Quantum Mechanics III — Michaelmas Term 2009

Lecturer: Dr. Benjamin Doyon

Homework 2 – due 19 November 2009

1. Prove that
$$\widehat{X^2P} = \frac{\hat{X}^2\hat{P} + \hat{X}\hat{P}\hat{X} + \hat{P}\hat{X}^2}{3}$$
by calculating the commutator $[\hat{X}^3, \hat{P}^2]$ and using Dirac's quantisation condition.

2. Consider a particle on a circle of circumference L. We showed in class that the momentum eigenvalues are $p_n = 2\pi n\hbar/L$ for $n \in \mathbb{Z}$, and that the corresponding eigenstates $|p_n\rangle$ have wave functions given by
$$\langle x|p_n\rangle = a\, e^{i2\pi nx/L} \quad (a \in \mathbb{C}).$$
   (a) Show that we have $\langle p_n|p_{n'}\rangle = \delta_{n,n'}$ for an appropriately chosen a (and calculate that a).
   (b) Using the completeness relations $\sum_{n\in\mathbb{Z}} |p_n\rangle\langle p_n| = \mathbf{1}$ and $\int_0^L dx\, |x\rangle\langle x| = \mathbf{1}$, derive the formulas that give the coefficients $\tilde{\psi}_n$ in terms of the wave function $\psi(x)$ and vice versa, in
$$|\psi\rangle = \sum_{n\in\mathbb{Z}} \tilde{\psi}_n|p_n\rangle = \int_0^L dx\, \psi(x)|x\rangle.$$

3. Consider the space of functions ψ supported on the interval $[0, L]$, with twisted periodicity condition $\psi(x + L) = e^{i\theta}\psi(x)$ for some fixed $\theta \in \mathbb{R}$, and with the usual inner product $\langle\psi_1|\psi_2\rangle = \int_0^L \psi_1^*(x)\psi_2(x)\, dx$.
   (a) Show that the momentum operator $\hat{P} = -i\hbar d/dx$ is Hermitian on that space.
   (b) Find the spectrum of $\hat{P}$ and its normalised eigenfunctions, and show that they are orthonormal.
   (c) Explain why the wave function
$$\psi(x) = Ae^{i\theta x/L}\cos(2\pi x/L)$$
is an example of a function in this space. Normalise this wave function. If a measurement of momentum is made, what values can be obtained and with what probabilities? Evaluate the expectation of the momentum $\langle\hat{P}\rangle$.

Answers

1. The most direct way of doing it is using the general formuli
$$[\hat{A}\hat{B}\hat{C}, \hat{D}] = \hat{A}\hat{B}[\hat{C}, \hat{D}] + \hat{A}[\hat{B}, \hat{D}]\hat{C} + [\hat{A}, \hat{D}]\hat{B}\hat{C} \qquad (1)$$

and

$$[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}. \tag{2}$$

We get

$$\begin{aligned} [\hat{X}^3, \hat{P}^2] &= \hat{X}^2[\hat{X}, \hat{P}^2] + \hat{X}[\hat{X}, \hat{P}^2]\hat{X} + [\hat{X}, \hat{P}^2]\hat{X}^2 \\ [\hat{X}, \hat{P}^2] &= \hat{P}[\hat{X}, \hat{P}] + [\hat{X}, \hat{P}]\hat{P} = 2i\hbar\hat{P} \end{aligned} \tag{3}$$

where we used the canonical commutation relations $[\hat{X}, \hat{P}] = i\hbar$. Hence

$$[\hat{X}^3, \hat{P}^2] = 2i\hbar(\hat{X}^2\hat{P} + \hat{X}\hat{P}\hat{X} + \hat{P}\hat{X}^2). \tag{4}$$

But also, according to the quantisation condition,

$$[\hat{X}^3, \hat{P}^2] = [\widehat{X^3}, \widehat{P^2}] = i\hbar\widehat{\{X^3, P^2\}} \tag{5}$$

and the Poisson bracket is

$$\{X^3, P^2\} = \frac{\partial X^3}{\partial X}\frac{\partial P^2}{\partial P} - \frac{\partial X^3}{\partial P}\frac{\partial P^2}{\partial X} = 6X^2P. \tag{6}$$

Hence, combining (4) with (5), we find

$$2i\hbar(\hat{X}^2\hat{P} + \hat{X}\hat{P}\hat{X} + \hat{P}\hat{X}^2) = 6\widehat{X^2P} \tag{7}$$

which proves it. Note that we could also have done

$$\begin{aligned} [\hat{X}^3, \hat{P}^2] &= \hat{P}[\hat{X}^3, \hat{P}] + [\hat{X}^3, \hat{P}]\hat{P} \\ [\hat{X}^3, \hat{P}] &= \hat{X}^2[\hat{X}, \hat{P}] + \hat{X}[\hat{X}, \hat{P}]\hat{X} + [\hat{X}, \hat{P}]\hat{X}^2 = 3i\hbar\hat{X}^2 \end{aligned} \tag{8}$$

so that

$$[\hat{X}^3, \hat{P}^2] = 3i\hbar(\hat{X}^2\hat{P} + \hat{P}\hat{X}^2). \tag{9}$$

How can that be the same as (4)? It's just using the canonical commutation relations again, as follows:

$$\begin{aligned} 3i\hbar(\hat{X}^2\hat{P} + \hat{P}\hat{X}^2) &= 3i\hbar\left(\frac{2}{3}\hat{X}^2\hat{P} + \frac{1}{3}\hat{X}^2\hat{P} + \frac{1}{3}\hat{P}\hat{X}^2 + \frac{2}{3}\hat{P}\hat{X}^2\right) \\ &= 3i\hbar\left(\frac{2}{3}\hat{X}^2\hat{P} + \frac{1}{3}(\hat{X}\hat{P}\hat{X} + \hat{X}[\hat{X}, \hat{P}]) + \frac{1}{3}(\hat{X}\hat{P}\hat{X} + [\hat{P}, \hat{X}]\hat{X}) + \frac{2}{3}\hat{P}\hat{X}^2\right) \\ &= 3i\hbar\left(\frac{2}{3}\hat{X}^2\hat{P} + \frac{1}{3}(\hat{X}\hat{P}\hat{X} + i\hbar\hat{X}) + \frac{1}{3}(\hat{X}\hat{P}\hat{X} - i\hbar\hat{X}) + \frac{2}{3}\hat{P}\hat{X}^2\right) \\ &= 2i\hbar(\hat{X}^2\hat{P} + \hat{X}\hat{P}\hat{X} + \hat{P}\hat{X}^2). \end{aligned}$$

In fact, generalising this process, we can write

$$[\hat{X}^3, \hat{P}^2] = 6i\hbar(a\hat{X}^2\hat{P} + (1 - 2a)\hat{X}\hat{P}\hat{X} + a\hat{P}\hat{X}^2). \tag{10}$$

for any a, so that

$$\widehat{X^2P} = a\hat{X}^2\hat{P} + (1 - 2a)\hat{X}\hat{P}\hat{X} + a\hat{P}\hat{X}^2. \tag{11}$$

For $a = 0$, we get the simpler result $\widehat{X^2P} = \hat{X}\hat{P}\hat{X}$, but the one we had to prove for this Question 1 is the more "standard" form.

2. (a) Since $\hat{P}$ is hermitian (as we showed in class), it is clear that $\langle p_n | p_{n'} \rangle = 0$ for $n \neq n'$, since they are eigenvectors corresponding to different eigenvalues. But we can work this out explicitly:

$$\begin{aligned} \langle p_n | p_{n'} \rangle &= \int_0^L dx\, \langle p_n | x \rangle \langle x | p_{n'} \rangle \\ &= \int_0^L dx\, |a|^2 e^{2\pi i (n'-n) x/L} \\ &\overset{n' \neq n'}{=} \frac{L|a|^2}{2\pi i (n'-n)} (e^{2\pi i (n'-n)} - 1) \\ &\overset{n' \neq n'}{=} 0. \end{aligned} \tag{12}$$

To get the value of a, we do the case $n = n'$ separately:

$$\begin{aligned} \langle p_n | p_n \rangle &= \int_0^L dx\, \langle p_n | x \rangle \langle x | p_n \rangle \\ &= \int_0^L dx\, |a|^2 \\ &= |a|^2 L \end{aligned} \tag{13}$$

so that we can choose $a = 1/\sqrt{L}$.

(b) We have

$$\begin{aligned} |\psi\rangle &= \sum_{n \in \mathbb{Z}} \tilde{\psi}_n | p_n \rangle \\ &= \sum_{n \in \mathbb{Z}} \tilde{\psi}_n \int_0^L dx\, | x \rangle \langle x | p_n \rangle \\ &= \int_0^L dx\, \frac{1}{\sqrt{L}} \sum_{n \in \mathbb{Z}} e^{2\pi i n x/L} \tilde{\psi}_n | x \rangle \end{aligned} \tag{14}$$

so that

$$\psi(x) = \frac{1}{\sqrt{L}} \sum_{n \in \mathbb{Z}} e^{2\pi i n x/L} \tilde{\psi}_n. \tag{15}$$

Likewise,

$$\begin{aligned} |\psi\rangle &= \int_0^L dx\, \psi(x) | x \rangle \\ &= \int_0^L dx\, \psi(x) \sum_{n \in \mathbb{Z}} | p_n \rangle \langle p_n | x \rangle \\ &= \sum_{n \in \mathbb{Z}} \frac{1}{\sqrt{L}} \int_0^L dx\, e^{-2\pi i n x/L} \psi(x) | p_n \rangle \end{aligned} \tag{16}$$

so that

$$\tilde{\psi}_n = \frac{1}{\sqrt{L}} \int_0^L dx\, e^{-2\pi i n x/L} \psi(x). \tag{17}$$

3. (a) In order to show hermiticity, we must show that $\langle\psi_1|\hat{P}|\psi_2\rangle^* = \langle\psi_2|\hat{P}|\psi_1\rangle$. We have, using integration by parts,

$$\begin{aligned}
\langle\psi_1|\hat{P}|\psi_2\rangle &= \int_0^L dx\,\psi_1^*(x)(-i\hbar)\frac{d}{dx}\psi_2(x) \\
&= i\hbar\int_0^L dx\,\frac{d}{dx}\psi_1^*(x)\psi_2(x) - i\hbar\left(\psi_1^*(x)\psi_2(x)\right)\Big|_{x=0}^{x=L} \\
&= i\hbar\int_0^L dx\,\frac{d}{dx}\psi_1^*(x)\psi_2(x) - i\hbar\left(\psi_1^*(L)\psi_2(L) - \psi_1^*(0)\psi_2(0)\right) \\
&= i\hbar\int_0^L dx\,\frac{d}{dx}\psi_1^*(x)\psi_2(x) - i\hbar\left(e^{-i\theta}\psi_1^*(0)e^{i\theta}\psi_2(0) - \psi_1^*(0)\psi_2(0)\right) \\
&= i\hbar\int_0^L dx\,\frac{d}{dx}\psi_1^*(x)\psi_2(x) \qquad (18)
\end{aligned}$$

where we used the twisted periodicity conditions. Hence, we find

$$\begin{aligned}
\langle\psi_1|\hat{P}|\psi_2\rangle^* &= -i\hbar\int_0^L dx\,\psi_2^*(x)\frac{d}{dx}\psi_1(x) \\
&= \langle\psi_2|\hat{P}|\psi_1\rangle \qquad (19)
\end{aligned}$$

which proves hermiticity.

(b) Certainly, the functions $\psi_p(x) = \langle x|p\rangle$ that are eigenfunctions of the differential operator $\hat{P} = -i\hbar d/dx$, with eigenvalue p, must be as usual, $\psi_p(x) = a_p\, e^{ipx/\hbar}$ (note that in general, the normalisation constant a_p may depend on the eigenvalue p). But then we must guarantee that they are in the space that we are looking at. That is, they must satisfy the condition $\psi_p(x+L) = e^{i\theta}\psi_p(x)$. Hence,

$$a_p\, e^{ip(x+L)/\hbar} = a_p\, e^{ipx/\hbar + i\theta} \quad \Rightarrow \quad e^{ipL/\hbar} = e^{i\theta} \qquad (20)$$

so that we find the eigenvalues

$$p = p_n := \frac{(2\pi n + \theta)\hbar}{L}, \quad n \in \mathbb{Z}. \qquad (21)$$

The set $\{p_n : n \in \mathbb{Z}\}$ is the spectrum of $\hat{P}$ on that space. For the eigenfunctions

$$\psi_{p_n}(x) = \langle x|p_n\rangle = a_{p_n}\, e^{(2\pi n+\theta)ix/L},$$

we know that they are orthogonal for different n, since they correspond to different eigenvalues of a Hermitian operator (and this is enough of a proof!). We can also check explicitly orthonality as in Question 2, by evaluating explicitly the integrals; it's exactly the same calculation, since the $e^{i\theta x/L}$ factors just cancel out. To get the value of a, we do the case $n = n'$ again, and the same cancellation occurs:

$$\begin{aligned}
\langle p_n|p_n\rangle &= \int_0^L dx\,\langle p_n|x\rangle\langle x|p_n\rangle \\
&= \int_0^L dx\,|a_{p_n}|^2 \\
&= |a_{p_n}|^2 L \qquad (22)
\end{aligned}$$

so that we can choose again $a_{p_n} = 1/\sqrt{L}$.

(c) The function $\psi(x)$ satisfies $\psi(x+L) = e^{i\theta}\psi(x)$, so it is in the space we are looking at. In order to normalise it, we must have

$$1 = \int_0^L dx\, \psi^*(x)\psi(x) = \int_0^L dx\, |A|^2 \cos^2(2\pi x/L) = L|A|^2/2 \tag{23}$$

hence we can choose $A = \sqrt{2/L}$. In order to assess the probabilities of momentum measurements, we must evaluate the overlap with the momentum eigenfunctions $\psi_{p_n}(x)$. The easiest way is to recognise that the cosine can be written as a sum of exponentials, and directly write $\psi(x)$ as a linear combination of momentum eigenfunctions:

$$\begin{aligned}
\psi(x) &= \sqrt{\frac{2}{L}} e^{i\theta x/L} \frac{e^{2\pi i x/L} + e^{-2\pi i x/L}}{2} \\
&= \frac{1}{\sqrt{2L}} \left(e^{(2\pi+\theta)ix/L} + e^{(-2\pi+\theta)ix/L} \right) \\
&= \frac{1}{\sqrt{2}} \left(\psi_{p_1}(x) + \psi_{p_{-1}}(x) \right).
\end{aligned} \tag{24}$$

Since the momentum eigenfunctions are orthonormal, we can immediately read-off the coefficients:

$$\langle p_n|\psi\rangle = \begin{cases} \frac{1}{\sqrt{2}} & (n = 1, -1) \\ 0 & (\text{otherwise}). \end{cases} \tag{25}$$

Hence, the probabilities are

$$P(\text{momentum} = (2\pi+\theta)\hbar/L) = \frac{1}{2}, \quad P(\text{momentum} = (-2\pi+\theta)\hbar/L) = \frac{1}{2} \tag{26}$$

other probabilities being zero (of course, since these two add to 1). The average is then simply

$$\mathbb{E}(P) = \frac{1}{2}p_1 + \frac{1}{2}p_{-1} = \frac{\theta\hbar}{L}. \tag{27}$$