Physics 606

Quantum Mechanics I

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Homework #6

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November 1st, 2015

1 Problem #1

(a) For a particle of charge, e, in an infinitely deep one-dimensional potential well from $0 \leq x \leq a$. We can find the matrix elements of the dipole moment $e\hat{x}$ in the energy representation by noting that the energy eigenfunctions in coordinate representation are

$$\langle x|E_n\rangle = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

This allows us to calculate

$$\begin{aligned}
\langle E_m|e\hat{x}|E_n\rangle &= \int dx\langle E_m|x\rangle e\hat{x}\langle x|E_n\rangle \\
&= \frac{2e}{a}\int_0^a \sin\left(\frac{m\pi}{a}x\right) x\sin\left(\frac{n\pi}{a}x\right) dx \\
&= \frac{e}{a}\left(\int_0^a x\cos\left(\frac{(n-m)\pi}{a}x\right) dx - \int_0^a x\cos\left(\frac{(m+n)\pi}{a}x\right) dx\right) \\
&= \frac{e}{a}\left(\frac{a^2(\cos((m-n)\pi) + (m-n)\pi\sin((m-n)\pi) - 1)}{(m-n)^2\pi^2}\right. \\
&\qquad \left. - \frac{a^2(\cos((m+n)\pi) + (m+n)\pi\sin((m+n)\pi) - 1)}{(m+n)^2\pi^2}\right) \\
&= \frac{ea}{\pi^2}\left(\frac{\cos((m-n)\pi) - 1}{(m-n)^2} - \frac{\cos((m+n)\pi) - 1}{(m+n)^2}\right)
\end{aligned}$$

Note the term with $\sin((n \pm m)\pi)$ is zero for all integers m, n so we see that for $n - m = 2i$ where $i = 1, 2, 3, ...$ we have

$$\begin{aligned}
\langle E_m|e\hat{x}|E_n\rangle &= \frac{2ea}{\pi^2}\left(\frac{\cos((2i)\pi) - 1}{(m-n)^2} - \frac{\cos(2(i+n)\pi) - 1}{(m+n)^2}\right) \\
&= \frac{ea}{\pi^2}\left(\frac{1-1}{(m-n)^2} - \frac{1-1}{(m+n)^2}\right) = 0
\end{aligned}$$

And for $m - n = 2i - 1$ where $i = 1, 2, 3, ...$ we have non-zero matrix elements given by

$$\begin{aligned}
\langle E_m|e\hat{x}|E_n\rangle &= \frac{2ea}{\pi^2}\left(\frac{\cos((2i-1)\pi) - 1}{(m-n)^2} - \frac{\cos(2(i+n) - 1\pi) - 1}{(m+n)^2}\right) \\
&= \frac{ea}{\pi^2}\left(\frac{-1-1}{(m-n)^2} - \frac{-1-1}{(m+n)^2}\right) \\
&= \frac{-2ea}{\pi^2}\left(\frac{1}{(m-n)^2} - \frac{1}{(m+n)^2}\right)
\end{aligned}$$

Note these are the matrix elements for $m \neq n$ for $n = m$ we have the integral

$$\begin{aligned}
\langle E_n|e\hat{x}|E_n\rangle &= \int dx\langle E_n|x\rangle e\hat{x}\langle x|E_n\rangle \\
&= \frac{e}{a}\left(\int_0^a x dx - \cancelto{0}{\int_0^a x\cos\left(\frac{2n\pi}{a}x\right) dx}\right) \\
&= \frac{e}{a}\frac{a^2}{2} = \frac{ea}{2}
\end{aligned}$$

So we have the value $ea/2$ along the diagonal of $\langle E_m|e\hat{x}|E_n\rangle$.

(b) We can repeat this process of the momentum operator $\hat{p}$ which in coordinate representation is

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

So the matrix elements can be calculated as

$$\begin{aligned}
\langle E_m|\hat{p}|E_n\rangle &= \int dx \langle E_m|x\rangle \hat{p}\langle x|E_n\rangle \\
&= -\frac{i2\hbar}{a}\int_0^a \sin\left(\frac{m\pi}{a}x\right)\frac{\partial}{\partial x}\sin\left(\frac{n\pi}{a}x\right)dx \\
&= -\frac{i2\hbar n\pi}{a^2}\int_0^a \sin\left(\frac{m\pi}{a}x\right)\cos\left(\frac{n\pi}{a}x\right)dx \\
&= \frac{i2\hbar n\pi}{a^2}\frac{a(m - m\cos(m\pi)\cos(n\pi) - n\sin(m\pi)\sin(n\pi))}{(m^2-n^2)\pi} \\
&= \frac{i2\hbar nm}{a(m^2-n^2)}(1-\cos(m\pi)\cos(n\pi))
\end{aligned}$$

Again we have the situation where $n - m = 2i$ for $i = 1, 2, 3, ...$ we have $\cos(m\pi)\cos(n\pi) = 1$ which implies that

$$\langle E_m|\hat{p}|E_n\rangle = 0 \qquad \text{for } n - m = 2i$$

and for $n - m = 2i - 1$ we have we have $\cos(m\pi)\cos(n\pi) = -1$ which imples

$$\langle E_m|\hat{p}|E_n\rangle = -\frac{i4\hbar nm}{a(m^2-n^2)} \qquad \text{for } n - m = 2i - 1$$

Note for the case where $m = n$ we have

$$\langle E_m|\hat{p}|E_n\rangle = -\frac{i2\hbar n\pi}{a^2}\int_0^a \sin\left(\frac{n\pi}{a}x\right)\cos\left(\frac{n\pi}{a}x\right)dx = 0$$

2 Problem #2

For a particle in a potential field $U(x)$ we have a Hamiltonian operator, $\hat{H}$, given by

$$\hat{H} = \frac{\mathbf{p}^2}{2m} + U(x)$$

this allows us to calculate the time variation of the operator $\hat{p}_x^2$ given by

$$\begin{aligned}
\frac{d(\hat{p}_x)^2}{dt} &= [\hat{p}_x^2, \hat{H}] \\
&= [\hat{p}_x^2, U(x)] \\
&= -[U(x), \hat{p}_x^2] \\
&= -i\hbar\frac{\partial U(x)}{\partial x}\hat{p}_x - \hbar^2\frac{\partial^2 U(x)}{\partial x^2}
\end{aligned}$$

Note that the calculate of the commutation relation between a potential, $U(x)$, and $\hat{p}_x^2$ we done in homework three.

3 Problem #3

We can find the Heisenberg representation for the position and momentum operators for a one-dimensional linear harmonic oscillator by the transformation

$$\hat{F}_H(t) = S^{-1}(t)\hat{F}_S S(t)$$

where $S(t) = \exp(-i/\hbar \hat{H} t)$. Note $\hat{H}$ is the Hamiltonian operator give by

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$$

in coordinate representation. We can find the time evolution of the operator $\hat{x}$ by taking the commutation with the Hamiltonian

$$\begin{aligned}
\frac{d\hat{x}}{dt} &= \frac{1}{i\hbar}[\hat{x}, \hat{H}] \\
&= -\frac{1}{i\hbar}[\hat{x}, \hat{p}^2] \\
&= -\frac{1}{i\hbar}\frac{-i\hbar}{m}\hat{p} \\
&= \frac{\hat{p}}{m}
\end{aligned}$$

where the time evolution of the momentum operator is found as

$$\begin{aligned}
\frac{d\hat{p}}{dt} &= \frac{1}{i\hbar}[\hat{p}, \hat{H}] \\
&= -\frac{1}{i\hbar}i\hbar\frac{\partial U(x)}{\partial dx} \\
&= -m\omega^2 x
\end{aligned}$$

Therefore we can combine these to get

$$\frac{d^2\hat{x}}{dt^2} = -\omega^2\hat{x}(t)$$

and

$$\frac{d^2\hat{p}}{dt^2} = -\omega^2\hat{p}(t)$$

We which are simple differentials with the solutions

$$\begin{aligned}
\hat{x}(t) &= A\sin(\omega t) + B\cos(\omega t) \\
\hat{p}(t) &= C\sin(\omega t) + D\cos(\omega t)
\end{aligned}$$

Where we apply the initial conditions

$$\begin{aligned}
\hat{x}(t=0) &= \hat{x}(0) \\
\frac{d\hat{x}(t=0)}{dt} &= \frac{\hat{p}(0)}{m} \\
\hat{p}(t=0) &= \hat{p}(0) \\
\frac{d\hat{p}(t=0)}{dt} &= -m\omega^2\hat{x}(0)
\end{aligned}$$

This implies that the constants of integration are

$$
\begin{aligned}
A &= \frac{\hat{p}(0)}{m\omega} \\
B &= \hat{x}(0) \\
C &= -m\omega\hat{x}(0) \\
D &= \hat{p}(0)
\end{aligned}
$$

so our operators are

$$
\begin{aligned}
\hat{x}(t) &= \frac{\hat{p}(0)}{m\omega}\sin(\omega t) + \hat{x}(0)\cos(\omega t) \\
\hat{p}(t) &= -m\omega\hat{x}(0)\sin(\omega t) + \hat{p}(0)\cos(\omega t)
\end{aligned}
$$

We can now use these to find the time evolution of the expectation values of these operators with an initial wave packet give by

$$\psi(x) A \exp\left(-\frac{(x-x_0)^2}{2a^2} + i\frac{p_0 x}{\hbar}\right)$$

We see that this wave packet is exactly localized at $x = x_0$ with a momentum of $p = p_0$ this implies that it's initial expectation value is $<\hat{x}(0)>= x_0$ and $<\hat{p}(0) = p_0$. There for we can find

$$
\begin{aligned}
<\hat{x}(t)> &= \left\langle \frac{\hat{p}(0)}{m\omega}\sin(\omega t) + \hat{x}(0)\cos(\omega t) \right\rangle \\
&= \frac{<\hat{p}(0)>}{m\omega}\sin(\omega t) + <\hat{x}(0)>\cos(\omega t) \\
&= \frac{p_0}{m\omega}\sin(\omega t) + x_0\cos(\omega t)
\end{aligned}
$$

and

$$
\begin{aligned}
<\hat{p}(t)> &= \langle -m\omega\hat{x}(0)\sin(\omega t) + \hat{p}(0)\cos(\omega t)\rangle \\
&= -m\omega <\hat{x}(0)> \sin(\omega t) + <\hat{p}(0)> \cos(\omega t) \\
&= -m\omega x_0 \sin(\omega t) + p_0\cos(\omega t)
\end{aligned}
$$

Next in order to calculate $<\Delta x>^2$ we need to find

$$
\begin{aligned}
<x^2(t)> &= \left\langle \left(\frac{\hat{p}(0)}{m\omega}\right)^2 \sin^2(\omega t) + \hat{x}(0)^2\cos^2(\omega t) + \frac{\hat{p}(0)\hat{x}(0) + \hat{x}(0)\hat{p}(0)}{m\omega}\sin(\omega t)\cos(\omega t) \right\rangle \\
&= \frac{<\hat{p}(0)^2>}{(m\omega)^2}\sin^2(\omega t) + <\hat{x}(0)^2>\cos^2(\omega t) + \frac{<2\hat{x}(0)\hat{p}(0) - [\hat{x}(0),\hat{p}(0)]>}{m\omega}\sin(\omega t)\cos(\omega t) \\
&= \frac{<\hat{p}(0)^2>}{(m\omega)^2}\sin^2(\omega t) + <\hat{x}(0)^2>\cos^2(\omega t) + \frac{<2\hat{x}(0)\hat{p}(0)> - i\hbar>}{m\omega}\sin(\omega t)\cos(\omega t) \\
&= \frac{<\hat{p}(0)^2>}{(m\omega)^2}\sin^2(\omega t) + <\hat{x}(0)^2>\cos^2(\omega t) + \frac{2x_0p_0 + i\hbar - i\hbar}{m\omega}\sin(\omega t)\cos(\omega t) \\
&= \frac{<\hat{p}(0)^2>}{(m\omega)^2}\sin^2(\omega t) + <\hat{x}(0)^2>\cos^2(\omega t) + \frac{2x_0p_0}{m\omega}\sin(\omega t)\cos(\omega t)
\end{aligned}
$$

This yields

$$
\begin{aligned}
< \Delta x(t) >^2 &=< x(t)^2 > - < x(t) >^2 \\
&= \frac{< \hat{p}(0)^2 >}{(m\omega)^2} \sin^2(\omega t) + < \hat{x}(0)^2 > \cos^2(\omega t) + \frac{2x_0 p_0}{m\omega} \sin(\omega t)\cos(\omega t) - \frac{p_0^2}{(m\omega)^2} \sin^2(\omega t) - x_0^2 \cos^2(\omega t) \\
&\quad - \frac{2x_0 p_0}{m\omega} \sin(\omega t)\cos(\omega t) \\
&= \frac{< \hat{p}(0)^2 > - p_0^2}{(m\omega)^2} \sin^2(\omega t) + < \hat{x}(0)^2 > - x_0^2 \cos^2(\omega t) \\
&= \frac{< \Delta\hat{p}(0) >^2}{(m\omega)^2} \sin^2(\omega t) + < \hat{x}(0) >^2 \cos^2(\omega t) \\
&= \frac{\hbar^2}{(2m\omega)^2 < \Delta x(0) >^2} \sin^2(\omega t) + < \hat{x}(0) >^2 \cos^2(\omega t)
\end{aligned}
$$

Note we use the limited case of Heisenberg's uncertainty relation

$$
< \Delta p(0) >^2 < \Delta x(0) >^2 = \frac{\hbar^2}{4}
$$

Now all we need is the variance of $x(0)$ which is just the variance of our initial wave packet with gives us

$$
< \Delta x(0) >^2 = \frac{a^2}{2}
$$

So we can find

$$
\begin{aligned}
< \Delta x(t) >^2 &= \frac{\hbar^2}{(2m\omega)^2 < \Delta x(0) >^2} \sin^2(\omega t) + < \hat{x}(0) >^2 \cos^2(\omega t) \\
&= \frac{2\hbar^2}{(2am\omega)^2} \sin^2(\omega t) + \frac{a^2}{2} \cos^2(\omega t)
\end{aligned}
$$

Now we repeat this process for $< \delta p(t) >^2$ by noting that

$$
\begin{aligned}
< \delta p(t)^2 > &= (m\omega)^2 < \hat{x}(0)^2 > \sin^2(\omega t) + < \hat{p}(0)^2 > \cos(\omega t) + m\omega(< \hat{p}(0)\hat{x}(0) + \hat{x}(0)\hat{p}(0) >) \sin(\omega t)\cos(\omega t) \\
&= (m\omega)^2 < \hat{x}(0)^2 > \sin^2(\omega t) + < \hat{p}(0)^2 > \cos(\omega t) + 2m\omega x_0 p_0 \sin(\omega t)\cos(\omega t)
\end{aligned}
$$

So it follows like before that

$$
\begin{aligned}
< \Delta p(t) >^2 &=< p(t)^2 > - < p(t) >^2 \\
&= (m\omega)^2 < \hat{x}(0)^2 > \sin^2(\omega t) + < \hat{p}(0)^2 > \cos(\omega t) + 2m\omega x_0 p_0 \sin(\omega t)\cos(\omega t) \\
&\quad - (m\omega)^2 x_0^2 \sin^2(\omega t) - p_0^2 \cos(\omega t) - 2m\omega x_0 p_0 \sin(\omega t)\cos(\omega t) \\
&= (m\omega)^2 < \hat{x}(0) >^2 \sin^2(\omega t) + < \Delta\hat{p}(0) >^2 \cos(\omega t) \\
&= (m\omega)^2 < \hat{x}(0) >^2 \sin^2(\omega t) + \frac{\hbar^2}{4 < \Delta\hat{x}(0) >^2} \cos(\omega t) \\
&= \frac{(ma\omega)^2}{2} \sin^2(\omega t) + \frac{\hbar^2}{2a^2} \cos(\omega t)
\end{aligned}
$$