

# 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,

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

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.

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

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

$$N^2 \int_{-\infty}^{\infty} \exp \left( -2 \left( \frac{x - x_0}{2\sigma} \right)^2 \right) dx = \sqrt{2}\sigma N^2 \int_{-\infty}^{\infty} e^{-t^2} dt \quad (3)$$

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

$$\int_{-\infty}^{\infty} e^{-(x^2+y^2)} dx dy = \int_0^{2\pi} \int_0^{\infty} e^{-r^2} r dr d\theta \quad (4)$$

$$= \int_0^{2\pi} \frac{1}{2} d\theta = \pi. \quad (5)$$

First double integration about coordinate space can be decomposed.

$$\int_{-\infty}^{\infty} e^{-(x^2+y^2)} dx dy = \int_{-\infty}^{\infty} e^{-x^2} dx \int_{-\infty}^{\infty} e^{-y^2} dy = \left( \int_{-\infty}^{\infty} e^{-x^2} dx \right)^2 \quad (6)$$

From this result,

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}, \quad \sqrt{2\pi}\sigma N^2 = 1. \quad (7)$$

Finally we obtain the normalization constant,

$$N = \left( \frac{1}{2\pi\sigma^2} \right)^{\frac{1}{4}}. \quad (8)$$

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

$$\phi(p, 0) = \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x, 0) e^{-\frac{i}{\hbar}px} dx = \frac{N}{\sqrt{2\pi\hbar}} \int \exp \left( i \frac{p_0 x}{\hbar} - \left( \frac{x - x_0}{2\sigma} \right)^2 \right) e^{-\frac{i}{\hbar}px} dx \quad (9)$$

$$= \frac{N}{\sqrt{2\pi\hbar}} \int \exp \left( - \left( \frac{x - x_0}{2\sigma} \right)^2 - \frac{i}{\hbar}(p - p_0)x \right) dx \quad (10)$$

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

$$u \equiv \frac{x - x_0}{2\sigma}, \quad du = \frac{1}{2\sigma} dx \quad (11)$$

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

$$\phi(p, 0) = \frac{2\sigma N}{\sqrt{2\pi\hbar}} \int \exp \left( -u^2 - \frac{i}{\hbar}(p - p_0)(2\sigma u + x_0) \right) du \quad (12)$$

$$= \left( \frac{2\sigma^2}{\pi^3 \hbar^2} \right)^{\frac{1}{4}} e^{-\frac{i}{\hbar}(p - p_0)x_0} \int \exp \left( -u^2 - 2\frac{i}{\hbar}\sigma(p - p_0)u \right) du. \quad (13)$$

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

$$-u^2 - 2\frac{i}{\hbar}\sigma(p - p_0)u = - \left( u + \frac{i}{\hbar}\sigma(p - p_0) \right)^2 - \frac{\sigma^2}{\hbar^2}(p - p_0)^2 \quad (14)$$

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

$$\phi(p, 0) = \left( \frac{2\sigma^2}{\pi^3 \hbar^2} \right)^{\frac{1}{4}} e^{-\frac{i}{\hbar}(p - p_0)x_0} \int \exp \left( -u^2 - 2\frac{i}{\hbar}\sigma(p - p_0)u \right) du \quad (15)$$

$$= \left( \frac{2\sigma^2}{\pi^3 \hbar^2} \right)^{\frac{1}{4}} e^{-\frac{i}{\hbar}(p - p_0)x_0} \int \exp \left( - \left( u + \frac{i}{\hbar}\sigma(p - p_0) \right)^2 - \frac{\sigma^2}{\hbar^2}(p - p_0)^2 \right) du \quad (16)$$

$$= \left( \frac{2\sigma^2}{\pi^3 \hbar^2} \right)^{\frac{1}{4}} \exp \left( -\frac{i}{\hbar}(p - p_0)x_0 - \frac{\sigma^2}{\hbar^2}(p - p_0)^2 \right) \int e^{-u^2} du \quad (17)$$

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

$$\phi(p,0) = \left(\frac{2\sigma^2}{\pi^3\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\frac{i}{\hbar}(p-p_0)x_0 - \frac{\sigma^2}{\hbar^2}(p-p_0)^2\right) \int e^{-u^2} du \quad (18)$$

$$= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\frac{i}{\hbar}(p-p_0)x_0 - \frac{\sigma^2}{\hbar^2}(p-p_0)^2\right) \quad (19)$$

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

$$\phi(0,0) = \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\frac{\sigma^2}{\hbar^2}p_0^2 + \frac{i}{\hbar}p_0x_0\right). \quad (20)$$

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

$$\phi(p,t) = \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\frac{\sigma^2}{\hbar^2}(p-p_0)^2 - i\frac{p^2}{2m\hbar}t - \frac{i}{\hbar}(p-p_0)x_0\right) \quad (21)$$

$$= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\left(\frac{\sigma^2}{\hbar^2} + \frac{it}{2m\hbar}\right)p^2 + \left(\frac{2\sigma^2}{\hbar^2}p_0 - \frac{i}{\hbar}x_0\right)p - \frac{\sigma^2}{\hbar^2}p_0^2 - \frac{i}{\hbar}p_0x_0\right) \quad (22)$$

$$= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\frac{2m\sigma^2 + i\hbar t}{2m\hbar^2}p^2 - \frac{2\sigma^2p_0 - i\hbar x_0}{\hbar^2}p - \frac{(\sigma^2p_0 + i\hbar x_0)p_0}{\hbar^2}\right) \quad (23)$$

The complete square form of  $\phi(p,t)$  is,

$$\phi(p,t) = \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} \exp\left(-\frac{2m\sigma^2 + i\hbar t}{2m\hbar^2}p^2 - \frac{2\sigma^2p_0 - i\hbar x_0}{\hbar^2}p - \frac{(\sigma^2p_0 + i\hbar x_0)p_0}{\hbar^2}\right) \quad (24)$$

$$= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} \exp\left(\alpha(t)(p + \beta(t))^2 + \gamma(t)\right) \quad (25)$$

$$\alpha(t) = -\frac{2m\sigma^2 + i\hbar t}{2m\hbar^2}, \quad \beta(t) = \frac{2m\sigma^2p_0 - i\hbar x_0}{2m\sigma^2 + i\hbar t}, \quad (26)$$

$$\gamma(t) = \frac{-mx_0\left(\frac{1}{2}\hbar x_0 + 4i\sigma^2p_0\right) - (\hbar x_0 - i\sigma^2p_0)p_0t}{2m\hbar\sigma^2 + i\hbar^2t}. \quad (27)$$

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

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int \phi(p,t) e^{\frac{i}{\hbar}px} dp = \quad (28)$$

(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,

$$\phi(p, t) = e^{-i \frac{p^2}{2m\hbar} t} \phi(p, 0). \quad (29)$$

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

$$\langle p_x \rangle = \int \phi^*(p, t) p_x \phi(p, t) d^3 p = \int e^{i \frac{p^2}{2m\hbar} t} \phi^*(p, 0) p_x e^{-i \frac{p^2}{2m\hbar} t} \phi(p, 0) d^3 p \quad (30)$$

The time evolutions are canceled out.

$$\langle p_x \rangle = \int \phi^*(p, 0) p_x \phi(p, 0) d^3 p = \langle p_x \rangle_{t=0}. \quad (31)$$

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

$$\langle x \rangle = i\hbar \int \phi^*(p, t) \frac{\partial \phi(p, t)}{\partial p_x} d^3 p = i\hbar \int e^{i \frac{p^2}{2m\hbar} t} \phi^*(p, 0) \frac{\partial}{\partial p_x} \left( e^{-i \frac{p^2}{2m\hbar} t} \phi(p, 0) \right) d^3 p \quad (32)$$

$$= i\hbar \int e^{i \frac{p^2}{2m\hbar} t} \phi^*(p, 0) \left( -i \frac{p_x}{m\hbar} t e^{-i \frac{p^2}{2m\hbar} t} \phi(p, 0) + e^{-i \frac{p^2}{2m\hbar} t} \frac{\partial \phi(p, 0)}{\partial p_x} \right) d^3 p \quad (33)$$

$$= i\hbar \int -i \frac{p_x}{m\hbar} t |\phi(p, 0)|^2 + \phi^*(p, 0) \frac{\partial \phi(p, 0)}{\partial p_x} d^3 p \quad (34)$$

$$= \frac{\langle p_x \rangle_{t=0}}{m} t + \langle x \rangle_{t=0} \quad (35)$$

(3) The definition of the deviation is,

$$(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2. \quad (36)$$

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 a (31).

$$\langle p_x^2 \rangle = \int \phi^*(p, t) p_x^2 \phi(p, t) d^3 p \quad (37)$$

From a (29),

$$\int \phi^*(p, t) p_x^2 \phi(p, t) d^3 p = \int e^{i \frac{p^2}{2m\hbar} t} \phi^*(p, 0) p_x^2 e^{-i \frac{p^2}{2m\hbar} t} \phi(p, 0) d^3 p \quad (38)$$

$$= \int \phi^*(p, 0) p_x^2 \phi(p, 0) d^3 p = \langle p_x^2 \rangle_{t=0} \quad (39)$$

So, we obtain that,

$$\langle p_x^2 \rangle = \langle p_x^2 \rangle_{t=0}. \quad (40)$$

Finally, the result is,

$$(\Delta p_x)^2 = \langle p_x^2 \rangle_{t=0} - \langle p_x \rangle_{t=0}^2 = (\Delta p_x)_{t=0}^2, \quad (\Delta p_x)^2 = (\Delta p_x)_{t=0}^2. \quad (41)$$

(4) From a (36), the derivative of the deviation is,

$$\frac{d}{dt}(\Delta x)^2 = \frac{d}{dt}\langle x^2 \rangle - \frac{d}{dt}(\langle x \rangle^2). \quad (42)$$

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

$$\begin{aligned} \langle x^2 \rangle &= -\hbar^2 \int \phi^*(p, t) \frac{\partial^2 \phi(p, t)}{\partial p_x^2} d^3p = -\hbar^2 \int e^{i\frac{p^2}{2m\hbar}t} \phi^*(p, 0) \frac{\partial^2}{\partial p_x^2} \left( e^{-i\frac{p^2}{2m\hbar}t} \phi(p, 0) \right) d^3p \\ &= -\hbar^2 \int e^{i\frac{p^2}{2m\hbar}t} \phi^*(p, 0) \frac{\partial}{\partial p_x} \left( -i\frac{p_x}{m\hbar} t e^{-i\frac{p^2}{2m\hbar}t} \phi(p, 0) + e^{-i\frac{p^2}{2m\hbar}t} \frac{\partial \phi(p, 0)}{\partial p_x} \right) d^3p \end{aligned} \quad (43)$$

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

$$\begin{aligned} \langle x^2 \rangle &= -\hbar^2 \int \phi^*(p, 0) \left[ \left( -i\frac{t}{m\hbar} + \left( -i\frac{p_x}{m\hbar} t \right)^2 \right) \phi(p, 0) - \left( 2i\frac{p_x}{m\hbar} t \frac{\partial \phi(p, 0)}{\partial p_x} - \frac{\partial^2 \phi(p, 0)}{\partial p_x^2} \right) \right] d^3p \\ &= -\hbar^2 \int \phi^*(p, 0) \left( -i\frac{t}{m\hbar} + \left( -i\frac{p_x}{m\hbar} t \right)^2 \right) \phi(p, 0) d^3p \\ &\quad + \hbar^2 \int \phi^*(p, 0) \left( 2i\frac{p_x}{m\hbar} t \frac{\partial \phi(p, 0)}{\partial p_x} - \frac{\partial^2 \phi(p, 0)}{\partial p_x^2} \right) d^3p \end{aligned} \quad (44)$$

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

$$\begin{aligned} -\hbar^2 \int \phi^*(p, 0) \left( -i\frac{t}{m\hbar} + \left( -i\frac{p_x}{m\hbar} t \right)^2 \right) \phi(p, 0) d^3p &= \frac{t}{m} \int i\hbar |\phi(p, 0)|^2 d^3p + \frac{t^2}{m^2} \int p_x^2 |\phi(p, 0)|^2 d^3p \\ &= \frac{\langle [x, p_x] \rangle_{t=0}}{m} t + \frac{\langle p_x^2 \rangle_{t=0}}{m^2} t^2 \end{aligned} \quad (45)$$

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

$$\begin{aligned} \hbar^2 \int \phi^*(p, 0) \left( 2i\frac{p_x}{m\hbar} t \frac{\partial \phi(p, 0)}{\partial p_x} - \frac{\partial^2 \phi(p, 0)}{\partial p_x^2} \right) d^3p &= \frac{2t}{m} \int \phi^*(p, 0) p_x \left( i\hbar \frac{\partial \phi(p, 0)}{\partial p_x} \right) d^3p \\ &\quad + \int \phi^*(p, 0) \left( -\hbar^2 \frac{\partial^2 \phi(p, 0)}{\partial p_x^2} \right) d^3p \\ &= \frac{2\langle p_x x \rangle_{t=0}}{m} t + \langle x^2 \rangle_{t=0} \end{aligned} \quad (46)$$

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

$$\langle x^2 \rangle = \frac{\langle [x, p_x] \rangle_{t=0}}{m} t + \frac{\langle p_x^2 \rangle_{t=0}}{m^2} t^2 + \frac{2\langle p_x x \rangle_{t=0}}{m} t + \langle x^2 \rangle_{t=0} \quad (47)$$

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

$$\frac{d}{dt}\langle x^2 \rangle = \frac{\langle [x, p_x] \rangle_{t=0}}{m} + \frac{2\langle p_x^2 \rangle_{t=0}}{m^2} t + \frac{2\langle p_x x \rangle_{t=0}}{m} \quad (48)$$

$$= \frac{\langle xp_x \rangle_{t=0} + \langle p_x x \rangle_{t=0}}{m} + \frac{2\langle p_x^2 \rangle_{t=0}}{m^2} t \quad (49)$$

expectation value 의 square 를 계산하자.

$$\begin{aligned} \frac{d}{dt}(\langle x \rangle^2) &= 2\langle x \rangle \frac{d\langle x \rangle}{dt} = 2 \left( \frac{\langle p_x \rangle_{t=0}}{m} t + \langle x \rangle_{t=0} \right) \left( \frac{\langle p_x \rangle_{t=0}}{m} \right) \\ &= \frac{2\langle p_x \rangle_{t=0}^2}{m^2} t + \frac{2\langle p_x \rangle_{t=0} \langle x \rangle_{t=0}}{m} \end{aligned} \quad (50)$$

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

$$\begin{aligned}
 \frac{d}{dt}(\Delta x)^2 &= \frac{d}{dt}\langle x^2 \rangle - \frac{d}{dt}(\langle x \rangle^2) \\
 &= \frac{\langle xp_x \rangle_{t=0} + \langle p_x x \rangle_{t=0}}{m} + \frac{2\langle p_x^2 \rangle_{t=0}}{m^2}t - \left( \frac{2\langle p_x \rangle_{t=0}^2}{m^2}t + \frac{2\langle p_x \rangle_{t=0}\langle x \rangle_{t=0}}{m} \right) \\
 &= \frac{\langle xp_x \rangle_{t=0} + \langle p_x x \rangle_{t=0} - 2\langle p_x \rangle_{t=0}\langle x \rangle_{t=0}}{m} + \frac{2(\Delta p_x)_{t=0}^2}{m^2}t
 \end{aligned} \tag{51}$$

$\frac{d}{dt}(\Delta x)^2$  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  $\sigma$  are real parameters.

- (1) Find the normalization constant  $C$ .
- (2) Find the mean values of  $x$  and  $p$ .
- (3) Find the standard deviations  $\Delta x$  and  $\Delta p$ .

**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  $\Omega_1$  and  $\Omega_2$ , respectively.

- (1) (a) Show that, if the particle is initially in region  $\Omega_1$  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  $\Omega_1$  and  $\Omega_2$  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  $\Omega_1$  and  $\Omega_2$  to be two concentric spheres of radii  $R_1 > R_2$ . Compute the probability current that flows through  $\Omega_1$ .

(Problem 4 is a bit difficult. To solve (3), introduce phase factors for  $\psi_1(\mathbf{x})$  and  $\psi_2(\mathbf{x})$  and consider the interference term when one computes the probability density. To solve (4), consider the current density and continuity equation.