Quantum Mechanics III — Epiphany Term 2008

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Homework 2 – due 20 February 2008

Question 1. Consider a particle of mass m moving in a one-dimensional infinite square well potential

$$V(x) = \begin{cases} \infty & (x < 0) \\ 0 & (0 < x < a) \\ \infty & (x > a). \end{cases}$$

(a) Determine the energy levels and the corresponding wavefunctions.

(b) Calculate $\langle \hat{x} \rangle$, $\Delta \hat{x}$, $\langle \hat{p} \rangle$ and $\Delta \hat{p}$, where $\hat{x}$ and $\hat{p}$ are the position and momentum operators, respectively.

Question 2. Consider the operator $\hat{\mathcal{P}}_a$ defined by $\hat{\mathcal{P}}_a|x\rangle = |a-x\rangle$. Evaluate $\hat{\mathcal{P}}_a^2$, $\hat{\mathcal{P}}_a\hat{x}\hat{\mathcal{P}}_a$, $\hat{\mathcal{P}}_a f(\hat{x})\hat{\mathcal{P}}_a$ (for some function $f(\hat{x})$), $\hat{\mathcal{P}}_a\hat{p}\hat{\mathcal{P}}_a$, and $\hat{\mathcal{P}}_a\hat{p}^2\hat{\mathcal{P}}_a$. Is the hamiltonian of question 1 invariant under this transformation? If yes, what is the $\hat{\mathcal{P}}_a$ eigenvalue associated to the n^{th} energy level?

ANSWERS

1.

(a) The wave function is non-zero only in the region $0 < x < a$, where we will denote it $\psi(x)$. There, the potential is flat and 0, so the wave function is that of a free particle, given in general by

$$\psi(x) = A\cos(kx) + B\sin(kx)$$

with $k = \sqrt{2mE}/\hbar$ where E is the energy. Continuity of the wave function at $x = 0$ and $x = a$ gives

$$\psi(0) = 0\ , \quad \psi(a) = 0$$

and there is no continuity of the derivative of the wave function, because the potential is infinite at $x < 0$ and $x > a$. The first equation means that we must have $A = 0$, and the second, that

$$\sin(ka) = 0$$

This gives

$$k = k_n \equiv \frac{n\pi}{a}\ , \quad n = 1, 2, 3, \ldots$$

so that the energy levels are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

and the corresponding (unnormalised) wave functions are

$$\psi(x) = \psi_n(x) = B\sin(k_n x)$$

In order to normalise them, we impose

$$1 = \int_0^a \psi^*(x)\psi(x) = |B|^2 \int_0^a \sin(k_n x)^2 = \frac{a|B|^2}{2}$$

so that we can take

$$B = \sqrt{\frac{2}{a}}$$

(b) We may make use of the formulas

$$\int e^{ux}dx = \frac{e^{ux}}{u}\,, \quad \int xe^{ux}dx = \frac{\partial}{\partial u}\frac{e^{ux}}{u} = (xu-1)\frac{e^{ux}}{u^2}\,, \quad \int x^2e^{ux}dx = \frac{\partial^2}{\partial u^2}\frac{e^{ux}}{u} = (x^2u^2-2xu+2)\frac{e^{ux}}{u^3}$$

We have

$$\begin{aligned}
\langle\hat{x}\rangle &= \int_0^a \psi^*(x)x\psi(x)dx \\
&= \frac{2}{a}\int_0^a x\sin^2(k_n x)dx \\
&= \frac{1}{2a}\int_0^a x(2 - e^{2ik_n x} - e^{-2ik_n x})dx \\
&= \frac{1}{2a}\left(x^2 - 2\mathrm{Re}\left(e^{2ik_n x}\frac{1-2ik_n x}{4k_n^2}\right)\right)_{x=0}^{x=a} \\
&= \frac{a}{2}
\end{aligned}$$

where we used $e^{2ik_n a} = 1$. Also,

$$\begin{aligned}
\langle\hat{x}^2\rangle &= \int_0^a \psi^*(x)x^2\psi(x)dx \\
&= \frac{1}{2a}\int_0^a x^2(2 - e^{2ik_n x} - e^{-2ik_n x})dx \\
&= \frac{1}{2a}\left(\frac{2x^3}{3} - 2\mathrm{Re}\left(e^{2ik_n x}\frac{-4k_n^2x^2 - 4ik_n x + 2}{-8ik_n^3}\right)\right)_{x=0}^{x=a} \\
&= \frac{a^2}{3} - \frac{1}{2k_n^2}
\end{aligned}$$

and we find

$$\Delta\hat{x} = \sqrt{\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2} = a\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}$$

Continuing,

$$\begin{aligned}
\langle\hat{p}\rangle &= \int_0^a \psi^*(x)(-i\hbar)\frac{d}{dx}\psi(x)dx \\
&= -\frac{2i\hbar}{a}\int_0^a \sin(k_n x)\frac{d}{dx}\sin(k_n x)dx \\
&= -\frac{i\hbar}{a}\int_0^a \frac{d}{dx}\sin^2(k_n x)dx \\
&= -\frac{i\hbar}{a}\left(\sin^2(k_n x)\right)_0^a \\
&= 0
\end{aligned}$$

This was to be expected, since the average momentum in any bound state is exactly zero. Also,

$$\begin{aligned}
\langle\hat{p}^2\rangle &= \int_0^a \psi^*(x)(-\hbar^2)\frac{d^2}{dx^2}\psi(x)dx \\
&= \frac{2\hbar^2 k_n^2}{a}\int_0^a \sin^2(k_n x)dx \\
&= \hbar^2 k_n^2 \\
&= \frac{n^2\pi^2\hbar^2}{a^2}
\end{aligned}$$

This was to be expected, since the energy operator in the interval $0 < x < a$ is just the kinetic energy, $\hat{p}^2/(2m)$, and we are evaluating averages in energy eigenstates, $\langle\hat{H}\rangle = E_n$. That is, $\langle\hat{p}^2/(2m)\rangle = n^2\pi^2\hbar^2/(2ma^2)$. Hence

$$\Delta\hat{p} = \sqrt{\langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2} = \frac{n\pi\hbar}{a}$$

Note that $\Delta\hat{p}\Delta\hat{x}$ takes the value $(0.56786...)\hbar$ for $n = 1$, and this is indeed larger than $\hbar/2$, in agreement with the general theorem. For $n > 1$, $\Delta\hat{p}\Delta\hat{x}$ becomes even larger.

2.

By definition, $\hat{\mathcal{P}}_a|x\rangle = |a - x\rangle$. Then,

$$\begin{aligned}
\hat{\mathcal{P}}_a^2|x\rangle &= \hat{\mathcal{P}}_a|a - x\rangle \\
&= |a - (a - x)\rangle \\
&= |x\rangle
\end{aligned}$$

This is valid for all $|x\rangle$, which form a basis of the Hilbert space. Hence we conclude that $\hat{\mathcal{P}}_a^2 = 1$, the identity on the Hilbert space.

We have

$$\begin{aligned}
\hat{\mathcal{P}}_a\hat{x}\hat{\mathcal{P}}_a|x\rangle &= \hat{\mathcal{P}}_a\hat{x}|a - x\rangle \\
&= \hat{\mathcal{P}}_a(a - x)|a - x\rangle \\
&= (a - x)\hat{\mathcal{P}}_a|a - x\rangle \\
&= (a - x)|x\rangle \\
&= (a - \hat{x})|x\rangle
\end{aligned}$$

Again, this is valid for all vectors $|x\rangle$, hence we find the operator equation

$$\hat{\mathcal{P}}_a \hat{x} \hat{\mathcal{P}}_a = a - \hat{x}$$

Here, the number a on the right-hand side just means the scalar a times the identity operator on the Hilbert space.

In order to evaluate $\hat{\mathcal{P}}_a f(\hat{x}) \hat{\mathcal{P}}_a$, let us take $f(\hat{x}) = \hat{x}^n$ for some integrer power $n \geq 0$. We have

$$\begin{aligned} \hat{\mathcal{P}}_a \hat{x}^n \hat{\mathcal{P}}_a &= \hat{\mathcal{P}}_a \hat{x} \hat{\mathcal{P}}_a \hat{\mathcal{P}}_a \hat{x} \hat{\mathcal{P}}_a \cdots \hat{\mathcal{P}}_a \hat{x} \hat{\mathcal{P}}_a \ (n \text{ times}) \\ &= (\hat{\mathcal{P}}_a \hat{x} \hat{\mathcal{P}}_a)^n \\ &= (a - \hat{x})^n \end{aligned}$$

where in the first line, we used $\hat{\mathcal{P}}_a^2 = 1$. Hence, for any function $f(x)$ that has a Taylor series expansion at $x = 0$, we have

$$\hat{\mathcal{P}}_a f(\hat{x}) \hat{\mathcal{P}}_a = f(a - \hat{x})$$

This is then true for $f(x) = (x - x_0)^n$ for any number x_0. Hence we conclude that this stays true for any function that has a Taylor series expansion around some point x_0 – any function which is analytic in some domain! More precisely, this will stay true when applied on any state which involves position eigenstates $|x\rangle$ for x points where $f(x)$ is analytic. For instance, this also holds if $f(x)$ is defined by part (i.e. it is some analytic function in some region, another analytic function in another region, etc., like the potential of Question 1).

Now consider

$$\begin{aligned} \hat{\mathcal{P}}_a \hat{p} \hat{\mathcal{P}}_a |x\rangle &= \hat{\mathcal{P}}_a \hat{p} |a - x\rangle \\ &= \hat{\mathcal{P}}_a \left(i\hbar \frac{d}{dx'} |x'\rangle \right)_{x'=a-x} \\ &= -\hat{\mathcal{P}}_a i\hbar \frac{d}{dx} |a - x\rangle \\ &= -i\hbar \frac{d}{dx} \hat{\mathcal{P}}_a |a - x\rangle \\ &= -i\hbar \frac{d}{dx} |x\rangle \\ &= -\hat{p} |x\rangle \end{aligned}$$

so that, again for the same reasons, $\hat{\mathcal{P}}_a \hat{p} \hat{\mathcal{P}}_a = -\hat{p}$.

Finally,

$$\hat{\mathcal{P}}_a \hat{p}^2 \hat{\mathcal{P}}_a = (\hat{\mathcal{P}}_a \hat{p} \hat{\mathcal{P}}_a)^2 = \hat{p}^2$$

Then, with the hamiltonian being given by $\hat{H} = \hat{p}^2/(2m) + V(\hat{x})$, we have

$$\hat{\mathcal{P}}_a \hat{H} \hat{\mathcal{P}}_a = \hat{p}^2/(2m) + V(a - \hat{x})$$

The potential given in Question 1 is invariant under $x \to a - x$, so that $\hat{\mathcal{P}}_a \hat{H} \hat{\mathcal{P}}_a = \hat{H}$: the hamiltonian is invariant under this transformation. For the n^{th} eigenstate, $\psi_n(x) = B \sin(k_n x)$.

The action of $\hat{\mathcal{P}}_a$ on a wave function is obtained through $\hat{\mathcal{P}}_a\psi(x) = \langle x|\hat{\mathcal{P}}_a|\psi\rangle$ if $\psi(x) = \langle x|\psi\rangle$. This give $\hat{\mathcal{P}}_a\psi(x) = \psi(a-x)$ (here we are using $\hat{\mathcal{P}}_a^\dagger = \hat{\mathcal{P}}_a$ – which is proved by $\langle x|\hat{\mathcal{P}}_a|x'\rangle = \delta(x+x'-a) = \langle x'|\hat{\mathcal{P}}_a|x\rangle^* = \langle x|\hat{\mathcal{P}}_a^\dagger|x'\rangle$ – then we are using $\langle x|\hat{\mathcal{P}}_a = (\hat{\mathcal{P}}_a|x\rangle)^\dagger = (|a-x\rangle)^\dagger = \langle a-x|$). We then have

$$\hat{\mathcal{P}}_a\psi_n(x) = \psi_n(a-x) = B\sin(n\pi(a-x)/a) = (-1)^{n+1}\psi_n(x)$$

That is, the eigenvalue of $\hat{\mathcal{P}}_a$ on $\psi_n(x)$ is $(-1)^{n+1}$. Note that the ground state, with $n=1$, has eigenvalue 1 (that is, is invariant under the transformation).