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.

PROBLEMS CLASS 1

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

$$\int_{\text{orbit}} p\text{dx} = nh\,, \quad n \in \mathbb{Z}\,, \tag{2}$$

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

2 Problems: The Double Slit Experiment

2.1. Approximations:

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

$$I(x) = 4C^2 \cos^2\left(\frac{k}{2}(r_1 - r_2)\right) \,. \tag{3}$$

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?

PROBLEMS CLASS 1

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.

Consider first a single slit of width b as in the figure below, centered on the x-axis. You can view this as a superposition of a continuum of sources, so that the wave is given by

$$\psi(x,t) = C \int_{s=-b/2}^{b/2} e^{ikr(x,s) - i\omega t} \text{d}s \,. \tag{4}$$

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

$$|\psi(x,t)|^2 = \tilde{C}^2 \frac{\sin^2 \beta}{\beta^2}\,, \quad \beta = \frac{bkx}{2L}\,. \tag{5}$$

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

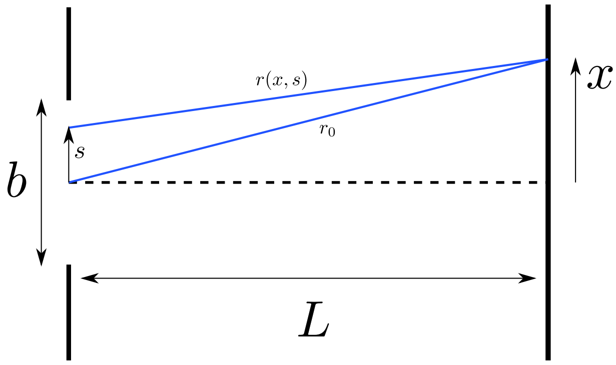

Figure 1: Finite-width single slit experiment, with a slit of width b.

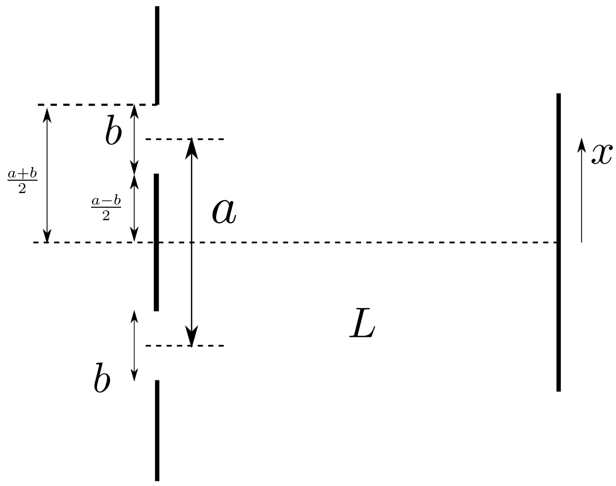

Figure 2: Finite-width double slit experiment, with slits of width b with their midpoints separated by a distance a.

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 (4) over $(a-b)/2$ to $(a+b)/2$, and then add the contribution from the second slit. 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.

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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

$$\psi(x) = \begin{cases} C\,\dfrac{x}{a} & 0 \le x \le a \\ C\,\dfrac{b-x}{b-a} & a < x \le b \\ 0 & \text{otherwise} \end{cases} \tag{6}$$

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 $x < a$?

3.2. More practice with wave functions:
Consider the wave function

$$\psi(x,t) = Ce^{-\lambda|x|}e^{-i\omega t} \tag{7}$$

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?

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

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

3.4. Another wave packet:
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,

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

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

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

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 $e^{ixp_0/\hbar}$?

4.3. Non-normalisable wave functions: TUTORIAL 1

Consider the wave function

$$\psi_1(x) = Ce^{ikx}\,, \tag{8}$$

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

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \mathrm{d}x \tag{9}$$

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 $\langle p^2\rangle$.

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?

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.

5.2. Heat equation: TUTORIAL 1

Consider the Schrödinger equation with, for simplicity, $\hbar = 1$ and $m = 1$, and vanishing potential,

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial\psi}{\partial x^2}\,. \tag{10}$$

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

$$\psi(x,\tilde{t}) = \frac{1}{\sqrt{2\pi\tilde{t}}}\exp\Big(-\frac{x^2}{2\tilde{t}}\Big)\,, \tag{11}$$

   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 $|\psi(x,t|^2$.

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 $\psi(x) = 0$ PROBLEMS CLASS 2

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

6.2. Inconsistent?:

Consider the canonical commutation relation

$$[\hat{x}, \hat{p}] = i\hbar \,. \tag{12}$$

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,

$$\mathrm{Tr}\Big([\hat{x}, \hat{p}]\Big) = \mathrm{Tr}\Big(i\hbar\Big) \,. \tag{13}$$

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?

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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. $(A_1 A_2)^\dagger = A_2^\dagger A_1^\dagger$
4. $(A^n)^\dagger = (A^\dagger)^n$ for any $n \in \mathbb{N}$
5. If $f(x)$ is a real analytic function of $x \in \mathbb{R}$, $f(A)^\dagger = f(A^\dagger)$.

7.2. Properties of Hermitian operators:

Hermitian operators satisfy various properties which will be important in later chapters: **TUTORIAL 2**

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. **TUTORIAL 2**

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 $n > 0$.

7.3. Eigenfunctions have zero uncertainty:
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?

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?

TUTORIAL 2

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

$$\frac{\mathrm{d}\theta(x)}{\mathrm{d}x} = \delta(x)\,, \tag{14}$$

Also prove

$$\delta\big(f(x)\big) = \sum_{x_0 \text{ s.t. } f(x_0)=0} \frac{\delta(x - x_0)}{\left|\frac{\mathrm{d}f(x)}{\mathrm{d}x}\right|}\,. \tag{15}$$

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

$$\int_{-\infty}^{\infty} \delta(x^2 - 4) g(x) \mathrm{d}x\,, \tag{16}$$

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

TUTORIAL 2

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.

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

$$\psi(t=0,x) = C\left(\frac{1}{\sqrt{2}}\psi_{E=1}(x) + e^{i\alpha}\psi_{E=2}(x)\right)\,, \tag{17}$$

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?

10 Problems: Commutators and Uncertainty Principle

10.1. Generalised uncertainty principle:
Derive the generalised uncertainty principle,

$$(\Delta A)^2\,(\Delta B)^2 \geq \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2\,, \tag{18}$$

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

$$\Delta x\,\Delta E \geq \frac{\hbar}{2m}\big|\langle p\rangle\big|\,. \tag{19}$$

10.3. Time-energy uncertainty relation (sort of):
For an operator $\hat{Q}$ which does not depend on time explicitly, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{Q}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle\,. \tag{20}$$

TUTORIAL 3

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

$$\Delta Q \approx \left|\frac{\mathrm{d}\langle\hat{Q}\rangle}{\mathrm{d}t}\right|\Delta t\,. \tag{21}$$

What is the meaning of Δt here? Use (21) to derive the "time-energy uncertainty relation" $\Delta H\,\Delta t \geq \hbar/2$. What does this 'uncertainty relation' express?

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

$$V(x) = -\alpha\,\delta(x)\,, \tag{22}$$

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).

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.

TUTORIAL 3

12.2. Time evolution on a circle:

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

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

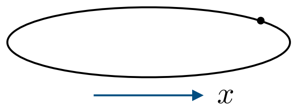

Figure 3: A particle on a circle.

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.

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

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* $n \in \mathbb{Z}_{>0}$.

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.

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

$$\begin{aligned}\psi(x, t + \mathrm{d}t) &= \psi(x, t - \mathrm{d}t) \\ &\quad + i\mathrm{d}t\Big[\psi(x - \mathrm{d}x, t) + \psi(x + \mathrm{d}x, t) - 2\big(1 + V(x)\big)\psi(x, t)\Big] . \end{aligned} \tag{23}$$

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

$$\Delta(t) = \Delta\sqrt{1 + \frac{\hbar^2 t^2}{4m^2\Delta^4}} , \tag{24}$$

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,

$$\psi(x_1, x_2) = \sqrt{\frac{18}{5}}\frac{1}{L}\left[\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{3\pi x_2}{L}\right) + \frac{1}{3}\sin\left(\frac{3\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right)\right] . \tag{25}$$

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

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

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

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 $t > 0$.

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 $\langle\psi_1, a^\dagger\psi_2\rangle = \langle a\psi_1, \psi_2\rangle$.

15.4. Properties of Hamiltonian eigenfunctions:

TUTORIAL 4

The ladder operators are defined by

$$a = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} + i\hat{p}) \qquad (26)$$
$$a^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} - i\hat{p}) .$$

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.

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 $t = 0$?

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 $J(x,t)$.

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.

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?

16.4. Time-dependence of the probability current: TUTORIAL 4

Consider the infinite potential well $0 < x < L$ with wavefunction

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

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

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

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 $E \to V_0$.

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 $x = 0$,
$$\lim_{\epsilon \to 0}\left(\phi'(\epsilon) - \phi'(-\epsilon)\right) = -\frac{2m\alpha}{\hbar^2}\phi(0) .$$
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 $E \to \infty$.

17.3. Critical scattering off a potential barrier:

Consider the potential barrier with $V_0 > 0$,

$$V(x) = \begin{cases} 0 & x \leq 0 \\ V_0 & 0 < x < L \\ 0 & x \geq L \end{cases} . \tag{27}$$

1. Show that the wavefunction

$$\phi(x) = \begin{cases} e^{ikx} + re^{-ikx} & x < 0 \\ A + Bx & 0 < x < L \\ te^{ikx} & x > L \end{cases} \tag{28}$$

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 $\gamma \to \infty$.

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.

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

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

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 $V_0 \to \infty$.

19 Problems: Momentum-space Wave function

19.1. Gaussian in momentum space:
Consider the normalized Gaussian wave function

$$\psi(x) = \frac{1}{(2\pi\Delta^2)^{1/4}} e^{-x^2/4\Delta^2} e^{ip_0 x/\hbar}$$

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!