**THE UNIVERSITY OF QUEENSLAND**
**SCHOOL OF MATHEMATICS AND PHYSICS**
**PHYS2041 – Quantum Physics**

**Tutorial 3 Solutions**

## Problem 3.1

For an arbitrary wave function $\Psi(x,t)$, show that the expectation value of the momentum is equal to

$$\langle p\rangle = m\langle v\rangle = m\frac{d\langle x\rangle}{dt} = -i\hbar\int_{-\infty}^{\infty}\Psi^*\,\frac{\partial\Psi}{\partial x}\,dx \tag{1}$$

Let's start with $\langle x\rangle = \int_{-\infty}^{\infty} x|\Psi(x,t)|^2\mathrm{d}x$

$$\begin{aligned}
\frac{d\langle x\rangle}{dt} &= \frac{d}{dt}\int_{-\infty}^{\infty} x|\Psi(x,t)|^2\mathrm{d}x && (2)\\
&= \int_{-\infty}^{\infty} x\frac{\partial}{\partial t}|\Psi(x,t)|^2\mathrm{d}x && (3)\\
&= \int_{-\infty}^{\infty} x\left(\Psi^*\frac{\partial\Psi}{\partial t}+\frac{\partial\Psi^*}{\partial t}\Psi\right)\mathrm{d}x && (4)
\end{aligned}$$

Where in the second line exploited the fact that $x$ and $t$ are independent variables, and in the final line we used $|\Psi|^2 = \Psi^*\Psi$ with the product rule. We can then rearrange the Schrödinger equation for expressions for $\frac{\partial\Psi}{\partial t}$ and $\frac{\partial\Psi^*}{\partial t}$,

$$\begin{aligned}
\frac{\partial\Psi}{\partial t} &= \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi && (5)\\
\frac{\partial\Psi^*}{\partial t} &= \frac{-i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^* && (6)
\end{aligned}$$

Substituting these into (4) and expanding (the potential terms cancel),

$$\frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2}-\frac{\partial^2\Psi^*}{\partial x^2}\Psi\right)\mathrm{d}x \tag{7}$$

Identifying that this can be simplified by using the product rule in reverse (it's easy to check this using the product rule),

$$\frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)\mathrm{d}x \tag{8}$$

$$\tag{9}$$

We can integrate this by parts using

$$\int_a^b f(x)\frac{dg(x)}{dx}\mathrm{d}x = [f(x)g(x)]_a^b - \int_a^b \frac{df(x)}{dx}g(x)\mathrm{d}x \tag{10}$$

if we let $f = x$ and $dg/dx = \frac{\partial}{\partial x}(...)$ then we get

$$\int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\mathrm{d}x = \left[x\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\mathrm{d}x \quad (11)$$

Here, the first term (which we call the boundary term, because it's evaluated at the boundary of the domain) is zero because if $\Psi$ is normalised it must go to zero at $\pm\infty$, and the derivatives must be finite.

So now we have,

$$\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\mathrm{d}x \quad (12)$$

Integrating the first term in the integrand by parts, and setting the boundary term to 0,

$$\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\mathrm{d}x = -\int_{-\infty}^{\infty}\frac{\partial\Psi^*}{\partial x}\Psi\mathrm{d}x \quad (13)$$

which gives,

$$\frac{d\langle x\rangle}{dt} = \frac{i\hbar}{m}\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\mathrm{d}x \quad (14)$$

Multiplying by $m$ gives the required result:

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = -i\hbar\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\mathrm{d}x. \quad (15)$$

**Problem 3.2**

It will be useful to define the normalisation integral

$$A(t) = \int_{-\infty}^{\infty}|\Psi(x,t)|^2 dx. \quad (16)$$

If the wavefunction is normalised at $t = 0$, then we have $A(0) = 1$. We wish to show that it remains normalised at all later times. Let's proceed by learning how the normalisation changes with time,

$$\frac{dA}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty}|\Psi(x,t)|^2\mathrm{d}x = \int_{-\infty}^{\infty}\left(\Psi^*\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^*}{\partial t}\Psi\right)\mathrm{d}x \quad (17)$$

using the same reasoning as (4) from the previous question. Also as in the previous question, we know the wavefunction must obey the Schrödinger equation, so we again use (5) and (6) to evaluate the time derivatives, cancel the potential terms and apply product rule to deduce

$$\frac{dA}{dt} = \frac{i\hbar}{2m}\int_{-\infty}^{\infty}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right)\mathrm{d}x \quad (18)$$

$$= \frac{i\hbar}{2m}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\mathrm{d}x \quad (19)$$

The final line is simply the integral of a derivative, which from the fundamental theorem of calculus is simply

$$\frac{dA}{dt} = \frac{i\hbar}{2m}\left[\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right]_{-\infty}^{\infty} = 0 \tag{20}$$

which must go to 0, as both terms contain $\Psi$. As discussed in the previous question, due to normalisation $\Psi$ must vanish at the boundaries, and the derivatives must be finite.

Since we have shown that $dA/dt = 0$, the normalisation integral is conserved. This means that at all later times $t$, $A(t) = A(0) = 1$, i.e. the wavefunction will remain normalised, as required.

**Problem 3.3** *

For an arbitrary wave function $\Psi(x,t)$, calculate $d\langle p\rangle/dt$, *i.e.*, the derivative of the expectation value of the momentum with respect to time, and eventually show that it can be written as

$$\frac{d\langle p\rangle}{dt} = -\left\langle \frac{\partial V(x,t)}{\partial t}\right\rangle, \tag{21}$$

We start with writing $\langle p\rangle$ in integral form

$$\langle p\rangle = -i\hbar \int_{-\infty}^{\infty} \Psi^* \frac{\partial}{\partial x}\Psi \; dx, \tag{22}$$

and we take its time derivative

$$\frac{d\langle p\rangle}{dt} = -i\hbar \int_{-\infty}^{\infty} \frac{\partial}{\partial t}\left(\Psi^* \frac{\partial \Psi}{\partial x}\right) \; dx. \tag{23}$$

We expand inside the integral by using the product rule

$$\frac{\partial}{\partial t}\left(\Psi^* \frac{\partial \Psi}{\partial x}\right) = \frac{\partial \Psi^*}{\partial t}\frac{\partial \Psi}{\partial x} + \Psi^* \frac{\partial}{\partial x}\left(\frac{\partial \Psi}{\partial t}\right) \tag{24}$$

Note: In the second term of the right hand side we used $\frac{\partial^2 \Psi}{\partial t \partial x} = \frac{\partial^2 \Psi}{\partial x \partial t}$.

Then we use Schrodinger equation to write the time derivative of $\Psi$ in terms of potential and position derivative.

$$\frac{\partial}{\partial t}\left(\Psi^* \frac{\partial \Psi}{\partial x}\right) = \left[-\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^*\right]\frac{\partial \Psi}{\partial x} + \Psi^* \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi\right] \tag{25}$$

$$= \frac{i\hbar}{2m}\left[\Psi^* \frac{\partial^3 \Psi}{\partial x^3} - \frac{\partial^2 \Psi^*}{\partial x^2}\frac{\partial \Psi}{\partial x}\right] + \frac{i}{\hbar}\left[V\Psi^* \frac{\partial \Psi}{\partial x} - \Psi^* \frac{\partial}{\partial x}(V\Psi)\right] \tag{26}$$

Now we need to integrate equation (26). The first term can be evaluated by integration by parts,

$$\int_{-\infty}^{\infty} \frac{\partial^2 \Psi^*}{\partial x^2}\frac{\partial \Psi}{\partial x} dx = -\int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial x}\frac{\partial^2 \Psi}{\partial x^2} dx = \int_{-\infty}^{\infty} \Psi^* \frac{\partial^3 \Psi}{\partial x^3} dx \tag{27}$$

and it is equal to zero. We expand the second term using the product rule and take the integral

$$\begin{aligned}
\frac{d\langle p\rangle}{dt} &= -i\hbar \int_{-\infty}^{\infty} \frac{i}{\hbar}\left[V\Psi^* \frac{\partial \Psi}{\partial x} - \Psi^* \frac{\partial}{\partial x}(V\Psi)\right] dx &(28)\\
&= \int_{-\infty}^{\infty} \left[V\Psi^* \frac{\partial \Psi}{\partial x} - \Psi^* V \frac{\partial \Psi}{\partial x} - |\Psi|^2 \frac{\partial V}{\partial x}\right] dx &(29)\\
&= -\int_{-\infty}^{\infty} |\Psi|^2 \frac{\partial V}{\partial x} dx &(30)\\
&= -\left\langle \frac{\partial V}{\partial x}\right\rangle, &(31)
\end{aligned}$$

as required.

This result is known as **Ehrenfest's theorem**, and it states that quantum mechanics obeys Newton's laws *on average*.

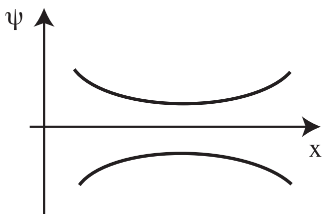
## <u>Problem 3.4</u> [FOR ASSIGNMENT 2; max 10 points]

Use Eqs. [1.23] and [1.24], and integration by parts: (Here, [1.23]=[Schroedinger eq.]; [1.24]=[its conjugate].)

$$\begin{aligned}
\frac{d}{dt}\int_{-\infty}^{\infty} \Psi_1^* \Psi_2 \, dx &= \int_{-\infty}^{\infty} \frac{\partial}{\partial t}\left(\Psi_1^*\Psi_2\right) dx = \int_{-\infty}^{\infty} \left(\frac{\partial \Psi_1^*}{\partial t}\Psi_2 + \Psi_1^* \frac{\partial \Psi_2}{\partial t}\right) dx \\
&= \int_{-\infty}^{\infty} \left[\left(\frac{-i\hbar}{2m}\frac{\partial^2 \Psi_1^*}{\partial x^2} + \frac{i}{\hbar} V \Psi_1^*\right)\Psi_2 + \Psi_1^*\left(\frac{i\hbar}{2m}\frac{\partial^2 \Psi_2}{\partial x^2} - \frac{i}{\hbar} V\Psi_2\right)\right] dx \\
&= -\frac{i\hbar}{2m}\int_{-\infty}^{\infty} \left(\frac{\partial^2 \Psi_1^*}{\partial x^2}\Psi_2 - \Psi_1^* \frac{\partial^2 \Psi_2}{\partial x^2}\right) dx \\
&= -\frac{i\hbar}{2m}\left[\frac{\partial \Psi_1^*}{\partial x}\Psi_2\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial \Psi_1^*}{\partial x}\frac{\partial \Psi_2}{\partial x} dx - \Psi_1^* \frac{\partial \Psi_2}{\partial x}\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{\partial \Psi_1^*}{\partial x}\frac{\partial \Psi_2}{\partial x} dx\right] = 0. \text{ QED}
\end{aligned}$$

**Problem 3.5** **[FOR ASSIGNMENT 2; max 10 points]**

Given $\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[V(x) - E]\psi$, if $E < V_{\min}$, then $\psi''$ and $\psi$ always have the same sign: If $\psi$ is positive(negative), then $\psi''$ is also positive(negative). This means that $\psi$ always curves away from the axis (see Figure). However, it has got to go to zero as $x \to -\infty$ (else it would not be normalizable). At some point it's got to *depart* from zero (if it *doesn't*, it's going to be identically zero *everywhere*), in (say) the positive direction. At this point its slope is positive, and *increasing*, so $\psi$ gets bigger and bigger as $x$ increases. It can't ever "turn over" and head back toward the axis, because that would require a negative second derivative—it always has to bend away from the axis. By the same token, if it starts out heading negative, it just runs more and more negative. In neither case is there any way for it to come back to zero, as it must (at $x \to \infty$) in order to be normalizable. QED




Expanded version of the solution:

The time independent Schrödinger equation for an arbitrary, time independent potential $V(x)$ can be written as

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}\left[V(x) - E\right]\psi \tag{32}$$

where the solution $\psi$ is an energy eigenfunction. To show that the energy must *exceed* the minimum value of $V_{\min}$ we will use proof by contradiction.

So, let's assume for the moment that the energy $E$ is *less* than $V_{\min}$, i.e. $E < V_{\min}$. This means that $(V(x) - E) > 0$. From Eq. 1, this inequality implies that the second derivative $\psi''$ always has the same sign as $\psi$, for all $x$. What this means is that for all $x$, $\psi$ curves *away* from the $x$ axis, (i.e. $\psi$ is *convex*, as opposed to concave). This is the logic behind the well known "second derivative test" for classifying stationary points.

However, we also need $\psi$ to approach zero at $\pm\infty$ if the normalisation integral is to converge. As $\psi$ is curving away from the $x$ axis, this would require $\psi$ to turn around, and head back towards the $x$ axis. This will introduce another stationary point which is locally a maximum (i.e. concave), which would change the sign of $\psi''$, but not $\psi$, so now $\psi''$ and $\psi$ will have *opposite* sign. However if $E < V_{\min}$ then the time independent Schrödinger equation forbids this, hence a contradiction. Additionally, if $E = V_{\min}$, then at this point we would be left with $\psi'' = 0$, which also yields un-normalisable solutions (check this!).

Therefore we can conclude that $E > V_{\min}$ for all $x$, as required.

Let's think about a *classical* particle moving under a potential $V(x)$. So long as the total energy $E = T + V$ is conserved, then when the potential is a minimum the kinetic energy $T$ must be at a maximum, i.e. $E = T_{\max} + V_{\min}$. The only way for $E < V_{\min}$ is if $T_{\max}$ is negative, which is impossible. Therefore, similarly to a quantum particle, a classical particle must always have $E > V_{\min}$.