Quantum Mechanics Spring 2023
Exercise Sheet 4 Solutions

Problem 1 (15 marks)

Let's consider one spatial dimension and time. Remember, we have defined the position and momentum operators in the class, $\hat{x}$ and $\hat{p}$, respectively. The momentum operator is the derivative operator defined as :

$$\hat{p} = -i\hbar \frac{d}{dx} \tag{1}$$

where $\hbar$ is the modified Planck's constant. You now know that if $\psi(x,t)$ is the wavefunction of the quantum system, then $|\psi(x,t)|^2$ is the probability distribution function. For any operator $\hat{Q}$, the expectation of it is defined by the following equation :

$$\langle \hat{Q} \rangle = \int dx \psi(x,t)^* \hat{Q} \psi(x,t) \tag{2}$$

1. Calculate the expectations of the position and momentum operators, $\langle \hat{x} \rangle$ and $\langle \hat{p} \rangle$.
2. Calculate the time derivative of the position expectation, $d\langle \hat{x} \rangle / dt$.
3. We define the time derivative of the position expectation by $\hat{v}$. Show that $\langle p \rangle = m \langle v \rangle$.
4. The kinetic energy is defined as $T = \frac{p}{2m}$. Define the kinetic energy operator and calculate the expectation value of the kinetic energy operator $\langle \hat{T} \rangle$.
5. Show that
$$\frac{\langle \hat{p} \rangle}{dt} = \langle -\frac{dV}{dx} \rangle \tag{3}$$
This is known as **Ehrenfest's Theorem**, which shows that the expectation values obey Newton's Second law.

Solutions

1. The expectation value of the position operator $\hat{x}$ is :
$$\begin{aligned} \langle \hat{x} \rangle &= \int dx \psi(x,t) \hat{x} \psi(x,t) \\ &= \int dx \psi(x,t) x \psi(x,t) \end{aligned}$$
The expectation value of the momentum operator $\hat{p}$ is :
$$\begin{aligned} \langle \hat{p} \rangle &= \int dx \psi(x,t) \hat{p} \psi(x,t) \\ &= \int dx \psi(x,t) \left(-i\hbar \frac{d}{dx} \right) \psi(x,t) \end{aligned}$$
2. Taking the derivative with respect to time, we get :
$$\begin{aligned} \frac{d\langle \hat{x} \rangle}{dt} &= \frac{d}{dt} \int dx \psi(x,t) x \psi(x,t) \\ &= \int dx \frac{\partial}{\partial t} \left(\psi(x,t) x \psi(x,t) \right) \\ &= \int dx \left(\frac{\partial \psi(x,t)}{\partial t} x \psi(x,t) + \psi(x,t) x \frac{\partial \psi(x,t)}{\partial t} \right) \end{aligned}$$

3. We define the time derivative of the position expectation as $\hat{v}$:

$$\begin{aligned}\hat{v} = \frac{d\langle\hat{x}\rangle}{dt} &= \int dx \left(\frac{\partial\psi(x,t)}{\partial t}x\psi(x,t) + \psi(x,t)x\frac{\partial\psi(x,t)}{\partial t}\right) \\ &= \frac{1}{m}\int dx \left(\psi(x,t)\hat{p}\psi(x,t) + \psi(x,t)\hat{p}\psi(x,t)\right) \\ &= \frac{1}{m}\langle\hat{p}\rangle\end{aligned}$$

Therefore, we have $\langle p\rangle = m\langle v\rangle$.

4. The kinetic energy operator is defined as $\hat{T} = \frac{\hat{p}^2}{2m}$. The expectation value of the kinetic energy operator is :

$$\begin{aligned}\langle\hat{T}\rangle &= \int dx\psi(x,t)\hat{T}\psi(x,t) \\ &= \int dx\psi(x,t)\frac{\hat{p}^2}{2m}\psi(x,t) \\ &= \frac{1}{2m}\int dx\psi(x,t)\hat{p}\hat{p}\psi(x,t) \\ &= \frac{1}{2m}\langle\hat{p}^2\rangle\end{aligned}$$

5. To show Ehrenfest's Theorem, we start by taking the time derivative of the momentum operator :

$$\begin{aligned}\frac{d\hat{p}}{dt} &= -i\hbar\frac{d^2}{dx^2}\frac{d}{dt} \\ &= -i\hbar\frac{d}{dx}\frac{\partial}{\partial t}\end{aligned}$$

Next, we take the expectation value of this expression :

$$\begin{aligned}\frac{d}{dt}\langle\hat{p}\rangle &= \frac{d}{dt}\int dx\psi^*(x,t)\hat{p}\psi(x,t) \\ &= -i\hbar\int dx\psi^*(x,t)\frac{\partial}{\partial x}\left(\frac{\partial}{\partial t}\psi(x,t)\right) \\ &= -i\hbar\int dx\psi^*(x,t)\frac{\partial}{\partial x}\left(\frac{i}{\hbar}H\psi(x,t)\right) \\ &= -\int dx\psi^*(x,t)\frac{\partial}{\partial x}H\psi(x,t) \\ &= -\int dx\psi^*(x,t)\frac{\partial}{\partial x}V(x)\psi(x,t) \\ &= \langle-\frac{\partial V}{\partial x}\rangle\end{aligned}$$

where H is the Hamiltonian operator, $V(x)$ is the potential energy function. We have used the time-dependent Schrodinger equation, $\frac{\partial}{\partial t}\psi(x,t) = -\frac{i}{\hbar}H\psi(x,t)$, and the fact that the momentum operator is related to the Hamiltonian by $\hat{p} = -i\hbar\frac{\partial}{\partial x}$.

Thus, we have shown that the expectation value of the time derivative of the momentum operator is equal to the expectation value of the negative spatial derivative of the potential energy function, which is precisely Newton's second law for a one-dimensional system. This is Ehrenfest's Theorem, which shows that the expectation values of quantum mechanical observables obey classical mechanics.

Problem 2 (15 marks)

In class, we derived the Probability conservation law in QM. The probability conservation tells us that the particle is conserved "locally" and is stable. Suppose you want to describe an "unstable" particle that spontaneously disintegrates with a lifetime of τ. In that case, the total probability of finding the particle somewhere should not be constant but decrease exponentially :

$$P(t) \equiv \int dx|\psi(x,t)|^2 = e^{-t/\tau} \tag{4}$$

In our derivation, we used the fact that the potential energy V is **real**. This leads to the conservation of probability. What if we assign to V an imaginary part :

$$V = V_0 - i\Gamma \tag{5}$$

where V_0 is the true potential energy and Γ is the positive real constant.

1. Calculate $\frac{dP}{dt}$.
2. Solve for $P(t)$ and find the lifetime of the particle in terms of Γ.

Solution

(a) The time derivative of the wavefunction is given by $\dfrac{\partial \Psi}{\partial t} = -\dfrac{i\hbar}{2m}\dfrac{\partial^2 \Psi^*}{\partial x^2} + i(V^*\Psi^*)$, and therefore, the time derivative of the mode-squared of the wavefunction now picks up an extra term :

$$\frac{\partial}{\partial t}|\Psi|^2 = \cdots + i\frac{|\Psi|^2(V^* - V)}{\hbar} \qquad = \cdots + i\frac{|\Psi|^2(V_0 + i\Gamma - V_0 + i\Gamma)}{\hbar} \qquad = \cdots - 2\Gamma\frac{|\Psi|^2}{\hbar},$$

This implies that $\dfrac{dP}{dt} = -2\Gamma \int_{-\infty}^{\infty} |\Psi|^2 dx = -2\Gamma P$. QED

1. Integrating both sides with respect to time, we get

$$\begin{aligned} \int_{P(0)}^{P(t)} \frac{dP}{P} &= \int_0^t -2\Gamma dt \\ \ln\frac{P(t)}{P(0)} &= -\frac{2\Gamma}{\hbar}t \\ P(t) &= P(0)e^{-\frac{2\Gamma}{\hbar}t}. \end{aligned}$$

Comparing this with the given equation $P(t) = e^{-t/\tau}$, we see that $\tau = \hbar/(2\Gamma)$.