

Tutorial 3 - Wave Function

Question 1:

Given the wave function

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

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

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

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

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

This result suggests that $|\tilde{\psi}(k)|^2$ 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

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

hence

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

Using this expression it is easy to find

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

thus

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

5. The expectation value for k^n is

$$\langle k^n \rangle = \int_{-\infty}^{\infty} \tilde{\psi}^*(k) k^n \tilde{\psi}(k) dk = \frac{1}{x_0 \pi} \int_{-\infty}^{\infty} \frac{\sin^2 kx_0}{k^2} k^n dk,$$

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

$$\int_{-\infty}^{\infty} \sin^2 kx_0 dk = \frac{1}{2} \int_{-\infty}^{\infty} (1 - \cos 2kx_0) dk \rightarrow \infty.$$

Therefore

$$\langle k \rangle = 0 \quad \text{and} \quad \langle k^2 \rangle \rightarrow \infty,$$

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

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

1. Find N .
2. Find the expectation values $\langle \mathbf{r} \rangle$, $\langle r \rangle$, $\langle r^2 \rangle$.
3. Find the variances $(\Delta \mathbf{r})^2$ 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 $(\Delta \mathbf{k})^2$ and $(\Delta k)^2$.
7. Show that the wave function is isotropic at all times, i.e. $\psi(\mathbf{r}, t) = \psi(r, t)$.
8. Find $\langle \mathbf{r}(t) \rangle$.

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 \mathbf{r} vanishes due to symmetry, as can be shown from

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

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 $\mathbf{r}^2 = \mathbf{r} \cdot \mathbf{r} = r^2$ we have $\langle \mathbf{r}^2 \rangle = \langle r^2 \rangle$, leaving us

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

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

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

5. The Fourier transform in the free particle scenario is

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

thus

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

which is isotropic as well.

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

$\tilde{\psi}(\mathbf{k})$ 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

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

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 $\boxed{(\Delta \mathbf{k})^2 = \alpha^2}$, 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 θ and φ , 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 $\langle \mathbf{r}(t) \rangle = 0$.