

Homework H10 Solution

1. In lecture, we talked about how the vibrating molecule Hamiltonian (energy operator) is symmetrical in p and x because it depends on the square of both. We made use of this symmetry to find out that a Gaussian is the lowest energy state (ground state) of the harmonic oscillator, and its energy is $\hbar\omega/2$. We also derived an expression for the Hamiltonian in terms of the raising operator $\hat{a}^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{\frac{1}{2}} \left(x - \frac{i\hat{p}}{m\omega}\right)$ and lowering operator $\hat{a} = \left(\frac{m\omega}{2\hbar}\right)^{\frac{1}{2}} \left(x + \frac{i\hat{p}}{m\omega}\right)$: $\hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2}\right)$

Now, work out $\hat{a}\hat{a}^\dagger$ to derive an equivalent representation for the Hamiltonian

$$\hat{H} = \hbar\omega \left(\hat{a}\hat{a}^\dagger - \frac{1}{2}\right).$$

That formula looks very similar to the one we derived in class, but the order of \hat{a}^\dagger and \hat{a} has switched.

Solution:

Recall the expression for $\hat{a}^\dagger \hat{a}$ from lecture:

$$\hat{a}^\dagger \hat{a} = \left(\frac{m\omega}{2\hbar}\right) \left\{ x^2 + \frac{i}{m\omega} (x\hat{p} - \hat{p}x) + \frac{\hat{p}^2}{m^2\omega^2} \right\} \quad (1)$$

Writing $\hat{a}\hat{a}^\dagger$ we have

$$\hat{a}\hat{a}^\dagger = \left(\frac{m\omega}{2\hbar}\right) \left\{ x^2 + \frac{i}{m\omega} (\hat{p}x - x\hat{p}) + \frac{\hat{p}^2}{m^2\omega^2} \right\} \quad (2)$$

The expression for $\hat{a}\hat{a}^\dagger$ looks very similar to that of $\hat{a}^\dagger \hat{a}$ except in the middle part of eq. (2) the order of x and \hat{p} are switched. We know that the commutator $[x, \hat{p}] = i\hbar$ and that $[\hat{p}, x] = -i\hbar$ so no terms change from eq. (1) to eq. (2) but there **is a sign change** and we write

$$\hat{a}\hat{a}^\dagger = \left(\frac{1}{\hbar\omega}\right) \left\{ \frac{\hat{p}^2}{2m} + \frac{k}{2} x^2 + \frac{\hbar\omega}{2} \right\} \quad (3)$$

where we have followed the same procedure outlined in lecture. From here, it is a simple algebraic rearrangement to obtain

$$\hat{H} = \hbar\omega \left(\hat{a}\hat{a}^\dagger - \frac{1}{2}\right) \quad (4)$$

Turn in 2. Remember, in quantum mechanics order matters: $x\hat{p} \neq \hat{p}x$ because momentum is a derivative. We showed $x\hat{p} - \hat{p}x = i\hbar$ several lectures ago.

a. What is $\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}$ equal to? Is it zero, or does order matter? The ‘leftover’ difference is called a ‘commutator’ and is often abbreviated with square brackets as $[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}$. When you see $[a,b]$ in quantum mechanics, think $ab-ba$!

BIG HINT: To make this really easy, use the two formulas for \hat{H} from the previous problem!

Solution:

Take advantage of the hint! Isolate $\hat{a}\hat{a}^\dagger$ and $\hat{a}^\dagger\hat{a}$ in the two respective formulas for \hat{H} to obtain

$$\hat{a}\hat{a}^\dagger = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2} \quad (5)$$

$$\hat{a}^\dagger\hat{a} = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2} \quad (6)$$

Now, subtract eq. (6) from eq. (5) to get the desired result

$$[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = \left(\frac{\hat{H}}{\hbar\omega} + \frac{1}{2}\right) - \left(\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right) = 1 \quad (7)$$

The commutator of the raising and lowering operator product is just the number 1!

b. Use your result above and the fact that $\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$ to show that $\hat{H}\hat{a}^\dagger = \hat{a}^\dagger\hat{H} + \hbar\omega\hat{a}^\dagger$, the formula we used in lecture. **HINT:** $\hat{H}\hat{a}^\dagger = \hbar\omega\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hbar\omega\frac{1}{2}\hat{a}^\dagger$; now use the commutator from (a) to replace the $\hat{a}\hat{a}^\dagger$ in the first part by $\hat{a}^\dagger\hat{a}$ plus other stuff to get the answer.

Solution:

From the hint, we know we should be playing around with the given equality

$$\hat{H}\hat{a}^\dagger = \hbar\omega\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hbar\omega\frac{1}{2}\hat{a}^\dagger \quad (8)$$

Using the second part of the hint and the result from part (a) we know that

$$[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1 \rightarrow \hat{a}\hat{a}^\dagger = 1 + \hat{a}^\dagger\hat{a} \quad (9)$$

Substituting the result from eq. (9) into equation (8) we have

$$\begin{aligned}\hat{H}\hat{a}^\dagger &= \hbar\omega\hat{a}^\dagger(1 + \hat{a}^\dagger\hat{a}) + \hbar\omega\frac{1}{2}\hat{a}^\dagger = \hbar\omega\hat{a}^\dagger\left\{1 + \hat{a}^\dagger\hat{a} + \frac{1}{2}\right\} \\ &= \hbar\omega\hat{a}^\dagger + \hat{a}^\dagger(\hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})) = \hbar\omega\hat{a}^\dagger + \hat{a}^\dagger\hat{H}\end{aligned}\quad (10)$$

which is what we set out to prove!

c. What is $[\hat{a}^\dagger, \hat{a}^\dagger]$ equal to? **HINT: yes, this is easy!**

Solution:

Indeed this is easy; the answer is $[\hat{a}^\dagger, \hat{a}^\dagger] = 0$. An operator always commutes with itself! You can prove this to yourself for any specific case if you like, but it should be intuitive. It is like saying “Does it matter if I differentiate with respect to x and then differentiate with respect to x , or differentiate with respect to x and then differentiate with respect to x ”. They are *identical* operations.

3. Prove that the Gaussian stationary state of the vibrating molecule that we derived in lecture L9 really is the lowest energy state, or ground state: the Heisenberg principle forbids the wavefunction from having a smaller Δx and ‘squeezing down further’ in energy.

To do this, recall from lecture that raising operator ‘raises’ an eigenstate to the next higher energy eigenstate, while the lowering operator ‘lowers’ an eigenstate to the next lower one. Simply show that for the Gaussian $\psi_0(x)$,

$$\hat{a}\psi_0 = 0.$$

This proves that there IS NO state lower in energy than the Gaussian, so the lowest eigenstate is the gaussian ψ_0 with energy $E_0 = \hbar\omega/2 = \hbar\omega(0 + \frac{1}{2})$. The next higher state, as we saw, is Ψ_1 with energy $E_1 = \hbar\omega(1 + \frac{1}{2})$, and so on up to $E_n = \hbar\omega(n + \frac{1}{2})$.

Solution:

As suggested in the problem, apply \hat{a} to ψ_0 :

$$\begin{aligned}\hat{a}\psi_0 &= \left(\frac{m\omega}{2\hbar}\right)^{\frac{1}{2}}\left(x + \frac{i\hat{p}}{m\omega}\right)\psi_0 = \left(\frac{m\omega}{2\hbar}\right)^{\frac{1}{2}}\left(x + \frac{\hbar}{m\omega}\frac{\partial}{\partial x}\right)\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}e^{-\frac{m\omega x^2}{2\hbar}} \\ &= \left(\frac{m\omega}{2\hbar}\right)^{\frac{1}{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\left(xe^{-\frac{m\omega x^2}{2\hbar}} - xe^{-\frac{m\omega x^2}{2\hbar}}\right) = 0\end{aligned}$$

Again, this implies that there is no lower energy state than the Gaussian $\psi_0(x)$ and so this must be the ground state of the vibrating molecule = harmonic oscillator.