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,

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

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.

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

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

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

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

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

$$= \int_0^{2\pi} \frac{1}{2}\,d\theta = \pi. \tag{5}$$

First double integration about coordinate space can be decomposed.

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

From this result,

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

Finally we obtain the normalization constant,

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

(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

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

(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,

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

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

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

The time evolutions are canceled out.

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

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

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

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

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

$$= \frac{\langle p_x\rangle_{t=0}}{m}t + \langle x\rangle_{t=0} \tag{35}$$

(3) The definition of the deviation is,

$$(\Delta p_x)^2 = \langle p_x^2\rangle - \langle p_x\rangle^2. \tag{36}$$

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 a (31).

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

From a (29),

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

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

So, we obtain that,

$$\langle p_x^2\rangle = \langle p_x^2\rangle_{t=0}. \tag{40}$$

Finally, the result is,

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

expectation value 의 square 를 계산하자.

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

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

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

$\frac{d}{dt}(\Delta x)^2$ 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 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.

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.

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