Tutorial 4 - Wave Function

Question 1:

Show that $\tilde{\rho}(k) = \left|\tilde{\psi}(k)\right|^2$ is the probability distribution function for the variable k.

Solution:

If $\tilde{\rho}$ is the probability density for k then it must yield 1 when integrated over the entire k-space,

$$\begin{aligned}
\int_{\tilde{\Omega}} \tilde{\psi}^* \tilde{\psi} dk &= \int_{\tilde{\Omega}} \left(\frac{1}{\sqrt{2\pi}} \int_{\Omega} \psi^*(y) e^{iky} dy\right) \left(\frac{1}{\sqrt{2\pi}} \int_{\Omega} \psi(x) e^{-ikx} dx\right) dk \\
&= \int_{\Omega} \psi(x) dx \int_{\Omega} \psi^*(y) dy \underbrace{\frac{1}{2\pi} \int_{\tilde{\Omega}} e^{-ik(x-y)} dk}_{\delta(x-y)} \\
&= \int_{\Omega} \psi(x) dx \underbrace{\int_{\Omega} \psi^*(y) \delta(x-y) dy}_{\psi^*(x)} \\
&= \int_{\Omega} \psi^*(x) \psi(x) dx,
\end{aligned}$$

which is exactly the integral over $\rho(x)$ over all space which is by definition 1.

Normalization

The statistical interpretation of the wave function requires it must follow the probability normalization condition

$$\boxed{\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1},$$

But this is not enough, since the wave function must remain normalized as time evolves as well, which means that

$$\frac{d}{dt} \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = \int_{-\infty}^{\infty} \frac{\partial}{\partial t} |\Psi(x,t)|^2 dx = 0$$

must hold always. Let us massage the integral a bit

$$\frac{\partial}{\partial t} |\Psi|^2 = \frac{\partial}{\partial t} (\Psi^* \Psi) = \Psi^* \frac{\partial}{\partial t} \Psi + \frac{\partial}{\partial t} \Psi^* \Psi,$$

using the Schrodinger equation and its complex conjugate

$$\begin{aligned}
i\hbar \frac{\partial \Psi}{\partial t} &= -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \quad \rightarrow \quad \frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V\Psi \\
-i\hbar \frac{\partial \Psi^*}{\partial t} &= -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + V\Psi^* \quad \rightarrow \quad \frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V\Psi^*
\end{aligned}$$

we get

$$\begin{aligned}
\frac{\partial}{\partial t}\left|\Psi\right|^2 &= \Psi^*\left(\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \cancel{\frac{i}{\hbar}V\Psi}\right) + \left(-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \cancel{\frac{i}{\hbar}V\Psi^*}\right)\Psi \\
&= \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right) \\
&= \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\right].
\end{aligned}$$

Plugging this expression into the integral above we get

$$\frac{d}{dt}\int_{-\infty}^{\infty}\left|\Psi\left(x,t\right)\right|^2 dx = \int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\right]dx = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\Bigg|_{-\infty}^{\infty},$$

but since the wave function must vanish at $x \to \pm\infty$ it follows that

$$\underline{\frac{d}{dt}\int_{-\infty}^{\infty}\left|\Psi\left(x,t\right)\right|^2 = 0,}$$

so that if Ψ is normalized at $t = 0$, it stays normalized for all future times. We call the quantity

$$\boxed{J\left(x,t\right) \equiv \frac{i\hbar}{2m}\left(\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right)},$$

the *probability current*. Note that $J\left(x,t\right) = \frac{\hbar}{m}\mathrm{Im}\left[\Psi^*\frac{\partial\Psi}{\partial x}\right]$.

Question 2:

Consider the one-dimensional normalized wave functions $\psi_0\left(x\right)$ and $\psi_1\left(x\right)$ which satisfy:

$$\psi_0\left(-x\right) = \psi_0\left(x\right) = \psi_0^*\left(x\right) \qquad \text{and} \qquad \psi_1\left(x\right) = N\frac{d\psi_0}{dx}.$$

Consider the linear combination

$$\psi\left(x\right) = c_0\psi_0\left(x\right) + c_1\psi_1\left(x\right),$$

with $\left|c_0\right|^2 + \left|c_1\right|^2 = 1$. The complex constants N, c_0 and c_1 are known.

1. Show that $\psi_0\left(x\right)$ and $\psi_1\left(x\right)$ are orthogonal and that $\psi\left(x\right)$ is normalized.
2. Compute the expectation values $\langle x\rangle$, $\langle p\rangle$ in the states $\psi_0\left(x\right)$, $\psi_1\left(x\right)$ and $\psi\left(x\right)$.
3. Compute the expectation value of the kinetic energy $\hat{T} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ in the state ψ_0 and demonstrate that

$$\left\langle\psi_0, \hat{T}^2\psi_0\right\rangle = \left\langle\psi_0, \hat{T}\psi_0\right\rangle\left\langle\psi_1, \hat{T}\psi_1\right\rangle,$$

   and that

$$\left\langle\psi_1, \hat{T}\psi_1\right\rangle \geq \left\langle\psi, \hat{T}\psi\right\rangle \geq \left\langle\psi_0, \hat{T}\psi_0\right\rangle.$$

4. Show that

$$\left\langle\psi_0, \hat{x}^2\psi_0\right\rangle\left\langle\psi_1, \hat{p}^2\psi_1\right\rangle \geq \frac{\hbar^2}{4}.$$

Solution:

1. Taking the inner product of the two functions we have

$$\langle \psi_0, \psi_1 \rangle = \int_\Omega \psi_0^* \psi dx = N \int_\Omega \psi_0 \frac{d\psi_0}{dx} dx,$$

but ψ_0 is a symmetric function, whereas

$$\psi(-x) = N \frac{d\psi_0(-x)}{d(-x)} = -N \frac{d\psi_0(x)}{dx} = -\psi(x).$$

Therefore the integral above, over a the multiplication of an even function and an odd function, which yields an odd function, vanishes when integrating over all space, meaning $\boxed{\langle \psi_0, \psi_1 \rangle = 0}$.
Taking the inner product of ψ with itself yields

$$\begin{aligned} \langle \psi, \psi \rangle &= \int_\Omega \psi^* \psi dx \\ &= \int_\Omega \left(c_0^* \psi_0^* + c_1^* \psi_1^*\right)\left(c_0 \psi_0 + c_1 \psi_1\right) dx \\ &= \int_\Omega \left(c_0^* c_0 \underbrace{\psi_0 \psi_0^*}_{\to 1} + c_1^* c_0 \underbrace{\cancel{\psi_0 \psi_1^*}}_{\text{odd}} + c_0^* c_1 \underbrace{\cancel{\psi_1 \psi_0^*}}_{\text{odd}} + c_1^* c_1 \underbrace{\psi_1 \psi_1^*}_{\to 1} \right) dx \\ &= |c_0|^2 + |c_1|^2, \end{aligned}$$

thus

$$\boxed{\langle \psi, \psi \rangle = 1}.$$

2. The expectation values for the space operator $\hat{x}$ are

$$\begin{aligned} \langle \psi_0, \hat{x}\psi_0 \rangle &= \int_\Omega \psi_0^* \hat{x} \psi_0 dx = \int_\Omega \underbrace{\psi_0^2 x}_{\text{odd}} dx = 0, \\ \langle \psi_1, \hat{x}\psi_1 \rangle &= \int_\Omega \psi_1^* \hat{x} \psi_1 dx = -\int_\Omega \underbrace{\psi_1^2 x}_{\text{odd}} dx = 0. \\ \langle \psi, \hat{x}\psi \rangle &= \int_\Omega \left(c_0^* \psi_0^* + c_1^* \psi_1^*\right) \hat{x} \left(c_0 \psi_0 + c_1 \psi_1\right) dx \\ &= \int_\Omega \left(c_0^* c_0 \underbrace{\cancel{\psi_0 \psi_0^* x}}_{\text{odd}} + c_1^* c_0 \psi_0 \psi_1^* x + c_0^* c_1 \psi_1 \psi_0^* x + c_1^* c_1 \underbrace{\psi_1 \psi_1^* x}_{\text{odd}} \right) dx \\ &= \left(N c_0^* c_1 + N^* c_1^* c_0\right) \int_\Omega \frac{d\psi_0}{dx} \psi_0 x dx \\ &= \left(N c_0^* c_1 + \left(N c_0^* c_1\right)^*\right) \int_\Omega \left[\frac{1}{2} \frac{d}{dx}\left(\psi_0^2 x\right) - \psi_0^2 \right] dx \\ &= 2\mathrm{Re}\left[N c_0^* c_1\right] \left[\cancel{\frac{1}{2}\left(\psi_0^2 x\right)\Big|_{-\infty}^{\infty}} - 1 \right] \\ &= -2\mathrm{Re}\left[N c_0^* c_1\right]. \end{aligned}$$

Therefore

$$\boxed{\langle \psi_0, \hat{x}\psi_0 \rangle \qquad \langle \psi_1, \hat{x}\psi_1 \rangle = 0 \qquad \langle \psi, \hat{x}\psi \rangle = -2\mathrm{Re}\left[N c_0^* c_1\right]}.$$

Whereas the expectation values for the space operator $\hat{p}$ are

$$\langle\psi_0,\hat{p}\psi_0\rangle = \int_\Omega \psi_0^*\hat{p}\psi_0 dx = \int_\Omega \psi_0\left(-i\hbar\frac{d}{dx}\right)\psi_0 dx = -i\hbar\int_\Omega \frac{1}{2}\frac{d}{dx}\left(\psi_0^2\right)dx = -\frac{i\hbar}{2}\psi_0^2\Big|_{-\infty}^{\infty} = 0,$$

$$\langle\psi_1,\hat{p}\psi_1\rangle = \int_\Omega \psi_1^*\hat{p}\psi_1 dx = \int_\Omega \frac{N^*}{N}\psi_1\left(-i\hbar\frac{d}{dx}\right)\psi_1 dx = -i\hbar\frac{N^*}{N}\int_\Omega \frac{1}{2}\frac{d}{dx}\psi_1^2 dx = -\frac{i\hbar}{2}\frac{N^*}{N}\psi_1^2\Big|_{-\infty}^{\infty} = 0,$$

$$\begin{aligned}
\langle\psi,\hat{p}\psi\rangle &= \int_\Omega \left(c_0^*\psi_0^* + c_1^*\psi_1^*\right)\hat{p}\left(c_0\psi_0 + c_1\psi_1\right)dx \\
&= -i\hbar\int_\Omega \left(c_0^*c_0\underbrace{\cancel{\psi_0'\psi_0}}_{\text{odd}} + c_1^*c_0\psi_0'\psi_1^* + c_0^*c_1\psi_1'\psi_0 + c_1^*c_1\underbrace{\cancel{\psi_1'\psi_1^*}}_{\text{odd}}\right)dx \\
&= -i\hbar\int_\Omega \left[c_1^*c_0\psi_0'\psi_1^* + c_0^*c_1\frac{d}{dx}\left(\psi_1\psi_0\right) - c_0^*c_1\psi_1\psi_0'\right]dx \\
&= -i\hbar\left[\int_\Omega\left(\frac{c_1^*c_0}{N} - \frac{c_0^*c_1}{N^*}\right)\psi_1\psi_1^* dx + \cancel{c_0^*c_1(\psi_1\psi_0)\Big|_{-\infty}^{\infty}}\right] \\
&= 2\hbar\,\mathrm{Im}\left[\frac{c_0c_1^*}{N}\right],
\end{aligned}$$

where we used the fact that $\psi_0' = \psi_1/N$ and its complex conjugate. Therefore

$$\boxed{\langle\psi_0,\hat{p}\psi_0\rangle \qquad \langle\psi_1,\hat{p}\psi_1\rangle = 0 \qquad \langle\psi,\hat{p}\psi\rangle = 2\hbar\,\mathrm{Im}\left[\frac{c_0c_1^*}{N}\right]}.$$

3. The expectation value for $\hat{T}^2$ in the ψ_0 state is

$$\begin{aligned}
\left\langle\psi_0,\hat{T}\psi_0\right\rangle &= \int_\Omega \psi_0^*\hat{T}\psi_0 dx \\
&= -\frac{\hbar^2}{2m}\int_\Omega \psi_0^*\frac{d^2}{dx^2}\psi_0 dx \\
&= -\frac{\hbar^2}{2m}\int_\Omega\left[\frac{d}{dx}\left(\psi_0^*\frac{d}{dx}\psi_0\right) - \frac{d}{dx}\psi_0^*\frac{d}{dx}\psi_0\right]dx \\
&= -\frac{\hbar^2}{2m}\left[\cancel{\left(\frac{1}{N}\psi_0^*\psi_1\right)\Big|_{-\infty}^{\infty}} - \frac{1}{|N|^2}\underbrace{\int_\Omega \psi_1^*\psi_1 dx}_{=1}\right],
\end{aligned}$$

thus

$$\boxed{\left\langle\psi_0,\hat{T}\psi_0\right\rangle = \frac{\hbar^2}{2m|N|^2}}.$$

Taking a look at the expectation value of $\hat{T}^2$ we find

$$\begin{aligned}
\left\langle\psi_0,\hat{T}^2\psi_0\right\rangle &= \int_\Omega \psi_0^*\hat{T}^2\psi_0 dx \\
&= \frac{\hbar^4}{4m^2}\int_\Omega \psi_0\frac{d^4}{dx^4}\psi_0 dx \\
&= \frac{\hbar^4}{4m^2}\int_\Omega\left[\frac{d}{dx}\left(\psi_0\frac{d^3}{dx^3}\psi_0\right) - \frac{d}{dx}\psi_0^*\frac{d^3}{dx^3}\psi_0\right]dx \\
&= \frac{\hbar^2}{2m}\left[\cancel{\left(\psi_0\frac{d^3}{dx^3}\psi_0\right)\Big|_{-\infty}^{\infty}} - \frac{1}{|N|^2}\int_\Omega \psi_1^*\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_1 dx\right] \\
&= \frac{\hbar^2}{2m|N|^2}\left\langle\psi_1,\hat{T}\psi_1\right\rangle,
\end{aligned}$$

therefore, using the result we had for $\left\langle \psi_0, \hat{T}\psi_0 \right\rangle$, we immediately see that

$$\boxed{\left\langle \psi_0, \hat{T}^2\psi_0 \right\rangle = \left\langle \psi_0, \hat{T}\psi_0 \right\rangle \left\langle \psi_1, \hat{T}\psi_1 \right\rangle}.$$

In order to prove the inequality, let us consider the following wave function

$$\psi_2 \equiv \hat{T}\psi_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_0,$$

such that

$$\left|\langle \psi_0 \psi_2 \rangle\right|^2 = \left\langle \psi_0, \hat{T}\psi_0 \right\rangle^2 \le \underbrace{\langle \psi_0 \psi_0 \rangle}_{=1} \langle \psi_2 \psi_2 \rangle = \langle \psi_2 \psi_2 \rangle,$$

where we used the Cauchy–Schwarz inequality. The term on the right-hand-side can be written as

$$\langle \psi_2 \psi_2 \rangle = \left\langle \hat{T}\psi_0, \hat{T}\psi_0 \right\rangle = \left\langle \psi_0, \hat{T}^2\psi_0 \right\rangle = \left\langle \psi_0, \hat{T}\psi_0 \right\rangle \left\langle \psi_1, \hat{T}\psi_1 \right\rangle.$$

Plugging the last equation into the inequality we get

$$\left\langle \psi_0, \hat{T}\psi_0 \right\rangle^2 \le \left\langle \psi_0, \hat{T}\psi_0 \right\rangle \left\langle \psi_1, \hat{T}\psi_1 \right\rangle \quad \text{or} \quad \boxed{\left\langle \psi_0, \hat{T}\psi_0 \right\rangle \le \left\langle \psi_1, \hat{T}\psi_1 \right\rangle}.$$

Finally, the expectation value of $\hat{T}$ in the ψ state is

$$\begin{aligned}\left\langle \psi, \hat{T}\psi \right\rangle &= \left\langle \left(c_0\psi_0 + c_1\psi_1\right), \hat{T}\left(c_0\psi_0 + c_1\psi_1\right) \right\rangle \\ &= |c_0|^2 \left\langle \psi_0, \hat{T}\psi_0 \right\rangle + c_0^* c_1 \cancel{\left\langle \psi_0, \hat{T}\psi_1 \right\rangle} + c_0 c_1^* \cancel{\left\langle \psi_1, \hat{T}\psi_0 \right\rangle} + |c_1|^2 \left\langle \psi_1, \hat{T}\psi_1 \right\rangle\end{aligned}$$

but since $\left\langle \psi_0, \hat{T}\psi_0 \right\rangle \le \left\langle \psi_1, \hat{T}\psi_1 \right\rangle$ and $|c_0|^2 + |c_1|^2 = 1$, then

$$\boxed{\left\langle \psi, \hat{T}\psi \right\rangle \le \left\langle \psi_1, \hat{T}\psi_1 \right\rangle \quad \text{and} \quad \left\langle \psi, \hat{T}\psi \right\rangle \ge \left\langle \psi_0, \hat{T}\psi_0 \right\rangle},$$

That is

$$\boxed{\left\langle \psi_1, \hat{T}\psi_1 \right\rangle \ge \left\langle \psi, \hat{T}\psi \right\rangle \ge \left\langle \psi_0, \hat{T}\psi_0 \right\rangle}.$$

4. This is a manifestation of the position-momentum uncertainty principle $(\Delta x)^2 (\Delta p)^2 \ge \hbar^2/4$, where $(\Delta q)^2 = \langle q^2 \rangle - \langle q \rangle^2$. But we've already calculated $\langle \psi_i, \hat{x}\psi_i \rangle = \langle \psi_i, \hat{p}\psi_i \rangle = 0$, thus

$$(\Delta x)_i^2 = \langle \hat{x}^2 \rangle_i \quad \text{and} \quad (\Delta p)_i^2 = \langle \hat{p}^2 \rangle_i.$$

Recalling that $\hat{T} = \hat{p}^2/2m$, the left-hand-side term follows

$$\langle \psi_0, \hat{x}^2\psi_0 \rangle \langle \psi_1, \hat{p}^2\psi_1 \rangle \ge \langle \psi_0, \hat{x}^2\psi_0 \rangle \langle \psi_0, \hat{p}^2\psi_0 \rangle = (\Delta x)_0^2 (\Delta p)_0^2 \ge \frac{\hbar^2}{4},$$

hence

$$\boxed{\langle \psi_0, \hat{x}^2\psi_0 \rangle \langle \psi_1, \hat{p}^2\psi_1 \rangle \ge \frac{\hbar^2}{4}}.$$

Question 3:

A system is made so that in time $t = 0$ the wave function is given by

$$\psi(x) = N e^{ik_0 x} e^{-\frac{x^2}{2a^2}}.$$

The dispersion relation is given by $\omega(k) = \hbar k^2/2m$ (i.e. a free particle). Find:

1. $|N|$.
2. $\tilde{\psi}(k)$.
3. $\rho(x,0)$, $\langle x\rangle(t=0)$, $\Delta x(t=0)$ and $J(x,0)$.

Solution:

1. Using the normalization condition

$$\langle\psi,\psi\rangle = \int_{-\infty}^{\infty}\psi^*\psi dx = |N|^2\int_{-\infty}^{\infty} e^{-\frac{x^2}{a^2}}dx = |N|^2\sqrt{\pi a^2} = 1,$$

we get

$$\boxed{|N| = \left(\pi a^2\right)^{-1/4}}.$$

2. The Fourier transform is

$$\tilde{\psi}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x)\,e^{-ikx}dx = \frac{N}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{x^2}{2a^2}}e^{-i(k-k_0)x}dx,$$

using the common form of the integral

$$\int_{-\infty}^{\infty} e^{-ax^2-ikx}dx = \sqrt{\frac{\pi}{a}}e^{-\frac{k^2}{4a}},$$

with $a\to 1/2a^2$ and $k\to k-k_0$, we find

$$\boxed{\tilde{\psi}(k) = Na^2e^{-\frac{a^2(k-k_0)^2}{2}}}.$$

3. The initial position probability density is

$$\boxed{\rho(x,0) = |\psi|^2 = |N|^2\,e^{-\frac{x^2}{a^2}}}.$$

The initial position expectation value is

$$\boxed{\langle x\rangle(t=0) = \int_{-\infty}^{\infty}\psi^* x\psi dx = |N|^2\int_{-\infty}^{\infty}\underbrace{xe^{-\frac{x^2}{a^2}}}_{\text{odd}}dx = 0},$$

thus the initial uncertainty in the position is

$$\boxed{\Delta x(t=0) = \left\langle x^2\right\rangle^{1/2} = \left[|N|^2\int_{-\infty}^{\infty}x^2e^{-\frac{x^2}{a^2}}dx\right]^{1/2} = \frac{a}{\sqrt{2}}}.$$

The initial probability density current is

$$\boxed{J(x,0) = \frac{\hbar}{m}\text{Im}\left[\psi^*\frac{d\psi}{dx}\right] = \frac{\hbar}{m}\text{Im}\left[|N|^2\left(ik_0-\frac{x}{a^2}\right)e^{-\frac{x^2}{a^2}}\right] = \frac{\hbar k_0}{m}|N|^2\,e^{-\frac{x^2}{a^2}} = v_g(k_0)\,\rho(x,0)}.$$