# PH20013/60 – Quantum and Atomic Physics – 2022-23
# Problem Sheet 1

## Wavefunctions, probability densities, and normalisation

1. A particle is constrained to move along the $x$-axis and has a time-independent wavefunction

$$\psi(x) = \begin{cases} Cx(2-x) & 0 \leq x \leq 2 \\ 0 & \text{otherwise} \end{cases}$$

where C is a constant.

   (a) Normalise the wavefunction $\psi(x)$.

   (b) Sketch the wavefunction and its associated probability density $|\psi(x)|^2$.

   (c) Calculate the probability of finding the particle between $x = 0.95$ and $x = 1.05$.

   (d) Find $\langle x \rangle$, the expectation value of the particle's position.

2. A particle of mass $m$ has a time-independent wavefunction given by

$$\psi(x) = A\mathrm{e}^{-\frac{|x|}{a}},$$

where $A$ and $a$ are constants.

   (a) Sketch the wavefunction $\psi(x)$ and find the normalisation constant $A$.

   (b) Calculate the probability of finding the particle in the region $-a \leq x \leq a$.

3. Prove that the probability density $P(x,t) = \psi^*(x,t)\psi(x,t)$ associated with a general wavefunction $\psi(x,t)$ is always real and non-negative.

## The Schrödinger equation

4. After separation of variables in the time-dependent Schrödinger equation, the time-dependent part becomes

$$\frac{i\hbar}{\phi(t)}\frac{\mathrm{d}\phi(t)}{\mathrm{d}t} = E.$$

Solve this first-order differential equation to find the time-dependent part of the solution to the Schrödinger equation.

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5. If $\psi$ is a solution of the time-independent Schrödinger equation with energy $E$, show that $\tilde{\psi} = A\psi$ is also a solution with the same energy. What does this imply about the relationship between normalising a wavefunction and its energy?

6. $\psi_1(x)$ and $\psi_2(x)$ are stationary-state solutions of the one-dimensional time-independent Schrödinger equation with energy $E_1$ and $E_2$ respectively.

   (a) Show that $\psi(x) = A\psi_1 + B\psi_2$ is a solution to the time-independent Schrödinger equation only if $E_1 = E_2$.

   (b) If $E_1 = E_2$ the two eigenfunctions $\psi_1$ and $\psi_2$ have the same energy. Given that we are solving the Schrödinger equation in one spatial dimension only with no other degrees of freedom, what relationship does this imply between $\psi_1$ and $\psi_2$?

   (c) Assuming $E_1 \neq E_2$, show that $\Psi(x,t) = A\psi_1 \mathrm{e}^{-\frac{iE_1 t}{\hbar}} + B\psi_2 \mathrm{e}^{-\frac{iE_2 t}{\hbar}}$ is a solution to the time-dependent Schrödinger equation.

## The infinite potential well

7. A particle of mass $m$ is confined to the region $0 \leq x \leq a$ by a time-independent potential $V(x)$. Within this region the potential energy of the particle is zero.

   (a) Write down the time-independent Schrödinger equation for the region between $x = 0$ and $x = a$.

   (b) Show that the allowed energy levels and normalised eigenfunctions of the particle form a discrete set given by

   $$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}, \qquad \psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a},$$

   where $n = 1, 2, 3, \ldots$

   (c) What is the de Broglie wavelength of the particle in the $n^{\text{th}}$ energy level?

   (d) Sketch the eigenfunctions and probability densities of the ground and first excited states.

   (e) Calculate the probability of finding the particle between $0.45a$ and $0.55a$ in each case.

   (f) Show that as $n \to \infty$ the probability of finding the particle between these two points approaches 0.1. How does this compare with the value for a classical particle?

8. An electron is strictly confined to a one-dimensional region in which its ground-state energy is 2 eV.

   (a) What is the width of the region?

   (b) How much energy is required to promote the electron to its first excited state?

9. An electron with an energy of approximately 6 eV moves between rigid walls exactly 1 nm apart.

   (a) Find the quantum number of the energy state that the electron occupies.

   (b) Find the exact value of the electron's energy.

10. By making an appropriate change of variable in equation (4.20) from the lecture notes, show mathematically that the eigenfunctions of the infinite square well have definite parity.

11. (a) Find the energy of the ground state and first two excited states of a proton in a one-dimensional box of length 0.2 nm (roughly the diameter of an $H_2$ molecule).

    (b) Calculate the wavelength of electromagnetic radiation emitted when the proton makes a transition from

       (i) $n = 2$ to $n = 1$;

       (ii) $n = 3$ to $n = 1$;

       (iii) $n = 3$ to $n = 2$.

12. For an electron in a one-dimensional infinite square well:

    (a) Show that two eigenfunctions with different quantum numbers and opposite parity are orthogonal;

    (b) Show that two eigenfunctions with different quantum numbers and the same parity are orthogonal.

13. During the lectures we wrote down an equally-weighted superposition state of the ground state and first excited state eigenfunctions of the infinite square well:

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\psi_1(x)\mathrm{e}^{-\frac{iE_1 t}{\hbar}} + \frac{1}{\sqrt{2}}\psi_2(x)\mathrm{e}^{-\frac{iE_2 t}{\hbar}}.$$

   (a) Show that the probability density of this state can be written as

$$\Psi(x,t) = \frac{1}{2}\left(\psi_1^2 + \psi_2^2\right) + \psi_1\psi_2 \cos\left(\frac{\Delta E\, t}{\hbar}\right)$$

   where $\Delta E = E_2 - E_1$.

   (b) Sketch the probability density at times $t = 0$, $t = \frac{\pi\hbar}{2\Delta E}$, and $t = \frac{\pi\hbar}{\Delta E}$.

## Quantum vs. Classical

14. A particle of mass $m$ is trapped in a one-dimensional box of length $L$.

   (a) Write down the probability distribution $P(x)$ for the particle assuming it obeys:

      (i) classical (Newtonian) equations of motion;

      (ii) the time-independent Schrödinger equation.

   (b) Show that the expectation value of $x^2$ according to the classical probability distribution is $L^2/3$.

   (c) Find the expectation value of $x^2$ for the $n^{\text{th}}$ quantum state of the particle. Show that it tends to the classical limit for $n \gg 1$.

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