Quantum Mechanics

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PROBLEM SET 1

Problem 1. The wave function for a free particle is given by

$$\psi(x,\,0) = N\exp\left(i\frac{p_0 x}{\hbar} - \frac{(x-x_0)^2}{4\sigma^2}\right),$$

where $\sigma \in \mathbb{R}$ is a contant and N is a normalization constant.

(1) Derive the normalization constant N.

(2) Derive the wave function $\phi(0,\,0)$ in momentum space.

(3) Find $\phi(p,\,t)$.

(4) Find $\psi(x\,t)$.

(5) Show that the the spread in the spatial probability distribution increases with time t. Note that the spread is defined as

$$\mathcal{S}(t) = \frac{|\psi(x,\,t)|^2}{|\psi(0,t)|^2}.$$

Solution :

(1) From the normalization of the wave function,

$$\int_{-\infty}^{\infty} |\psi(x,0)|^2\,dx = N^2\int_{-\infty}^{\infty}\exp\left(-2\left(\frac{x-x_0}{2\sigma}\right)^2\right)\,dx = 1.$$

Since a range of integration is all space, the translation about x can be ignored. To make a compact form, it needs to change an integral variable.

$$t \equiv \left(\frac{x-x_0}{\sqrt{2}\sigma}\right), \quad dt = \frac{1}{\sqrt{2}\sigma}dx$$

Then the wave function changes into more comfort form to integrate.

$$\int_{-\infty}^{\infty}\exp\left(-2\left(\frac{x-x_0}{2\sigma}\right)^2\right)\,dx = \sqrt{2}\sigma\int_{-\infty}^{\infty} e^{-t^2}\,dt \tag{1}$$

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To calcualte this integration, we use a idea of double integration,

$$\int_{-\infty}^{\infty} e^{-(x^2+y^2)}\,dx\,dy = \int_0^{2\pi}\int_0^{\infty} e^{-r^2} r\,dr\,d\theta$$
$$= \int_0^{2\pi} \frac{1}{2}\,d\theta = \pi.$$

First double integration about coordinate space can be decomposed.

$$\int_{-\infty}^{\infty} e^{-(x^2+y^2)}\,dx\,dy = \int_{-\infty}^{\infty} e^{-x^2}\,dx \int_{-\infty}^{\infty} e^{-y^2}\,dy = \left(\int_{-\infty}^{\infty} e^{-x^2}\,dx\right)^2$$

From this result,

$$\int_{-\infty}^{\infty} e^{-x^2}\,dx = \sqrt{\pi}, \quad \sqrt{2\pi}\sigma N^2 = 1.$$

Finally we obtain the normalization constant,

$$N = \left(\frac{1}{2\pi\sigma^2}\right)^{\frac{1}{4}}. \tag{2}$$

(2) We will find $\phi(p,0)$ first. $\phi(p,0)$ is the Fourier transform of $\psi(x,0)$.

$$\phi(p,0) = \frac{1}{\sqrt{2\pi\hbar}}\int \psi(x,0)e^{-\frac{i}{\hbar}px}\,dx = \frac{N}{\sqrt{2\pi\hbar}}\int \exp\left(i\frac{p_0 x}{\hbar} - \left(\frac{x-x_0}{2\sigma}\right)^2\right)e^{-\frac{i}{\hbar}px}\,dx$$
$$= \frac{N}{\sqrt{2\pi\hbar}}\int \exp\left(-\left(\frac{x-x_0}{2\sigma}\right)^2 - \frac{i}{\hbar}(p-p_0)x\right)\,dx$$

To make it compact form, let us erase the translation term and change the variable.

$$u \equiv \frac{x-x_0}{2\sigma}, \quad du = \frac{1}{2\sigma}dx$$

Then, a $\phi(p,0)$ is,

$$\phi(p,0) = \frac{2\sigma N}{\sqrt{2\pi\hbar}}\int \exp\left(-u^2 - \frac{i}{\hbar}(p-p_0)(2\sigma u + x_0)\right)\,du$$
$$= \left(\frac{2\sigma^2}{\pi^3\hbar^2}\right)^{\frac{1}{4}} e^{-\frac{i}{\hbar}(p-p_0)x_0}\int \exp\left(-u^2 - 2\frac{i}{\hbar}\sigma(p-p_0)u\right)\,du.$$

And, a exponential of integrated function can be expressed in terms of complete square form about u.

$$-u^2 - 2\frac{i}{\hbar}\sigma(p-p_0)u = -\left(u + \frac{i}{\hbar}\sigma(p-p_0)\right)^2 - \frac{\sigma^2}{\hbar^2}(p-p_0)^2 \tag{3}$$

$\frac{i}{\hbar}\sigma p$ is the translation term that can be ignored since the integration range is from $-\infty$ to ∞,

$$\phi(p,0) = \left(\frac{2\sigma^2}{\pi^3\hbar^2}\right)^{\frac{1}{4}} e^{-\frac{i}{\hbar}(p-p_0)x_0}\int \exp\left(-u^2 - 2\frac{i}{\hbar}\sigma(p-p_0)u\right)\,du$$
$$= \left(\frac{2\sigma^2}{\pi^3\hbar^2}\right)^{\frac{1}{4}} e^{-\frac{i}{\hbar}(p-p_0)x_0}\int \exp\left(-\left(u + \frac{i}{\hbar}\sigma(p-p_0)\right)^2 - \frac{\sigma^2}{\hbar^2}(p-p_0)^2\right)\,du$$
$$= \left(\frac{2\sigma^2}{\pi^3\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\frac{i}{\hbar}(p-p_0)x_0 - \frac{\sigma^2}{\hbar^2}(p-p_0)^2\right)\int e^{-u^2}\,du$$

So, we obtain a $\phi(p.0)$.

$$\phi(p,0) = \left(\frac{2\sigma^2}{\pi^3\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\frac{i}{\hbar}(p-p_0)x_0 - \frac{\sigma^2}{\hbar^2}(p-p_0)^2\right)\int e^{-u^2}\,du$$
$$= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\frac{i}{\hbar}(p-p_0)x_0 - \frac{\sigma^2}{\hbar^2}(p-p_0)^2\right)$$

Finally, $\phi(0,0)$ is,

$$\phi(0,0) = \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\frac{\sigma^2}{\hbar^2}{p_0}^2 + \frac{i}{\hbar}p_0x_0\right). \tag{4}$$

(3) Because it is a free particle, the time evolution of $\phi(p,0)$ is $\phi(p,t) = e^{-i\omega t}\phi(p,0)$ and $\omega = \frac{p^2}{2m\hbar}$.

$$\phi(p,t) = \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\frac{\sigma^2}{\hbar^2}(p-p_0)^2 - i\frac{p^2}{2m\hbar}t - \frac{i}{\hbar}(p-p_0)x_0\right)$$
$$= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\left(\frac{\sigma^2}{\hbar^2} + \frac{it}{2m\hbar}\right)p^2 + \left(\frac{2\sigma^2}{\hbar^2}p_0 - \frac{i}{\hbar}x_0\right)p - \frac{\sigma^2}{\hbar^2}p_0^2 + \frac{i}{\hbar}p_0x_0\right)$$
$$= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\frac{2m\sigma^2 + i\hbar t}{2m\hbar^2}p^2 + \frac{2\sigma^2p_0 - i\hbar x_0}{\hbar^2}p - \frac{\left(\sigma^2p_0 - i\hbar x_0\right)p_0}{\hbar^2}\right)$$

(4) $\psi(x,t)$ is the Fourier transform of $\phi(p,t)$.

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int \phi(p,t)e^{\frac{i}{\hbar}px}\,dp$$
$$= \left(\frac{\sigma^2}{2\pi^3\hbar^4}\right)^{\frac{1}{4}} \int \exp\left(-\frac{2m\sigma^2 + i\hbar t}{2m\hbar^2}p^2 + \frac{2\sigma^2p_0 + i\hbar(x-x_0)}{\hbar^2}p - \frac{\left(\sigma^2p_0 - i\hbar x_0\right)p_0}{\hbar^2}\right)dp \tag{5}$$
$$= \left(\frac{\sigma^2}{2\pi^3\hbar^4}\right)^{\frac{1}{4}} \int \exp\left(-\alpha(t)p^2 + \beta(x)p + \gamma\right)dp$$

$\alpha(t)$, $\beta(t)$ and $\gamma(x,t)$ are the replacement factors that,

$$\alpha(t) = \frac{2m\sigma^2 + i\hbar t}{2m\hbar^2},\ \ \beta(t) = \frac{2\sigma^2p_0 + i\hbar(x-x_0)}{\hbar^2},\ \ \gamma = \frac{\left(\sigma^2p_0 - i\hbar x_0\right)p_0}{\hbar^2} \tag{6}$$

This integration is a type of guassian integration.

$$\int \exp\left(-\alpha(t)p^2 + \beta(x)p + \gamma\right)dp = \sqrt{\frac{\pi}{\alpha(t)}}\exp\left(\frac{(\beta(x))^2}{4\alpha(t)} - \gamma\right) \tag{7}$$

Finally, we obtain $\psi(x,t)$,

$$\psi(x,t) = \left(\frac{\sigma^2}{2\pi\hbar^4}\right)^{\frac{1}{4}}\sqrt{\frac{1}{\alpha(t)}}\exp\left(\frac{(\beta(x))^2}{4\alpha(t)} - \gamma\right) \tag{8}$$
$$= \left(\frac{\sigma^2}{2\pi}\right)^{\frac{1}{4}}\sqrt{\frac{2m}{2m\sigma^2 + i\hbar t}}\exp\left(\frac{m\left(2\sigma^2p_0 + i\hbar(x-x_0)^2\right)\left(2m\sigma^2 - i\hbar t\right)}{2\hbar^2\left(4m^2\sigma^4 + \hbar^2t^2\right)} - \frac{\left(\sigma^2p_0 - i\hbar x\right)p_0}{\hbar^2}\right) \tag{9}$$

(5) Set $\hbar = 1$. Then the probability density is,

$$|\psi(x,t)|^2 = \left(\frac{\sigma^2}{2\pi}\right)^{\frac{1}{2}}\frac{2m}{\sqrt{4m^2\sigma^4 + t^2}}\exp\left(\frac{2m^2\sigma^2\left(4\sigma^4p_0^2 - (x-x_0)^2\right) + 4m\sigma^2p_0(x-x_0)t}{4m^2\sigma^4 + t^2} - 2\sigma^2p_0^2\right)$$
$$= \left(\frac{\sigma^2}{2\pi}\right)^{\frac{1}{2}}\frac{2m}{\sqrt{4m^2\sigma^4 + t^2}}\exp\left(\frac{k(x) + 4m\sigma^2p_0(x-x_0)t}{4m^2\sigma^4 + t^2} - 2\sigma^2p_0^2\right), \tag{10}$$

and $k(x)$ is the replacement factor,

$$k(x) = 2m^2\sigma^2 \left(4\sigma^4 p_0^2 - (x - x_0)^2\right). \tag{11}$$

The spread is,

$$\mathcal{S}(t) = \frac{|\psi(x,\, t)|^2}{|\psi(x, 0)|^2} = \sqrt{\frac{4m^2\sigma^4}{4m^2\sigma^4 + t^2}} \exp\left(\frac{k(x) + 4m\sigma^2 p_0(x - x_0)t}{4m^2\sigma^4 + t^2} - \frac{k(x)}{4m^2\sigma^4}\right) \tag{12}$$

Suppose that $\sigma = 0.6$, $m = 2$, $x_0 = 2$ and $p_0 = 2$. Through the FIG. 1 and FIG. 2, we can confirm that $|\psi|^2$ is spread and the spread $\mathcal{S}(t)$ is increases with time t.

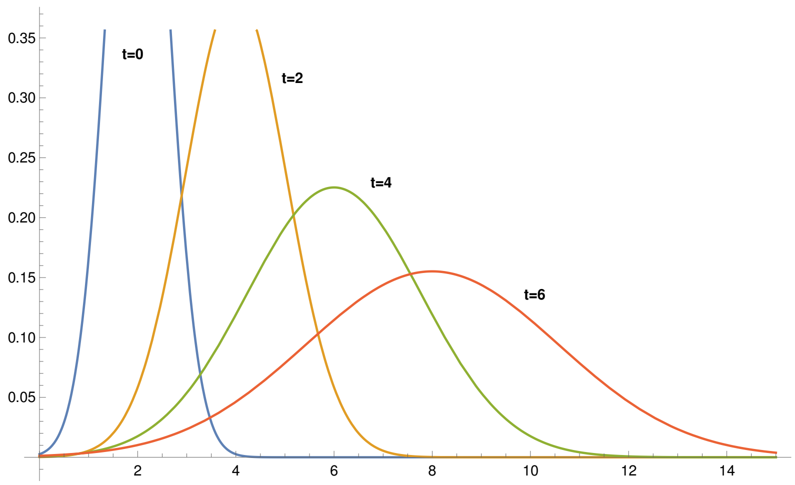

FIG. 1. Normalized $|\psi|^2$ in different time

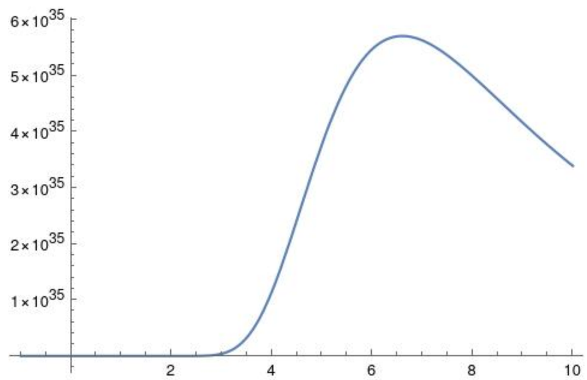

FIG. 2. $\mathcal{S}(t)$ with $x = 10$

Problem 2. The Hamiltonian for a free particle is given by

$$H = \frac{p^2}{2m}.$$

(1) Show

$$\langle p_x \rangle = \langle p_x \rangle_{t=0}.$$

(2) Show

$$\langle x \rangle = \frac{\langle p_x \rangle_{t=0}}{m} t + \langle x \rangle_{t=0}.$$

(3) Show

$$(\Delta p_x)^2 = (\Delta p_x)^2_{t=0}.$$

(4) Find $d(\Delta x)^2/dt$ as a function of time and initial conditions.

Solution :

(1) The expectation value of physical quantity can be expressed in coordinate space and momentum space each other. For free particle, the $\phi(p,t)$ is,

$$\phi(p,t) = e^{-i\frac{p^2}{2m\hbar}t}\phi(p,0). \tag{13}$$

And the expectation value of p_x in the momentum space is,

$$\langle p_x \rangle = \int \phi^*(p,t)\, p_x\, \phi(p,t)\, d^3p = \int e^{i\frac{p^2}{2m\hbar}t}\phi^*(p,0)\, p_x\, e^{-i\frac{p^2}{2m\hbar}t}\phi(p,0)\, d^3p$$

The time evolutions are canceled out.

$$\langle p_x \rangle = \int \phi^*(p,0)\, p_x\, \phi(p,0)\, d^3p = \langle p_x \rangle_{t=0}. \tag{14}$$

(2) The expectation value of x also can be described in the momentum space regarding as the operator in the integration.

$$\begin{aligned}
\langle x \rangle &= i\hbar \int \phi^*(p,t)\frac{\partial \phi(p,t)}{\partial p_x}\, d^3p = i\hbar \int e^{i\frac{p^2}{2m\hbar}t}\phi^*(p,0)\frac{\partial}{\partial p_x}\left(e^{-i\frac{p^2}{2m\hbar}t}\phi(p,0)\right) d^3p \\
&= i\hbar \int e^{i\frac{p^2}{2m\hbar}t}\phi^*(p,0)\left(-i\frac{p_x}{m\hbar}t\, e^{-i\frac{p^2}{2m\hbar}t}\phi(p,0) + e^{-i\frac{p^2}{2m\hbar}t}\frac{\partial \phi(p,0)}{\partial p_x}\right) d^3p \\
&= i\hbar \int -i\frac{p_x}{m\hbar}t\,|\phi(p,0)|^2 + \phi^*(p,0)\frac{\partial \phi(p,0)}{\partial p_x}\, d^3p \\
&= \frac{\langle p_x \rangle_{t=0}}{m}t + \langle x \rangle_{t=0}
\end{aligned} \tag{15}$$

(3) The definition of the deviation is,

$$(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2. \tag{16}$$

We calculate $\langle p_x^2 \rangle$ in the momentum space and $\langle p_x \rangle^2 = \langle p_x \rangle^2_{t=0}$ because of (14).

$$\langle p_x^2 \rangle = \int \phi^*(p,t)\, p_x^2\, \phi(p,t)\, d^3p$$

From (13),

$$\begin{aligned}
\int \phi^*(p,t)\, p_x^2\, \phi(p,t)\, d^3p &= \int e^{i\frac{p^2}{2m\hbar}t}\phi^*(p,0)p_x^2 e^{-i\frac{p^2}{2m\hbar}t}\phi(p,0)\, d^3p \\
&= \int \phi^*(p,0)p_x^2\phi(p,0)\, d^3p = \langle p_x^2 \rangle_{t=0}
\end{aligned}$$

So, we obtain that,

$$\langle p_x^2 \rangle = \langle p_x^2 \rangle_{t=0}. \tag{17}$$

Finally, the result is,

$$(\Delta p_x)^2 = \langle p_x^2 \rangle_{t=0} - \langle p_x \rangle^2_{t=0} = (\Delta p_x)^2_{t=0}, \;\; (\Delta p_x)^2 = (\Delta p_x)^2_{t=0}. \tag{18}$$

(4) From (16), the derivative of the deviation is,

$$\frac{d}{dt}(\Delta x)^2 = \frac{d}{dt}\langle x^2\rangle - \frac{d}{dt}\left(\langle x\rangle^2\right). \tag{19}$$

Before derivation, let us calculate the expectation value $\langle x^2\rangle$ first.

$$\begin{aligned}\langle x^2\rangle =& -\hbar^2\int \phi^*(p,t)\frac{\partial^2\phi(p,t)}{\partial p_x^2}\,d^3p = -\hbar^2\int e^{i\frac{p^2}{2m\hbar}t}\phi^*(p,0)\frac{\partial^2}{\partial p_x^2}\left(e^{-i\frac{p^2}{2m\hbar}t}\phi(p,0)\right)d^3p\\ =& -\hbar^2\int e^{i\frac{p^2}{2m\hbar}t}\phi^*(p,0)\frac{\partial}{\partial p_x}\left(-i\frac{p_x}{m\hbar}te^{-i\frac{p^2}{2m\hbar}t}\phi(p,0)+e^{-i\frac{p^2}{2m\hbar}t}\frac{\partial\phi(p,0)}{\partial p_x}\right)d^3p.\end{aligned}$$

Operate differentiative again,

$$\begin{aligned}\langle x^2\rangle =& -\hbar^2\int \phi^*(p,0)\left[\left(-i\frac{t}{m\hbar}+\left(-i\frac{p_x}{m\hbar}t\right)^2\right)\phi(p,0)-\left(2i\frac{p_x}{m\hbar}t\,\frac{\partial\phi(p,0)}{\partial p_x}-\frac{\partial^2\phi(p,0)}{\partial p_x^2}\right)\right]d^3p\\ =& -\hbar^2\int \phi^*(p,0)\left(-i\frac{t}{m\hbar}+\left(-i\frac{p_x}{m\hbar}t\right)^2\right)\phi(p,0)\,d^3p\\ &+\hbar^2\int \phi^*(p,0)\left(2i\frac{p_x}{m\hbar}t\,\frac{\partial\phi(p,0)}{\partial p_x}-\frac{\partial^2\phi(p,0)}{\partial p_x^2}\right)d^3p.\end{aligned}$$

$i\hbar$ can be ragarded as the canonical commute relation $[x,p_x]$ in the momentum space.

$$\begin{aligned}&-\hbar^2\int \phi^*(p,0)\left(-i\frac{t}{m\hbar}+\left(-i\frac{p_x}{m\hbar}t\right)^2\right)\phi(p,0)\,d^3p = \frac{t}{m}\int i\hbar|\phi(p,0)|^2\,d^3p+\frac{t^2}{m^2}\int p_x^2|\phi(p,0)|^2\,d^3p\\ &=\frac{\langle[x,p_x]\rangle_{t=0}}{m}t+\frac{\langle p_x^2\rangle_{t=0}}{m^2}t^2.\end{aligned}$$

Since x is a operator in the momentum space, the second integration term is,

$$\begin{aligned}\hbar^2\int \phi^*(p,0)\left(2i\frac{p_x}{m\hbar}t\,\frac{\partial\phi(p,0)}{\partial p_x}-\frac{\partial^2\phi(p,0)}{\partial p_x^2}\right)d^3p =& \frac{2t}{m}\int\phi^*(p,0)p_x\left(ih\frac{\partial\phi(p,0)}{\partial p_x}\right)d^3p\\ &+\int\phi^*(p,0)\left(-\hbar^2\frac{\partial^2\phi(p,0)}{\partial p_x^2}\right)d^3p\\ =&\frac{2\langle p_x x\rangle_{t=0}}{m}t+\langle x^2\rangle_{t=0}.\end{aligned}$$

We obtain the expectation value $\langle x^2\rangle$ summing these two result.

$$\langle x^2\rangle = \frac{\langle[x,p_x]\rangle_{t=0}}{m}t+\frac{\langle p_x^2\rangle_{t=0}}{m^2}t^2+\frac{2\langle p_x x\rangle_{t=0}}{m}t+\langle x^2\rangle_{t=0}. \tag{20}$$

What we want is $\frac{d}{dt}(\Delta x)^2$. Differentiative (20),

$$\begin{aligned}\frac{d}{dt}\langle x^2\rangle &= \frac{\langle[x,p_x]\rangle_{t=0}}{m}+\frac{2\langle p_x^2\rangle_{t=0}}{m^2}t+\frac{2\langle p_x x\rangle_{t=0}}{m}\\ &=\frac{\langle xp_x\rangle_{t=0}+\langle p_x x\rangle_{t=0}}{m}+\frac{2\langle p_x^2\rangle_{t=0}}{m^2}t.\end{aligned} \tag{21}$$

Calculate the expectation value of the square.

$$\begin{aligned}\frac{d}{dt}\left(\langle x\rangle^2\right) &= 2\langle x\rangle\frac{d\langle x\rangle}{dt} = 2\left(\frac{\langle p_x\rangle_{t=0}}{m}t+\langle x\rangle_{t=0}\right)\left(\frac{\langle p_x\rangle_{t=0}}{m}\right)\\ &=\frac{2\langle p_x\rangle_{t=0}^2}{m^2}t+\frac{2\langle p_x\rangle_{t=0}\langle x\rangle_{t=0}}{m}.\end{aligned} \tag{22}$$

$\frac{d}{dt}(\Delta x)^2$ is the difference of two values.

$$\begin{aligned}\frac{d}{dt}(\Delta x)^2 &= \frac{d}{dt}\langle x^2\rangle - \frac{d}{dt}\left(\langle x\rangle^2\right)\\ &= \frac{\langle xp_x\rangle_{t=0} + \langle p_x x\rangle_{t=0}}{m} + \frac{2\langle p_x^2\rangle_{t=0}}{m^2}t - \left(\frac{2\langle p_x\rangle_{t=0}^2}{m^2}t + \frac{2\langle p_x\rangle_{t=0}\langle x\rangle_{t=0}}{m}\right)\\ &= \frac{\langle xp_x\rangle_{t=0} + \langle p_x x\rangle_{t=0} - 2\langle p_x\rangle_{t=0}\langle x\rangle_{t=0}}{m} + \frac{2\left(\Delta p_x\right)_{t=0}^2}{m^2}t.\end{aligned} \tag{23}$$

Problem 3. The state of a particle is described by the following wavefunction:

$$\psi(x) = C\exp\left[i\frac{p_0 x}{\hbar} - \frac{(x-x_0)^2}{2\sigma^2}\right].$$

where p_0, x_0, and a are real parameters.

(1) Find the normalization constant C.

(2) Find the mean values of x and p.

(3) Find the standard deviations Δx and Δp.

Solution :

(1) The constant C is calculable from the normalization.

$$C^2\int_{-\infty}^{\infty}\exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right)dx = C^2\int_{-\infty}^{\infty}\exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right)dx = C^2\sigma\sqrt{\pi}.$$

The result of the noramlizatoin is must be 1. So,

$$C = \left(\frac{1}{\sigma\sqrt{\pi}}\right)^{\frac{1}{2}}. \tag{24}$$

(2) First, let us find the mean value of x.

$$\langle x\rangle = \int_{-\infty}^{\infty}\psi^* x\psi\, dx = \frac{1}{\sigma\sqrt{\pi}}\int_{-\infty}^{\infty}x\exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right)dx$$

$$\int_{-\infty}^{\infty}x\exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right)dx = \int_{-\infty}^{\infty}xe^{-\left(\frac{x}{\sigma}\right)^2}dx + x_0\int_{-\infty}^{\infty}e^{-\left(\frac{x}{\sigma}\right)^2}dx.$$

The first term of the right-hand side is a zero because $xe^{-\left(\frac{x}{\sigma}\right)^2}$ is an even function and this integration is from $-\infty$ to ∞. The calculation of the second term is the gaussian integration.

$$x_0\int_{-\infty}^{\infty}e^{-\left(\frac{x}{\sigma}\right)^2}dx = x_0\,\sigma\sqrt{\pi}$$

So, the mean value is a x_0.

$$\langle x\rangle = \frac{1}{\sigma\sqrt{\pi}}x_0\,\sigma\sqrt{\pi} = x_0 \tag{25}$$

The mean value of p is,

$$\begin{aligned}\langle p\rangle &= -i\hbar\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}dx = \frac{-i\hbar}{\sigma\sqrt{\pi}}\int_{-\infty}^{\infty}\left(\frac{i}{\hbar}p_0 - \frac{x-x_0}{\sigma^2}\right)\exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right)dx\\ &= \frac{-i\hbar}{\sigma\sqrt{\pi}}\left[\frac{i}{\hbar}p_0\int_{-\infty}^{\infty}\exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right)dx - \int_{-\infty}^{\infty}\left(\frac{x-x_0}{\sigma^2}\right)\exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right)dx\right] = p_0\end{aligned} \tag{26}$$

Because the second term is a even function about $x = x_0$, it is a zero.

(3) From (16), we use the definition of the deviation.

$$(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2, \quad (\Delta p)^2 = \langle p^2\rangle - \langle p\rangle^2 \tag{27}$$

First we calculate $\langle x^2\rangle$.

$$\begin{aligned}\langle x^2\rangle &= \frac{1}{\sigma\sqrt{\pi}}\int_{-\infty}^{\infty} x^2 \exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right) dx = \frac{1}{\sigma\sqrt{\pi}}\int_{-\infty}^{\infty}(x-x_0)^2 e^{-\left(\frac{x}{\sigma}\right)^2} dx \\ &= \frac{1}{\sigma\sqrt{\pi}}\left[\int_{-\infty}^{\infty} x^2 e^{-\left(\frac{x}{\sigma}\right)^2} dx + 2x_0\int_{-\infty}^{\infty} x e^{-\left(\frac{x}{\sigma}\right)^2} dx + x_0^2\int_{-\infty}^{\infty} e^{-\left(\frac{x}{\sigma}\right)^2} dx\right]\end{aligned}$$

The middle term of the right-hand side is zero from a (2) and the last term is $x_0^2\sigma\sqrt{\pi}$.

$$\int_{-\infty}^{\infty} x^2 e^{-\left(\frac{x}{\sigma}\right)^2} dx = \sigma^3\int_{-\infty}^{\infty} x^2 e^{-x^2} dx = -\frac{1}{2}\sigma^3\left[xe^{-x^2}\right]_{-\infty}^{\infty} + \frac{1}{2}\sigma^3\int_{-\infty}^{\infty} e^{-x^2} dx = \frac{1}{2}\sigma^3\sqrt{\pi}$$

So,

$$\langle x^2\rangle = \frac{1}{\sigma\sqrt{\pi}}\left[x_0^2\sigma\sqrt{\pi} + \frac{1}{2}\sigma^3\sqrt{\pi}\right] = \frac{1}{2}\sigma^2 + x_0^2$$

Then $(\Delta x)^2$ is,

$$(\Delta x)^2 = \frac{1}{2}\sigma^2 + x_0^2 - x_0^2 = \frac{1}{2}\sigma^2 \tag{28}$$

the expectation value of p^2 is,

$$\langle p^2\rangle = -\hbar^2\int_{-\infty}^{\infty}\psi^*\frac{\partial^2\psi}{\partial x^2} dx = -\hbar^2\int_{-\infty}^{\infty}\left(\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x}\right) - \frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x}\right) dx$$

Some of the integration in calculation will be canceled out since these are even functions and the integration range is symmetric.

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x}\right) dx &= \frac{1}{\sigma\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left(\left(\frac{i}{\hbar}p_0 - \frac{x-x_0}{\sigma^2}\right)\exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right)\right) dx = 0 \\ \int_{-\infty}^{\infty}\frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x} dx &= \frac{1}{\sigma\sqrt{\pi}}\int_{-\infty}^{\infty}\left(\left(\frac{p_0}{\hbar}\right)^2 + \left(\frac{x-x_0}{\sigma^2}\right)^2\right)\exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right) dx \\ &= \left(\frac{p_0}{\hbar}\right)^2 + \frac{1}{\sigma^2\sqrt{\pi}}\int_{-\infty}^{\infty} x^2 e^{-x^2} dx\end{aligned}$$

It is the gaussian integration.

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} dx = -\frac{1}{2}\left[xe^{-x^2}\right]_{-\infty}^{\infty} + \frac{1}{2}\int_{-\infty}^{\infty} e^{-x^2} dx = \frac{\sqrt{\pi}}{2}$$

From these results, we can calculate $\langle p^2\rangle$.

$$\langle p^2\rangle = p_0^2 + \frac{\hbar^2}{2\sigma^2}$$

Finally, we can calculate $(\Delta p)^2$,

$$(\Delta p)^2 = p_0^2 + \frac{\hbar^2}{2\sigma^2} - p_0^2 = \frac{\hbar^2}{2\sigma^2}. \tag{29}$$

Confirm these result does satisfy Heisenberg's uncertainty principle.

$$\Delta x\Delta p = \sqrt{\frac{\hbar^2}{2\sigma^2}\frac{\sigma^2}{2}} = \frac{\hbar}{2} \tag{30}$$

We can confirm that this state does not violate Heisenberg's uncertainty principle.

Problem 4*. Consider a particle and two normalized energy eigenfunctions $\psi_1(\boldsymbol{x})$ and $\psi_2(\boldsymbol{x})$ corresponding to the eigenvalues $E_1 \neq E_2$. Assume that the eigenfunctions vanish outside the two non-overlapping regions Ω_1 and Ω_2, respectively.

(1) (a) Show that, if the particle is initially in region Ω_1 then it will stay there forever.

(b) If, initially, the particle is in the state with wave function

$$\psi(\boldsymbol{x}, 0) = \frac{1}{\sqrt{2}}[\psi_1(\boldsymbol{x}) + \psi_2(\boldsymbol{x})]$$

show that the probability density $|\psi(\boldsymbol{x}, t)|^2$ is independent of time.

(c) Now assume that the two regions Ω_1 and Ω_2 overlap partially. Starting with the initial wave function of case (b), show that the probability density is a periodic function of time. ($E_2 - E_1 = \hbar\omega$).

(d) Starting with the same initial wave function and assuming that the two eigenfunctions are real and isotropic, take the two partially overlapping regions Ω_1 and Ω_2 to be two concentric spheres of radii $R_1 > R_2$. Compute the probability current that flows through Ω_1.

Solution :

(a) The initial state is,

$$\psi(\boldsymbol{x}, 0) = c_1\psi_1(\boldsymbol{x}) + c_2\psi_2(\boldsymbol{x})$$

Since this particle is in region Ω_1, $c_1 = 1$ and $c_2 = 0$. The time evolutoin of this particle is,

$$\psi(\boldsymbol{x}, t) = c_1 e^{-\frac{i}{\hbar}E_1 t}\psi_1(\boldsymbol{x}) + c_2 e^{-\frac{i}{\hbar}E_2 t}\psi_2(\boldsymbol{x}) = e^{-\frac{i}{\hbar}E_1 t}\psi_1(\boldsymbol{x})$$

Since the time evolution is dependent to only $\psi_1(\boldsymbol{x})$, it will stay region Ω_1, forever.

(b) The time evolution is,

$$\psi(\boldsymbol{x}, t) = \frac{1}{\sqrt{2}}\left[e^{-\frac{i}{\hbar}E_1 t}\psi_1(\boldsymbol{x}) + e^{-\frac{i}{\hbar}E_2 t}\psi_2(\boldsymbol{x})\right]$$

Consider the probability density of this particle.

$$|\psi(\boldsymbol{x}, t)|^2 = \frac{1}{2}\left[|\psi_1(\boldsymbol{x})|^2 + |\psi_2(\boldsymbol{x})|^2 + e^{-\frac{i}{\hbar}(E_2-E_1)t}\psi_1(\boldsymbol{x})^*\psi_2(\boldsymbol{x}) + e^{-\frac{i}{\hbar}(E_1-E_2)t}\psi_1(\boldsymbol{x})\psi_2(\boldsymbol{x})^*\right] \tag{31}$$

The last two terms are zero. To prove this, consider three divided regions, Ω_1, Ω_2, and Ω_3. The union of three regions is a universal space and there is no intersection of each region. In Ω_1, ψ_2 and ψ_2^* are zero. In Ω_2, ψ_1 and ψ_1^* are zero. Finally, ψ_1 and ψ_2 are zero in Ω_3. For these reason, terms $e^{-\frac{i}{\hbar}(E_2-E_1)t}\psi_1^*\psi_2 + e^{-\frac{i}{\hbar}(E_1-E_2)t}\psi_1\psi_2^*$ are always zero. Therefore,

$$|\psi(\boldsymbol{x}, t)|^2 = \frac{1}{2}\left[|\psi_1(\boldsymbol{x})|^2 + |\psi_2(\boldsymbol{x})|^2\right]. \tag{32}$$

And the probability density is time-independent.

(c) In this case, the last two terms of (31) are not zero. The probability density is,

$$|\psi(\boldsymbol{x}, t)|^2 = \frac{1}{2}\left[|\psi_1(\boldsymbol{x})|^2 + |\psi_2(\boldsymbol{x})|^2 + e^{-i\omega t}\psi_1(\boldsymbol{x})^*\psi_2(\boldsymbol{x}) + e^{i\omega t}\psi_1(\boldsymbol{x})\psi_2^*(\boldsymbol{x})\right]$$

since $E_2 - E_1 = \hbar\omega$. ψ_1 and ψ_2 are the complex function that can be introduced phase factor.

$$\psi_1(\boldsymbol{x}) = |\psi_1(\boldsymbol{x})|e^{i\alpha_1}, \quad \psi_2(\boldsymbol{x}) = |\psi_2(\boldsymbol{x})|e^{i\alpha_2}$$

Then the probability density is,

$$\begin{aligned}|\psi(\boldsymbol{x}, t)|^2 &= \frac{1}{2}\left[|\psi_1(\boldsymbol{x})|^2 + |\psi_2(\boldsymbol{x})|^2 + |\psi_1(\boldsymbol{x})||\psi_2(\boldsymbol{x})|\left(e^{-i(\omega t+\alpha_1-\alpha_2)} + e^{i(\omega t+\alpha_1-\alpha_2)}\right)\right] \\ &= \frac{1}{2}\left[|\psi_1(\boldsymbol{x})|^2 + |\psi_2(\boldsymbol{x})|^2 + 2|\psi_1(\boldsymbol{x})||\psi_2(\boldsymbol{x})|\cos(\omega t + \alpha_1 - \alpha_2)\right].\end{aligned}$$

This result is a periodic function about time because the last term is a periodic function of time and other terms are constant about time.

(d) From the continuity equation, We use the integration of this equation because of the right hand side.

$$\int_{\Omega_2} \frac{\partial \rho}{\partial t}\, dr^3 = \int_{\Omega_2} \nabla \cdot \boldsymbol{J}\, dr^3$$

The left term can be calculated using the result of (c),

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial t}|\psi(\boldsymbol{x}, t)|^2 = -\omega|\psi_1(\boldsymbol{x})||\psi_2(\boldsymbol{x})| \sin(\omega t + \alpha_1 - \alpha_2)$$

If we integrate this about the surface that includes the Ω_2, it will be a zero since ψ_1 and ψ_2 are orthogonal in Ω_2 to each other. Consider the right hand side. This integration is changed into the surface integration following Green's Theorem. Suppose that surfaces of Ω_1 and Ω_2 are S_1 and S_2 respectively. Then,

$$\int_{S_2} \nabla \cdot \boldsymbol{J}\, dr^3 = \int_{S_2} \boldsymbol{J} \cdot d\boldsymbol{S}.$$

Because wave functions are isotropic, a current has the same value in a different direction. It means that this integration is replaced by the just inner product.

$$\int_{\Omega_2} \boldsymbol{J} \cdot d\boldsymbol{S} = 4\pi R_2^2 \boldsymbol{J} \cdot \hat{n}$$

$\hat{n}$ is a vector that is vertical to the surface of a sphere Ω_2. Fianlly,

$$0 = 4\pi R_2^2 \boldsymbol{J} \cdot \hat{n}$$

This means that there is no probability current between region Ω_1 and Ω_2.