Quantum Mechanics I

Week 7 (Solutions)

Spring Semester 2025

1 Representation in momentum space

We consider a particle whose state is described by the following wave function

$$\psi(x) = (2\pi d^2)^{-\frac{1}{4}} \exp\left(i\frac{p_0}{\hbar}x - \frac{(x-x_0)^2}{4d^2}\right), \tag{1.1}$$

where p_0, x_0, and d are real parameters.

(a) Find the representation of this state in the momentum space.

The Fourier transform of $\psi(x)$ is given by

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dx\, \psi(x) e^{-i\frac{px}{\hbar}} \tag{1.2}$$

By substituting $\psi(x)$, we find:

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(2\pi d^2)^{\frac{1}{4}}} \int_{-\infty}^{+\infty} dx \exp\left(-i\frac{(p-p_0)x}{\hbar} - \frac{(x-x_0)^2}{4d^2}\right) \tag{1.3}$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(2\pi d^2)^{\frac{1}{4}}} e^{-i\frac{(p-p_0)x_0}{\hbar}} \int_{-\infty}^{+\infty} dx \exp\left(-i\frac{(p-p_0)x}{\hbar} - \frac{x^2}{4d^2}\right). \tag{1.4}$$

where in the second equality we have performed a change of variables $x - x_0 \to x$. Using the Gaussian integral,

$$\int_{-\infty}^{+\infty} dx\, e^{-ax^2+\beta x} = \sqrt{\frac{\pi}{a}} e^{\frac{\beta^2}{4a}}, \tag{1.5}$$

we obtain

$$\psi(p) = \left(\frac{2d^2}{\pi\hbar^2}\right)^{\frac{1}{4}} e^{-i\frac{(p-p_0)x_0}{\hbar}} \exp\left(-\frac{d^2(p-p_0)^2}{\hbar^2}\right). \tag{1.6}$$

(b) Show that $\langle\hat{p}\rangle = p_0$.

The expectation value of the momentum operator $\hat{p}$ is given by

$$\langle\psi|\hat{p}|\psi\rangle = \int_{-\infty}^{+\infty} dp\, |\psi(p)|^2\, p. \tag{1.7}$$

Substituting $|\psi(p)|^2$,

$$\langle \hat{p} \rangle = \frac{2d}{\hbar}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dp\, p e^{-2\frac{d^2(p-p_0)^2}{\hbar^2}} \tag{1.8}$$

$$= \frac{2d}{\hbar}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dp\,(p+p_0) e^{-2\frac{d^2p^2}{\hbar^2}}. \tag{1.9}$$

Since the integral of an odd function over symmetric limits is zero, we obtain

$$\langle \hat{p} \rangle = p_0. \tag{1.10}$$

(c) Show that $\langle \hat{p}^2 \rangle = \frac{\hbar^2}{4d^2} + p_0^2$.

The expectation value of $\hat{p}^2$ is given by

$$\langle \psi | \hat{p}^2 | \psi \rangle = \int_{-\infty}^{+\infty} dp\, |\psi(p)|^2\, p^2. \tag{1.11}$$

Following a similar approach,

$$\langle \hat{p}^2 \rangle = \frac{2d}{\hbar}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dp\, p^2 e^{-2\frac{d^2(p-p_0)^2}{\hbar^2}} \tag{1.12}$$

$$= \frac{2d}{\hbar}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dp\,(p+p_0)^2 e^{-2\frac{d^2p^2}{\hbar^2}}. \tag{1.13}$$

Using the Gaussian integral result

$$\int_{-\infty}^{+\infty} dx\, x^2 e^{-ax^2} = \frac{\sqrt{\pi}}{2}\frac{1}{a^{3/2}}, \tag{1.14}$$

we obtain

$$\langle \hat{p}^2 \rangle = \frac{\hbar^2}{4d^2} + p_0^2. \tag{1.15}$$

Note that the variance of the probability distribution $|\psi(p)|^2$ in momentum space is then $(\Delta p)^2 = \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2 = \hbar^2/(4d^2)$. By similar calculations, it can be shown that the variance of the probability distribution in coordinate space, $|\psi(x)|^2$ is given by $(\Delta x)^2 = d^2$. The wavefunction considered in the problem is a state of minimal uncertainty. It saturates the bound imposed by the Heisenberg uncertainty principle: $\Delta x \Delta p \geq \hbar/2$. The uncertainty relations are analyzed in more details in the following problems.

2 Uncertainty relation

The commutator of two Hermitian operators $\hat{A}$ and $\hat{B}$ always has the form

$$[\hat{A}, \hat{B}] = i\hat{C},$$

where $\hat{C}$ is a Hermitian operator.

(a) Prove the uncertainty relation

$$\langle \Delta \hat{A}^2 \rangle \langle \Delta \hat{B}^2 \rangle \geq \frac{1}{4} \langle \hat{C} \rangle^2, \tag{2.1}$$

where

$$\langle \Delta \hat{X}^2 \rangle = \langle \hat{X}^2 \rangle - \langle \hat{X} \rangle^2,$$

and all expectations $\langle \cdot \rangle$ refer to the same wave function.

Hint: Consider the integral

$$J(\lambda) = \int dx \left| \left(\lambda \hat{A}_1 - i\hat{B}_1 \right) \psi(x) \right|^2 \geq 0,$$

where $\hat{A}_1 = \hat{A} - a$, $\hat{B}_1 = \hat{B} - b$ and λ, a and b are real parameters.

First, we find that:

- $[\hat{A}_1, \hat{B}_1] = [\hat{A}, \hat{B}] = i\hat{C}$
- $\langle (\Delta \hat{A})^2 \rangle = \langle A_1^2 \rangle$
- $\langle (\Delta \hat{B})^2 \rangle = \langle B_1^2 \rangle$.

In the above, we have used the fact that a, b are the expectation values of A, B in the given state, respectively.

Then we calculate the integral:

$$\begin{aligned}
J(\lambda) &= \int \left| (\lambda \hat{A}_1 - i\hat{B}_1)\psi(x) \right|^2 dx \\
&= \int \left((\lambda \hat{A}_1 - i\hat{B}_1)\psi(x) \right)^* (\lambda \hat{A}_1 - i\hat{B}_1)\psi(x) dx \\
&= \int \psi^*(x)(\lambda \hat{A}_1 + i\hat{B}_1)(\lambda \hat{A}_1 - i\hat{B}_1)\psi(x) dx \\
&= \int \psi^*(x) \left(\lambda^2 \hat{A}_1^2 + i\lambda \hat{B}_1 \hat{A}_1 - i\lambda \hat{A}_1 \hat{B}_1 + \hat{B}_1^2 \right) \psi(x) dx \\
&= \int \psi^*(x) \left(\lambda^2 \hat{A}_1^2 + \lambda \hat{C} + \hat{B}_1^2 \right) \psi(x) dx \\
&= \lambda^2 \langle \hat{A}_1^2 \rangle + \lambda \langle \hat{C} \rangle + \langle \hat{B}_1^2 \rangle \geq 0.
\end{aligned}$$

Since the integral is non-negative, the discriminant of the quadratic equation of λ must satisfy:

$$\Delta_\lambda = \langle \hat{C} \rangle^2 - 4 \langle \hat{A}_1^2 \rangle \langle \hat{B}_1^2 \rangle \leq 0. \tag{2.2}$$

Therefore, we obtain the uncertainty relation:

$$\langle \Delta \hat{A}^2 \rangle \langle \Delta \hat{B}^2 \rangle \geq \frac{1}{4} \langle \hat{C} \rangle^2. \tag{2.3}$$

(b) Consider specifically the operators $\hat{x}$ and $\hat{p}$ of position and momentum, respectively. Find an explicit form of a wave function that minimizes the uncertainty product $\langle \Delta \hat{x}^2 \rangle \langle \Delta \hat{p}^2 \rangle$.

The equality in the uncertainty relation is achieved when $(\lambda \hat{A}_1 - i\hat{B}_1)\psi(x) = 0$. We set $\hat{A} = \hat{x}$, $\hat{B} = \hat{p} = -i\hbar \frac{d}{dx}$, and $\hat{C} = \hbar$, with $a = x_0$ and $b = p_0$. Substituting, we get:

$$\left[\lambda(x - x_0) - \hbar \frac{d}{dx} + ip_0 \right] \psi(x) = 0. \tag{2.4}$$

Rearranging,

$$\frac{d\psi(x)}{dx} = \frac{\lambda(x - x_0) + ip_0}{\hbar} \psi(x). \tag{2.5}$$

Integrating, we find the general form of a wave function that minimizes the uncertainty on $\hat{x}$ and $\hat{p}$:

$$\psi(x) \propto \exp\left(i\frac{p_0 x}{\hbar} + \lambda \frac{(x - x_0)^2}{2\hbar} \right). \tag{2.6}$$

First, note that for $\psi(x)$ to be normalizable (i.e., $\int dx |\psi(x)|^2 = 1$), λ needs to be negative, resulting in $\psi(x)$ being a Gaussian wave function. Interestingly, we find not a single wave function that minimizes $\langle \Delta \hat{x}^2 \rangle \langle \Delta \hat{p}^2 \rangle$, but rather a continuum of states, parameterized by λ.

To understand this, we compute the uncertainties individually. Through similar calculations, we obtain:

$$\langle \Delta \hat{x}^2 \rangle = \frac{\hbar}{2|\lambda|}, \quad \langle \Delta \hat{p}^2 \rangle = \frac{\hbar |\lambda|}{2}. \tag{2.7}$$

Their product is:

$$\langle \Delta \hat{x}^2 \rangle \langle \Delta \hat{p}^2 \rangle = \frac{\hbar^2}{4}, \tag{2.8}$$

which confirms that $\psi(x)$ saturates the uncertainty relation.

Additionally, this provides insight into the role of λ: the uncertainty relation bounds only the product $\langle \Delta \hat{x}^2 \rangle \langle \Delta \hat{p}^2 \rangle$, not their individual values. We can have states with large uncertainty in $\hat{p}$ and small uncertainty in $\hat{x}$ ($|\lambda| \gg 1$), as well as the opposite case ($|\lambda| \approx 0$) and all those in between. In particular, for $\lambda = -1$, the uncertainties are equal.

3 Wavepackets in one dimension

A free particle of mass m is moving in a one-dimensional space. At time $t = 0$, its normalized wave function reads

$$\psi(x;\mu = 0, \sigma_x^2) = \frac{1}{(2\pi\sigma_x^2)^{1/4}} e^{-\frac{x^2}{4\sigma_x^2}}, \tag{3.1}$$

where $\sigma_x^2 \equiv \langle x^2 \rangle$ and $\mu = \langle x \rangle$ denotes its mean value.

(a) Calculate the wave function in momentum representation $\psi(p, t = 0)$.

By Fourier transforming, we obtain:

$$\psi(p, 0) = \frac{1}{\sqrt{2\pi\hbar}} \int dx\, e^{-ipx/\hbar} \psi(x, 0) = \frac{1}{\sqrt{2\pi\hbar}} \int dx\, e^{-ipx/\hbar} \frac{1}{(2\pi\sigma_x^2)^{1/4}} e^{-\frac{x^2}{4\sigma_x^2}}. \tag{3.2}$$

Using the Gaussian integral formula, we get:

$$\psi(p, 0) = \left(\frac{2\sigma_x^2}{\pi\hbar^2} \right)^{1/4} \exp\left\{ -\frac{\sigma_x^2 p^2}{\hbar^2} \right\}. \tag{3.3}$$

(b) Calculate the uncertainty in momentum associated with this wavepacket ($\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2$).

The expectation value of momentum in its respective representation is found by the following integral:

$$\langle p \rangle = \int_{-\infty}^{+\infty} dp\, \psi^*(p) p \psi(p). \tag{3.4}$$

Since p is odd and the Gaussian function $e^{-2\sigma_x^2 p^2/\hbar^2}$ is even, we conclude that the expectation value of the momentum is zero, i.e. $\langle p \rangle = 0$.

Similarly, for $\langle p^2 \rangle$, we compute:

$$\langle p^2 \rangle = \int_{-\infty}^{+\infty} \psi^*(p) p^2 \psi(p) dp. \tag{3.5}$$

Using the substitution $q = \frac{\sqrt{2}\sigma_x}{\hbar} p$ in the resulting integrals, we obtain:

$$\langle p^2 \rangle = \frac{\hbar^2}{4\sigma_x^2}. \tag{3.6}$$

Thus, the uncertainty in the momentum is:

$$\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \frac{\hbar}{2\sigma_x}. \tag{3.7}$$

(c) Show that at time $t > 0$ the probability density of the particle is of the form

$$|\psi(x,t)|^2 = |\psi(x;0,\sigma_x^2 + \sigma_p^2 t^2/m^2)|^2. \tag{3.8}$$

Since the energy of a free particle is given by $E = \frac{p^2}{2m}$, we evolve the wave function in time as:

$$\psi(p,t) = \psi(p,0)e^{-iEt/\hbar} = \psi(p,0)e^{-ip^2 t/2m\hbar}.$$

By inverse Fourier transform, we obtain:

$$\begin{aligned}
\psi(x,t) &= \frac{1}{\sqrt{2\pi\,\hbar}} \int e^{\frac{i\,p\,x}{\hbar}}\,\psi(p,t)\,dp \\
&= \sqrt[4]{\frac{2\,\sigma_x^2}{\pi\,\hbar^2}}\,\frac{1}{\sqrt{2\pi\,\hbar}} \int e^{\frac{i\,p\,x}{\hbar}}\,\exp\Big[-\big(\sigma_x^2 + i\,\tfrac{\hbar\,t}{2m}\big)\,\tfrac{p^2}{\hbar^2}\Big]\,dp \\
&= \sqrt[4]{\frac{2\,\sigma_x^2}{\pi\,\hbar^2}}\,\frac{1}{\sqrt{2\pi\,\hbar}}\,\frac{\sqrt{\pi}\hbar}{\sqrt{\sigma_x^2 + i\,\frac{\hbar\,t}{2m}}}\,\exp\Big[-\frac{x^2}{4\,\big(\sigma_x^2 + i\,\frac{\hbar\,t}{2m}\big)}\Big] \\
&= \sqrt[4]{\frac{\sigma_x^2}{2\,\pi}}\,\frac{1}{\sqrt{\sigma_x^2 + i\,\frac{\hbar\,t}{2m}}}\,\exp\Big[-\frac{x^2}{4\,\big(\sigma_x^2 + i\,\frac{\hbar\,t}{2m}\big)}\Big].
\end{aligned}$$

Considering now the probability density, we find:

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi}\big(\sigma_x^2 + \frac{\sigma_p^2\,t^2}{m^2}\big)}\,\exp\Bigg(-\frac{x^2}{2\big(\sigma_x^2 + \frac{\sigma_p^2\,t^2}{m^2}\big)}\Bigg) = \Big|\psi\big(x;0,\sigma_x^2 + \sigma_p^2\,t^2/m^2\big)\Big|^2$$

(d) Interpret the results of (b) and (c) with respect to Heisenberg's uncertainty principle.

The results indicates that the Gaussian wave-packet's width changes with time.

$$\sigma_x \to \sqrt{\sigma_x^2 + \sigma_p^2 t^2/m^2}. \tag{3.9}$$

where $\sigma_p^2 = \hbar^2/(4\sigma_x^2)$. This result demonstrates that as $t \to \infty$, the wave packet completely spreads over space.

Hints: You might use the following integrals:

$$\int_{-\infty}^{+\infty} e^{-ax^2} e^{-ikx} dx = \sqrt{\frac{\pi}{a}} e^{-\frac{k^2}{4a}},$$

$$\int_{-\infty}^{+\infty} x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{2a^{3/2}}.$$

4 Space Translations

(a) Let x and p_x be the coordinate and linear momentum in one dimension. Evaluate the classical Poisson bracket

$$[x, F(p_x)]_{\rm cl}. \tag{4.1}$$

We use the definition of the Poisson bracket and we find:

$$[x, F(p_x)]_{\rm cl} = \frac{\partial x}{\partial x}\frac{\partial F}{\partial p_x} - \frac{\partial x}{\partial p_x}\frac{\partial F}{\partial x} = \frac{\partial F}{\partial p_x},$$

since $\partial x/\partial p_x = 0$.

(b) Let x and p_x be the corresponding quantum-mechanical operators this time. Evaluate the commutator

$$\left[x, \exp\left(\frac{ip_x a}{\hbar}\right)\right]. \tag{4.2}$$

Hint: Use your result from Question (a).

Now since $\{x, F(p_x)\}_{\rm cl} \to [x, F(p_x)]_{\rm QM}/i\hbar$, hence

$$[x, \exp(ip_x a/\hbar)]_{\rm QM} = i\hbar\frac{\partial}{\partial p_x}\exp(ip_x a/\hbar) = -a\exp(ip_x a/\hbar).$$

(c) Using the result obtained in Question (b), prove that

$$\exp\left(\frac{ip_x a}{\hbar}\right)|x'\rangle \tag{4.3}$$

is an eigenket of the coordinate operator x. What is the corresponding eigenvalue?

Using the result from Question (b), we have

$$[x, \exp(ip_x a/\hbar)]|x'\rangle = -a\exp(ip_x a/\hbar)|x'\rangle.$$

Hence

$$x\exp(ip_x a/\hbar)|x'\rangle - \exp(ip_x a/\hbar)x|x'\rangle = -a\exp(ip_x a/\hbar)|x'\rangle.$$

so

$$x[\exp(ip_x a/\hbar)|x'\rangle] = (x' - a)[\exp(ip_x a/\hbar)|x'\rangle].$$

This eigenvalue equation implies that $\exp(ip_x a/\hbar)|x'\rangle$ is an eigenstate of the coordinate operator x, with corresponding eigenvalue $(x' - a)$. The operator $\exp\{ip_x a/\hbar\}$ clearly corresponds to a space translation by a.