

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 constant 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 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.

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

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

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

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To calculate 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,

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

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

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

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 .

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

$\frac{i}{\hbar} \sigma p$ 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,

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

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

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

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

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int \phi(p,t) e^{\frac{i}{\hbar}px} dp \quad (5)$$

$$= \left(\frac{\sigma^2}{2\pi^3\hbar^4}\right)^{\frac{1}{4}} \int \exp\left(-\frac{2m\sigma^2 + i\hbar t}{2m\hbar^2}p^2 - \frac{2\sigma^2p_0 - i\hbar(x_0 + x)}{\hbar^2}p - \frac{(\sigma^2p_0 + i\hbar x_0)p_0}{\hbar^2}\right) dp \quad (6)$$

$$= \left(\frac{\sigma^2}{2\pi^3\hbar^4}\right)^{\frac{1}{4}} \int \exp\left(-\frac{2m\sigma^2 + i\hbar t}{2m\hbar^2}p^2 - \frac{2\sigma^2p_0 - i\hbar(x_0 + x)}{\hbar^2}p - \frac{(\sigma^2p_0 + i\hbar x_0)p_0}{\hbar^2}\right) dp \quad (7)$$

$$= \left(\frac{\sigma^2}{2\pi^3\hbar^4}\right)^{\frac{1}{4}} \int \exp\left(\alpha(t)(p + \beta(t))^2 + \gamma(t)\right) dp \quad (8)$$

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

$$\begin{aligned}\alpha(t) &= -\frac{2m\sigma^2 + i\hbar t}{2m\hbar^2}, \quad \beta(t) = \frac{m(2\sigma^2p_0 - i\hbar(x_0 + x))}{2m\sigma^2 + i\hbar t}, \\ \gamma(t) &= -\frac{m\hbar^2(x_0 + x_0)^2 + 4im\hbar\sigma^2p_0 + 2\hbar^2x_0p_0 + 2i\hbar\sigma^2p_0^2}{2\hbar^2(2m\sigma^2 + i\hbar t)}.\end{aligned} \quad (9)$$

This integration is a type of gaussian integration.

$$\int \exp\left(\alpha(t)(p + \beta(t))^2 + \gamma(t)\right) dp = e^{\gamma(t)} \sqrt{\frac{\pi}{\alpha(t)}} \quad (10)$$

(5)

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

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

(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,

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

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.

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

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

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

(3) The definition of the deviation is,

$$(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2. \quad (13)$$

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,

$$\langle p_x^2 \rangle = \langle p_x^2 \rangle_{t=0}. \quad (14)$$

Finally, the result is,

$$(\Delta p_x)^2 = \langle p_x^2 \rangle_{t=0} - \langle p_x \rangle_{t=0}^2 = (\Delta p_x)_{t=0}^2, \quad (\Delta p_x)^2 = (\Delta p_x)_{t=0}^2. \quad (15)$$

(4) From (13), the derivative of the deviation is,

$$\frac{d}{dt}(\Delta x)^2 = \frac{d}{dt}\langle x^2 \rangle - \frac{d}{dt}(\langle x \rangle^2). \quad (16)$$

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

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

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

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

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.

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

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

$$\langle x^2 \rangle = \frac{\langle [x, p_x] \rangle_{t=0}}{m} t + \frac{\langle p_x^2 \rangle_{t=0}}{m^2} t^2 + \frac{2\langle p_x x \rangle_{t=0}}{m} t + \langle x^2 \rangle_{t=0} \quad (17)$$

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

$$\begin{aligned} \frac{d}{dt} \langle x^2 \rangle &= \frac{\langle [x, p_x] \rangle_{t=0}}{m} + \frac{2\langle p_x^2 \rangle_{t=0}}{m^2} t + \frac{2\langle p_x x \rangle_{t=0}}{m} \\ &= \frac{\langle xp_x \rangle_{t=0} + \langle p_x x \rangle_{t=0}}{m} + \frac{2\langle p_x^2 \rangle_{t=0}}{m^2} t \end{aligned} \quad (18)$$

expectation value 의 square 를 계산하자.

$$\begin{aligned} \frac{d}{dt} (\langle x \rangle^2) &= 2\langle x \rangle \frac{d\langle x \rangle}{dt} = 2 \left(\frac{\langle p_x \rangle_{t=0}}{m} t + \langle x \rangle_{t=0} \right) \left(\frac{\langle p_x \rangle_{t=0}}{m} \right) \\ &= \frac{2\langle p_x \rangle_{t=0}^2}{m^2} t + \frac{2\langle p_x \rangle_{t=0} \langle x \rangle_{t=0}}{m} \end{aligned} \quad (19)$$

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

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

$\frac{d}{dt}(\Delta x)^2$ 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 normalization must be 1. So,

$$C = \left(\frac{1}{\sigma \sqrt{\pi}} \right)^{\frac{1}{2}} \quad (21)$$

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

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

The first term of the right-hand side is a zero because $x e^{-\left(\frac{x}{\sigma}\right)^2}$ is an odd 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 .

$$\langle x \rangle = \frac{1}{\sigma \sqrt{\pi}} x_0 \sigma \sqrt{\pi} = x_0 \quad (22)$$

The mean value of p is,

$$\begin{aligned} \langle p \rangle &= -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx = \frac{-i\hbar}{\sigma \sqrt{\pi}} \int_{-\infty}^{\infty} \left(\frac{i}{\hbar} p_0 - \frac{x - x_0}{\sigma^2} \right) \exp \left(- \left(\frac{x - x_0}{\sigma} \right)^2 \right) dx \\ &= \frac{-i\hbar}{\sigma \sqrt{\pi}} \left[\frac{i}{\hbar} p_0 \int_{-\infty}^{\infty} \exp \left(- \left(\frac{x - x_0}{\sigma} \right)^2 \right) dx - \int_{-\infty}^{\infty} \left(\frac{x - x_0}{\sigma^2} \right) \exp \left(- \left(\frac{x - x_0}{\sigma} \right)^2 \right) dx \right] = p_0 \end{aligned} \quad (23)$$

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

- (3) From (13), we use the definition of the deviation.

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2, \quad (\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2 \quad (24)$$

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 $x_0^2 \sigma\sqrt{\pi}$.

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

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,

$$(\Delta x)^2 = \frac{1}{2}\sigma^2 + x_0^2 - x_0^2 = \frac{1}{2}\sigma^2 \quad (25)$$

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.

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

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 $(\Delta p)^2$,

$$(\Delta p)^2 = p_0^2 + \frac{\hbar^2}{2\sigma^2} - p_0^2 = \frac{\hbar^2}{2\sigma^2}. \quad (26)$$

Confirm these result does satisfy Heisenberg's uncertainty principle.

$$\Delta x \Delta p = \sqrt{\frac{\hbar^2}{2\sigma^2} \frac{\sigma^2}{2}} = \frac{\hbar}{2} \quad (27)$$

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

Problem 4*. Consider a particle and two normalized energy eigenfunctions $\psi_1(\mathbf{x})$ and $\psi_2(\mathbf{x})$ 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

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

show that the probability density $|\psi(\mathbf{x}, t)|^2$ 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,

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

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

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

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

- (b) The time evolution is,

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

Consider the probability density of this particle.

$$|\psi(\mathbf{x}, t)|^2 = \frac{1}{2} \left[|\psi_1(\mathbf{x})|^2 + |\psi_2(\mathbf{x})|^2 + e^{-\frac{i}{\hbar}(E_2 - E_1)t} \psi_1(\mathbf{x})^* \psi_2(\mathbf{x}) + e^{-\frac{i}{\hbar}(E_1 - E_2)t} \psi_1(\mathbf{x}) \psi_2(\mathbf{x})^* \right] \quad (28)$$

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,

$$|\psi(\mathbf{x}, t)|^2 = \frac{1}{2} [|\psi_1(\mathbf{x})|^2 + |\psi_2(\mathbf{x})|^2]. \quad (29)$$

And the probability density is time-independent.

- (c) In this case, the last two terms of (28) are not zero. The probability density is,

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

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

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

Then the probability density is,

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

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.

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

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

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

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,

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

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.

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

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

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

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