The harmonic oscillator

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In what follows, we will be making use of the following key results:

$$\hat{a}_{\pm} = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} \mp i\hat{p}) \tag{1}$$

$$[\hat{a}_-, \hat{a}_+] = 1 \tag{2}$$

$$\hat{a}_+\psi_n = \sqrt{n+1}\,\psi_n, \quad \hat{a}_-\psi_n = \sqrt{n}\psi_{n-1} \tag{3}$$

$$\int \psi_m^*\psi_n \,\mathrm{d}x = \delta_{mn} \tag{4}$$

$$\hat{H} = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right) \tag{5}$$

We can use (1) to rewrite $\hat{x}$ and $\hat{p}$ in terms of $\hat{a}_+$ and $\hat{a}_-$:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_+ + \hat{a}_-) \tag{6}$$

$$\hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}_+ - \hat{a}_-) \tag{7}$$

1 A superposition of states

In lecture we discussed finding $\langle x\rangle_n$ and $\langle p\rangle_n$ for energy eigenstates, and found that they where both zero. In this section we look at calculating $\langle x\rangle$ and $\langle p\rangle$ for a state that is *not* an energy eigenstate.

Let us consider the state that is initially a superposition of ψ_0 and ψ_1:

$$\Psi(x,0) = \frac{1}{\sqrt{2}}\left(\psi_0(x) + \psi_1(x)\right) \tag{8}$$

We know how to make this into a time-dependent equation by attaching the appropriate phase factors:

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left(\psi_0(x)e^{-iE_0t/\hbar} + \psi_1(x)e^{-iE_1t/\hbar}\right) \tag{9}$$

To get the expectation value of $\langle x\rangle$ and $\langle p\rangle$ we need to know what the ladder operators do. Looking at $\hat{a}_+$ first:

$$\begin{aligned}\hat{a}_+\Psi(x,t) &= \frac{1}{\sqrt{2}}\left((\hat{a}_+\psi_0)e^{-iE_0t/\hbar} + (\hat{a}_+\psi_1)e^{-iE_1t/\hbar}\right) &(10)\\ &= \frac{1}{\sqrt{2}}\left(\psi_1(x)e^{-iE_0t/\hbar} + \sqrt{2}\psi_2(x)e^{-iE_1t/\hbar}\right), &(11)\end{aligned}$$

where in the last line I have used (3). Doing $\hat{a}_-$ is even easier (as $\hat{a}_-\psi_0 = 0$):

$$\hat{a}_-\Psi(x,t) = \frac{1}{\sqrt{2}}\left(\psi_0(x)e^{-iE_1t/\hbar}\right) \tag{12}$$

1.1 Calculating $\langle x\rangle$

The procedure is almost identical for what was done for stationary states. We start by replacing the operator $\hat{x}$

$$\begin{aligned}\langle x\rangle &= \int \Psi(x,t)^*\hat{x}\Psi(x,t)\,\mathrm{d}x\\ &= \sqrt{\frac{\hbar}{2m\omega}}\int \Psi(x,t)^*(\hat{a}_+\Psi(x,t) + \hat{a}_-\Psi(x,t))\,\mathrm{d}x\\ &= \sqrt{\frac{\hbar}{2m\omega}}\frac{1}{\sqrt{2}}\int \Psi(x,t)^*\left(\psi_1e^{-iE_0t/\hbar} + \sqrt{2}\psi_2e^{-iE_1t/\hbar} + \psi_0e^{-iE_1t/\hbar}\right)\mathrm{d}x\end{aligned}$$

where we have simply substituted $\hat{a}_+\Psi$ and $\hat{a}_-\Psi$. Taking the complex conjugate of Ψ gives

$$\Psi(x,t)^* = \frac{1}{\sqrt{2}}\left(\psi_0(x)^*e^{iE_0t/\hbar} + \psi_1(x)^*e^{+iE_1t/\hbar}\right) \tag{13}$$

from (9). Note the signs on the exponentials!

Placing this back into the expression for $\langle x\rangle$ gives

$$\begin{aligned}\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}}\frac{1}{2}\int &\left(\psi_0(x)^*e^{iE_0t/\hbar} + \psi_1(x)^*e^{+iE_1t/\hbar}\right)\\ &\times\left(\psi_0e^{-iE_1t/\hbar} + \psi_1e^{-iE_0t/\hbar} + \sqrt{2}\psi_2e^{-iE_1t/\hbar}\right)\mathrm{d}x\end{aligned} \tag{14}$$

Now we exploit orthonormality (equation (4)), as all the x dependence lies in the $\psi_i(x)$. The only non-zero pieces are

$$\langle x \rangle = \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}} \left[e^{i(E_0-E_1)t/\hbar} \int \psi_0(x)^* \psi_0(x)\,\mathrm{d}x + e^{i(E_1-E_0)t/\hbar} \int \psi_1(x)^* \psi_1(x)\,\mathrm{d}x \right] \tag{15}$$

$$= \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}} \left[e^{i(E_0-E_1)t/\hbar} + e^{-i(E_0-E_1)t/\hbar} \right] \tag{16}$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \cos\left(\frac{(E_1-E_0)t}{\hbar}\right) \tag{17}$$

Finally, we use the result that $E_1 = E_0 + \hbar\omega$ as we showed from the ladder operators to get

$$\langle x \rangle = \sqrt{\frac{\hbar}{2m\omega}} \cos(\omega t) \tag{18}$$

1.2 Calculating $\langle p \rangle$

This is very much the same and will be done in much less detail. We have

$$\langle p \rangle = \int \Psi^* \hat{p} \Psi \,\mathrm{d}x \tag{19}$$

$$= i\sqrt{\frac{m\hbar\omega}{2}} \int \Psi^* (\hat{a}_+ \Psi - \hat{a}_- \Psi) \tag{20}$$

$$= i\sqrt{\frac{m\hbar\omega}{2}} \frac{1}{2} \int \left(\psi_0(x)^* e^{iE_0 t/\hbar} + \psi_1(x)^* e^{+iE_1 t/\hbar} \right) \times \left(\psi_1(x) e^{-iE_0 t/\hbar} + \sqrt{2}\psi_2(x) e^{-iE_1 t/\hbar} - \psi_0(x) e^{-iE_1 t/\hbar} \right) \mathrm{d}x \tag{21}$$

Again, we exploit orthonormality to get

$$\langle p \rangle = \sqrt{\frac{m\hbar\omega}{2}} \frac{i}{2} \left[-e^{i(E_0-E_1)t/\hbar} \int \psi_0(x)^* \psi_0(x)\,\mathrm{d}x + e^{i(E_1-E_0)t/\hbar} \int \psi_1(x)^* \psi_1(x)\,\mathrm{d}x \right] \tag{22}$$

$$= \sqrt{\frac{m\hbar\omega}{2}} \frac{i}{2} \left[e^{i(E_1-E_0)t/\hbar} - e^{i(E_0-E_1)t/\hbar} \right] \tag{23}$$

$$= \sqrt{\frac{m\hbar\omega}{2}} \frac{i}{2} \times 2i \sin\left(\frac{(E_1-E_0)t}{\hbar}\right) \tag{24}$$

$$= -\sqrt{\frac{m\hbar\omega}{2}} \sin(\omega t) \tag{25}$$

1.3 Relationship between $\langle x \rangle$ and $\langle p \rangle$

We see that unlike the energy eigenstates, that now the expectation values are non-zero and depend on time. In particular, we can look at the rate of change of the expectation value of position:

$$\frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t} = -\sqrt{\frac{\hbar}{2m\omega}}\omega\sin(\omega t) = -\sqrt{\frac{\hbar\omega}{2m}}\sin(\omega t) \tag{26}$$

Looking back at the expression for $\langle p \rangle$ we see

$$\langle p \rangle = m\frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t}! \tag{27}$$

The expectation values are behaving much like the way that we expect particles in *classical mechanics* to behave[1]. In some sense, we should have expected that the laws of classical mechanics to work out for averages, as the classical world is an approximation for a large (decoherent) quantum system[2]. This result is known as *Ehrenfest's theorem*. It will be proved to you later, but this is a nice example of it.

You have to be a little bit careful when applying Ehrenfest's theorem. If I asked you what the expectation value of the kinetic energy was, is it

$$\langle \mathrm{KE} \rangle \stackrel{?}{=} \frac{\langle p^2 \rangle}{2m} \quad \text{or} \quad \langle \mathrm{KE} \rangle \stackrel{?}{=} \frac{\langle p \rangle^2}{2m}$$

From the work that you have done so far, we know the operator for KE is $\hat{p}^2/2m$ and so the expression on the left is correct. When using Ehrenfest's theorem, you have to take the expectation value of the entire left and right hand side. So what we should have is

$$\langle p \rangle = m\left\langle \frac{\mathrm{d}x}{\mathrm{d}t} \right\rangle \tag{28}$$

as m is a constant. In this case we are lucky because

$$\left\langle \frac{\mathrm{d}x}{\mathrm{d}t} \right\rangle = \frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t}$$

[1] This happened in energy eigenstates too, except the relationship was $\langle p \rangle = 0 = m\mathrm{d}0/\mathrm{d}t$, and did not catch our attention at the time.

[2] The decoherence is needed so that I am not looking at many copies of the same system. This means that I am allowed to interpret the many body average as the same thing as the *ensemble* average. The ensemble average is what I mean when I write $\langle x \rangle$ etc.