PHY 137A
October 31, 2023

Discussion 9

Background

The harmonic oscillator is super important. Let's get a little practice with it. The quantum harmonic oscillator is defined by a Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + m\omega^2\hat{x}^2$. In the position basis, the momentum operator is $\hat{p} \to -i\hbar\partial/\partial x$, and the position operator is $\hat{x} \to x$. The system is exactly solvable, meaning we can determine the energy spectrum and the stationary states. This is done most economically by introducing the raising and lowering operators:

$$a_+ = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{i}{m\omega}\hat{p})$$
$$a_- = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{i}{m\omega}\hat{p})$$

It was shown in lecture that the nth energy eigenstate has energy

$$E_n = \hbar\omega(n + \frac{1}{2}) \quad n = 0, 1, 2, 3, ...$$

and can be generated by repeatedly applying the raising operator to the ground state

$$|n\rangle = \frac{1}{\sqrt{n!}}(a_+)^n |0\rangle$$

The Hamiltonian can be written in terms of the raising and lower operators as

$$\hat{H} = \hbar\omega(a_+a_- + \frac{1}{2}).$$

Finally, it is useful to have the inverse relation, giving the position and momentum operators in terms of the raising and lowering operators:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-)$$
$$\hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(a_+ - a_-).$$

Warm-Up

1. Using $[\hat{x}, \hat{p}] = i\hbar$, show that $[a_-, a_+] = a_-$.

2. Using the above result, show that $[\hat{n}, a_-] = -a_-$ and $[\hat{n}, a_+] = a_+$, where $\hat{n} \equiv a_+a_-$ is the number operator, not to be confused with the number n which does not have a hat on it!

Discussion 9

Problems

3. Confirm that the Hamiltonian of the simple harmonic oscillator can be written as $H = \hbar\omega(\hat{n} + \frac{1}{2})$.

4. We have the formula $a_+ |n\rangle = \sqrt{n+1}\,|n+1\rangle$ which describes the action of the raising operator on a stationary state. By writing this equation in the position basis, generate the first excited state's wavefunction $\phi_1(x)$ from the ground state wavefunction

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$$

Verify that the procedure generates a normalized wavefunction.

5. A particle of mass m is trapped in a harmonic oscillator potential $V(x) = \frac{1}{2}m\omega^2 x^2$. At time $t = 0$, we are told that the state of the system is

$$\Psi(x, 0) = c_0\phi_0(x) + c_1\phi_1(x)$$

for some complex numbers c_0 and c_1, and where $\phi_0(x)$ and $\phi_1(x)$ are the normalized ground state and first excited state of the harmonic oscillator, respectively.

(a) Write an expression for the state of the system at a later time, t.

(b) Compute $\langle x\rangle$ as a function of time, using the explicit forms

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$$
$$\phi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}} x e^{-m\omega x^2/2\hbar}$$

(c) Compute $\langle x\rangle$ as a function of time, using only the properties of the raising and lowering operators.

(d) Compute $\langle p\rangle$ as a function of time (by any method you prefer).

(e) Confirm that Erenfest's theorem holds here

$$\langle p\rangle = m\frac{d}{dt}\langle x\rangle$$
$$\frac{d}{dt}\langle p\rangle = -\langle\frac{dV}{dx}\rangle$$

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Solutions

1. Simply insert the definitions of a_- and a_+ into $[a_-, a_+]$. Because the commutator $[A, B] = AB - BA$ is linear in both slots, it is distributive $[A+B, C] = [A, C] + [B, C]$, and numerical factors can be pulled out $[cA, B] = c[A, B]$. So we can write

$$\begin{aligned}
[a_-, a_+] &= \frac{m\omega}{2\hbar}\left([x + \frac{i}{m\omega}p, x - \frac{i}{m\omega}p]\right) \\
&= \frac{m\omega}{2\hbar}\left([x, x] + \frac{i}{m\omega}[p, x] - \frac{i}{m\omega}[x, p] + \frac{1}{m^2\omega^2}[p, p]\right)
\end{aligned}$$

   The commutator of anything with itself is zero. On the other hand, $[x, p] = i\hbar$ and $[p, x] = -i\hbar$. Putting these in and simplifying leads to the answer of 1 (the identity operator).

2. Let me show a useful trick for evaluating commutators. I claim that

$$[AB, C] = A[B, C] + [A, C]B$$

   To prove this, lets just write out the definition of each term:

$$\begin{aligned}
[AB, C] &= ABC - CAB \\
A[B, C] &= ABC - ACB \\
[A, C]B &= ACB - CAB
\end{aligned}$$

   Clearly the second two sum to the first, which proves the identity.

   OK, with that established the exercise becomes very straightforward. Write

$$[\hat{n}, a_-] = [a_+a_-, a_-] = a_+\cancelto{0}{[a_-, a_-]} + \cancelto{-1}{[a_+, a_-]}a_- = -a_-$$

   Similarly,

$$[\hat{n}, a_+] = [a_+a_-, a_+] = a_+\cancelto{1}{[a_-, a_+]} + \cancelto{0}{[a_+, a_+]}a_- = a_+$$

3. This one is another simple plug-and-chug. Take the Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$ and just insert the expression for $\hat{x}$ and $\hat{p}$ in terms of the ladder operators. The first term is:

$$\begin{aligned}
\frac{1}{2m}p^2 &= \frac{1}{2m}(i)^2\frac{m\omega\hbar}{2}(a_+ - a_-)^2 \\
&= -\frac{\hbar\omega}{4}(a_+a_+ - a_-a_+ - a_+a_- + a_-a_-)
\end{aligned}$$

The second term is

$$\begin{aligned}\frac{1}{2}m\omega^2 x^2 &= \frac{1}{2}m\omega^2\frac{\hbar}{2m\omega}(a_+ + a_-)^2 \\ &= \frac{\hbar\omega}{4}(a_+a_+ + a_+a_- + a_-a_+ + a_-a_-)\end{aligned}$$

They add to make

$$H = \frac{\hbar\omega}{2}(a_+a_- + a_-a_+) = \hbar\omega(\hat{n} + \frac{1}{2})$$

after using $[a_-, a_+] = 1$.

4. Specializing to the case $n = 0$, the raising equations says $a_+\phi_0 = \sqrt{1}\phi_1$. In the position basis, this equation becomes

$$\sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{i}{m\omega}\frac{\hbar}{i}\frac{d}{dx}\right)\phi_0(x) = \phi_1(x).$$

Applying this to $\phi_0(x) = (m\omega/\pi\hbar)^{1/4}e^{-m\omega x^2/2\hbar}$ leads to

$$\phi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}xe^{-m\omega x^2/2\hbar}$$

I'll let you check that it is normalized.

5. (a) $\Psi(x,t) = c_0\phi_0(x)e^{-iE_0t\hbar} + c_1\phi_1(x)e^{-iE_1t/\hbar}$.

(b) The expectation value of x at time t for this state is

$$\langle x\rangle = \int_{-\infty}^{\infty} dx\Psi(x,t)^* x\Psi(x,t) = \int dxx|\Psi(x,t)|^2 \tag{1}$$

Let's get an expression for the probability density $|\Psi(x,t)|^2$ at time t. Using $|z|^2 = z^*z$ we have

$$\begin{aligned}|\Psi(x,t)|^2 &= (c_0^*\phi_0(x)e^{+iE_0t\hbar} + c_1^*\phi_1(x)e^{+iE_1t/\hbar})(c_0\phi_0(x)e^{-iE_0t\hbar} + c_1\phi_1(x)e^{-iE_1t/\hbar}) \\ &= |c_0|^2|\phi_0|^2 + |c_1|^2|\phi_1|^2 + \phi_0\phi_1(c_0^*c_1e^{-i\omega t} + c_0c_1^*e^{+i\omega t})\end{aligned}$$

where I used $E_n = \hbar\omega(n + 1/2)$ to simplify the exponent. Let's do the integral in equation 1 one term at a time. First we have

$$\int dxx|c_0|^2|\phi_0|^2$$

But this is zero because the integrand is an odd function and we are integrating over all space. The second term dissapears for the same reason. We are left with the last term. I will only write the part that depends on x, and tack the rest on later. We want to compute:

$$\int dx x\phi_0(x)\phi_1(x) = \sqrt{\frac{m\omega}{\pi\hbar}}\sqrt{\frac{2m\omega}{\hbar}}\int_{-\infty}^{\infty} dx x^2 e^{-m\omega x^2/\hbar}$$

Let $u = \sqrt{m\omega/\hbar}x$, and $du = \sqrt{m\omega/\hbar}dx$. Then the integral becomes

$$= \sqrt{\frac{2}{\pi}}\frac{m\omega}{\hbar}\left(\frac{\hbar}{m\omega}\right)^{3/2}\int_{\infty}^{\infty} du u^2 e^{-u^2}$$

The integral itself evaluates to $\sqrt{\pi}/2$, leaving $\sqrt{\hbar/2m\omega}$. Tacking back on the rest of the expression, we have

$$\boxed{\langle x\rangle = \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}\{c_0^* c_1 e^{-i\omega t}\}}.$$

where I used $\mathrm{Re}\{z\} = (z + z^*)/2$.

(c) Let's do it again! But this time no integrals allowed. I promise you'll like it. All I will use is the fact that the inner product is linear (so it distributes), and the action of a_- and a_+ on the stationary states. Namely I will use

$$\begin{aligned} a_-\phi_0 &= 0 \\ a_+\phi_0 &= \phi_1 \\ a_-\phi_1 &= \phi_0 \\ a_+\phi_1 &= \sqrt{2}\phi_2 \end{aligned}$$

The expectation value of x with respect to the state Ψ is

$$\begin{aligned} \langle x\rangle &= \langle\Psi(t)|\,\hat{x}\,|\Psi(t)\rangle \\ &= \langle\Psi(t)|\sqrt{\frac{\hbar}{2m\omega}}(a_- + a_+)\left(c_0\,|\phi_0(x)\rangle\, e^{-iE_0 t\hbar} + c_1\,|\phi_1(x)\rangle\, e^{-iE_1 t/\hbar}\right) \end{aligned}$$

Now allow the ladder operators to distribute over the states and act on them. This will generate four terms out of the two terms, leaving:

$$= \sqrt{\frac{\hbar}{2m\omega}}\,\langle\Psi(t)|\left(\cancelto{0}{c_0(0)e^{-iE_0 t\hbar}} + c_1\,|\phi_0(x)\rangle\, e^{-iE_1 t/\hbar} + c_0\,|\phi_1(x)\rangle\, e^{-iE_0 t\hbar} + c_1\sqrt{2}\,|\phi_2(x)\rangle\, e^{-iE_1 t/\hbar}\right).$$

Now distribute the inner product, using $\langle\phi_0|\phi_0\rangle = 1$, $\langle\phi_0|\phi_1\rangle = 0$, etc. When the dust settles,

$$\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(c_0^* c_1 e^{-i\omega t}\cancelto{1}{\langle\phi_0|\phi_0\rangle} + c_0 c_1^2 e^{i\omega t}\cancelto{1}{\langle\phi_1|\phi_1\rangle}\right)$$

I neglected to write some terms which are zero due to the states being orthogonal. Once again we find

$$\boxed{\langle x\rangle = \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}\big\{c_0^* c_1 e^{-i\omega t}\big\}}.$$

Notice that this procedure would not have been any harder if we were working with the $n = 75$ and $n = 122$ states, while the integral version would be an absolute nightmare in that case!

(d) Allow me to use the ladder operator method. We have:

$$\begin{aligned}
\langle p\rangle &= \langle\Psi(t)|\,\hat{p}\,|\Psi(t)\rangle \\
&= \langle\Psi(t)|\,i\sqrt{\frac{m\omega\hbar}{2}}(a_+ - a_-)\,|\Psi(t)\rangle \\
&= \langle\Psi(t)|\,i\sqrt{\frac{m\omega\hbar}{2}}(a_+ - a_-)\left(c_0\,|\phi_0(x)\rangle\, e^{-iE_0 t\hbar} + c_1\,|\phi_1(x)\rangle\, e^{-iE_1 t/\hbar}\right) \\
&= \langle\Psi(t)|\,i\sqrt{\frac{m\omega\hbar}{2}}\left(0 + c_0 e^{-iE_0 t/\hbar}\,|\phi_1\rangle - c_1 e^{-iE_1 t/\hbar}\,|\phi_0\rangle + c_1 e^{-iE_1 t/\hbar}\sqrt{2}\,|\phi_2\rangle\right) \\
&= -i\sqrt{\frac{m\omega\hbar}{2}}\left(c_0^* c_1 e^{-i\omega t} - c_0 c_1^* e^{i\omega t}\right) \\
&= \boxed{\sqrt{2m\omega\hbar}\,\mathrm{Im}\big\{c_0^* c_1 e^{-i\omega t}\big\}}.
\end{aligned}$$

(e) Now for some payoff. To simplify matters let's set $c_0 = c_1 = 1/\sqrt{2}$ (you can show it in general if you'd like, it's not much harder). With this, we have

$$\begin{aligned}
\mathrm{Re}\big\{c_0^* c_1 e^{-i\omega t}\big\} &= \frac{1}{2}\cos(\omega t) \\
\mathrm{Im}\big\{c_0^* c_1 e^{-u\omega t}\big\} &= -\frac{1}{2}\sin(\omega t)
\end{aligned}$$

and so

$$\begin{aligned}
\langle x\rangle &= \sqrt{\frac{2\hbar}{m\omega}}\frac{1}{2}\cos(\omega t) \\
\langle p\rangle &= -\sqrt{2m\omega\hbar}\frac{1}{2}\sin(\omega t)
\end{aligned}$$

Then to establish the first of Erenfest's relations, compute

$$\begin{aligned}
m\frac{d}{dt}\langle x\rangle &= m\frac{d}{dt}\sqrt{\frac{2\hbar}{m\omega}}\frac{1}{2}\cos(\omega t) \\
&= -\sqrt{2m\omega\hbar}\frac{1}{2}\sin(\omega t)
\end{aligned}$$

which does agree with our calculation of $\langle p \rangle$. Next up, since $V(x) = \frac{1}{2}m\omega^2 x^2$, $dV/dx = m\omega^2 x$, and upon taking the expectation value of both sides, we have $\langle dV/dx \rangle = m\omega^2 \langle x \rangle$. Meanwhile,

$$\begin{aligned}
\frac{d}{dt}\langle p \rangle &= -\sqrt{2m\omega\hbar}\frac{1}{2}\frac{d}{dt}\sin(\omega t) \\
&= -m\omega^2\sqrt{\frac{2\hbar}{m\omega}}\frac{1}{2}\cos t \\
&= -m\omega^2\langle x \rangle \\
&= -\langle\frac{dV}{dx}\rangle
\end{aligned}$$

The expectation values follow their classical equations of motion.