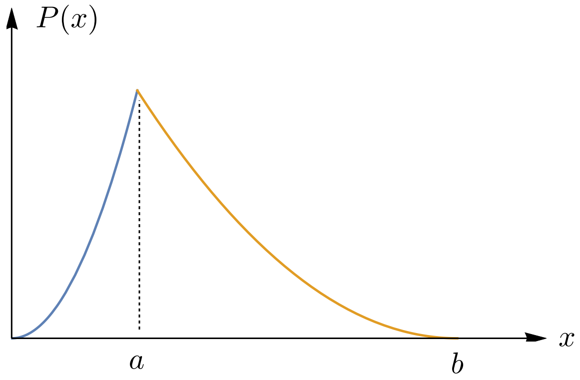
1. What principle fixes the normalisation C?
2. Find C in terms of a and b.
3. Sketch the probability density $P(x) = |\psi(x)|^2$.
4. Where is the particle most likely to be found?
5. Compute the position expectation value $\langle x \rangle$. Does it coincide with your previous answer?
6. What is the probability of finding the particle in the region $x < a$?

Solution:

1. The probability to find the particle anywhere should be 1.
2. The total probability is

$$1 = \int_{-\infty}^{\infty} dx |\psi(x)|^2 = |C|^2 \int_0^a dx \left(\frac{x}{a}\right)^2 + |C|^2 \int_a^b dx \left(\frac{b-x}{b-a}\right)^2 = \frac{b}{3}|C|^2 \,.$$

   Therefore $C = \sqrt{\frac{3}{b}}$ up to a phase.
3. Plot of probability density:



4. The most likely value (mode) is $x = a$.
5. The expectation value of x (mean) is

$$\langle x\rangle = \int_0^b dx\, x|\psi(x)|^2 = \frac{3}{b}\int_0^a dx\, x\left(\frac{x}{a}\right)^2 + \frac{3}{b}\int_a^b dx\, x\left(\frac{b-x}{b-a}\right)^2 = \frac{1}{4}(2a+b)\,.$$

The probability distribution is skewed for generic constants $0 < a < b$ and therefore the mode and mean to not coincide. However, for $a = \frac{b}{2}$ the probability distribution is symmetric and both answers give the same result, $\frac{b}{2}$.
6. The probability to find the particle in the region $x < a$ is

$$P(x<a) = \int_0^a |\psi(x)|^2 = \frac{3}{b}\int_0^a \left(\frac{x}{a}\right)^2 = \frac{a}{b}\,.$$

3.2. More practice with wave functions:

Consider the wave function

$$\psi(x,t) = Ce^{-\lambda|x|}e^{-i\omega t} \tag{22}$$

where C, λ, $\omega \in \mathbb{R}_{>0}$.

1. Find the normalisation C.
2. Find the expectation values $\langle x\rangle$ and $\langle x^2\rangle$ and the uncertainty Δx.
3. Sketch the probability density $P(x)$ and mark the points $x_\pm := \langle x\rangle \pm \Delta x$.
4. What is the probability to find the particle in the region $x_- < x < x_+$?
5. Can the wave function be physical if ω has an imaginary part?

Solution:

1. The probability to find the particle anywhere must be 1.

$$1 = \int_{\infty}^{\infty} |\psi(x,t)|^2 dx = |C|^2\int_{-\infty}^{\infty} e^{-2\lambda|x|}dx = 2|C|^2\int_0^{\infty} e^{-2\lambda x}dx = \frac{|C|^2}{\lambda}\,.$$

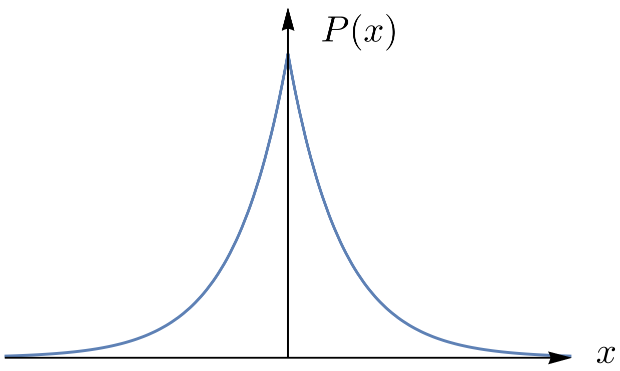
Therefore $C = \sqrt{\lambda}$ up to a phase.

2. First, $\langle x \rangle = 0$ since the integrand is an odd function of x. Second,

$$\begin{aligned}
\langle x^2 \rangle &= \lambda \int_{-\infty}^{\infty} x^2 e^{-2\lambda|x|} dx \qquad (23)\\
&= 2\lambda \int_0^{\infty} x^2 e^{-2\lambda x} dx \\
&= \frac{\lambda}{2} \frac{\partial^2}{\partial \lambda^2} \int_0^{\infty} e^{-2\lambda x} dx \qquad (24)\\
&= \frac{1}{2\lambda^2} \,. \qquad (25)
\end{aligned}$$

Finally, $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = 1/\sqrt{2}\lambda$.

3. The probability density is $P(x,t) = \lambda e^{-2\lambda|x|}$.



4. We have $x_\pm = \pm 1/\sqrt{2}\lambda$. The probability to find the particle in the region $x_- < x < x_+$ is therefore

$$\int_{-1/\sqrt{2}\lambda}^{1/\sqrt{2}\lambda} \lambda e^{-2\lambda|x|} dx = 2\lambda \int_0^{1/\sqrt{2}\lambda} e^{-2\lambda x} dx = 1 - e^{-\sqrt{2}} \,.$$

5. If ω had an imaginary part, the probability density would become

$$\begin{aligned}
P(x,t) &= |C|^2 e^{-2\lambda|x|} e^{-i(\omega-\omega^*)t} \\
&= |C|^2 e^{-2\lambda|x|} e^{2\Im(\omega)t} \,. \qquad (26)
\end{aligned}$$

Attempting to normalise the wave function we would find

$$1 = \frac{|C|^2}{\lambda} e^{2\Im(\omega)t} \,,$$

which cannot be satisfied for all time t unless $\Im(\omega) = 0$. Therefore the wave function is not physical if $\Im(\omega) \neq 0$.

3.3. Gaussian wave function:

The quantum mechanical wave function of a particle at time $t = 0$ is

$$\psi(x) = Ce^{-(x-x_0)^2/4\Delta^2}$$

1. Find the normalisation C.
2. Sketch the probability density $P(x) = |\psi(x)|^2$.
3. Find the expectation values $\langle x \rangle$ and $\langle x^2 \rangle$ and the uncertainty Δx.
4. Which parameter controls how well the particle is localised in position space?

You may use the Gaussian integrals

$$\int_{-\infty}^{\infty} e^{-y^2} dy = \sqrt{\pi} \qquad \int_{-\infty}^{\infty} y^2 e^{-y^2} dy = \frac{\sqrt{\pi}}{2}\,.$$

Solution:

1. Probability to find the particle anywhere should be 1. We find,

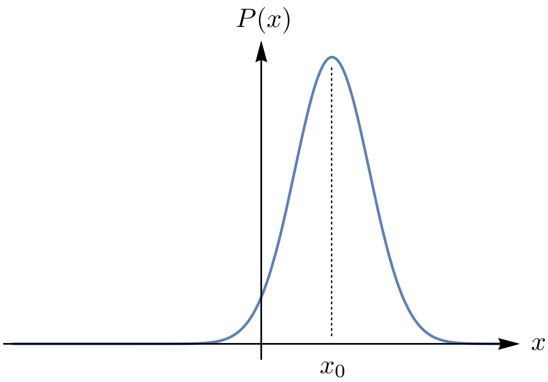
$$1 = |C|^2 \int_{-\infty}^{\infty} dx\, e^{-(x-x_0)^2/2\Delta^2} \tag{27}$$
$$= \sqrt{2\Delta^2}|C|^2 \int_{-\infty}^{\infty} dy\, e^{-y^2}$$
$$= \sqrt{2\pi\Delta^2}\,|C|^2\,, \tag{28}$$

where we defined $y = (x - x_0)/\sqrt{2\Delta^2}$. Therefore

$$C = 1/(2\pi\Delta^2)^{1/4}$$

up to a phase.

2. Sketch of the probability density.



3. First,

$$\langle x \rangle = \frac{1}{\sqrt{2\pi\Delta^2}} \int_{-\infty}^{\infty} dx\, x\, e^{-(x-x_0)^2/2\Delta^2} \tag{29}$$
$$= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dy\, (x_0 + \sqrt{2\Delta^2}\, y)\, e^{-y^2}$$
$$= \frac{x_0}{\sqrt{\pi}} \int_{-\infty}^{\infty} dy\, e^{-y^2} \tag{30}$$
$$= x_0\,. \tag{31}$$

Second,

$$\langle x^2 \rangle = \frac{1}{\sqrt{2\pi\Delta^2}} \int_{-\infty}^{\infty} dx\, x^2\, e^{-(x-x_0)^2/2\Delta^2} \tag{32}$$

$$= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dy\, (x_0 + \sqrt{2\Delta^2}\, y)^2\, e^{-y^2}$$

$$= \frac{x_0^2}{\sqrt{\pi}} \int_{-\infty}^{\infty} dy\, e^{-y^2} + \frac{2\Delta^2}{\sqrt{\pi}} \int_{-\infty}^{\infty} dy\, y^2\, e^{-y^2} \tag{33}$$

$$= x_0^2 + \Delta^2\,. \tag{34}$$

Finally,

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \Delta\,.$$

4. $\Delta x = \Delta$ is a measure of how well localised the particle is in space.

3.4. Another wave packet:

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Consider the following wave function

$$\psi(x) = \sqrt{\frac{1}{4\pi\hbar\delta p}} \int_{p_0-\delta p}^{p_0+\delta p} e^{ipx/\hbar} dp\,.$$

1. Compute and sketch the probability density $P(x)$.
2. Verify that the wave function is normalised.
3. What happens if you try to compute Δx?
4. Instead compute the distance δx between the zeroes of $P(x)$ closest to the origin and show that

$$\delta x\, \delta p = 2\pi\hbar\,.$$

You may assume the following integral,

$$\int_{-\infty}^{\infty} \frac{\sin^2(y)}{y^2} = \pi\,.$$

Solution:

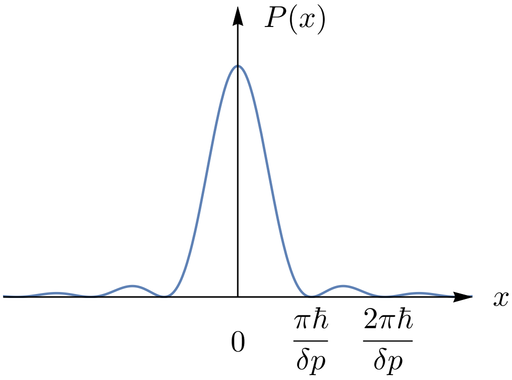
1. We first compute the integral

$$\psi(x) = \sqrt{\frac{1}{4\pi\hbar\delta p}} \int_{p_0-\delta p}^{p_0+\delta p} e^{ipx/\hbar} dp \tag{35}$$

$$= \sqrt{\frac{\hbar}{\pi\delta p}}\, \frac{e^{ip_0 x/h} \sin\left(x\delta p/\hbar\right)}{x}\,.$$

The probability density is therefore

$$P(x) = \frac{\hbar}{\pi\delta p} \frac{\sin^2\left(x\delta p/\hbar\right)}{x^2}\,.$$



2. Changing variables to $y = x\delta p/\hbar$, we have

$$\int_{-\infty}^{\infty} P(x)dx = \frac{\hbar}{\pi\delta p}\int_{-\infty}^{\infty}\frac{\sin^2(x\delta p/\hbar)}{x^2}dx$$
$$= \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\sin^2(y)}{y^2} = 1\,. \qquad (36)$$

3. The integrals required to compute $\langle x^n\rangle$ for $n > 0$ do not converge. Therefore we cannot compute the uncertainty Δx.
4. The zeroes closest to the origin are at $\pm\pi\hbar/\delta p$. We therefore take $\delta x = 2\pi\hbar/\delta p$.
5. Hence $\delta x\delta p = 2\pi\hbar$.

4 Problems: Momentum and Planck's constant

4.1. Momentum expectation value:

The expectation value of momentum measurements on a particle with wave function $\psi(x)$ is

$$\langle p\rangle = -i\hbar\int_{-\infty}^{\infty} dx\,\overline{\psi(x)}\,\partial_x\psi(x)\,.$$

You may assume the wave function is normalised, $\int_{-\infty}^{\infty} dx|\psi(x)|^2 = 1$.

1. Show that $\langle p\rangle$ is real.
2. Show that if $\psi(x)$ is real then $\langle p\rangle = 0$.
3. Suppose a wave function $\phi(x)$ has momentum expectation value $\langle p\rangle_\phi = P$. Compute the expectation value $\langle p\rangle_\psi$ for

$$\psi(x) = e^{ixp_0/\hbar}\phi(x)\,.$$

Solution:

1. We compute the conjugate

$$\begin{aligned}
\overline{\langle p\rangle} &= +i\hbar\int_{-\infty}^{\infty} dx\,\psi(x)\partial_x\overline{\psi(x)} \\
&= -i\hbar\int_{-\infty}^{\infty} dx\,\partial_x\psi(x)\overline{\psi(x)} + i\hbar\left[|\psi(x)|^2\right]_{-\infty}^{\infty} && (37)\\
&= -i\hbar\int_{-\infty}^{\infty} dx\,\overline{\psi(x)}\partial_x\psi(x) && (38)\\
&= \langle p\rangle\,. && (39)
\end{aligned}$$

   In passing to the second line we have integrated by parts. The boundary term vanishes provided the probability density $|\psi(x)|^2$ vanishes at $x\to\pm\infty$. This is a necessary condition for the wave function to be normalizable, $\int_{-\infty}^{\infty}|\psi(x)|^2<\infty$.

2. Assuming the wave function is real $\overline{\psi(x)}=\psi(x)$, then

$$\begin{aligned}
\langle p\rangle &= -i\hbar\int_{-\infty}^{\infty} dx\,\psi(x)\partial_x\psi(x) && (40)\\
&= -\frac{i\hbar}{2}\int_{-\infty}^{\infty} dx\,\partial_x(\psi(x)^2) \\
&= -\frac{i\hbar}{2}\left[\psi(x)^2\right]_{-\infty}^{\infty}\,, && (41)
\end{aligned}$$

   which vanishes for the same reason as the boundary term in part (a).

3. By direct computation

$$\begin{aligned}
\langle p\rangle_\psi &= -i\hbar\int_{-\infty}^{\infty} dx\,\overline{\psi(x)}\partial_x\psi(x) && (42)\\
&= -i\hbar\int_{-\infty}^{\infty} dx\,e^{-ixp_0/\hbar}\overline{\phi(x)}\,\partial_x\left(e^{ixp_0/\hbar}\phi(x)\right) \\
&= -i\hbar\int_{-\infty}^{\infty} dx\,\overline{\phi(x)}\left(\partial_x\phi(x)+\frac{ip_0}{\hbar}\phi(x)\right) && (43)\\
&= -i\hbar\int_{-\infty}^{\infty} dx\,\overline{\phi(x)}\partial_x\phi(x) + p_0\int_{-\infty}^{\infty} dx|\phi(x)|^2 && (44)\\
&= P + p_0 && (45)
\end{aligned}$$

   where in the last step we used that the wave function is normalized.

4.2. Gaussian wave function:

Reconsider the Gaussian wave function which you have seen in one of the problems in the previous chapter.

1. Explain why the momentum expectation value is zero, $\langle p\rangle = 0$.
2. Compute the momentum uncertainty Δp.
3. Show that the wave function saturates Heisenberg's uncertainty principle,

$$\Delta x\,\Delta p \geq \frac{\hbar}{2}\,.$$

4. What happens to Δp when the particle is localised in space?
5. What changes if you multiply the wave function by $e^{ixp_0/\hbar}$?

Solution:

1. The wave function is real.
2. First compute the action of the momentum operator $p = -i\hbar\frac{\partial}{\partial x}$ on the wave function,

$$p\,\psi(x) = -i\hbar\frac{\partial}{\partial x}\left(Ce^{-(x-x_0)^2/4\Delta^2}\right)$$

$$= \frac{i\hbar}{2\Delta^2}(x-x_0)\,Ce^{-(x-x_0)^2/4\Delta^2} \tag{46}$$

$$= \frac{i\hbar}{2\Delta^2}(x-x_0)\,\psi(x)\,. \tag{47}$$

Acting again, we find

$$p^2\,\psi(x) = -\frac{\hbar^2}{4\Delta^4}\left((x-x_0)^2 - 2\Delta^2\right)\psi(x)\,.$$

We can now re-use the position expectation values $\langle x\rangle = x_0$ and $\langle x^2\rangle = x_0^2+\Delta^2$ computed in question 3 (together with the normalisation condition $\langle 1\rangle = 1$) to compute the momentum expectation values,

$$\langle p\rangle = \frac{i\hbar}{2\Delta^2}\langle x-x_0\rangle = 0 \tag{48}$$

$$\langle p^2\rangle = -\frac{\hbar^2}{4\Delta^2}\langle (x-x_0)^2 - 2\Delta^2\rangle$$

$$= -\frac{\hbar^2}{4\Delta^2}\left(\langle x^2\rangle - 2x_0\langle x\rangle + x_0^2 - 2\Delta^2\right) \tag{49}$$

$$= \frac{\hbar^2}{4\Delta^2}\,. \tag{50}$$

If you are uncomfortable with the above manipulations, you can first compute the momentum expectation values using the integral definitions

$$\langle p\rangle = -i\hbar\int_{-\infty}^{\infty} dx\,\overline{\psi(x)}\partial_x\psi(x)$$

$$\langle p^2\rangle = -\hbar^2\int_{-\infty}^{\infty} dx\,\overline{\psi(x)}\partial_x^2\psi(x)\,. \tag{51}$$

You will find that the computation is equivalent to the one above! Finally, $\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \hbar/2\Delta$.

3. Recalling that $\Delta x = \Delta$, we have $\Delta x\Delta p = \hbar/2$.
4. The uncertainty in momentum increases.
5. If you multiply the wave function by $e^{ixp_0/\hbar}$, the momentum expectation value changes to $\langle p\rangle = p_0$.

4.3. Non-normalisable wave functions:

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Consider the wave function

$$\psi_1(x) = Ce^{ikx}\,, \tag{52}$$

for some constant C and k. The total integrated probability is not defined, because the integral

$$\int_{-\infty}^{\infty}|\psi(x)|^2\mathrm{d}x \tag{53}$$

does not exist for any non-zero value of C. However, we can make sense of it by 'cutting off' the integral so that $-L < x < L$ ('putting the particle in a box'), doing all computations at finite L, and then taking the limit $L \to \infty$. If you use this 'regularisation', what is the expectation value $\langle \hat{p} \rangle$ when the system is described by the wave function above? Also compute $\langle p^2 \rangle$.

Solution:

If we cut off the integrals,

$$C^{-2} = \int_{-L}^{L} \mathrm{d}x = 2L\,, \quad \to \quad C = 1/\sqrt{2L}\,, \tag{54}$$

and the expectation value of the momentum becomes

$$\langle p \rangle = C^2 \int_{-L}^{L} (-i\hbar)(ik)\mathrm{d}x = \hbar k\,. \tag{55}$$

This is independent of L. *However*, manipulations like these are on a shoddy mathematical ground (we e.g. did not discuss the boundary conditions on the wave function), and we will see some examples where naive reasoning like this goes flat on its face.

4.4. Momentum in a box:

Consider a particle in an infinite potential well, so that $-L/2 < x < L/2$. If you want to show that $\langle p \rangle$ is real (see above), you will encounter boundary terms which need to vanish. Do they? Why?

Solution:

The boundary term you encounter when computing $\overline{\langle p \rangle} - \langle p \rangle$ reads

$$i\hbar \Big[\psi(x)\bar{\psi}(x)\Big]_{-L/2}^{L/2}\,. \tag{56}$$

For generic wave functions $\psi(x)$ this would not vanish. It will, however, vanish if the wave function vanishes at the edge of the box, which is precisely the condition we have used in the chapter where we first introduced the wave function.

5 Problems: Schrödinger's Equation

5.1. Conservation of the inner product:

Consider two square normalizable solutions $\psi_1(x,t)$ and $\psi_2(x,t)$ of Schrödinger's equation.

1. Show that the inner product of these wavefunctions is conserved,

$$\partial_t \langle \psi_1, \psi_2 \rangle = 0\,.$$

2. Hence explain why
    1. a normalized wavefunction remains normalized,
    2. a pair of orthogonal wavefunctions remain orthogonal.

Solution:

1. Schrödinger's equation is
$$i\hbar\partial_t\psi = \hat{H}\cdot\psi$$
and therefore
$$\partial_t\psi = -\frac{i}{\hbar}\hat{H}\cdot\psi\,.$$
Computing the time derivative of the inner product,
$$\begin{aligned}\partial_t\langle\psi_1,\psi_2\rangle &= \langle\partial_t\psi_1,\psi_2\rangle + \langle\psi_1,\partial_t\psi_2\rangle \qquad (57)\\ &= \langle -\frac{i}{\hbar}\hat{H}\cdot\psi_1,\psi_2\rangle + \langle\psi_1, -\frac{i}{\hbar}\hat{H}\cdot\psi_2\rangle\\ &= \frac{i}{\hbar}\Big(\langle\hat{H}\cdot\psi_1,\psi_2\rangle - \langle\psi_1,\hat{H}\cdot\psi_2\rangle\Big) = 0 \qquad (58)\end{aligned}$$
To see that this last line is true, write out what the pointy bracket notation means:
$$\langle\hat{H}\cdot\psi_1,\psi_2\rangle = \int_{-\infty}^{\infty}\left(-\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi_1(x) + V(x)\psi_1(x)\right)^*\psi_2(x) \qquad (59)$$
$$= \text{bdy. terms} + \int_{-\infty}^{\infty}\psi_1^*(x)\left(-\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi_2(x) + V(x)\right)\psi_2(x) \qquad (60)$$
$$= \langle\psi_1,\hat{H}\cdot\psi_2\rangle\,. \qquad (61)$$
In going to the pre-last line, we have integrated by parts twice to move the derivative to the $\psi_2(x)$ factor, and we have used that $V(x)$ is real.
The cancellation of these two terms in 58 is a manifestation of the fact that $\hat{H}$ is a so-called *Hermitian operator*. We will discuss this in more detail in chapter 7 & 8.
2. We conclude that $\langle\psi_1,\psi_2\rangle$ is constant in time for any square-normalizable solutions ψ_1 and ψ_1 of Schrödinger's equation. The results follow immediately.

5.2. Heat equation:

TUTORIAL 1

Consider the Schrödinger equation with, for simplicity, $\hbar = 1$ and $m = 1$, and vanishing potential,
$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial\psi}{\partial x^2}\,. \qquad (62)$$

1. Make the change of variable $t = -i\tilde{t}$ and show that this leads to the *heat equation* with diffusivity $1/2$ (look up these terms if you do not know them).
2. The heat equation has the well-known solution
$$\psi(x,\tilde{t}) = \frac{1}{\sqrt{2\pi\tilde{t}}}\exp\Big(-\frac{x^2}{2\tilde{t}}\Big)\,, \qquad (63)$$
What does this solution describe? (make some plots at various fixed values of $\tilde{t}$).
3. Do the inverse transformation $\tilde{t} = it$ on this solution, to obtain your first time-dependent solution to the Schrödinger equation. Make plots or sketches at a fixed value of t for the real and imaginary part, as well as the norm $|\psi(x,t|^2$.

Solution:

1. Under this transformation, and using

$$\frac{\partial}{\partial t} = \frac{\partial \tilde{t}}{\partial t} \frac{\partial}{\partial \tilde{t}}, \tag{64}$$

we get

$$\frac{\partial \psi(x, \tilde{t})}{\partial \tilde{t}} = \frac{1}{2} \frac{\partial^2 \psi(x, \tilde{t})}{\partial x^2}, \tag{65}$$

the heat equation with coefficient $1/2$.

2. The solution looks like a Gaussian blob which spreads out in time,

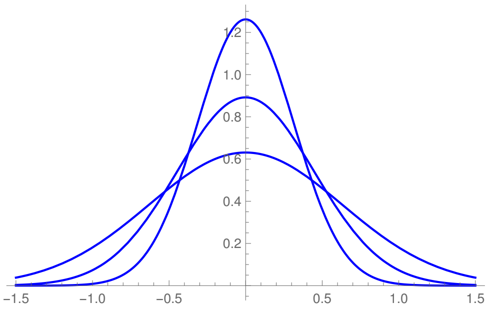


Figure 6: Solution of the heat equation, describing a localised high-temperature region at $\tilde{t} = 0.1, 0.2, 0.4$, showing how it spreads out.

3. The inverse transform yields

$$\psi(x, t) = \frac{1}{\sqrt{2\pi i t}} \exp\left(\frac{i x^2}{2t}\right), \tag{66}$$

which for $t = 0.1$ produces the plot below.

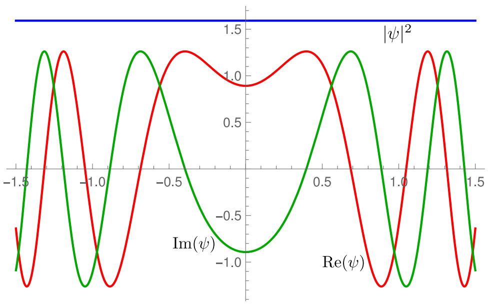


Figure 7: Solution of the Schrödinger equation.

We will discuss the use of this solution later when we discuss the free particle in quantum mechanics.

6 Problems: The Hilbert Space

6.1. Properties of the inner product:

The inner product on continuous square-integrable functions is

$$\langle \psi_1, \psi_2 \rangle = \int_{-\infty}^{\infty} \overline{\psi_1(x)} \psi_2(x) dx \,.$$

Show that

1. $\langle \psi_1, \psi_2 \rangle = \overline{\langle \psi_2, \psi_1 \rangle}$
2. $\langle \psi_3, a_1\psi_1 + a_2\psi_2 \rangle = a_1 \langle \psi_3, \psi_1 \rangle + a_2 \langle \psi_3, \psi_2 \rangle$
3. $\langle a_1\psi_1 + a_2\psi_2, \psi_3 \rangle = \bar{a}_1 \langle \psi_1, \psi_3 \rangle + \bar{a}_2 \langle \psi_2, \psi_3 \rangle$
4. $\langle \psi, \psi \rangle \geq 0$
5. $\langle \psi, \psi \rangle = 0$ implies $\psi(x) = 0$

for any constants $a_1, a_2 \in \mathbb{C}$.

Solution:

1. We have

$$\begin{aligned} \langle \psi_1, \psi_2 \rangle &= \int_{-\infty}^{\infty} \overline{\psi_1(x)} \psi_2(x) \, dx & (67) \\ &= \overline{\int_{-\infty}^{\infty} \overline{\psi_2(x)} \psi_1(x) \, dx} \\ &= \overline{\langle \psi_2, \psi_1 \rangle} \,. & (68) \end{aligned}$$

2. We have

$$\begin{aligned} \langle \psi_3, a_1\psi_1 + a_2\psi_2 \rangle &= \int_{-\infty}^{\infty} \overline{\psi_3(x)} \left(a_1\psi_1(x) + a_2\psi_2(x) \right) dx & (69) \\ &= a_1 \int_{-\infty}^{\infty} \overline{\psi_3(x)} \psi_1(x) dx + a_2 \int_{-\infty}^{\infty} \overline{\psi_3(x)} \psi_2(x) dx \\ &= a_1 \langle \psi_3, \psi_1 \rangle + a_2 \langle \psi_3, \psi_2 \rangle \,. & (70) \end{aligned}$$

3. This follows from parts (a) and (b).
4. We have $\langle \psi, \psi \rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 dx \geq 0$ since $|\psi(x)|^2 \geq 0$ for all $x \in \mathbb{R}$.
5. Suppose $\langle \psi, \psi \rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 0$. Then $|\psi(x)|^2$ can be non-zero at most on a set of measure zero in $\mathbb{R}$. But since the wavefunction is continuous, $|\psi(x)|^2 = 0$ everywhere and therefore $\psi(x) = 0$.

6.2. Inconsistent?: PROBLEMS CLASS 2

Consider the canonical commutation relation

$$[\hat{x}, \hat{p}] = i\hbar \,. \qquad (71)$$

We have argued that wave functions are vectors in Hilbert space, and operators are 'matrices' acting on those vectors. In this case, the operators $\hat{x}$ and $\hat{p}$ are then both matrices, and the right hand side should be read as '$i\hbar$ times the unit matrix'. All fine so far.

Now let use take the trace of the above equation,

$$\mathrm{Tr}\Big([\hat{x},\hat{p}]\Big) = \mathrm{Tr}\Big(i\hbar\Big)\,. \tag{72}$$

The left-hand side vanishes by virtue of cyclicity of the trace. The right-hand side clearly does not vanish, as it is the trace over the unit operator. How can this be consistent?

Solution:

This argument shows that Hilbert space cannot be finite-dimensional, as the trace of a commutator of finite-dimensional matrices definitely vanishes, and the trace of a finite-dimensional unit matrix does not.

If you write this in terms of wave functions, you can see the kind of trouble we get into. The left-hand side would be an integral or infinite sum over all normalisable wave functions,

$$\mathrm{Tr}\Big([\hat{x},\hat{p}]\Big) \text{``=''} -i\hbar \sum_{\text{all normalisable } \phi(x)} \int_{-\infty}^{\infty} \overline{\phi(x)} \left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x} x \right) \phi(x)\,\mathrm{d}x\,, \tag{73}$$

where the derivatives act on everything to the right, and the 'sum' of course needs careful definition. However, the key point is that e.g. in the second term, the derivative acts on $x\phi(x)$, which may **not** be a normalisable function!

For more details on this and related tricky points, see e.g. F. Gieres. "Dirac's formalism and mathematical surprises in quantum mechanics". In: *Rept. Prog. Phys.* 63 (2000), p. 1893. arXiv: `quant-ph/9907069`.

7 Problems: Hermitian Operators

7.1. Properties of the adjoint:

The adjoint $A^\dagger$ of a linear operator A is defined by

$$\langle \psi_1, A\psi_2\rangle = \langle A^\dagger \psi_1, \psi_2\rangle$$

for any continuous square-integrable wavefunctions $\psi_1(x)$ and $\psi_2(x)$. Show that

1. $(A_1 + A_2)^\dagger = A_1^\dagger + A_2^\dagger$
2. $(aA)^\dagger = \bar{a}A^\dagger$ for any constant $a \in \mathbb{C}$
3. $(A_1A_2)^\dagger = A_2^\dagger A_1^\dagger$
4. $(A^n)^\dagger = (A^\dagger)^n$ for any $n \in \mathbb{N}$
5. If $f(x)$ is a real analytic function of $x \in \mathbb{R}$, $f(A)^\dagger = f(A^\dagger)$.

Solution:

These properties can be shown algebraically using the properties of the inner product in question 2.1.

1. We have

$$\langle \psi, (A_1 + A_2)\psi' \rangle = \langle \psi, A_1\psi' + A_2\psi' \rangle \tag{74}$$
$$= \langle \psi, A_1\psi' \rangle + \langle \psi, A_2\psi' \rangle$$
$$= \langle A_1^\dagger \psi, \psi' \rangle + \langle A_2^\dagger \psi, \psi' \rangle \tag{75}$$
$$= \langle A_1\psi + A_2\psi, \psi' \rangle \tag{76}$$
$$= \langle (A_1^\dagger + A_2^\dagger)\psi, \psi' \rangle \tag{77}$$

and therefore $(A_1 + A_2)^\dagger = A_1^\dagger + A_2^\dagger$.

2. We have

$$\langle \psi, (aA)\psi' \rangle = \langle \psi, a(A\psi') \rangle \tag{78}$$
$$= a\langle \psi, A\psi' \rangle$$
$$= a\langle A^\dagger \psi, \psi' \rangle \tag{79}$$
$$= \langle \bar{a}(A^\dagger \psi, \psi' \rangle \tag{80}$$
$$= \langle (\bar{a}A^\dagger)\psi, \psi' \rangle \tag{81}$$

and therefore $(aA)^\dagger = \bar{a}A^\dagger$.

3. We have

$$\langle \psi, (A_1A_2)\psi' \rangle = \langle \psi, A_1(A_2\psi') \rangle \tag{82}$$
$$= \langle A_1^\dagger \psi, A_2\psi' \rangle$$
$$= \langle A_2^\dagger (A_1^\dagger)\psi, \psi' \rangle \tag{83}$$
$$= \langle (A_2^\dagger A_1^\dagger)\psi, \psi' \rangle \tag{84}$$

and therefore $(A_1A_2)^\dagger = A_2^\dagger A_1^\dagger$.

4. From part (c), we have immediately $(A^2)^\dagger = (A^\dagger)^2$. We now proceed by induction on n. Let us assume $(A^n)^\dagger = (A^\dagger)^n$. Then

$$(A^{n+1})^\dagger = (AA^n)^\dagger = (A^n)^\dagger A^\dagger = (A^\dagger)^n A^\dagger = (A^\dagger)^{n+1}$$

where have again used part (c) with $A_1 = A$ and $A_2 = A^n$.

5. A real analytic function $f(x)$ has a convergent power series expansion

$$f(x) = \sum_{n=0}^{\infty} f_n x^n$$

with real coefficients $f_n \in \mathbb{R}$. The result now follows from parts (a), (b), and (d).

7.2. Properties of Hermitian operators:

TUTORIAL 2

Hermitian operators satisfy various properties which will be important in later chapters:

1. Show that any linear operator A can be expressed as a sum

$$A = U + V$$

where $U^\dagger = U$ is Hermitian and $V^\dagger = -V$ is anti-Hermitian.

2. Show that if A and B are Hermitian then $A + B$ is Hermitian.
3. Show that if A is Hermitian then aA is Hermitian if and only if $a \in \mathbb{R}$. What happens if $a \in i\mathbb{R}$?

4. Show that if A and B are Hermitian then the commutator

$$[A, B] := AB - BA$$

is anti-Hermitian.

5. Suppose A and B are Hermitian. Under what condition is AB Hermitian?
6. Show that if A is Hermitian then A^n is Hermitian for $n > 0$.

Solution:

For this question, you will need to use properties of the adjoint from question 2.

1. We can express any linear operator as $A = U + V$ where

$$U = \frac{1}{2}(A + A^\dagger) \qquad V = \frac{1}{2}(A - A^\dagger)\,.$$

It is straightforward to see that $U^\dagger = U$ and $V^\dagger = -V$.

2. Suppose A and B are Hermitian, then $(A + B)^\dagger = A^\dagger + B^\dagger = A + B$ and therefore $A + B$ is Hermitian.
3. Suppose A is Hermitian and $a \in \mathbb{C}$. Then $(aA)^\dagger = \bar{a}A^\dagger = \bar{a}A$. Therefore aA is Hermitian if $a \in \mathbb{R}$ and anti-Hermitian if $a \in i\mathbb{R}$.
4. The commutator is $[A, B] = AB - BA$. Computing the adjoint

$$[A, B]^\dagger = (AB)^\dagger - (BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger = BA - AB = -[A, B]\,.$$

5. Suppose A and B are Hermitian then $(AB)^\dagger = B^\dagger A^\dagger = BA$. So AB is Hermitian if $AB = BA$, or equivalently if $[A, B] = 0$.
6. If A is Hermitian, we have $(A^n)^\dagger = (A^\dagger)^n = A^n$. This implies $f(A)$ is also Hermitian where $f(a)$ is a real analytic function.

7.3. Eigenfunctions have zero uncertainty:

TUTORIAL 2

Consider a eigenfunction of a Hermitian operator A with eigenvalue a. You may assume the wavefunction is normalised.

1. Show that $\langle A^n \rangle = a^n$ for any $n > 0$.
2. Hence show that $\Delta A = 0$.
3. What is the physical interpretation of these results?

Solution:

1. Since $A \cdot \psi = a\psi$ we also have $A^n \cdot \psi = a^n\psi$ for any $n > 0$ and therefore

$$\langle A^n \rangle = \langle \psi, A^n \cdot \psi \rangle = a^n \langle \psi, \psi \rangle = a^n$$

since $\langle \psi, \psi \rangle = 1$ for a normalised wavefunction.

2. Using part (a), $(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2 = a^2 - a^2 = 0$.
3. An eigenfunction of a Hermitian operator A has zero uncertainty for measurements of A. In fact a measurement of A will yield the eigenvalue a with probability 1.

8 Problems: The Spectrum of a Hermitian Operator

8.1. More on Hermitian operators:

A Hermitian operator obeys $A^\dagger = A$ or equivalently $\langle A\psi_1, \psi_2\rangle = \langle \psi_1, A\psi_2\rangle$ for any square-normalizable $\psi_1(x)$, $\psi_2(x)$.

1. Show that eigenvalues of Hermitian operators are real.
2. Show that two eigenfunctions of a Hermitian operator with different eigenvalues are orthogonal.
3. Show that position $\hat{x}$ and momentum $\hat{p}$ are Hermitian.
4. Show that $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$ is Hermitian.
5. Why are measurable quantities represented by Hermitian operators?

Solution:

1. Suppose $A\psi = a\psi$. We have,

$$\begin{aligned} \langle \psi, A\psi\rangle &= \langle \psi, a\psi\rangle = a\langle \psi, \psi\rangle \qquad (85) \\ \langle A\psi, \psi\rangle &= \langle a\psi, \psi\rangle = \bar{a}\langle \psi, \psi\rangle \,. \end{aligned}$$

Subtracting these equations we find $(a-\bar{a})\langle\psi,\psi\rangle = 0$. Assuming $\psi \neq 0$, we find $a = \bar{a}$ and therefore $a \in \mathbb{R}$.

2. Suppose $A\psi_1 = a_1\psi_1$ and $A\psi_2 = a_2\psi_2$ with $a_1 \neq a_2$. We have

$$\begin{aligned} \langle \psi_1, A\psi_2\rangle &= \langle \psi_1, a_2\psi_2\rangle = a_2\langle \psi_1, \psi_2\rangle \qquad (86) \\ \langle A\psi_1, \psi_2\rangle &= \langle a_1\psi_1, \psi_2\rangle = \bar{a}_1\langle \psi_1, \psi_2\rangle = a_1\langle \psi_1, \psi_2\rangle \,. \end{aligned}$$

Subtracting these equations we find $(a_2 - a_1)\langle\psi_1,\psi_2\rangle = 0$ and therefore $\langle\psi_1,\psi_2\rangle = 0$ since $a_1 \neq a_2$.

3. For position, using the fact that $x \in \mathbb{R}$,

$$\begin{aligned} \langle \hat{x}\cdot\psi_1, \psi_2\rangle &= \int_{-\infty}^{\infty} \overline{x\psi_1(x)}\,\psi_2(x)\,dx \qquad (87) \\ &= \int_{-\infty}^{\infty} \overline{\psi_1(x)}\,x\psi_2(x)\,dx \\ &= \langle \psi_1, \hat{x}\cdot\psi_2\rangle \qquad (88) \end{aligned}$$

For momentum, integrating by parts,

$$\begin{aligned} \langle \hat{p}\cdot\psi_1, \psi_2\rangle &= \int_{-\infty}^{\infty} \overline{-i\hbar\frac{\partial\psi_1(x)}{\partial x}}\psi_2(x)dx \qquad (89) \\ &= \int_{-\infty}^{\infty} i\hbar\frac{\partial\overline{\psi_1(x)}}{\partial x}\psi_2(x)dx \\ &= \int_{-\infty}^{\infty} \overline{\psi_1(x)}\left(-i\hbar\frac{\partial\psi_2(x)}{\partial x}\right)dx \qquad (90) \\ &= \langle \psi_1, \hat{p}\cdot\psi_2\rangle \,. \qquad (91) \end{aligned}$$

where in passing to the third line we have integrated by parts and discarded the boundary term since $\overline{\psi_1(x)}\psi_2(x)$ must vanish as $x \to \pm\infty$ for square-normalizable wavefunctions.

4. For the hamiltonian, we can use the properties of the adjoint together with the fact that x and p are Hermitian to show

$$\hat{H}^\dagger = \frac{(\hat{p}^2)^\dagger}{2m} + V(x)^\dagger \tag{92}$$
$$= \frac{(\hat{p}^\dagger)^2}{2m} + V(x^\dagger)$$
$$= \frac{\hat{p}^2}{2m} + V(x) = \hat{H}\,. \tag{93}$$

where we assume the potential $V(x)$ is a real analytic function. You can also show this directly using the differential operator

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

inside the inner product and integrating by parts twice.

5. In quantum mechanics, the possible outcomes of a measurement are the eigenvalues of the corresponding linear operator A. Measurements must yield real numbers. If A is Hermitian, this is guaranteed from part (a).

   In quantum mechanics, if a measurement of A yields the result a_1, then the probability another measurement will yield a different result $a_2 \neq a_1$ immediately afterwards is zero. If A is Hermitian, this is guaranteed from part (b).

8.2. Delta function:

TUTORIAL 2

Prove the following property of the Dirac delta function $\delta(x)$ and the Heaviside step function $\theta(x)$ by integrating with a test function $g(x)$.

$$\frac{\mathrm{d}\theta(x)}{\mathrm{d}x} = \delta(x)\,, \tag{94}$$

Also prove

$$\delta\big(f(x)\big) = \sum_{x_0 \text{ s.t. } f(x_0)=0} \frac{\delta(x-x_0)}{\left|\frac{\mathrm{d}f(x)}{\mathrm{d}x}\right|}\,. \tag{95}$$

You may want to start by doing an explicit example, e.g. by rewriting

$$\int_{-\infty}^{\infty} \delta(x^2-4)g(x)\mathrm{d}x\,, \tag{96}$$

as the sum of *two* integrals over $y = x^2 - 4$. Be careful with signs and the order of integration limits.

Solution:

1. For a smooth test function $g(x)$ we have

$$\int_{-\infty}^{\infty} g(x)\frac{\mathrm{d}}{\mathrm{d}x}\theta(x)\mathrm{dx} = -\int_{-\infty}^{\infty}\frac{\mathrm{d}}{\mathrm{d}x}g(x)\theta(x)\mathrm{dx} = -\int_0^{\infty}\frac{\mathrm{d}}{\mathrm{d}x}g(x)\mathrm{dx} = -g(x)\Big|_0^{\infty} = g(0)\,, \tag{97}$$

   from which the conclusion follows.

2. Change variables to $y = f(x)$ so that $\mathrm{d}y = |f'(x)|\mathrm{d}x$ (where the absolute sign is used so we can keep the integration limits for integration over y in natural

order). This gives

$$\int_{-\infty}^{\infty} g(x)\delta\big(f(x)\big)\mathrm{dx} = \int g\big(x = f^{-1}(y)\big)\frac{\delta(y)}{\big|f'(x)\big|}\mathrm{d}y\,. \tag{98}$$

The integral on the right-hand side may consist of of multiple integrals if $f(x)$ is not monotonic. The integrals get contributions at $y = 0$ only, where the integral will lead to replacement of x with the value of x at which $y = 0$. That can also be done in terms of an integral over x,

$$= \int_{-\infty}^{\infty} \sum_{x \text{ s.t. f(x)=0}} \frac{\delta(x - x_0)}{\big|f'(x)\big|} g(x)\mathrm{d}x\,, \tag{99}$$

from which the requested result follows.
The example would give $f(x) = x^2 - 4$ so that $f'(x) = 2x$, and $f'(-2) = -4$ and $f'(2) = 4$. If you use $\mathrm{d}y = f'(x)\mathrm{d}x$ and keep track of the integration direction, you get

$$\begin{aligned}\int_{-\infty}^{\infty} \delta(x^2 - 4)g(x)\mathrm{d}x &= \int_{\infty}^{-4} \delta(y)\frac{g(x = -\sqrt{y+4})}{-4}\mathrm{d}y + \int_{-4}^{\infty} \delta(y)\frac{g(x = \sqrt{y+4})}{4}\mathrm{d}y \\ &= \int_{-4}^{\infty} \delta(y)\left[\frac{g(x = -\sqrt{y+4})}{4} + \frac{g(x = \sqrt{y+4})}{4}\right]\mathrm{d}y \\ &= \frac{1}{4}\Big(g(x = -2) + g(x = 2)\Big)\,.\end{aligned} \tag{100}$$

9 Problems: Postulates of Quantum Mechanics

9.1. Momentum space representation:

Recall that classically there is a symmetry between position and momentum. In fact, we could also have formulated the postulates of quantum mechanics in terms of a so-called momentum wave function $\widetilde{\psi}(p)$ with momentum operator $\hat{p} = p$ and position operator $\hat{x} = i\hbar\partial_p$. Can you work out the commutator $[\hat{x}, \hat{p}]$ in this representation? We will return to this formulation in a later chapter.

Solution:

In this representation, we get

$$\begin{aligned}[\hat{x}, \hat{p}]\,\widetilde{\psi}(p) &= \hat{x}(\hat{p}\,\psi(x)) - \hat{p}(\hat{x}\,\psi(x)) \\ &= i\hbar\frac{\partial}{\partial p}\left(p\psi(p)\right) - p\left(i\hbar\frac{\partial}{\partial p}\psi(p)\right) \quad = i\hbar\,\psi(p)\,.\end{aligned} \tag{101}$$

Which of course gives the same result as we derived before using the position representation.

9.2. Wave function collapse:

TUTORIAL 2

A quantum mechanical system is, at $t = 0$, prepared in a state described by the wave function

$$\psi(t = 0, x) = C\left(\frac{1}{\sqrt{2}}\psi_{E=1}(x) + e^{i\alpha}\psi_{E=2}(x)\right)\,, \tag{102}$$

where the wave functions on the right-hand side are orthonormal energy eigenfunctions. Both C and α are real constants.

1. Determine the constant C.
2. An energy measurement is made. What are the possible outcomes, and what are the probabilities of those outcomes?
3. Subsequently, the position of the particle is measured. What do you know about the wave function of the system immediately after this measurement?

Solution:

1. Because $\langle\psi_1|\psi_2\rangle = 0$ and each of the wave functions is normalised, we have

$$\langle\psi|\psi\rangle = C^2\left(\frac{1}{2}|\psi_1|^2 + |\psi_2|^2\right) = C^2\frac{3}{2}\,, \quad \Rightarrow \quad C = \sqrt{2/3}\,. \tag{103}$$

2. Either $E = 1$ with probability $1/3$, or $E = 2$ with probability $2/3$.
3. The position operator does not commute with the energy operator, and in particular the energy eigenstates are not position eigenstates. Rather, the wave function will now be an eigenfunction of the position operator, which is a Dirac delta function at the position at which the particle was measured to be.

10 Problems: Commutators and Uncertainty Principle

10.1. Generalised uncertainty principle:

Derive the generalised uncertainty principle,

$$(\Delta A)^2\,(\Delta B)^2 \geq \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2\,, \tag{104}$$

where $(\Delta\hat{A})^2 = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$ and similar for $\hat{B}$.

10.2. Energy-position uncertainty relation:

Show that measurements of position and measurements of energy of a particle in one dimension satisfy the uncertainty relation

$$\Delta x\,\Delta E \geq \frac{\hbar}{2m}\big|\langle p\rangle\big|\,. \tag{105}$$

10.3. Time-energy uncertainty relation (sort of): TUTORIAL 3

For an operator $\hat{Q}$ which does not depend on time explicitly, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{Q}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle\,. \tag{106}$$

For small Δt and small standard-deviation ΔQ we can write

$$\Delta Q \approx \left|\frac{\mathrm{d}\langle\hat{Q}\rangle}{\mathrm{d}t}\right|\Delta t\,. \tag{107}$$

What is the meaning of Δt here? Use (107) to derive the "time-energy uncertainty relation" $\Delta H \Delta t \geq \hbar/2$. What does this 'uncertainty relation' express?

Solution:

1. Writing

$$a(x) := (\hat{A} - \langle\psi \hat{A} \psi\rangle)\psi(x) \qquad (108)$$

and ditto for $\hat{B}$ we can write

$$(\Delta A)^2 (\Delta B)^2 = \langle a, a\rangle \langle b, b\rangle \geq |\langle a, b\rangle|^2 \,. \qquad (109)$$

Setting $z = \langle a, b\rangle$ we then have

$$|z|^2 \geq \mathrm{Im}(z)^2 = \left(\frac{1}{2i}(z - z^*)\right)^2 \,, \qquad (110)$$

For the particular z we have

$$\langle a, b\rangle = \langle \hat{A}\hat{B}\rangle - \langle \hat{A}\rangle\langle \hat{B}\rangle \qquad (111)$$

and similar for the conjugate. Using that for the difference $z - z^*$ then gives the requested result.

2. This requires computing

$$[\hat{x}, \hat{H}] = \frac{1}{2m}[\hat{x}, \hat{p}^2] = \frac{i\hbar}{m}\hat{p} \,. \qquad (112)$$

and thus

$$(\Delta x)^2 (\Delta E)^2 \geq \left(\frac{\hbar}{2m}\langle \hat{p}\rangle\right)^2 \,, \qquad (113)$$

from which the relation follows.

3. Insertion of the Schrödinger equation into the uncertainty relation gives

$$\Delta H \, \Delta Q \geq \frac{\hbar}{2}\left|\frac{\mathrm{d}\langle \hat{Q}\rangle}{\mathrm{d}t}\right| \,. \qquad (114)$$

Then inserting the definition of Δt and rearranging factors produces the $E - t$ uncertainty relation.

The symbol Δt is the time it takes the expectation value of the (arbitrary) operator $\hat{Q}$ to change by one standard deviation.

The uncertainty relation expresses the fact that if all observables change rapidly (Δt small), then the uncertainty in the energy must be large, and if all observables change slowly, the uncertainty in the energy is small.

See Griffiths for more detail and discussion.

11 Problems: Energy Revisited

11.1. Delta function potential:

TUTORIAL 3

So far we have seen only situations in which the energy spectrum is either continuous (when e.g. $V(x) = 0$ everywhere) *or* discrete (e.g. the infinite square well). That is not the generic situation, however. Most potentials lead to spectra which have both a discrete and a continuous part.

Consider particle on a real line with potential given by

$$V(x) = -\alpha\,\delta(x) \,, \qquad (115)$$

where $\alpha > 0$.

1. Solve for the most general $\psi(x)$ in the region $x < 0$ which is an eigenfunction of the Hamiltonian with *negative* eigenvalue E. This should have one unknown parameter (in addition to the constant E).
2. Do the same for the region $x > 0$. This again should have one unknown parameter (again, in addition to E).
3. Impose that the wave function is continuous. Integrate the Hamiltonian eigenfunction equation over an interval $-\epsilon < x < \epsilon$ with $\epsilon \to 0$. Use this to relate E to α.
4. Unit-normalise the wave function to completely fix $\psi(x)$.

There is thus a single (bound) state with $E < 0$.

We will look at the continuum part of the spectrum (eigenfunctions with $E > 0$) later (problem in chapter 17).

Solution:

1. The eigenvalue equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) = E(x)\psi(x)\,. \tag{116}$$

   For $x < 0$ the potential $V(x) = -\alpha\delta(x)$ vanishes, and the general solution reads

$$x < 0: \qquad \psi(x) = Ae^{-\kappa x} + Be^{\kappa x}\,, \quad \kappa = \sqrt{-\frac{2mE}{\hbar^2}}\,. \tag{117}$$

   For a normalisable solution $A = 0$.

2. For $x > 0$ the story is similar, now we get

$$\psi(x) = \tilde{B}e^{-\kappa x}\,. \tag{118}$$

3. Continuity implies $B = \tilde{B}$. Integrating the eigenfunction equation over an infinitesimal region around $x = 0$ yields

$$\int_{-\epsilon}^{\epsilon}\Big(-\frac{\hbar^2}{2m}\psi''(x) - \alpha\delta(x)\psi(x) - E\psi(x)\Big)\mathrm{d}x\,. \tag{119}$$

   The last term vanishes in the limit $\epsilon \to 0$, while the second term gives $-\alpha\psi(0) = -\alpha B$. The first term is a total derivative, equal to

$$-\frac{\hbar^2}{2m}\psi'(x)\Big|_{x=-\epsilon}^{\epsilon} = -\frac{\hbar^2}{2m}2B\kappa\,. \tag{120}$$

   Together we thus find

$$\kappa = \frac{m\alpha}{\hbar^2}\,, \quad \text{or} \quad E = -\frac{m\alpha^2}{2\hbar^2}\,. \tag{121}$$

4. Integrating the norm-squared of the wave function over all of space gives

$$\int |\psi^2| = 2|B|^2\int_0^\infty e^{-2\kappa x}\mathrm{d}x = \frac{|B|^2}{\kappa} = 1\,, \quad \to \quad |B| = \sqrt{\kappa}\,. \tag{122}$$

12 Problems: Stationary states

12.1. Properties of stationary states:

Suppose $\{\phi_j(x)\}$ is an orthonormal basis of eigenfunctions of the Hamiltonian $\hat{H}$ with eigenvalues $\{E_j\}$. Consider the stationary wavefunctions

$$\psi_j(x,t) := e^{-E_j t/\hbar}\phi_j(x)\,.$$

1. Show that $\langle\psi_i,\psi_j\rangle = \delta_{ij}$ for all t.
2. Show that $\psi(x,t)$ satisfy Schödinger's equation.
3. Hence explain why

$$\psi(x,t) = \sum_j c_j\psi_j(x,t)$$

is a solution of Schrödinger's equation for any $c_j \in \mathbb{C}$.

4. What equation do c_j obey if the wavefunction is normalised, $\langle\psi,\psi\rangle = 1$?
5. Show that the probability of measuring energy E_j is independent of t.

Solution:

See chapter "Energy Revisited".

12.2. Time evolution on a circle:

TUTORIAL 3

An orthonormal basis of Hamiltonian eigenfunctions for a free particle on a circle of circumference L is

$$\phi_n(x) = \frac{1}{\sqrt{L}}\exp\left(\frac{2\pi i n x}{L}\right) \qquad n \in \mathbb{Z}$$

with energy eigenvalues

$$E_n = \frac{\hbar^2}{2m}\left(\frac{2\pi n}{L}\right)^2\,.$$

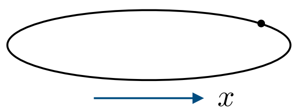


Figure 8: A particle on a circle.

1. The normalised initial wavefunction is

$$\psi(x,0) = \sqrt{\frac{2}{L}}\cos\left(\frac{2\pi x}{L}\right)\,.$$

Find the wavefunction $\psi(x,t)$ at $t > 0$ and explain why the solution is a stationary wavefunction.

2. Suppose the Hamiltonian operator is deformed to

$$\hat{H} = \frac{1}{2m}(\hat{p}+\alpha)^2\,,$$

where $0 < \alpha < \frac{\pi\hbar}{L}$ is a constant. Find the new wavefunction $\psi(x,t)$ at $t > 0$ and explain why the solution is no longer stationary.

Solution:

1. Following the recipe described in the lectures, we first expand the initial wavefunction as a linear combination

$$\psi(x,0) = \frac{1}{\sqrt{2L}}\left(e^{2\pi i x/L} + e^{-2\pi i x/L}\right) = \frac{1}{\sqrt{2}}\left(\phi_1(x) + \phi_{-1}(x)\right) . \tag{123}$$

The wavefunction at later times is therefore

$$\psi(x,t) = \frac{1}{\sqrt{2}}\left(\phi_1(x)e^{-iE_1 t/\hbar} + \phi_{-1}(x)e^{-iE_{-1}t/\hbar}\right) = \sqrt{\frac{2}{L}}\cos\left(\frac{2\pi x}{L}\right)e^{-i\frac{2\hbar\pi^2}{mL^2}t} , \tag{124}$$

where we have used

$$E_1 = E_{-1} = \frac{2\hbar^2\pi^2}{mL^2} .$$

We could also have noticed that since $E_1 = E_{-1}$, the initial wavefunction $\psi(x,0)$ is a Hamiltonian eigenfunction. The time evolution is therefore a stationary solution of Schrödinger's equation.

2. The energy eigenvalues become

$$E_n = \frac{\hbar^2}{2m}\left(\frac{2\pi n}{L} + \frac{\alpha}{\hbar}\right)^2 .$$

The wavefunction at later times is now

$$\psi(x,t) = \frac{1}{\sqrt{2}}\left(\phi_1(x)e^{-iE_1 t/\hbar} + \phi_{-1}(x)e^{-iE_{-1}t/\hbar}\right) = \sqrt{\frac{2}{L}}\cos\left(\frac{2\pi}{L}\left(x - \frac{\alpha t}{m}\right)\right)\exp\left[-i\frac{\hbar t}{2m}\left(\left(\frac{2\pi}{L}\right)^2 + \left(\frac{\alpha}{\hbar}\right)^2\right)\right] . \tag{125}$$

As a consistency check, this reduces to the previous result when $\alpha \to 0$. Since now $E_1 \neq E_{-1}$ the initial wavefunction $\psi(x,0)$ is no longer a Hamiltonian eigenfunction and so the wavefunction at later times is not a stationary solution of Schrödinger's equation.

12.3. Time dependence in a square well I:

PROBLEMS CLASS 3

The wavefunction of an infinite square well $0 < x < L$ at time $t = 0$ is

$$\psi(x,0) = C(\phi_1(x) + \phi_2(x))$$

1. Write down the normalisation factor C.
2. Write down the wave function $\psi(x,t)$ at $t \geq 0$.
3. What are the possible outcomes of an energy measurement and their probabilities? Why do they not depend on time?
4. Show that the position expectation value has the form

$$\langle x \rangle = \frac{L}{2} - A\cos(\omega t)$$

and determine the constants A and ω.

5. Sketch $\langle x \rangle$ as a function of t.
6. How would your sketch change if the initial wavefunction were

$$\psi(x,0) = C(\phi_1(x) + \phi_3(x))\,?$$

You may use the integral $\displaystyle\int_0^\pi dy\, y\, \cos(ny) = \frac{(-1)^n - 1}{n^2}$ *for* $n \in \mathbb{Z}_{>0}$.

Solution:

1. The normalisation is $C = 1/\sqrt{2}$ up to a constant phase.
2. The wavefunction at time $t \geq 0$ is

$$\psi(x,t) = \frac{1}{\sqrt{2}}(\phi_1(x)e^{-iE_1t/\hbar} + \phi_2(x)e^{-iE_2t/\hbar})\,.$$

3. The possible outcomes and probabilities are

$$\begin{aligned} E_1 \quad &: \quad P_1 = \frac{1}{2} \\ E_2 \quad &: \quad P_2 = \frac{1}{2}\,. \end{aligned} \tag{126}$$

The probabilities of energy measurements are always independent of time because the phases $e^{-iE_jt/\hbar}$ cancel out in computing $P_j = |\langle \phi_j, \psi\rangle|^2$.

4. Using the inner product notation, the position expectation value is

$$\begin{aligned} \langle x \rangle &= \langle \psi, \hat{x}\,\psi\rangle \\ &= \frac{1}{2}\langle \phi_1 e^{-iE_1t/\hbar} + \phi_2 e^{-iE_2t/\hbar}, \phi_1 e^{-iE_1t/\hbar} + \phi_2 e^{-iE_2t/\hbar}\rangle && (127) \\ &= \langle \phi_1, \hat{x}\,\phi_1\rangle + \langle \phi_2, \hat{x}\,\phi_2\rangle + e^{-i(E_2-E_1)t/\hbar}\langle \phi_1, \hat{x}\,\phi_2\rangle + e^{-i(E_1-E_2)t/\hbar}\langle \phi_2, \hat{x}\,\phi_1\rangle && (128) \\ &= \langle \phi_1, \hat{x}\,\phi_1\rangle + \langle \phi_2, \hat{x}\,\phi_2\rangle + e^{-i\omega t}\langle \phi_1, \hat{x}\,\phi_2\rangle + e^{i\omega t}\langle \phi_2, \hat{x}\,\phi_1\rangle && (129) \end{aligned}$$

where

$$\omega = (E_1 - E_2)/\hbar\,.$$

We know that

$$\langle \phi_1, \hat{x}\,\phi_1\rangle = \langle \phi_2, \hat{x}\,\phi_2\rangle = \frac{L}{2}$$

because the Hamiltonian eigenfunctions are either symmetric or anti-symmetric around the centre of the potential well. Using the definite integral given in the question, the cross term is

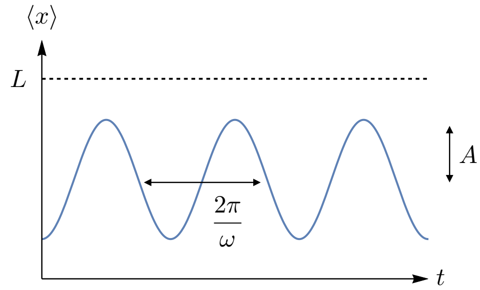
$$\begin{aligned} \langle \phi_1, \hat{x}\,\phi_2\rangle &= \frac{1}{L}\int_0^L dx\, x \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) \\ &= \frac{L}{\pi^2}\int_0^\pi dy\, y \sin(y)\sin(2y) && (130) \\ &= \frac{L}{\pi^2}\int_0^L dy\, y\,(\cos(y) - \cos(3y)) && (131) \\ &= -\frac{L}{\pi^2}\left(\frac{1}{1^2} - \frac{1}{3^2}\right) = -\frac{8L}{9\pi^2}\,, \end{aligned}$$

with the same result for $\langle \phi_2, \hat{x}\, \phi_1 \rangle$. Putting these results together, we find

$$\langle x \rangle = \frac{L}{2} - \frac{16L}{9\pi^2} \cos(\omega t)$$

and can identify $A = 16L/9\pi^2$.

5. The sketch should look like the following.



6. If we replace $\phi_2(x) \to \phi_3(x)$ in the initial wavefunction, the cross term in the computation of $\langle x \rangle$ vanishes,

$$\begin{aligned} \langle \phi_1, \hat{x}\, \phi_3 \rangle &= \frac{1}{L} \int_0^L dx\, x \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{3\pi x}{L}\right) \\ &= \frac{L}{\pi^2} \int_0^\pi dy\, y \sin(y) \sin(3y) \qquad (132) \\ &= \frac{L}{\pi^2} \int_0^L dy\, y \left(\cos(2y) - \cos(4y)\right) \qquad (133) \\ &= 0 \end{aligned}$$

and therefore $\langle x \rangle = L/2$ independent of time.

12.4. Time dependence in a square well II:

The initial wavefunction in an infinite square well $0 < x < L$ is

$$\psi(x, 0) = C \sin^3\left(\frac{\pi x}{L}\right).$$

1. Express $\psi(x, 0)$ as a linear combination of an orthonormal basis of Hamiltonian eigenfunctions $\phi_n(x)$.
   Hint: express $\sin^3(z)$ *as a linear combination of* $\sin(3z)$ *and* $\sin(z)$.
2. Using the orthonormality of $\phi_n(x)$, determine C.
3. What are the possible outcomes of an energy measurement and their probabilities?
4. Hence find the expectation value $\langle H \rangle$.
5. Write down the wavefunction $\psi(x, t)$ for arbitrary later time $t > 0$.
6. Show that the probability density has the form

$$P(x, t) = f(x) + g(x) \cos(\omega t)$$

   and determine the functions $f(x)$ and $g(x)$ and the constant ω.
7. Sketch $P(x, t)$ in the region $0 < x < L$ at times

$$t = 0, \frac{\pi}{\omega}, \frac{2\pi}{\omega}.$$

8. Show that $\langle x \rangle = \frac{L}{2}$ independent of t. Is this consistent with your sketches?

You may use the integral $\int_0^\pi dy\, y\, \cos(ny) = \frac{(-1)^n - 1}{n^2}$ *for* $n \in \mathbb{Z}_{>0}$.

Solution:

1. We first expand

$$\sin(x) = \frac{1}{2i}(e^{ix} - e^{-ix}) \tag{134}$$

$$\begin{aligned} \sin^3(x) &= -\frac{1}{8i}(e^{ix} - e^{-ix})^3 \\ &= -\frac{1}{8i}(e^{3ix} - 3e^{ix} + 3e^{-ix} - e^{-3ix}) \quad (135) \\ &= \frac{3}{4}\sin(x) - \frac{1}{4}\sin(3x) \quad (136) \end{aligned}$$

and therefore

$$\psi(x) = C\sqrt{\frac{L}{2}}\left(\frac{3}{4}\phi_1(x) - \frac{1}{4}\phi_3(x)\right) .$$

2. We now compute inner product using the orthonormal property of the eigenfunctions,

$$\langle \psi, \psi \rangle = \frac{L|C|^2}{2}\left(\left(\frac{3}{4}\right)^2 + \left(\frac{1}{4}\right)^2\right) = \frac{5L}{16}|C|^2 .$$

For the wavefunction to be normalised, we therefore require $C = \sqrt{\frac{16}{5L}}$, up to a constant phase.

3. Substituting the normalisation C back in, the wavefunction is

$$\begin{aligned} \psi(x) &= \sqrt{\frac{8}{5}}\left(\frac{3}{4}\phi_1(x) - \frac{1}{4}\phi_3(x)\right) \quad (137) \\ &= \sqrt{\frac{9}{10}}\phi_1(x) - \sqrt{\frac{1}{10}}\phi_3(x) . \end{aligned}$$

The possible outcomes and an energy measurement and their probabilities are therefore given by

$$\begin{aligned} E_1 &\quad : \quad P_1 = \frac{9}{10} \quad (138) \\ E_3 &\quad : \quad P_3 = \frac{1}{10} . \end{aligned}$$

4. The expectation value of the hamiltonian is

$$\langle H \rangle = P_1 E_1 + P_2 E_2 = \frac{9}{10}E_1 + \frac{1}{10}E_3 = \frac{9\hbar^2\pi^2}{10mL^2} .$$

5. The wave function for $t > 0$ is

$$\psi(x, 0) = \frac{3}{\sqrt{10}}\phi_1(x)e^{-iE_1 t/\hbar} - \frac{1}{\sqrt{10}}\phi_3(x)e^{-iE_3 t/\hbar} .$$

6. Noting that the wavefunctions $\phi_n(x)$ are real, the probability density is

$$\begin{aligned} P(x,t) &= |\psi(x,t)|^2 \quad (139)\\ &= \frac{9}{10}\phi_1(x)^2 + \frac{1}{10}\phi_3(x)^2 - \frac{3}{10}\phi_1(x)\phi_3(x)\left(e^{-i(E_1-E_3)t/\hbar} + \text{c.c.}\right)\\ &= \frac{9}{10}\phi_1(x)^2 + \frac{1}{10}\phi_3(x)^2 - \frac{6}{10}\phi_1(x)\phi_3(x)\cos(\omega t)\,, \quad (140) \end{aligned}$$

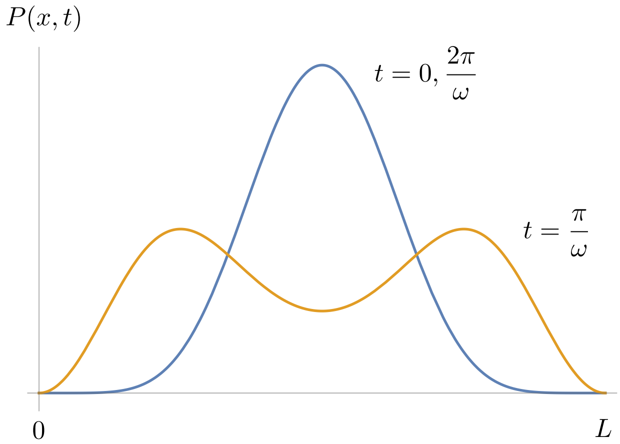
where

$$\omega = \frac{E_3 - E_1}{\hbar} = \frac{4\hbar\pi^2}{mL^2}\,.$$

Therefore

$$\begin{aligned} f(x) &= \frac{9}{10}\phi_1(x)^2 + \frac{1}{10}\phi_3(x)^2 = \frac{9}{5L}\sin^2\left(\frac{\pi x}{L}\right) + \frac{1}{5L}\sin^2\left(\frac{3\pi x}{L}\right)\\ g(x) &= -\frac{6}{10}\phi_1(x)\phi_3(x) = -\frac{6}{5L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{3\pi x}{L}\right)\,. \quad (141) \end{aligned}$$

7. The sketch looks like the following.



8. To compute the expectation value first note that

$$\int_0^L dx\, x\, \phi_n(x)^2 = \frac{L}{2}$$

for any $n > 0$ since $\phi_n(x)^2$ is symmetric around $x = L/2$. You may check this explicitly using the hint if you are not convinced. The remaining integral we need is

$$\begin{aligned} \int_0^L dx\, x\, \phi_1(x)\phi_3(x) dx &= \frac{2}{L}\int_0^L x \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{3\pi x}{L}\right)\\ &= \frac{1}{L}\int_0^L x\left(\cos\left(\frac{2\pi x}{L}\right) - \cos\left(\frac{4\pi x}{L}\right)\right) \quad (142)\\ &= 0\,, \quad (143) \end{aligned}$$

using the hint. We therefore find

$$\langle x \rangle = \int_0^L dx\, x\, f(x) = \frac{9}{10}\cdot\frac{L}{2} + \frac{1}{10}\cdot\frac{L}{2} = \frac{L}{2}$$

independent of t. This is consistent with the sketch: $P(x,t)$ is clearly symmetric around $x = L/2$ for the values sketched.

13 Problems: Case Study: The Free Particle

13.1. Time evolution of a free particle:
Consider a free particle with initial wavefunction $\psi(x,0)$.

1. Assuming all relevant integrals converge, show that

$$\psi(x,t) = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \int_{-\infty}^{\infty} dx' \exp\left(\frac{im}{2\hbar t}(x-x')^2\right)\psi(x',0)$$

is a solution of Schrödinger's equation for a free particle,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)\,.$$

2. Consider the initial wavefunction

$$\psi(x,0) = \begin{cases} C & \text{if } -a < x < a \\ 0 & \text{else} \end{cases}$$

where C is a normalisation constant you should determine. Write down an integral for the wavefunction $\psi(x,t)$ at later times.

Solution:

1. We compute both sides of Schrödinger's equation by differentiating under the integral and compare.

First computing derivatives with respect to x:

$$\begin{aligned}\partial_x\psi(x,t) &= \sqrt{\frac{m}{2\pi i\hbar t}}\int_{-\infty}^{\infty} dx'\,\partial_x \exp\left(\frac{im}{2\hbar t}(x-x')^2\right)\psi(x',0) \\ &= \sqrt{\frac{m}{2\pi i\hbar t}}\int_{-\infty}^{\infty} dx'\,\frac{im}{\hbar t}(x-x')\exp\left(\frac{im}{2\hbar t}(x-x')^2\right)\psi(x',0)\end{aligned} \tag{144}$$

$$\partial_x^2\psi(x,t) = \sqrt{\frac{m}{2\pi i\hbar t}}\int_{-\infty}^{\infty} dx'\left[\frac{im}{\hbar t} + \left(\frac{im}{\hbar t}\right)^2(x-x')^2\right]\exp\left(\frac{im}{2\hbar t}(x-x')^2\right)\psi(x',0) \tag{145}$$

and hence

$$-\frac{\hbar^2}{2m}\partial_x^2\psi(x,t) = \sqrt{\frac{m}{2\pi i\hbar t}}\int_{-\infty}^{\infty} dx'\left[-\frac{i\hbar}{2t} + \frac{m}{2t^2}(x-x')^2\right]\exp\left(\frac{im}{2\hbar t}(x-x')^2\right)\psi(x',0)$$

Second computing the derivative with respect to t:

$$\partial_t \psi(x,t) = \partial_t \sqrt{\frac{m}{2\pi i\hbar t}} \int_{-\infty}^{\infty} dx' \exp\left(\frac{im}{2\hbar t}(x-x')^2\right) \psi(x',0) \tag{146}$$

$$+ \sqrt{\frac{m}{2\pi i\hbar t}} \int_{-\infty}^{\infty} dx' \, \partial_t \exp\left(\frac{im}{2\hbar t}(x-x')^2\right) \psi(x',0)$$

$$= \sqrt{\frac{m}{2\pi i\hbar t}} \int_{-\infty}^{\infty} dx' \left[-\frac{1}{2t} - \frac{im}{2\hbar t^2}(x-x')^2\right] \exp\left(\frac{im}{2\hbar t}(x-x')^2\right) \psi(x',0)\,, \tag{147}$$

and hence

$$i\hbar\partial_t \psi(x,t) = \sqrt{\frac{m}{2\pi i\hbar t}} \int_{-\infty}^{\infty} dx' \left[-\frac{i\hbar}{2t} + \frac{m}{2t^2}(x-x')^2\right] \exp\left(\frac{im}{2\hbar t}(x-x')^2\right) \psi(x',0)$$

We therefore see explicitly that

$$i\hbar\partial_t \psi(x,t) = -\frac{\hbar^2}{2m}\partial_x \psi(x,t)\,.$$

2. The normalisation constant is $C = 1/\sqrt{2a}$.

   The wavefunction at $t > 0$ is

$$\psi(x,t) = \left(\frac{m}{4\pi i\hbar a t}\right)^{1/2} \int_{-a}^{a} dx' \exp\left(\frac{im}{2\hbar t}(x-x')^2\right)\,.$$

   You are not expected to know how to compute this integral.

13.2. Numerical wave packets:

In the notebook linked in the margin, you will find some basic Python code to numerically solve the Schrödinger equation. It is used to compute the time-evolution of a Gaussian wave packet, based on the discretisation scheme

$$\psi(x, t+\mathrm{d}t) = \psi(x, t-\mathrm{d}t)$$

$$+ i\mathrm{d}t\Big[\psi(x-\mathrm{d}x, t) + \psi(x+\mathrm{d}x, t) - 2\big(1+V(x)\big)\psi(x,t)\Big]\,. \tag{148}$$

For more information on this, see section 3.3 of Schroeder's book.

Use this code to verify that width of the Gaussian wave function spreads as

$$\Delta(t) = \Delta\sqrt{1 + \frac{\hbar^2 t^2}{4m^2\Delta^4}}\,, \tag{149}$$

as we derived analytically.

Sample notebook to numerically evolve the Schrödinger equation.

13.3. Degenerate or non-degenerate?:

In an earlier chapter we have argued that the spectrum of the Hamiltonian operator on the real line is non-degenerate. However, the present chapter starts by arguing that there are two wave functions for every energy eigenvalue. Which assumption in that proof of non-degeneracy does not hold in the present chapter?

14 Problems: Two-particle systems

14.1. Verify the normalisation constant for the example wave function used in the notes,

$$\psi(x_1,x_2) = \sqrt{\frac{18}{5}}\frac{1}{L}\left[\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{3\pi x_2}{L}\right) + \frac{1}{3}\sin\left(\frac{3\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right)\right]. \tag{150}$$

Solution:

To avoid having to do integrals, write this function in terms of single-particle wave functions,

$$\psi(x_1,x_2) = \sqrt{\frac{18}{5}}\frac{1}{2}\left[\psi_1(x_1)\psi_3(x_2) + \frac{1}{3}\psi_3(x_1)\psi_2(x_2)\right]. \tag{151}$$

We can now use orthonormality of the $\psi_n(y)$ to compute the norm of the wave function,

$$\langle\psi,\psi\rangle = \frac{18}{5}\frac{1}{4}\int_0^L {\rm d}x_1 \int_0^L {\rm d}x_2 \left(\psi_1^2(x_1)\psi_3^2(x_2) + \frac{1}{9}\psi_3^2(x_1)\psi_2^2(x_2)\right)$$
$$= \frac{9}{10}\left(1+\frac{1}{9}\right) = 1\,, \tag{152}$$

where the cross-terms drop out because of orthonormality of the single-particle wave functions. The wave function is thus correctly normalised.

14.2. How does the wave function in the previous problem evolve in time?

Solution:

The two terms in the wave function are each eigenfunctions of the Hamiltonian, so we know their time evolution is simply multiplication with $\exp(-iEt/\hbar)$ with E the energy eigenvalue for each term. So we get

$$\psi(x_1,x_2,tt) = \sqrt{\frac{18}{5}}\frac{1}{L}\Big[e^{-iE_{1,3}t/\hbar}\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{3\pi x_2}{L}\right)$$
$$+\frac{1}{3}e^{-iE_{1,3}t/\hbar}\sin\left(\frac{3\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right)\Big]. \tag{153}$$

with the energy eigenvalues

$$E_{1,3} = \frac{\hbar^2\pi^2}{2mL^2}(1+3^2)\,,\quad E_{3,2} = \frac{\hbar^2\pi^2}{2mL^2}(3^2+2^2)\,. \tag{154}$$

15 Problems: Simple Harmonic Oscillator

15.1. Virial theorem:

(Do this problem only after you have read the last chapter, on Ehrenfest's theorem).

Consider the Hamiltonian $H = T+V$ where $T = \frac{p^2}{2m}$ is the kinetic energy and $V(x)$ is the potential energy.

1. Use Ehrenfest's theorem to show that $\partial_t\langle xp\rangle = 2\langle T\rangle - \langle x\partial_x V\rangle$.

2. Now consider a stationary solution of Schrödinger's equation in the simple harmonic oscillator with potential

$$V(x) = \frac{1}{2}m\omega^2 x^2 \,.$$

Show that

$$\langle T \rangle = \langle V \rangle \,.$$

Solution:

1. Ehrenfest's theorem is

$$\partial_t \langle A \rangle = \frac{i}{\hbar}\langle [H, A] \rangle$$

for any Hermitian operator A. We apply this theorem to $A = xp$. We therefore compute the commutator on the right,

$$[H, xp] = x[H, p] + [H, x]p \tag{155}$$

$$= x[V(x), p] + [\frac{p^2}{2m}, x]p$$

$$= i\hbar\left(x\partial_x V(x) - \frac{p^2}{m}\right)\,, \tag{156}$$

where we used the fundamental commutator $[x, p] = i\hbar$. We therefore find

$$\partial_t \langle xp \rangle = 2\langle T \rangle - \langle x\partial_x V \rangle$$

where $T = p^2/2m$ is the kinetic energy.

2. First, for the simple harmonic oscillator potential, $x\partial_x V(x) = 2V(x)$. Second, for a stationary solution of Schrödinger's equation, the expectation value of any observable is independent of time. Combining with part (a), we find $\langle T \rangle = \langle V \rangle$.

15.2. Ground state of the harmonic oscillator:

Consider the initial wavefunction

$$\psi(x, 0) = C \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \,.$$

In this question, there is no need to determine C!

1. Show that $\psi(x, 0)$ is an eigenfunction of a Hamiltonian of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2$$

and determine the constant k.

2. What is the corresponding energy eigenvalue?
3. Hence write down the wavefunction $\psi(x, t)$ for $t > 0$.

Solution:

1. Compute the action of the Hamiltonian operator on the initial wavefunction,

$$\hat{H}\cdot\psi(x,0) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2\right)\psi(x,0)$$

$$= -C\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}e^{-\frac{m\omega x^2}{2\hbar}} + \frac{1}{2}kx^2\psi(x,0) \tag{157}$$

$$= C\frac{\hbar\omega}{2}\left(e^{-\frac{m\omega x^2}{2\hbar}} - \frac{m\omega x^2}{\hbar}e^{-\frac{m\omega x^2}{2\hbar}}\right) + \frac{1}{2}kx^2\psi(x,0) \tag{158}$$

$$= \frac{\hbar\omega}{2}\psi(x,0) + \left(k - \frac{1}{2}m\omega^2\right)x^2\psi(x,0)\,. \tag{159}$$

For the initial wavefunction to be a Hamiltonian eigenfunction, this must equal $E\,\psi(x,0)$ where E is a real constant that is independent of x. We therefore require $k = m\omega^2$ to cancel the term proportional to $x^2\psi(x,0)$.

2. The energy is therefore $E = \hbar\omega/2$.
3. The wavefunction at later times is

$$\psi(x,t) = C\exp\left(-\frac{m\omega x^2}{2\hbar}\right)\exp\left(-\frac{iEt}{\hbar}\right) \tag{160}$$

$$= C\exp\left(-\frac{m\omega x^2}{2\hbar}\right)\exp\left(-\frac{i\omega t}{2}\right)\,.$$

The constant ω has units of inverse time and specifies the frequency of the harmonic oscillator.

15.3. The coherent state:

PROBLEMS CLASS 4

Jupyter notebook (on Google Colab) to explore the time-dependence of coherent states of the simple harmonic oscillator.

Consider a normalized wave function obeying

$$\hat{a}\psi(x,t) = \alpha_0 e^{-i\omega t}\psi(x,t)\,.$$

where

$$\hat{a} = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} + i\hat{p})$$

is the annihilation operator and $\alpha_0 \in \mathbb{R}$ is a real constant.

1. Show that $\langle H\rangle = \hbar\omega(\alpha_0^2 + \frac{1}{2})$.
2. Show that

$$\langle x\rangle = \sqrt{\frac{2\hbar}{m\omega}}\,\alpha_0\cos(\omega t) \qquad \langle p\rangle = -\sqrt{2m\hbar\omega}\,\alpha_0\sin(\omega t)\,.$$

3. Show that the above result is a solution of Hamilton's equations.
4. How does the classical energy of the solution of Hamilton's equations compare to $\langle H\rangle$?

Hint (a): use the form of the hamiltonian $H = \hbar\omega(a^\dagger a + \frac{1}{2})$.
Hint (b): first express x, p *in terms of* a, $a^\dagger$.
General hint: remember the definition of the adjoint $\langle\psi_1, a^\dagger\psi_2\rangle = \langle a\psi_1, \psi_2\rangle$.

Solution:

1. The Hamiltonian can be expressed $H = \hbar\omega(a^\dagger a + \frac{1}{2})$. The expectation value of

the hamiltonian is therefore

$$\langle H \rangle = \hbar\omega \langle a^\dagger a + \frac{1}{2} \rangle \, .$$

We evaluate the two terms in this expression as follows:

- First, $\langle 1 \rangle := \langle \psi, \psi \rangle = 1$ for a normalized wave function.
- Second, using the definition of the adjoint,

  $$\langle a^\dagger a \rangle := \langle \psi, a^\dagger a \psi \rangle = \langle a\psi, a\psi \rangle = \langle \alpha_0 e^{-i\omega t}\psi, \alpha_0 e^{-i\omega t}\psi \rangle = \alpha_0^2 \langle \psi, \psi \rangle = \alpha_0^2$$

  where in the final step we again used that the wave function is normalized.

We conclude that $\langle H \rangle = \hbar\omega(\alpha_0^2 + \frac{1}{2})$.

2. Let us first compute the expectation values of the ladder operators

$$\begin{aligned} \langle a \rangle &= \langle \psi, a\psi \rangle = \langle \psi, \alpha_0 e^{-i\omega t}\psi \rangle = \alpha_0 e^{-i\omega t} \\ \langle a^\dagger \rangle &= \langle \psi, a^\dagger \psi \rangle = \langle a\psi, \psi \rangle = \langle \alpha_0 e^{-i\omega t}\psi, \psi \rangle = \alpha_0 e^{+i\omega t} \, . \end{aligned} \tag{161}$$

We now express position and momentum in terms of the ladder operators

$$\begin{aligned} x &= \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \\ p &= -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger) \, . \end{aligned} \tag{162}$$

The expectation values of position and momentum are then

$$\begin{aligned} \langle x \rangle &= \sqrt{\frac{\hbar}{2m\omega}}\alpha_0(e^{-i\omega t} + e^{+i\omega t}) = \sqrt{\frac{2\hbar\alpha_0^2}{m\omega}}\cos(\omega t) \\ \langle p \rangle &= -i\sqrt{\frac{\hbar m\omega}{2}}(e^{-i\omega t} - e^{+i\omega t}) = -\sqrt{2m\hbar\omega\alpha_0^2}\sin(\omega t) \, . \end{aligned} \tag{163}$$

3. This is a solution of Hamilton's equations with classical energy $E = \hbar\omega\alpha_0^2 \geq 0$.
4. If $E \geq 0$ denotes the classical energy of the corresponding solution of Hamilton's equations then $\langle H \rangle = E + \frac{1}{2}\hbar\omega$. This is consistent with the fact that $\langle H \rangle > 0$ for normalizable wave functions in quantum mechanics. Note that in the limit $\alpha_0 \to 0$ we recover the ground state of the simple harmonic oscillator with 'zero-point' energy $\frac{1}{2}\hbar\omega$.

15.4. Properties of Hamiltonian eigenfunctions:

TUTORIAL 4

The ladder operators are defined by

$$\begin{aligned} a &= \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} + i\hat{p}) \\ a^\dagger &= \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} - i\hat{p}) \, . \end{aligned} \tag{164}$$

1. Using the canonical commutator $[\hat{x}, \hat{p}] = i\hbar$, show that $[a, a^\dagger] = 1$.
2. What property does the ground state $\phi_0(x)$ obey?
3. Write down an expression for the excited wave functions $\phi_n(x)$ in terms of creation operators acting on $\phi_0(x)$.
4. Compute the expectation values $\langle x \rangle$, $\langle x^2 \rangle$ and the uncertainty Δx for $\phi_n(x)$.
5. Compute the expectation values $\langle p \rangle$, $\langle p^2 \rangle$ and the uncertainty Δp for $\phi_n(x)$.

6. Check consistency with Heisenberg's uncertainty principle.
7. Check that $\langle T \rangle = \langle V \rangle$, where T is the kinetic energy.

Solution:

1. Using the canonical commutation relation $[x, p] = i\hbar$,

$$[a, a^\dagger] = \frac{1}{2\hbar m\omega}[m\omega x + ip, m\omega x - ip] = \frac{1}{2\hbar}\left(-i[x,p] + i[p,x]\right) = 1\,.$$

2. The ground state wave function obeys $a \cdot \phi_0(x) = 0$.
3. The Hamiltonian eigenfunctions are

$$\phi_n(x) := \frac{1}{\sqrt{n!}}(a^\dagger)^n \phi_0(x)\,.$$

They obey the following important properties

- Orthonormality: $\langle \phi_n, \phi\rangle_m = \delta_{nm}$
- Annihilation: $a\phi_n = \sqrt{n}\phi_{n-1}$
- Creation: $a^\dagger \phi_n = \sqrt{n+1}\phi_{n+1}$

which are used freely below.

4. We compute the expectation value of x using ladder operators as follows,

$$\begin{aligned}
\langle x \rangle &= \sqrt{\frac{\hbar}{2m\omega}}\langle \phi_n, (a + a^\dagger)\phi_n\rangle && (165)\\
&= \sqrt{\frac{\hbar}{2m\omega}}\langle \phi_n, \sqrt{n}\phi_{n-1} + \sqrt{n+1}\phi_{n+1}\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n}\delta_{n,n-1} + \sqrt{n+1}\delta_{n,n+1}) && (166)\\
&= 0\,. && (167)
\end{aligned}$$

The expectation value of x^2 is computed similarly,

$$\begin{aligned}
\langle x^2 \rangle &= \frac{\hbar}{2m\omega}\langle \phi_n, (a + a^\dagger)^2\phi_n\rangle && (168)\\
&= \frac{\hbar}{2m\omega}\langle \phi_n, (a^2 + a^{\dagger 2} + aa^\dagger + a^\dagger a)\phi_n\rangle \\
&= \frac{\hbar}{2m\omega}\langle \phi_n, (a^2 + a^{\dagger 2} + 2a^\dagger a + 1)\phi_n\rangle && (169)\\
&= \frac{\hbar}{2m\omega}(\sqrt{n(n-1)}\delta_{n,n-2} + \sqrt{(n+1)(n+1)}\delta_{n,n+2} + (2n+1)\delta_{n,n}) && (170)\\
&= \frac{\hbar}{2m\omega}(2n+1) && (171)\\
&= \frac{\hbar}{m\omega}(n + \frac{1}{2})\,. && (172)
\end{aligned}$$

The uncertainty is therefore

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\frac{\hbar}{m\omega}(n+\frac{1}{2})}\,.$$

Note that the hamiltonian eigenfunctions are even or odd functions of x, $\phi_n(-x) = (-1)^n \phi_n(x)$. We therefore have $|\phi_n(-x)|^2 = |\phi_n(x)|^2$ and should have expected $\langle x \rangle = 0$.

5. We compute the expectation values of p and p^2 in the same way,

$$\begin{aligned} \langle p \rangle &= -i\sqrt{\frac{\hbar m\omega}{2}} \langle \phi_n, (a - a^\dagger)\phi_n \rangle & (173) \\ &= -i\sqrt{\frac{\hbar m\omega}{2}} \langle \phi_n, \sqrt{n}\phi_{n-1} - \sqrt{n+1}\phi_{n+1} \rangle \\ &= -i\sqrt{\frac{\hbar m\omega}{2}} (\sqrt{n}\delta_{n,n-1} - \sqrt{n+1}\delta_{n,n+1}) & (174) \\ &= 0 & (175) \end{aligned}$$

$$\begin{aligned} \langle p^2 \rangle &= -\frac{\hbar m\omega}{2} \langle \phi_n, (a - a^\dagger)^2\phi_n \rangle & (176) \\ &= \frac{\hbar m\omega}{2} \langle \phi_n, (-a^2 - a^{\dagger 2} + aa^\dagger + a^\dagger a)\phi_n \rangle \\ &= \frac{\hbar m\omega}{2} \langle \phi_n, (-a^2 - a^{\dagger 2} + 2a^\dagger a + 1)\phi_n \rangle & (177) \\ &= \frac{\hbar m\omega}{2} (-\sqrt{n(n-1)}\delta_{n,n-2} - \sqrt{(n+1)(n+1)}\delta_{n,n+2} + (2n+1)\delta_{n,n}) & (178) \\ &= \frac{\hbar m\omega}{2}(2n+1) & (179) \\ &= \hbar m\omega(n + \frac{1}{2})\,. & (180) \end{aligned}$$

The uncertainty is therefore

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\hbar m\omega(n + \frac{1}{2})}\,.$$

Note that the hamiltonian eigenfunctions $\phi_n(x)$ are all real functions and therefore we should have expected $\langle p \rangle = 0$.

6. The product of position and momentum uncertainties is

$$\Delta x \Delta p = \hbar(n + \frac{1}{2}) \geq \frac{\hbar}{2}$$

for $n \geq 0$. Note that the ground state wave function $\phi_0(x)$ saturates the Heisenberg uncertainty principle - it is a Gaussian wave function.

7. The expectation values of kinetic and potential energy are

$$\begin{aligned} \langle T \rangle &= \frac{1}{2m}\langle p^2 \rangle = \frac{\hbar\omega}{2}(n + \frac{1}{2}) & (181) \\ \langle V \rangle &= \frac{1}{2}m\omega^2\langle x^2 \rangle = \frac{\hbar\omega}{2}(n + \frac{1}{2}) \end{aligned}$$

and therefore $\langle T \rangle = \langle V \rangle$ in agreement with the quantum mechanical Virial theorem.

15.5. Instantaneous shift of frequency:

TUTORIAL 4

For $t < 0$, a particle is in the ground state of a simple harmonic oscillator of frequency ω with stationary wave function

$$\psi(x,t) = e^{-it\omega/2}\phi_0(x)\,.$$

At $t = 0$ the frequency suddenly doubles to $\omega' = 2\omega$ leaving the wave function momentarily unchanged.

1. Explain why a measurement at $t < 0$ yields energy $\frac{1}{2}\hbar\omega$ with probability 1.
2. Explain why the probability of measuring energy $\frac{1}{2}\hbar\omega$ at $t > 0$ is zero.
3. What is the probability of measuring energy $\hbar\omega$ just after $t = 0$?

Solution:

The hamiltonian eigenvalues before are $E_n = \hbar\omega(n + \frac{1}{2})$ and after are $E' = \hbar\omega'(n + \frac{1}{2}) = \hbar\omega(2n + 1)$.

1. For $t < 0$, we have a stationary wave function for the ground state with energy $E_0 = \frac{1}{2}\hbar\omega$.
2. For $t > 0$, the possible outcomes of energy measurements are $E'_n = \hbar\omega(2n+1)$ with $n \geq 0$. The probability to measure $\frac{1}{2}\hbar\omega$ at $t > 0$ is therefore zero.
3. Note that $E'_0 = \frac{1}{2}\hbar\omega' = \hbar\omega$ is the energy of the ground state wave function for $t > 0$. Since the wave function is momentarily unchanged, the probability of measuring this energy just after $t = 0$ is

$$P = |\langle \phi_0, \phi'_0 \rangle|^2$$

where

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$$
$$\phi'_0(x) = \left(\frac{m\omega'}{\pi\hbar}\right)^{1/4} e^{-m\omega' x^2/2\hbar}\,. \tag{182}$$

are the ground state eigenfunctions functions before and after. We find

$$\langle \phi_0, \phi'_0 \rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \left(\frac{m\omega'}{\pi\hbar}\right)^{1/4} \int_{-\infty}^{\infty} dx e^{-m\omega x^2/2\hbar} e^{-m\omega' x^2/2\hbar}$$
$$= \left(\frac{m}{\pi\hbar}\right)^{1/2} (\omega\omega')^{1/4} \int_{-\infty}^{\infty} dx e^{-m(\omega+\omega')x^2/2\hbar} \tag{183}$$
$$= \left(\frac{m}{\pi\hbar}\right)^{1/2} (\omega\omega')^{1/4} \left(\frac{2\hbar}{m(\omega+\omega')}\right)^{1/2} \int_{-\infty}^{\infty} dy e^{-y^2} \tag{184}$$
$$= \left(\frac{m}{\pi\hbar}\right)^{1/2} (\omega\omega')^{1/4} \left(\frac{2\hbar}{m(\omega+\omega')}\right)^{1/2} \sqrt{\pi} \tag{185}$$
$$= \left[\frac{4\omega\omega'}{(\omega+\omega')^2}\right]^{1/4}\,. \tag{186}$$

The probability is therefore

$$P = \left[\frac{4\omega\omega'}{(\omega+\omega')^2}\right]^{1/2} = \frac{2\sqrt{\omega\omega'}}{\omega+\omega'} = \frac{2\sqrt{2}}{3} \sim 0.943\,.$$

16 Problems: The Continuity Equation

16.1. Interpretation of the probability current:

Let $P_{ab}(t)$ be the probability to find the particle in the interval $a < x < b$.

1. Write down a definite integral for $P_{ab}(t)$.
2. Write down the continuity equation and use it to show that

$$\partial_t P_{ab}(t) = J(a,t) - J(b,t)\,.$$

3. Hence discuss the physical interpretation of $J(x,t)$.

Solution:

1. The probability to find the particle in the interval $a \le x \le b$ is

$$P_{ab}(t) = \int_a^b dx\, P(x,t) = \int_a^b dx\, |\psi(x,t)|^2\,.$$

2. We compute the derivative with respect to time and use the continuity equation

$$\partial_t P_{ab}(t) = \int_a^b dx\, \partial_t P(x,t) \tag{187}$$
$$= -\int_a^b dx\, \partial_x J(x,t)$$
$$= J(a,t) - J(b,t)\,. \tag{188}$$

3. This equation represents the conservation of probability: the rate of change of the probability to find the particle in the region $a < x < b$, is equal to the rate the probability is flowing in / out at the boundaries $x = a$ and $x = b$.

16.2. Stationary probability current:

Consider a stationary solution of Schrödinger's equation,

$$\psi(x,t) = e^{-iEt/\hbar}\phi(x)\,.$$

1. Write down an expression for the probability density $P(x,t)$ and show that it is independent of t.
2. Write down an expression for the probability current $J(x,t)$ and show that it is independent of t.
3. Using the continuity equation and part (a), show that $J(x,t)$ is also independent of x.
4. Hence explain why $J(x,t) = 0$ if $\phi(x)$ is square-normalizable.

Solution:

1. For a stationary wavefunction, the probability density is

$$P(x,t) = |\psi(x,t)|^2 = |\phi(x)|^2$$

which is independent of time.

2. For a stationary wavefunction, the probability current is

$$J(x,t) = \frac{\hbar}{2mi}(\bar{\psi}(x,t)\partial_x\psi(x,t) - \psi(x,t)\partial_x\bar{\psi}(x,t))$$
$$= \frac{\hbar}{2mi}(\bar{\phi}(x)\partial_x\phi(x) - \phi(x)\partial_x\bar{\phi}(x))\,, \tag{189}$$

which is independent of time.

3. The continuity equation is
$$\partial_t P + \partial_x J = 0\,.$$
From part (a), we find $\partial_x J = 0$ and therefore the probability current is also independent of position.
4. For a square-normalizable wavefunction, $\phi(x) \to 0$ and therefore $J \to 0$ as $|x| \to \infty$. Since J is independent of position, $J = 0$ everywhere.

16.3. Probability current in an infinite potential well:
Consider an infinite potential well $0 < x < L$.

1. By integrating the continuity equation over $0 < x < L$, explain why
$$J(0,t) - J(L,t) = 0\,.$$
2. Show that the standard boundary conditions on the wavefunction $\psi(x,t)$ at $x = 0$ and $x = L$ imply the stronger conditions
$$J(0,t) = J(L,t) = 0\,.$$
3. What is the physical interpretation of these results?

Solution:

1. From the continuity equation $\partial_t P + \partial_x J = 0$, the time-derivative of the total probability to find the particle anywhere in $0 < x < L$ is
$$\frac{d}{dt}\int_0^L P dx = \int_0^L \partial_t P dx = -\int_0^L \partial_x J dx = J(0,t) - J(L,t)\,.$$
For the conservation of the total probability we therefore require $J(0,t) = J(L,t)$ for all t.
2. The standard boundary condition for the infinite-square well is
$$\psi(0,t) = \psi(L,t) = 0\,.$$
We do not set the spatial derivative of the wavefunction to vanish at $x = 0, L$ because the potential jumps by an infinite amount there. Nevertheless, from the definition of the probability current
$$J = \frac{\hbar}{2mi}(\bar{\psi}\partial_x\psi - \psi\partial_x\bar{\psi})$$
we find
$$J(0,t) = J(L,t) = 0\,.$$
This is stronger than the condition from part (a). Intuitively, the probability to find the particle in the regions $x < 0$ and $x > L$ is zero, so there should not be any probability flowing into or our of these regions.

16.4. Time-dependence of the probability current: TUTORIAL 4
Consider the infinite potential well $0 < x < L$ with wavefunction
$$\psi(x,t) = \frac{1}{\sqrt{2}}(\phi_1(x)e^{-iE_1 t/\hbar} + \phi_2(x)e^{-iE_2 t/\hbar})\,.$$

1. Show that the probability current has the form

$$J(x,t) = C \sin^3\left(\frac{\pi x}{L}\right) \sin(\omega t)$$

where $\omega = (E_2 - E_1)/\hbar$ and $C > 0$ is a constant.
2. Show that

$$J(0,t) = J(L,t) = 0\,.$$

What is the physical interpretation of this result?
3. Sketch the probability current $J(x,t)$ at times

$$t = 0,\ \frac{\pi}{2\omega},\ \frac{\pi}{\omega},\ \frac{3\pi}{2\omega},\ \frac{2\pi}{\omega}\,.$$

4. In which direction is the probability “flowing" when

$$\text{(i)}\quad 0 < t < \frac{\pi}{\omega} \qquad\qquad \text{(ii)}\quad \frac{\pi}{\omega} < t < \frac{2\pi}{\omega}\ ?$$

5. Compare this to a sketch of the expectation value

$$\langle x \rangle = \frac{L}{2} - A\cos(\omega t)\,,$$

where $0 < A < \frac{L}{2}$. Is it consistent?

Hint 1: For part (a), you may assume the result from section 16.5 of the lecture notes.

Hint 2: For part (a), you may use the trigonometric identity

$$2\sin^3 y = \sin(2y)\cos(y) - 2\cos(2y)\sin(y)\,.$$

Solution:

1. In the section “Example: Sum of Two Stationary Wave functions”, we derived the following formula for the probability current of a sum of Hamiltonian eigenfunctions of energies E_1 and E_2,

$$J(x,t) = \frac{\hbar}{2m}\left(\phi_2 \partial_x \phi_1 - \phi_1 \partial_x \phi_2\right)\sin(\omega t)$$

where $\omega = (E_2 - E_1)/\hbar$. In the present case,

$$\phi_1 = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right) \qquad \phi_2 = \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)$$

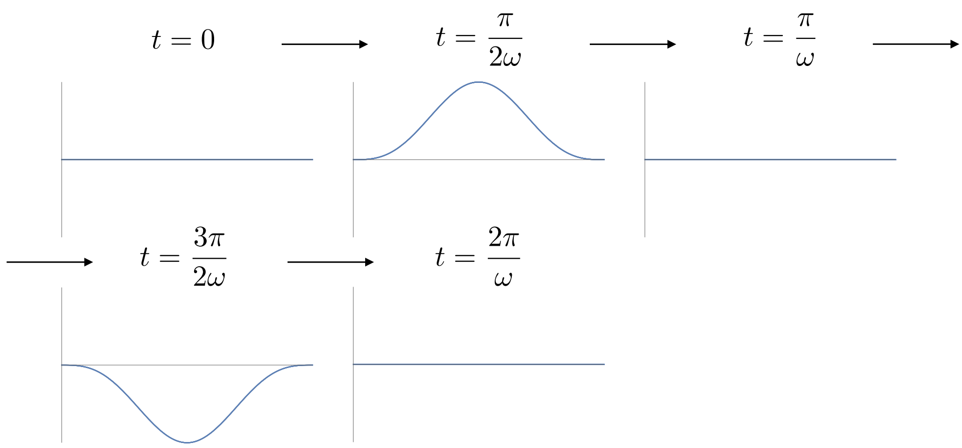
and hence

$$J(x,t) = \frac{\hbar}{2m}\left(\phi_2 \partial_x \phi_1 - \phi_1 \partial_x \phi_2\right)\sin(\omega t) \tag{190}$$

$$= \frac{\hbar\pi}{mL^2}\left(\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right) - 2\cos\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi x}{L}\right)\right)\sin(\omega t)$$

$$= \frac{2\hbar\pi}{mL^2}\sin^3\left(\frac{\pi x}{L}\right)\sin(\omega t) \tag{191}$$

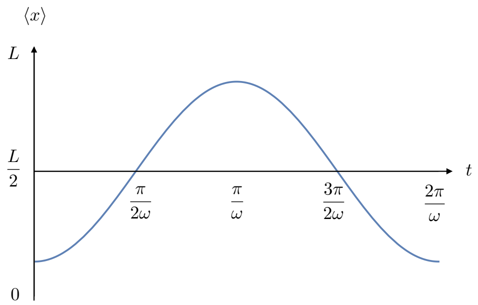
using the hint.
2. It is clear that $J(0,t) = J(L,t) = 0$ since $\sin(0) = \sin(\pi) = 0$. The physical explanation is that the wavefunction vanishes for $x < 0$ and $x > L$ so there cannot be any probability flowing into / out of these regions.
3. The sequence of sketches is



4. 1. For $0 < t < \frac{\pi}{\omega}$, $J > 0$ so the probability is flowing to the right.
   2. For $\frac{\pi}{\omega} < t < \frac{2\pi}{\omega}$, $J < 0$ so the probability is flowing to the left.
5. Let us compare this to the sketch below of the expectation value

$$\langle x \rangle = \frac{L}{2} - A\cos(\omega t)$$

where $A = 16L/9\pi^2$.



We see that whenever $J > 0$ the position expectation value is moving to the right and vice verse, as expected.

17 Problems: Scattering Problems

17.1. Scattering off a finite step potential:

Consider the potential

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

1. What are the boundary conditions on the wavefunction at $x = 0$?
2. Construct Hamiltonian eigenfunctions appropriate for incoming particles of energy $E > V_0$ sent from $x = -\infty$.
3. Compute the reflection and transmission probabilities R and T and sketch them as a function of E/V_0.
4. Check that $R + T = 1$. Explain!
5. Discuss the behaviour of R, T in the limits $E \gg V_0$ and $E \to V_0$.

Solution:

See lecture 17.

17.2. Scattering off a delta function potential:

Consider the potential well

$$V(x) = -\alpha\delta(x)$$

where $\alpha > 0$.

1. Show that a Hamiltonian eigenfunction with energy $E > 0$ obeys
$$\phi''(x) = -\frac{2m}{\hbar^2}\left(E + \alpha\delta(x)\right)\phi(x)\,.$$
2. The wavefunction $\psi(x)$ is continuous at $x = 0$. By integrating part (a) over an interval $(\epsilon, -\epsilon)$ show that the derivative of the wavefunction has a discontinuity at $x = 0$,
$$\lim_{\epsilon\to 0}\big(\phi'(\epsilon) - \phi'(-\epsilon)\big) = -\frac{2m\alpha}{\hbar^2}\phi(0)\,.$$
3. Find the constant k in terms of m, $\hbar$, E such that
$$\phi(x) = \begin{cases} e^{ikx} + re^{-ikx} & \text{if} \quad x < 0 \\ te^{ikx} & \text{if} \quad x > 0 \end{cases}$$
is a Hamiltonian eigenfunction with $E > 0$ for $x \neq 0$. What is the physical interpretation of the three terms?
4. Impose the boundary conditions from part (a) and show that
$$R = |r|^2 = \frac{1}{1 + 2\hbar^2 E/m\alpha^2} \qquad T = |t|^2 = \frac{2\hbar^2 E/m\alpha^2}{1 + 2\hbar^2 E/m\alpha^2}\,.$$
What is the physical interpretation of R, T and why does $R + T = 1$?
5. Sketch R, T as a function of energy $E > 0$ and explain intuitively their behaviour as $E \to \infty$.

Solution:

1. A Hamiltonian eigenfunction in the potential $V(x) = -\alpha\delta(x)$ obeys
$$-\frac{\hbar^2}{2m}\phi''(x) - \alpha\delta(x)\phi(x) = E\phi(x)\,.$$
Rearranging this equation,
$$\phi''(x) = -\frac{2m}{\hbar^2}\left(E + \alpha\delta(x)\right)\phi(x)\,.$$
2. Integrating this equation over an interval $(\epsilon, -\epsilon)$,
$$\int_{-\epsilon}^{\epsilon}\phi''(x)dx = -\frac{2m}{\hbar^2}\int_{-\epsilon}^{\epsilon}(E + \alpha\delta(x))\phi(x)\,.$$
Using the fundamental theorem of calculus and the defining property of the delta-function $\delta(x)$, we find
$$\phi'(\epsilon) - \phi'(-\epsilon) = -\frac{2m\alpha}{\hbar^2}\phi(0) - \frac{2mE}{\hbar^2}\int_{-\epsilon}^{\epsilon}\phi(x)dx\,.$$

In the limit $\epsilon \to 0$ the second term on the right tends to zero, leaving

$$\lim_{\epsilon \to 0} (\phi'(\epsilon) - \phi'(-\epsilon)) = -\frac{2m\alpha}{\hbar^2}\phi(0) .$$

3. A by now standard computation shows that $k = \sqrt{2mE/\hbar^2}$. The components e^{ikx}, re^{-ikx}, te^{ikx} correspond to the incident, reflected and transmitted waves.
4. Imposing the boundary conditions from part (b), we find

$$1 + r = t \qquad ik(1-r) - ikt = \frac{2m\alpha}{\hbar^2}t .$$

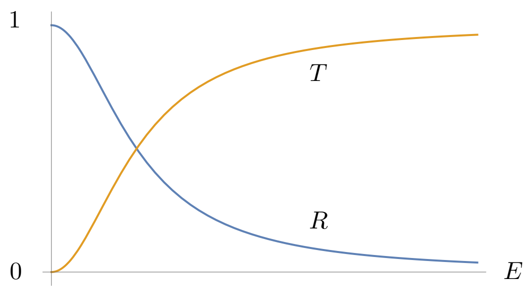
The solution for r, t is

$$r = -\frac{im\alpha}{\hbar^2 k + im\alpha} \qquad t = -\frac{\hbar^2 k}{\hbar^2 k + im\alpha} .$$

We therefore find

$$\begin{aligned} |r|^2 &= \frac{m^2\alpha^2}{k^2\hbar^4 + m^2\alpha^2} = \frac{1}{1 + 2\hbar^2 E/m\alpha^2} \\ |t|^2 &= \frac{k^2\hbar^4}{k^2\hbar^4 + m^2\alpha^2} = \frac{2\hbar^2 E/m\alpha^2}{1 + 2\hbar^2 E/m\alpha^2} . \end{aligned} \tag{192}$$

The quantities $R = |r|^2$, $T = |t|^2$ are the probabilities for a particle with energy E to be reflected transmitted. The relation $R+T = 1$ ensures that probabilities sum to 1.
5. The solutions look like the following.



As $E \to \infty$, $R \to 0$ and $T \to 1$. As the energy of the particle increases so does the probability of transmission.

17.3. Critical scattering off a potential barrier:
Consider the potential barrier with $V_0 > 0$,

$$V(x) = \begin{cases} 0 & x \leq 0 \\ V_0 & 0 < x < L \\ 0 & x \geq L \end{cases} . \tag{193}$$

1. Show that the wavefunction

$$\phi(x) = \begin{cases} e^{ikx} + re^{-ikx} & x < 0 \\ A + Bx & 0 < x < L \\ te^{ikx} & x > L \end{cases} \tag{194}$$

is a Hamiltonian eigenfunction with energy $E = V_0$ where

$$k = \sqrt{2mV_0/\hbar^2}\,.$$

2. What are the boundary conditions at $x = 0$ and $x = L$?
3. Imposing the boundary conditions, eliminate A, B and show that

$$|r|^2 = \frac{k^2L^2}{k^2L^2+4} \qquad |t|^2 = \frac{4}{k^2L^2+4}\,.$$

4. Show that $|r|^2 + |t|^2 = 1$ and discuss the physical significance of $|r|^2, |t|^2$.
5. Sketch $|r|^2$, $|t|^2$ as a function of the dimensionless ratio $\gamma = kL$ and explain the behaviour as $\gamma \to 0$ and $\gamma \to \infty$.

Solution:

1. For $x < 0$ and $x < L$ the Hamiltonian operator is $\hat{H} = \frac{\hat{p}^2}{2m}$ and therefore

$$\hat{H}\cdot e^{\pm ikx} = -\frac{\hbar^2}{2m}\partial_x^2 e^{\pm ikx} = \frac{\hbar^2k^2}{2m}e^{\pm ikx} = V_0 e^{\pm ikx}\,,$$

since $k = \sqrt{2mV_0/\hbar^2}$. For $0 \le x \le L$ the Hamiltonian operator is $\hat{H} = \frac{\hat{p}^2}{2m} + V_0$ and therefore

$$\hat{H}\cdot(A+Bx) = V_0(A+Bx)\,.$$

In all regions we therefore have Hamiltonian eigenfunctions with energy $E = V_0$.

2. Since the potential has a finite discontinuities at $x = 0$ and $x = L$, we require that the wavefunction $\psi(x)$ and its first derivative $\psi'(x)$ are continuous at $x = 0$ and $x = L$.
3. The boundary condition at $x = 0$ is

$$1 + r = A \qquad ik(1-r) = B\,.$$

The boundary condition at $x = L$ is

$$A + BL = te^{ikL} \qquad B = ikte^{iKL}\,.$$

There are four linear equations for four unkowns r, A, B, t. Eliminating A an B, the solution for r and t is

$$r = \frac{kL}{kL+2i} \qquad t = \frac{2ie^{-ikL}}{kL+2i}$$

and therefore

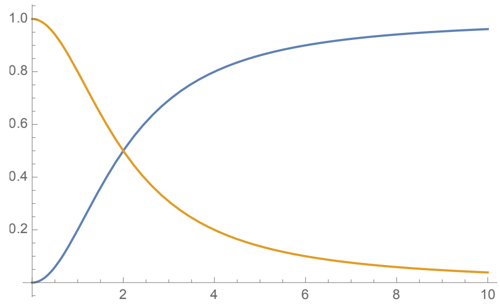
$$|r|^2 = \frac{k^2L^2}{k^2L^2+4} \qquad |t|^2 = \frac{4}{k^2L^2+4}\,.$$

4. It is clear that $|r|^2 + |t|^2 = 1$. The wavefunction describes the reflection and transmission of particles incoming from the left with definite energy $E = V_0$. The quantities $|r|^2$, $|t|^2$ are probabilities for an incoming particle to be reflected, transmitted. The relation $|r|^2 + |t|^2 = 1$ is the statement that the total probability is 1.

5. In terms of the dimensionless ration $\gamma = kL$,

$$|r|^2 = \frac{\gamma^2}{\gamma^2+4} \qquad |t|^2 = \frac{4}{\gamma^2+4}\,.$$

The sketch should shown $|r|^2$ starting at 0 when $\gamma = 0$, increasing monotonically for $0 < \gamma < \infty$, and asymptote to 1 as $\gamma \to \infty$.



1. The limit $\gamma \to 0$ corresponds to $L << \frac{1}{k}$, where $|r|^2 \to 0$, $|t|^2 \to 1$: tunnelling is inevitable. If the barrier length is much less than the incoming wavelength ($\propto \frac{1}{k}$), the particle does not resolve the barrier and so the probability of transmission is high.
2. The limit $\gamma \to \infty$ corresponds to $L >> \frac{1}{k}$, where $|r|^2 \to 1$ and $|t|^2 \to 0$: reflection is inevitable. If the barrier length is much greater than the incoming wavelength ($\propto \frac{1}{k}$), the probability density decays to near zero inside the barrier and the probability of transmission is high.

17.4. Scattering off a finite potential barrier:

Consider particles with definite energy $E > V_0 > 0$ incoming from the left on the potential barrier

$$V(x) = \begin{cases} V_0 & \text{if} \quad 0 < x < L \\ 0 & \text{otherwise} \end{cases}.$$

1. Write down appropriate Hamiltonian eigenfunctions in the regions $x < 0$, $0 < x < L$, and $x > L$.
2. Impose the boundary conditions at $x = 0$ and $x = L$ and hence compute the transmission and reflection coefficients R, T.
3. Verify that $R + T = 1$.
4. How do R, T behave when $E \to V_0^+$ and $E \to \infty$? Explain!
5. What happens to R, T when

$$E = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

for $n \in \mathbb{Z}_{>0}$ such that $E > V_0$? Why is this happening?

6. Sketch R, T as a function of energy.

Hint (b): after imposing boundary conditions, you should find four linear equations for four unknowns. At this stage you may use a computer to do the linear algebra.

Solution:

1. The hamiltonian eigenfunctions appropriate for the scattering of particles in-

coming from $x = -\infty$ with energy E are

$$\phi(x) = \begin{cases} e^{ik'x} + re^{-ik'x} & x < 0 \\ Ae^{ikx} + Be^{-ikx} & 0 < x < L \\ te^{ik'x} & x > L \end{cases},$$

where

$$k' = \sqrt{2mE/\hbar^2} \tag{195}$$
$$k = \sqrt{2m(E - V_0)/\hbar^2}$$

and r, t, A, B are constant we need to determine. For scattering problems, the wavefunctions are not normalizable and so the overall constant is not physically meaningful. We have used this freedom to set the coefficient of the incoming wave to 1.

2. We now impose $\phi(x)$ and $\partial_x \phi(x)$ are continuous at $x = 0$ and $x = L$. The boundary conditions at $x = 0$ give

$$1 + r = A + B \tag{196}$$
$$k'(1 - r) = k(A - B)$$

while those at $x = L$ give

$$Ae^{ikL} + Be^{-ikL} = te^{ik'L} \tag{197}$$
$$k(Ae^{ikL} - Be^{-ikL}) = k'te^{ik'L}.$$

This gives four linear equations for the four unknowns r, t, A, B. These are just simultaneous linear equations and the solution can of course be found by hand with some patience. Instead, you can use a computer. In any case, the solution for r and t is

$$r = \frac{(k'^2 - k^2)\sin(kL)}{(k'^2 + k^2)\sin(kL) + 2ik'k\cos(kL)} \tag{198}$$
$$t = \frac{2ik'ke^{-ik'L}}{(k'^2 + k^2)\sin(kL) + 2ik'k\cos(kL)}.$$

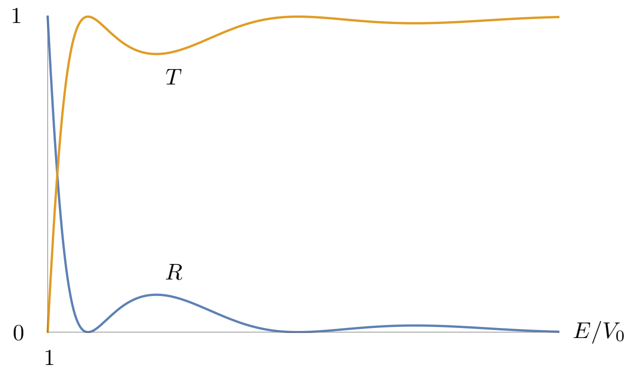
The reflection and transmission probabilities are

$$R = |r|^2 = \frac{\left(k'^2 - k^2\right)^2 \sin^2(kL)}{\left(k'^2 + k^2\right)^2 \sin^2(kL) + 4k'^2k^2\cos^2(kL)} \tag{199}$$
$$T = |t|^2 = \frac{4k'^2k^2}{\left(k'^2 + k^2\right)^2 \sin^2(kL) + 4k'^2k^2\cos^2(kL)}.$$

It is straightforward to see that $R + T = 1$ using $\sin^2 z + \cos^2 z = 1$.

3. 1. The limit $E \to V_0$ corresponds to $k' \to 0$. In this limit we find $R \to 1$ and $T \to 0$. We recover the classical expectation for $E \leq V_0$.
   2. The limit $E \to \infty$ corresponds to $k, k' \to \infty$ with $k/k' = 1$. We find $R \to 0$ and $T \to 1$. The potential well has effectively vanishes and the particle is transmitted with probability 1. We recover the classical expectation for $E > V_0$.

4. This corresponds to $kL = n\pi$ with $n \in \mathbb{Z}_{>0}$. At these points $R = 0$ and $T = 1$. They correspond to 'transmission resonances' where the particle is transmitted with probability 1. Roughly, at these points there is destructive interference between the waves reflected from the boundaries at $x = 0$ and $x = L$.
5. The reflection / transmission coefficients looks like:



18 Problems: Tunnelling

18.1. Tunneling through a finite step potential:

Consider the same problem but with $E < V_0$.

1. How do the hamiltonian eigenfunctions change in the region $x > 0$?
2. Explain why the probability current J vanishes for $x > 0$.
3. Show that $R = 1$ and $T = 0$.
4. Sketch the probability density in the region $x > 0$.

18.2. Bound States in a Finite Potential Well:

(This problem is similar to problem 9 of the May 2019 exam and provided here to illustrate the method required to solve it. This problem was not part of the 2020-2021 module). Consider the finite potential well

$$V(x) = \begin{cases} V_0 & x \le 0 \\ 0 & 0 < x < L \\ V_0 & x \ge L \end{cases} .$$

Consider the following ansatz for "bound state" wavefunctions,

$$\phi(x) = \begin{cases} Ae^{\kappa x} & x < 0 \\ B \sin kx + C\cos(kx) & 0 < x < L \\ De^{-\kappa x} & x > L\,. \end{cases}$$

1. Find constants κ, k in terms of E, V_0 such that this is a Hamiltonian eigenfunction with energy $0 < E < V_0$.
2. Explain why there are no terms in the ansatz proportional to $e^{-\kappa x}$ for $x < 0$ and $e^{\kappa x}$ for $x > L$.
3. What boundary conditions do the wavefunction obey at $x = 0$ and $x = L$?
4. Impose the boundary conditions and eliminate A, B, C, D to obtain the "quantisation condition"
$$\frac{\kappa}{k} = \frac{\tan kL - \frac{\kappa}{k}}{1 + \frac{\kappa}{k}\tan kL}\,.$$
5. Illustrate solutions of the quantisation condition *graphically* and show that
    1. There is at least one solution independent of L and V_0.
    2. Show that you reproduce the spectrum of the infinite potential well in the limit $V_0 \to \infty$.

Solution:

1. The Hamiltonian operator for $x < 0$ and $x > 0$ is
$$\hat{H} = -\frac{\hbar^2}{2m}\partial_x^2 + V_0$$
so the ansatz is a Hamiltonian eigenfunction with energy $0 < E < V_0$ provided $\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$. The Hamiltonian operator for $0 < x < L$ is
$$\hat{H} = -\frac{\hbar^2}{2m}\partial_x^2$$
and the ansatz is a Hamiltonian eigenfunction with energy $0 < E < V_0$ provided $k = \sqrt{2mE/\hbar^2}$.
2. These solutions diverge as $x \to -\infty$ and $x \to \infty$ respectively and are therefore not square-normalisable.

3. Since the potential remains finite both the wavefunction $\phi(x)$ and its derivative $\phi'(x)$ are continuous at $x = 0$ and $x = L$.

   Although not asked for in the question, we can show this as follows. First, continuity of $\phi(x)$ is required for a probabilistic interpretation. Second, consider the equation obeyed by a Hamiltonian eigenfunction
$$\phi''(x) = \frac{2m}{\hbar^2}(V(x) - E)\phi(x)\,.$$
   We now integrate this over a small interval $-\epsilon < x < \epsilon$ around the discontinuity in the potential at $x = 0$ to find
$$\phi'(x)|_\epsilon - \phi'(x)|_{-\epsilon} = \frac{2m}{\hbar^2}\int_{-\epsilon}^{\epsilon}(V(x) - E)\phi(x)dx\,,$$
   where we assume $\phi'(x)$ is continuous away from the discontinuity. Provided $V(x)$ remains finite in $-\epsilon < x < \epsilon$, the integral on right vanishes in the limit $\epsilon \to 0$. We conclude that $\psi'(x)$ also remains continuous across $x = 0$. The argument is identical at $x = L$.

4. We now impose the boundary conditions at $x = 0$ and $x = L$. First, from the requirement that the wavefunction and its derivative are continuous across $x = 0$, we have

$$A = C \qquad \kappa A = kB\,.$$

We can immediately eliminate A, leaving $\kappa C = kB$. Second, from the requirement that the wavefunction and its derivative are continuous across $x = 0$, we have

$$A' e^{-\kappa L} = B \sin kL + C \cos kL \tag{200}$$

$$= C\left(\frac{\kappa}{k} \sin kL + \cos kL\right) \tag{201}$$

$$-\kappa A' e^{-\kappa L} = k(B \cos kL - C \sin kL) \tag{202}$$

$$= \kappa C\left(\cos kL - \frac{k}{\kappa} \sin kL\right) \tag{203}$$

where we have eliminated B using $\kappa C = kB$. Dividing these equations, we can eliminate the remaining constants A' and C to find

$$\frac{\kappa}{k} = \frac{\sin kL - \frac{\kappa}{k} \cos kL}{\cos kL + \frac{\kappa}{k} \sin kL} \tag{204}$$

$$= \frac{\tan kL - \frac{\kappa}{k}}{1 + \frac{\kappa}{k} \tan kL}\,. \tag{205}$$

5. We first rearrange to find a quadratic equation for the ratio κ/k,

$$\tan kL \left(\frac{\kappa}{k}\right)^2 + 2\left(\frac{\kappa}{k}\right) - \tan kL = 0\,.$$

whose solution is

$$\frac{\kappa}{k} = \frac{1}{\tan kL}\left(-1 \pm \sqrt{1 + \tan^2 kL}\right) = \begin{cases} +\tan\left(\frac{kL}{2}\right) \\ -\cot\left(\frac{kL}{2}\right) \end{cases}$$

Since κ, k can be expressed in terms of E, this is a constraint or "quantisation condition" on the possible eigenvalues E. It is impossible to solve analytically. However, we can understand the solutions graphically. For this purpose, it is convenient to introduce the dimensionless variables

$$z = \frac{L}{2}\sqrt{\frac{2mE}{\hbar^2}} \qquad z_0 = \frac{L}{2}\sqrt{\frac{2mV_0}{\hbar^2}}\,.$$

The quantisation condition then becomes

$$\sqrt{z_0^2/z^2 - 1} = \begin{cases} +\tan z \\ -\cot z \end{cases} \quad .$$

We can now understand the solutions by plotting both sides of this equation on the same graph and looking for their intersection points.

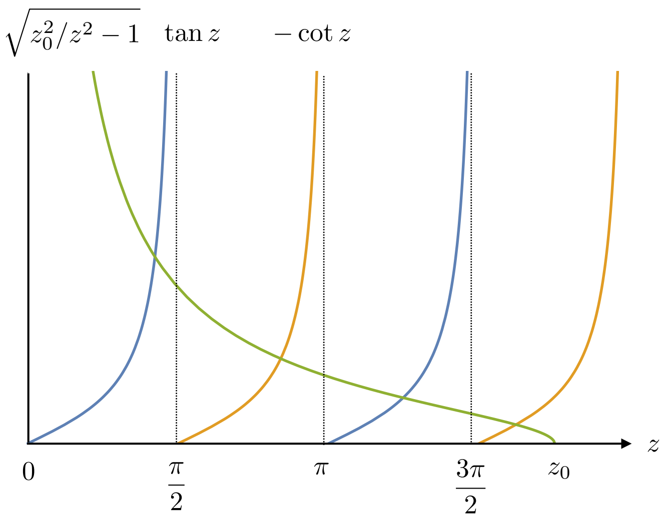


Figure 9: Graphical method to solve the non-linear equation which determines the energy spectrum.

1. There is a discrete number of solutions, which increases with the dimensionless parameter z_0. It is clear graphically that there is always at least one intersection point for $0 < z_0 < \infty$.
2. The limit $V_0 \to \infty$ corresponds to $z_0 \to \infty$. In this limit, there are an infinite number of intersection points that move closer to the asymptotes $z = \frac{n\pi}{2}$ for $n \in \mathbb{Z}_{>0}$. From the definition of z, the intersection points in this limit correspond to energies

$$E = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2,$$

which are those of an infinite square well.

19 Problems: Momentum-space Wave function

19.1. Gaussian in momentum space:

Consider the normalized Gaussian wave function

$$\psi(x) = \frac{1}{(2\pi\Delta^2)^{1/4}} e^{-x^2/4\Delta^2} e^{ip_0x/\hbar}$$

1. Compute the momentum expectation values $\langle p\rangle$, $\langle p^2\rangle$ and uncertainty Δp using the momentum operator $\hat{p} = -i\hbar\partial_x$.
2. Show that the momentum space wave function has the form

$$\widetilde{\psi}(p) = \frac{1}{(2\pi\widetilde{\Delta}^2)^{1/4}} e^{-(p-p_0)^2/4\widetilde{\Delta}^2}$$

up to a constant phase factor and determine $\widetilde{\Delta}$.

3. Repeat part (a) using the momentum probability density.

19.2. Momentum-space wavefunction for a particle in a box:

A particle confined to the region $-a < x < a$ has wave function

$$\psi(x) = \begin{cases} C\sin\left(\frac{\pi x}{a}\right) & \text{if } -a < x < a \\ 0 & \text{otherwise} \end{cases} .$$

1. Find the normalisation C.
2. Using the momentum operator $\hat{p} = -i\hbar\partial_x$ show that $\langle p \rangle = 0$.
3. Show that the momentum space wave function is

$$\widetilde{\psi}(p) = i\sqrt{\frac{2\pi\hbar^3}{a^3}}\,\frac{\sin(pa/\hbar)}{p^2 - (\hbar\pi/a)^2} .$$

4. Sketch the momentum probability density $|\widetilde{\psi}(p)|^2$ and hence explain why
   1. $\langle p \rangle = 0$, compatible with part (b).
   2. The mostly likely outcomes of a momentum measurement are
   $$p = \pm\frac{\pi\hbar}{a} .$$

Hints:

(c) Integrate by parts twice or convert the sine to complex exponentials.

(d) If you are having difficulty with the sketch, try Wolfram Alpha!

Solution:

1. To determine the normalisation,

$$\begin{aligned} 1 &= |C|^2 \int_{-a}^{a} \sin^2\left(\frac{\pi x}{a}\right) dx \\ &= \frac{|C|^2}{2}\int_{-a}^{a}\left(1 - \cos\left(\frac{2\pi x}{a}\right)\right) dx && (206) \\ &= |C|^2 a , && (207) \end{aligned}$$

so we can choose $C = 1/\sqrt{a}$.

2. The momentum expectation value is

$$\begin{aligned} \langle p \rangle &= -i\hbar \int_{-\infty}^{\infty} \overline{\psi(x)}\partial_x\psi(x) \\ &= -i\hbar\frac{\pi}{a^2}\int_{-a}^{a} \sin\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi x}{a}\right) && (208) \\ &= 0 && (209) \end{aligned}$$

because the integrand is odd. Alternatively, the wave function is normalised and real, which implies that $\langle p \rangle = 0$ by problem 1.3.

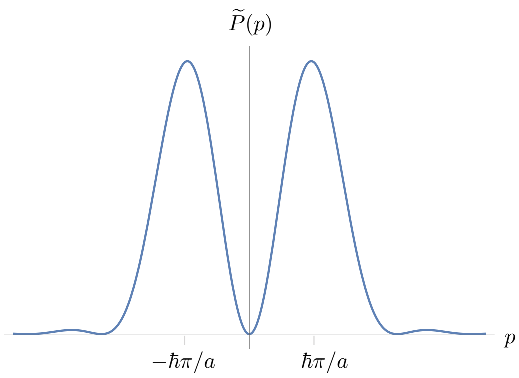
3. The momentum space wave function is

$$
\begin{aligned}
\widetilde{\psi}(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) dx \\
&= \frac{1}{\sqrt{2\pi\hbar a}} \int_{-a}^{a} e^{-ipx/\hbar} \sin\left(\frac{\pi x}{a}\right) && (210) \\
&= \frac{1}{\sqrt{2\pi\hbar a}} \frac{1}{2i} \int_{-a}^{a} \left(e^{-i(p/\hbar-\pi/a)x} - e^{-i(p/\hbar+\pi/a)x}\right) && (211) \\
&= \frac{1}{\sqrt{2\pi\hbar a}} \frac{1}{2} \left(\frac{e^{ipa/\hbar} - e^{-ipa/\hbar}}{p/\hbar - \pi/a} - \frac{e^{ipa/\hbar} - e^{-ipa/\hbar}}{p/\hbar + \pi/a}\right) && (212) \\
&= i\sqrt{\frac{2\pi\hbar^3}{a^3}} \frac{\sin(pa/\hbar)}{p^2 - (\hbar\pi/a)^2} \,. && (213)
\end{aligned}
$$

You may also integrate by parts twice to find the same result!

4. The probability density is

$$
\widetilde{P}(p) = \frac{2\pi\hbar^3}{a^3} \left(\frac{\sin(pa/\hbar)}{p^2 - (\hbar\pi/a)^2}\right)^2 \,.
$$



1. The momentum probability density is an even function so $\langle p \rangle = 0$.
2. The momentum probability density has global maxima at $p = \pm\hbar\pi/a$.