# Quantum Mechanics MT: Problem Sheet 3 (Christmas Break)

## Wave Mechanics

**3.1** Consider a free particle in one dimension with Hamiltonian

$$H = \frac{\hat{p}^2}{2m}. \tag{1}$$

Let the wave function of the particle at time $t = 0$ be a Gaussian wave packet

$$\psi(x, 0) = \langle x|\psi(0)\rangle = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} e^{-\frac{x^2}{4\sigma^2} + \frac{i}{\hbar} p_0 x} . \tag{2}$$

Show that in the momentum representation we have

$$\langle p|\psi(0)\rangle = \int dx\ \langle p|x\rangle\langle x|\psi(0)\rangle = \left[\frac{2\sigma^2}{\pi\hbar^2}\right]^{\frac{1}{4}} e^{-\frac{\sigma^2}{\hbar^2}(p-p_0)^2}. \tag{3}$$

Comment on the relation between the forms of the state in the position and momentum representations as a function of $\sigma$. By solving the TDSE show that the probability distribution function at time $t$ can be written in the form

$$|\psi(x,t)|^2 = \frac{\sigma}{\sqrt{2\pi\hbar^2|b(t)|^2}} e^{-\frac{\sigma^2}{2\hbar^2|b(t)|^2}(x - p_0 t/m)^2} , \tag{4}$$

and derive the form of the function $b(t)$. Explain what happens physically to the particle as time evolves.

**3.2** Particles move in the potential

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

Particles of mass $m$ and energy $E > V_0$ are incident from $x = -\infty$. Show that the probability that a particle is reflected is

$$\left(\frac{k-K}{k+K}\right)^2 ,$$

where $k \equiv \sqrt{2mE}/\hbar$ and $K \equiv \sqrt{2m(E-V_0)}/\hbar$. Show directly from the time-independent Schrödinger equation that the probability of transmission is

$$\frac{4kK}{(k+K)^2}$$

and check that the flux of particles moving away from the origin is equal to the incident particle flux.

**3.3** Show that the energies of bound, odd-parity stationary states of the square potential well

$$V(x) = \begin{cases} 0 & \text{for } |x| < a \\ V_0 > 0 & \text{otherwise} \end{cases},$$

are governed by

$$\cot(ka) = -\sqrt{\frac{W^2}{(ka)^2} - 1} \quad \text{where} \quad W \equiv \sqrt{\frac{2mV_0a^2}{\hbar^2}} \quad \text{and} \quad k^2 = 2mE/\hbar^2.$$

Show that for a bound odd-parity state to exist, we require $W > \pi/2$.

**3.4** A free particle of energy $E$ approaches a square, one-dimensional potential well of depth $V_0$ and width $2a$. Show that the probability of being reflected by the well vanishes when $Ka = n\pi/2$, where $n$ is an integer and $K = (2m(E+V_0)/\hbar^2)^{1/2}$. Explain this phenomenon in physical terms.

**3.5** Prove the following statements involving the delta-function and its derivative (and explain how these statements are to be understood):

(a)

$$\delta(cx) = \frac{1}{|c|}\delta(x), 0 \neq c \in \mathbb{R}. \tag{5}$$

(b)

$$\delta\big(x^2 - c^2\big) = \frac{1}{2|c|}\big(\delta(x-c) + \delta(x+c)\big). \tag{6}$$

(c)

$$\frac{d}{dx}\theta(x-c) = \delta(x-c)\ , \qquad \theta(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{else} \end{cases} \tag{7}$$

The function $\theta(x)$ is known as the Heaviside theta-function.

(d)

$$\delta(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ikx}. \tag{8}$$

(e)

$$\int dx\ f(x)\delta'(x-x_0) = -f'(x_0)\ . \tag{9}$$

(f)* (starred problem for students who have already taken the complex analysis short-option)
How would you show that $\delta(x) = \lim_{\epsilon\to 0}\frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2}$?

**3.6** A particle of energy $E$ approaches from $x < 0$ a barrier in which the potential energy is $V(x) = V_\delta\delta(x)$. Show that the probability of its passing the barrier is

$$P_{\text{tun}} = \frac{1}{1+(K/2k)^2} \quad \text{where} \quad k = \sqrt{\frac{2mE}{\hbar^2}}, \quad K = \frac{2mV_\delta}{\hbar^2}.$$

**3.7** Given that the wavefunction is $\psi = A\mathrm{e}^{\mathrm{i}(kz-\omega t)} + B\mathrm{e}^{-\mathrm{i}(kz+\omega t)}$, where $A$ and $B$ are constants, show that the probability current density is

$$\boldsymbol{J} = v\big(|A|^2 - |B|^2\big)\,\hat{\boldsymbol{z}},$$

where $v = \hbar k/m$. Interpret the result physically.

## More problems on basic quantum mechanics

**3.8** (a) Find the allowed energy values $E_n$ and the associated normalized eigenfunctions $\phi_n(x)$ for a particle of mass $m$ confined by infinitely high potential barriers to the region $0 \le x \le a$.

(b) For a particle with energy $E_n = \hbar^2 n^2\pi^2/2ma^2$ calculate $\langle x\rangle$.

(c) Without working out any integrals, show that

$$\langle (x - \langle x\rangle)^2\rangle = \langle x^2\rangle - \frac{a^2}{4}.$$

Hence find $\langle (x - \langle x \rangle)^2 \rangle$ using the result that $\int_0^a x^2 \sin^2(n\pi x/a)\,\mathrm{d}x = a^3(1/6 - 1/4n^2\pi^2)$.

(d) A classical analogue of this problem is that of a particle bouncing back and forth between two perfectly elastic walls, with uniform velocity between bounces. Calculate the classical average values $\langle x \rangle_{\mathrm{C}}$ and $\langle (x - \langle x \rangle)^2 \rangle_{\mathrm{C}}$, and show that for high values of $n$ the quantum and classical results tend to each other.

**3.9** A **Fermi oscillator** has Hamiltonian $\hat{H} = \hat{f}^\dagger \hat{f}$, where $\hat{f}$ is an operator that satisfies

$$\hat{f}^2 = 0, \quad \hat{f}\hat{f}^\dagger + \hat{f}^\dagger \hat{f} = 1.$$

Show that $\hat{H}^2 = \hat{H}$, and thus find the eigenvalues of $\hat{H}$. If the ket $|0\rangle$ satisfies $\hat{H}|0\rangle = 0$ with $\langle 0|0\rangle = 1$, what are the kets (a) $|a\rangle \equiv \hat{f}|0\rangle$, and (b) $|b\rangle \equiv \hat{f}^\dagger|0\rangle$?

In quantum field theory the vacuum is pictured as an assembly of oscillators, one for each possible value of the momentum of each particle type. A boson is an excitation of a harmonic oscillator, while a fermion in an excitation of a Fermi oscillator. Explain the connection between the spectrum of $\hat{f}^\dagger \hat{f}$ and the Pauli exclusion principle (which states that zero or one fermion may occupy a particular quantum state).

## Compute

**3.10** Using your favourite Large Language Model / AI model, develop Mathematica code (or Python or any other numerical lanaguage of your choice) which computes numerical solutions for the first 20 energy eigenstates $|\phi_n\rangle$ and eigenvalues $E_n$ of the Hamiltonian

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

where $V(\hat{x})$ is a infinite square well with the properties $V(x) = 0$ for $x < 0$, $V(x) = 0$ for $x > L$ and $V(x) = \sin^4(2\pi x/L)$ for $0 \le x \le L$.

Plot a representative sample of these eigenfunctions.

Consider an initial state $\psi(x, t = 0) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$. Using your favourite LLM/AI model, develop Mathematica code (or Python or any other numerical language of your choice) that decomposes this wavefunctions into energy eigenfunctions.

Hence develop code that evolves this wavefunction forward in time, and describe and plot the subsequent time evolution of the wavefunction.

**3.11** Redo question 3.3. Do *no* computations yourself. All calculations must be done by *either* posing a problem directly to an AI/LLM *or* asking an AI/LLM to construct Mathematica/Python/etc code that can then be run directly to solve a computation.