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,

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

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 $\psi(x,0)$.

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

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,

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

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 ∞,

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

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

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

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 $\omega = \frac{p^2}{2m\hbar}$.

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

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

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

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

$$\begin{aligned}&\alpha(t) = \frac{2m\sigma^2 + i\hbar t}{2m\hbar^2},\ \ \beta(t) = \frac{m(2\sigma^2p_0 - i\hbar(x+x_0))}{2m\sigma^2 + i\hbar t}, \\ &\gamma(x,t) = \frac{-m\left((x+x_0) + \frac{2i\sigma^2p_0}{\hbar}\right)^2}{4m\sigma^2 + 2i\hbar t} - \frac{(\sigma^2p_0 + i\hbar x_0)p_0}{\hbar^2}\end{aligned} \tag{6}$$

This integration is a type of guassian integration.

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

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

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

(5) The probability density is,

$$|\psi(x,t)|^2 = \sqrt{\frac{2}{\pi}}\left(\frac{m^2\sigma^2}{4m^2\sigma^4 + \hbar^2t^2}\right)e^{|\gamma(x,t)|^2} \tag{9}$$

Then, the spread is,

$$\mathcal{S}(t) = \frac{|\psi(x,\, t)|^2}{|\psi(x, 0)|^2} = \left(\frac{4m^2\sigma^4}{4m^2\sigma^4 + \hbar^2 t^2}\right) e^{|\gamma(x,t)|^2 - |\gamma(x,0)|^2} \tag{10}$$

From (6), $|\gamma(x,t)|^2$

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,

$$\phi(p,t) = e^{-i\frac{p^2}{2m\hbar}t}\phi(p,0). \tag{11}$$

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.

$$\langle p_x \rangle = \int \phi^*(p,0)\, p_x\, \phi(p,0)\, d^3p = \langle p_x \rangle_{t=0}. \tag{12}$$

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

$$\begin{aligned}
\langle x \rangle &= i\hbar \int \phi^*(p,t)\frac{\partial \phi(p,t)}{\partial p_x}\, d^3p = i\hbar \int e^{i\frac{p^2}{2m\hbar}t}\phi^*(p,0)\frac{\partial}{\partial p_x}\left(e^{-i\frac{p^2}{2m\hbar}t}\phi(p,0)\right) d^3p \\
&= i\hbar \int e^{i\frac{p^2}{2m\hbar}t}\phi^*(p,0)\left(-i\frac{p_x}{m\hbar}t\, e^{-i\frac{p^2}{2m\hbar}t}\phi(p,0) + e^{-i\frac{p^2}{2m\hbar}t}\frac{\partial \phi(p,0)}{\partial p_x}\right) d^3p \\
&= i\hbar \int -i\frac{p_x}{m\hbar}t\, |\phi(p,0)|^2 + \phi^*(p,0)\frac{\partial \phi(p,0)}{\partial p_x}\, d^3p \\
&= \frac{\langle p_x \rangle_{t=0}}{m} t + \langle x \rangle_{t=0}
\end{aligned} \tag{13}$$

(3) The definition of the deviation is,

$$(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2. \tag{14}$$

We calculate $\langle p_x^2 \rangle$ in the momentum space and $\langle p_x \rangle^2 = \langle p_x \rangle_{t=0}^2$ because of (12).

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

From (11),

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

So, we obtain that,

$$\langle p_x^2 \rangle = \langle p_x^2 \rangle_{t=0}. \tag{15}$$

Finally, the result is,

$$(\Delta p_x)^2 = \langle p_x^2 \rangle_{t=0} - \langle p_x \rangle_{t=0}^2 = (\Delta p_x)_{t=0}^2, \;\; (\Delta p_x)^2 = (\Delta p_x)_{t=0}^2. \tag{16}$$

(4) From (14), the derivative of the deviation is,

$$\frac{d}{dt}(\Delta x)^2 = \frac{d}{dt}\langle x^2 \rangle - \frac{d}{dt}\left(\langle x \rangle^2\right). \tag{17}$$

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

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

다시 p_x 에 대해 미분해주고, 미분이 존재하는 항과 그렇지 않은 항 끼리 묶어준다.

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

첫번째 적분 항을 먼저 계산해보자. $i\hbar$ 는 momentum space 에서도 canonical commute relation 으로 생각할 수 있다.

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

두번째 적분 항은 다음과 같다. x 는 momentum space 에서 연산자 $i\hbar\frac{\partial}{\partial p_x}$ 로 작용한다는 사실에 유의하자.

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

두 결과를 더해 expectation value $\langle x^2 \rangle$ 를 구할 수 있다.

$$\langle x^2 \rangle = \frac{\langle [x, p_x] \rangle_{t=0}}{m} t + \frac{\langle p_x^2 \rangle_{t=0}}{m^2} t^2 + \frac{2\langle p_x x \rangle_{t=0}}{m} t + \langle x^2 \rangle_{t=0} \tag{18}$$

결국 우리가 구하고자 하는 값 $\frac{d}{dt}(\Delta x)^2$ 을 구하기 위해, t 에 대해 $\langle x^2 \rangle$ 를 미분하자.

$$\begin{aligned}\frac{d}{dt}\langle x^2 \rangle &= \frac{\langle [x, p_x] \rangle_{t=0}}{m} + \frac{2\langle p_x^2 \rangle_{t=0}}{m^2} t + \frac{2\langle p_x x \rangle_{t=0}}{m} \\ &= \frac{\langle x p_x \rangle_{t=0} + \langle p_x x \rangle_{t=0}}{m} + \frac{2\langle p_x^2 \rangle_{t=0}}{m^2} t\end{aligned} \tag{19}$$

expectation value 의 square 를 계산하자.

$$\begin{aligned}\frac{d}{dt}\left(\langle x \rangle^2\right) &= 2\langle x \rangle \frac{d\langle x \rangle}{dt} = 2\left(\frac{\langle p_x \rangle_{t=0}}{m} t + \langle x \rangle_{t=0}\right)\left(\frac{\langle p_x \rangle_{t=0}}{m}\right) \\ &= \frac{2\langle p_x \rangle_{t=0}^2}{m^2} t + \frac{2\langle p_x \rangle_{t=0} \langle x \rangle_{t=0}}{m}\end{aligned} \tag{20}$$

최종적으로, $\frac{d}{dt}(\Delta x)^2$ 는 두 값을 뺀 값이다.

$$\begin{aligned}\frac{d}{dt}(\Delta x)^2 &= \frac{d}{dt}\langle x^2 \rangle - \frac{d}{dt}\left(\langle x \rangle^2\right) \\ &= \frac{\langle x p_x \rangle_{t=0} + \langle p_x x \rangle_{t=0}}{m} + \frac{2\langle p_x^2 \rangle_{t=0}}{m^2} t - \left(\frac{2\langle p_x \rangle_{t=0}^2}{m^2} t + \frac{2\langle p_x \rangle_{t=0} \langle x \rangle_{t=0}}{m}\right) \\ &= \frac{\langle x p_x \rangle_{t=0} + \langle p_x x \rangle_{t=0} - 2\langle p_x \rangle_{t=0} \langle x \rangle_{t=0}}{m} + \frac{2\left(\Delta p_x\right)_{t=0}^2}{m^2} t\end{aligned} \tag{21}$$

$\frac{d}{dt}(\Delta x)^2$ 를 initial conditions 와 t 에 대한 함수로서 나타냈다.

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,

$$C = \left(\frac{1}{\sigma\sqrt{\pi}}\right)^{\frac{1}{2}} \tag{22}$$

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

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

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.

$$\langle x \rangle = \frac{1}{\sigma\sqrt{\pi}} x_0 \, \sigma\sqrt{\pi} = x_0 \tag{23}$$

The mean value of p is,

$$\begin{aligned}\langle p \rangle &= -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx = \frac{-i\hbar}{\sigma\sqrt{\pi}} \int_{-\infty}^{\infty} \left(\frac{i}{\hbar}p_0 - \frac{x-x_0}{\sigma^2}\right) \exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right) dx \\ &= \frac{-i\hbar}{\sigma\sqrt{\pi}} \left[\frac{i}{\hbar}p_0 \int_{-\infty}^{\infty} \exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right) dx - \int_{-\infty}^{\infty} \left(\frac{x-x_0}{\sigma^2}\right) \exp\left(-\left(\frac{x-x_0}{\sigma}\right)^2\right) dx\right] = p_0\end{aligned} \tag{24}$$

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

(3) From (14), we use the definition of the deviation.

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2, \quad (\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2 \tag{25}$$

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

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

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

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

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,

$$(\Delta x)^2 = \frac{1}{2}\sigma^2 + x_0^2 - x_0^2 = \frac{1}{2}\sigma^2 \tag{26}$$

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.

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

It is the gaussian integration.

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

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 $(\Delta p)^2$,

$$(\Delta p)^2 = p_0^2 + \frac{\hbar^2}{2\sigma^2} - p_0^2 = \frac{\hbar^2}{2\sigma^2}. \tag{27}$$

Confirm these result does satisfy Heisenberg's uncertainty principle.

$$\Delta x \Delta p = \sqrt{\frac{\hbar^2}{2\sigma^2} \frac{\sigma^2}{2}} = \frac{\hbar}{2} \tag{28}$$

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.

$$|\psi(\boldsymbol{x},t)|^2 = \frac{1}{2}\left[|\psi_1(\boldsymbol{x})|^2 + |\psi_2(\boldsymbol{x})|^2 + e^{-\frac{i}{\hbar}(E_2-E_1)t}\psi_1(\boldsymbol{x})^*\psi_2(\boldsymbol{x}) + e^{-\frac{i}{\hbar}(E_1-E_2)t}\psi_1(\boldsymbol{x})\psi_2(\boldsymbol{x})^*\right] \tag{29}$$

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,

$$|\psi(\boldsymbol{x},t)|^2 = \frac{1}{2}\left[|\psi_1(\boldsymbol{x})|^2 + |\psi_2(\boldsymbol{x})|^2\right]. \tag{30}$$

And the probability density is time-independent.

(c) In this case, the last two terms of (29) 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.