# Tutorial 4 - Wave Function

## Question 1:

Given the wave function

$$\psi(x) = \begin{cases} N & |x| \le x_0 \\ 0 & |x| > x_0 \end{cases}$$

1. Find $N$.
2. The Fourier transform $\tilde{\psi}(k)$.
3. Show that $\int_{-\infty}^{\infty} \left|\tilde{\psi}(k)\right|^2 dk = 1$. What is the meaning of $\left|\tilde{\psi}(k)\right|^2$?
4. Write an expression for $\langle x^n \rangle$ and calculate $\langle x \rangle$, $\langle x^2 \rangle$ and $\Delta x$.
5. Write an expression for $\langle k^n \rangle$ and calculate $\langle k \rangle$, $\langle k^2 \rangle$ and $\Delta k$.
6. What is $\Delta x \Delta k$? Explain.

**Solution:**

1. Using the normalization condition

$$\int_{-x_0}^{x_0} |N|^2 dx = 1 \quad \rightarrow \quad \boxed{N = \sqrt{\frac{1}{2x_0}}}.$$

2. The Fourier transform is

$$\begin{aligned} \tilde{\psi}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx \\ &= \frac{N}{\sqrt{2\pi}} \int_{-x_0}^{x_0} e^{-ikx} dx \\ &= \frac{1}{2\sqrt{x_0\pi}} \left[ \frac{e^{ikx_0}}{ik} - \frac{e^{-ikx_0}}{ik} \right], \end{aligned}$$

thus

$$\boxed{\tilde{\psi}(k) = \frac{1}{\sqrt{x_0\pi}} \frac{\sin kx_0}{k}}.$$

3. Checking the normalization in $k$-space reads

$$\int_{-\infty}^{\infty} \left|\tilde{\psi}(k)\right|^2 dk = \frac{1}{\pi x_0} \int_{-\infty}^{\infty} \frac{\sin^2 kx_0}{k^2} dk = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\sin^2 u}{u^2} du,$$

using the definite integral $\int_{-\infty}^{\infty} \sin^2 x / x^2 dx = \pi$ we get

$$\boxed{\int_{-\infty}^{\infty} \left|\tilde{\psi}(k)\right|^2 dk = 1}.$$

This result suggests that $\left|\tilde{\psi}(k)\right|^2$ is a probability density $\tilde{\rho}(k)$ - in this case for finding the particle or system with momentum $p = \hbar k$.

4. The expectation value for $x^n$ is

$$\langle x^n \rangle = \int_{-\infty}^{\infty} \psi^* (x) x^n \psi (x) dx = \int_{-x_0}^{x_0} |N|^2 x^n dx = \frac{1}{2x_0} \frac{x_0^{n+1} \left[1 - (-1)^{n+1}\right]}{n+1}$$

hence

$$\boxed{\langle x^n \rangle = \frac{x_0^n}{2(n+1)} (1 + (-1)^n)}.$$

Using this expression it is easy to find

$$\boxed{\langle x \rangle = 0 \quad \text{and} \quad \left\langle x^2 \right\rangle = \frac{x_0^2}{3}},$$

thus

$$\boxed{\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{x_0}{\sqrt{3}}}.$$

5. The expectation value for $k^n$ is

$$\langle k^n \rangle = \int_{-\infty}^{\infty} \tilde{\psi}^* (k) k^n \tilde{\psi} (k) dk = \frac{1}{x_0 \pi} \int_{-\infty}^{\infty} \frac{\sin^2 k x_0}{k^2} k^n dk,$$

which can be solved for particular values of $n$. It is easy to see than for $n = 1$ the integrand is an odd function, hence the integral vanishes, whereas for $n = 2$ we need to solve the integral

$$\int_{-\infty}^{\infty} \sin^2 k x_0 dk = \frac{1}{2} \int_{-\infty}^{\infty} (1 - \cos 2 k x_0) dk \to \infty.$$

Therefore

$$\boxed{\langle k \rangle = 0 \quad \text{and} \quad \left\langle k^2 \right\rangle \to \infty},$$

so that even though the wave function is normalizable, its second moment diverges, which leads to $\boxed{\Delta k \to \infty}$.

6. The uncertainty principle, $\Delta x \Delta k \geq 1/2$ still holds in this case.

## Question 2:

The wave function of a particle is given

$$\psi (r) = N e^{-\alpha r},$$

where $r = |\boldsymbol{r}|$, $N$ is a constant and $\alpha > 0$ is a real constant.

1. Find $N$.
2. Find the expectation values $\langle \boldsymbol{r} \rangle$, $\langle r \rangle$, $\left\langle r^2 \right\rangle$.
3. Find the variances $(\Delta \boldsymbol{r})^2$ and $(\Delta r)^2$.
4. What is the probability to find the particle in the region $r > \Delta r$?
5. Find the time dependent Fourier transform $\tilde{\psi} (k, t)$, for a free particle (i.e. $\omega (k) = \hbar k^2 / 2m$)
6. Find the variance $(\Delta \boldsymbol{k})^2$ and $(\Delta k)^2$.
7. Show that the wave function is isotropic at all times, i.e. $\psi (\boldsymbol{r}, t) = \psi (r, t)$.
8. Find $\langle \boldsymbol{r} (t) \rangle$.

**Solution:**

1. Using the normalization condition

$$\int \psi^* (r) \psi (r) \, d^3r = 1,$$

where $d^3x = r^2 \sin\theta \, d\theta \, d\varphi \, dr$, we have

$$\begin{aligned} 4\pi |N|^2 \int_0^\infty r^2 e^{-2\alpha r} dr &= \pi |N|^2 \frac{\partial^2}{\partial \alpha^2} \int_0^\infty e^{-2\alpha r} dr \\ &= \pi |N|^2 \frac{\partial^2}{\partial \alpha^2} \left( \frac{1}{2\alpha} \right) \\ &= |N|^2 \frac{\pi}{\alpha^3}, \end{aligned}$$

thus

$$\boxed{|N| = \sqrt{\frac{\alpha^3}{\pi}}}.$$

2. The expectation value for $\boldsymbol{r}$ vanishes due to symmetry, as can be seen from

$$\langle \boldsymbol{r} \rangle = \int \psi^* (r) \, r \left( \sin\theta \cos\phi \hat{\boldsymbol{x}} + \sin\theta \sin\phi \hat{\boldsymbol{y}} + \cos\theta \hat{\boldsymbol{z}} \right) \psi (r) \, r^2 \sin\theta \, d\theta \, d\varphi \, dr = 0,$$

since

$$\int_0^\pi \cos\theta \sin\theta \, d\theta = \int_0^{2\pi} \sin\varphi \, d\varphi = \int_0^{2\pi} \cos\varphi \, d\varphi = 0.$$

While $r$'s $n$th moment is

$$\begin{aligned} \langle r^n \rangle &= \int \psi^* (r) \, r^n \psi (r) \, r^2 \sin\theta \, d\theta \, d\varphi \, dr \\ &= 4\alpha^3 \int_0^\infty r^{n+2} e^{-2\alpha r} dr \\ &= 4\alpha^3 \left( -\frac{1}{2} \right)^{n+2} \frac{\partial^{n+2}}{\partial \alpha^{n+2}} \int_0^\infty e^{-2\alpha r} dr \\ &= 4\alpha^3 \left( -\frac{1}{2} \right)^{n+2} \frac{\partial^{n+2}}{\partial \alpha^{n+2}} \left( \frac{1}{2\alpha} \right) \\ &= 2\alpha^3 \left( -\frac{1}{2} \right)^{n+2} (-1)^{n+2} \frac{(n+2)!}{\alpha^{n+3}} \end{aligned}$$

so that

$$\langle r^n \rangle = \frac{(n+2)!}{2^{n+1} \alpha^n}.$$

Therefore,

$$\boxed{\langle r \rangle = \frac{3}{2\alpha} \quad \text{and} \quad \langle r^2 \rangle = \frac{3}{\alpha^2}}.$$

3. Since $\boldsymbol{r}^2 = \boldsymbol{r} \cdot \boldsymbol{r} = r^2$ we have $\langle \boldsymbol{r}^2 \rangle = \langle r^2 \rangle$, leaving us

$$\boxed{(\Delta \boldsymbol{r})^2 = \langle \boldsymbol{r}^2 \rangle - \langle \boldsymbol{r} \rangle^2 = \langle r^2 \rangle = \frac{3}{\alpha^2} \quad \text{and} \quad (\Delta r)^2 = \langle r^2 \rangle - \langle r \rangle^2 = \frac{3}{4\alpha^2}}.$$

4. The probability for finding the particle in the region $r > \Delta r$ is

$$
\begin{aligned}
P(r > \Delta r) &= \int_{r>\Delta r} \psi^*(r)\,\psi(r)\,d^3r \\
&= 4\alpha^3 \int_{\Delta r}^{\infty} r^2 e^{-2\alpha r}\,dr \\
&= \alpha^3 \frac{\partial^2}{\partial\alpha^2} \int_{\Delta r}^{\infty} e^{-2\alpha r}\,dr \\
&= \alpha^3 \frac{\partial^2}{\partial\alpha^2} \left(\frac{e^{-2\alpha\Delta r}}{2\alpha}\right) \\
&= \alpha^3 \frac{\partial}{\partial\alpha} \left(-\Delta r \frac{e^{-2\alpha\Delta r}}{\alpha} - \frac{e^{-2\alpha\Delta r}}{2\alpha^2}\right) \\
&= \alpha^3 \left(2(\Delta r)^2 \frac{e^{-2\alpha\Delta r}}{\alpha} + 2\Delta r \frac{e^{-2\alpha\Delta r}}{\alpha^2} + \frac{e^{-2\alpha\Delta r}}{\alpha^3}\right),
\end{aligned}
$$

plugging $\Delta r = \sqrt{3}/2\alpha$ yields

$$
\boxed{P(r > \Delta r) = \left(\frac{3}{2} + \sqrt{3} + 1\right) e^{-\sqrt{3}} \approx 0.749}.
$$

5. The Fourier transform in the free particle scenario is

$$
\begin{aligned}
\tilde{\psi}(\boldsymbol{k}) &= \frac{1}{(2\pi)^{3/2}} \int \psi(r)\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\, d^3r \\
&= \frac{\sqrt{\alpha^3}}{\pi^2 2^{3/2}} \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\varphi \int_0^{\infty} e^{-\alpha r} e^{-ikr\cos\theta} r^2\, dr \\
&= \frac{\sqrt{\alpha^3}}{\pi 2^{1/2}} \int_0^{\infty} dr \int_{-1}^{1} e^{-\alpha r} e^{-ikr\cos\theta} r^2\, d\cos\theta \\
&= \frac{\sqrt{\alpha^3}}{\pi 2^{1/2}} \int_0^{\infty} e^{-\alpha r} \frac{e^{ikr} - e^{-ikr}}{ikr} r^2 dr \\
&= \frac{\sqrt{\alpha^3}}{ik\pi 2^{1/2}} \int_0^{\infty} \left(e^{(ik-\alpha)r} - e^{-(ik+\alpha)r}\right) r dr \\
&= \frac{\sqrt{\alpha^3}}{ik\pi 2^{1/2}} \frac{\partial}{\partial\lambda} \int_0^{\infty} \left(\frac{e^{(ik-\alpha)\lambda r}}{ik-\alpha} + \frac{e^{-(ik+\alpha)\lambda r}}{ik+\alpha}\right) dr \Bigg|_{\lambda=1} \\
&= \frac{\sqrt{\alpha^3}}{ik\pi 2^{1/2}} \frac{\partial}{\partial\lambda} \left(-\frac{1}{(ik-\alpha)^2\lambda} + \frac{1}{(ik+\alpha)^2\lambda}\right) \Bigg|_{\lambda=1} \\
&= \frac{\sqrt{\alpha^3}}{ik\pi 2^{1/2}} \left(\frac{1}{(ik-\alpha)^2} - \frac{1}{(ik+\alpha)^2}\right) \\
&= \frac{\sqrt{\alpha^3}}{ik\pi 2^{1/2}} \frac{4ik\alpha}{(k^2+\alpha^2)^2},
\end{aligned}
$$

thus

$$
\boxed{\tilde{\psi}(\boldsymbol{k}, t) = 4\sqrt{\frac{\alpha^5}{2\pi^2}} \frac{e^{-i\frac{\hbar k^2}{2m}t}}{(k^2+\alpha^2)^2}},
$$

which is isotropic as well.

6. As we saw for $\langle \boldsymbol{r} \rangle$, the expectation value for $\langle \boldsymbol{k} \rangle$ vanishes due to symmetry, whereas the first two moments of

$\tilde{\psi}(\boldsymbol{k})$ are

$$\begin{aligned}\langle k\rangle &= \int \tilde{\psi}^*(k)\,k\tilde{\psi}(k)\,k^2\sin\theta\,d\theta\,d\varphi\,dk\\ &= 32\frac{\alpha^5}{\pi}\int_0^\infty \frac{k^3}{(k^2+\alpha^2)^4}dk,\end{aligned}$$

changing variables to

$$u = k^2+\alpha^2 \quad \text{so that} \quad du = 2kdk, \quad \text{and} \quad k^2 = u-\alpha^2,$$

we get

$$\langle k\rangle = 16\frac{\alpha^5}{\pi}\int_{\alpha^2}^\infty \frac{u-\alpha^2}{u^4}du = 16\frac{\alpha^5}{\pi}\left(\frac{1}{2\alpha^4}-\frac{\alpha^2}{3\alpha^6}\right),$$

hence

$$\boxed{\langle k\rangle = \frac{8\alpha}{3\pi}}.$$

In the same manner

$$\begin{aligned}\langle k^2\rangle &= \int \tilde{\psi}^*(k)\,k^2\tilde{\psi}(k)\,k^2\sin\theta\,d\theta\,d\varphi\,dk\\ &= 32\frac{\alpha^5}{\pi}\int_0^\infty \frac{k^4}{(k^2+\alpha^2)^4}dk,\end{aligned}$$

which can be solved by using partial fractions and trigonometric variables to yield

$$\boxed{\langle k^2\rangle = \alpha^2}.$$

Therefore $\boxed{(\Delta\boldsymbol{k})^2 = \alpha^2}$, whereas $\boxed{(\Delta k)^2 = \alpha^2\left(1-\frac{64}{9\pi^2}\right)\approx 0.28\alpha^2}$.

7. It is clear that, since $\tilde{\psi}(k,t)$ is independent of $\theta$ and $\varphi$, that its inverse Fourier transform will be isotropic as well.
8. Since $\psi(r,t)$ is isotropic, it is, as we've seen before, clear that $\langle\boldsymbol{r}(t)\rangle = 0$.

# Question 3:

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 integrand a little

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

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

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

Plugging this expression into the integral above we get

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

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

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

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

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

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