Tutorial 5 - Wave Function

Question 1:

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

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

Consider the linear combination

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

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

1. Show that $\psi_0(x)$ and $\psi_1(x)$ are orthogonal and that $\psi(x)$ is normalized.
2. Compute the expectation values $\langle x\rangle$, $\langle p\rangle$ in the states $\psi_0(x)$, $\psi_1(x)$ and $\psi(x)$.
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

$$\psi_1(-x) = N\frac{d\psi_0(-x)}{d(-x)} = -N\frac{d\psi_0(x)}{dx} = -\psi_1(x).$$

   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 position operator $\hat{x}$ are

$$\langle \psi_0, \hat{x}\psi_0 \rangle = \int_\Omega \psi_0^* \hat{x} \psi_0 dx = \int_\Omega \underbrace{\psi_0^2 x}_{\text{odd}} \, dx = 0,$$

$$\langle \psi_1, \hat{x}\psi_1 \rangle = \int_\Omega \psi_1^* \hat{x} \psi_1 dx = -\int_\Omega \underbrace{\psi_1^2 x}_{\text{odd}} \, dx = 0.$$

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

Therefore

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

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

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

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

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

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

$$\boxed{\langle \psi_0, \hat{p}\psi_0 \rangle \qquad \langle \psi_1, \hat{p}\psi_1 \rangle = 0 \qquad \langle \psi, \hat{p}\psi \rangle = 2\hbar \mathrm{Im}\left[\frac{c_0 c_1^*}{N} \right]}.$$

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

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

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

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

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

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

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

$$\begin{aligned} \left\langle \psi, \hat{T}\psi \right\rangle &= \left(1 - |c_1|^2\right) \left\langle \psi_0, \hat{T}\psi_0 \right\rangle + |c_1|^2 \left\langle \psi_1, \hat{T}\psi_1 \right\rangle \\ &= \left\langle \psi_0, \hat{T}\psi_0 \right\rangle + |c_1|^2 \underbrace{\left(\left\langle \psi_1, \hat{T}\psi_1 \right\rangle - \left\langle \psi_0, \hat{T}\psi_0 \right\rangle\right)}_{>0}, \end{aligned}$$

$$\left\langle \psi, \hat{T}\psi \right\rangle = \left\langle \psi_1, \hat{T}\psi_1 \right\rangle + |c_0|^2 \underbrace{\left(\left\langle \psi_0, \hat{T}\psi_0 \right\rangle - \left\langle \psi_1, \hat{T}\psi_1 \right\rangle\right)}_{<0},$$

Hence

$$\boxed{\left\langle \psi, \hat{T}\psi \right\rangle \leq \left\langle \psi_1, \hat{T}\psi_1 \right\rangle \quad \text{and} \quad \left\langle \psi, \hat{T}\psi \right\rangle \geq \left\langle \psi_0, \hat{T}\psi_0 \right\rangle}.$$

That is

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

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

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

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

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

hence

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

Question 2:

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

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

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

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

thus the initial uncertainty in the position is

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

The initial probability density current is

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