QM4

Harmonic Oscillator

Discuss briefly why a harmonic oscillator (in one dimension) has the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

in terms of the classical angular fequency ω. We shall derive the eigenvalues of the harmonic oscillator as follows.

(i) Show that

$$[p, x] = -i\hbar$$

The operators a and $a^\dagger$ are defined by

$$a = \sqrt{\left(\frac{1}{2m\omega\hbar}\right)}(m\omega x + ip) \qquad a^\dagger = \sqrt{\left(\frac{1}{2m\omega\hbar}\right)}(m\omega x - ip)$$

Note that these are *not* Hermitian operators (why not?), but are an adjoint pair, which explains the symbols given to them. Find x and p in terms of these operators. We need not do any more differentiating but only algebra, using the commutator above. (Experience shows that students often do not understand this statement, thereby making a lot of work for themselves!) Show that the operators satisfy the commutation relation $[a, a^\dagger] = 1$.

(ii) Show that the harmonic oscillator Hamiltonian is given by $H = (\hbar\omega/2)(aa^\dagger + a^\dagger a)$ and, using the $[a, a^\dagger]$ commutator, that H can also be written $H = \hbar\omega(a^\dagger a + \frac{1}{2}) = \hbar\omega(aa^\dagger - \frac{1}{2})$.

(iii) Suppose that there exists an eigenket of the time-independent Schrodinger equation with energy E:

$$H|\psi\rangle = E|\psi\rangle.$$

Show that $a^\dagger|\psi\rangle$ and $a|\psi\rangle$ are also eigenkets, with energies $E + \hbar\omega$ and $E - \hbar\omega$. (Hint: try operating on these kets with H and see what you can do with the product using the commutation relations, or the different forms of H.) Note that all these eigenkets are time-independent, and thus solutions of the time-independent Schrodinger equation, not the time-dependent Schrodinger equation.

(iv) Show that all eigenvalues of H are positive. This is *not* because energy is positive! It isn't. Negative energy is just less than zero energy, and we can change our definition of which state has zero energy (at least non-relativistically). What is the zero energy state for this problem? Hence show there must be a state of least energy, the ground state, for which

$$a|0\rangle = 0.$$

By operating with $a^\dagger$ deduce that $E_0 = \frac{1}{2}\hbar\omega$, and hence that the eigenkets are $|n\rangle \propto (a^\dagger)^n|0\rangle$, with energy $E_n = (n + \frac{1}{2})\hbar\omega$.

(v) [Harder] The eigenvalues of a quantum-mechanical problem depend not only on the Hamiltonian, but also on the boundary conditions. What particular assumptions have we (implicitly) made about boundary conditions in the above derivation?

(vi) The reason for the proportional sign above is that if we assume all the $|n\rangle$ are normalised, $\langle n|n\rangle = 1$, then we can't assume that operating with $a^\dagger$ preseves the normalisation. Thus we can write

$$a|n\rangle = f|n-1\rangle \quad \text{and} \quad a^\dagger|n\rangle = g|n+1\rangle$$

for some, possibly complex, constants f and g. Deduce that $|f| = \sqrt{n}$, and similarly that $|g| = \sqrt{n+1}$. Why can we *choose* f and g to be real? The constants $f$and g are just matrix elements: $f = \langle n-1|a|n\rangle$. Illustrate the form of the a and $a^\dagger$ matrices.

(vii) Deduce the form of the x and p matrices. Can you work out what the x^2 and p^2 matrices look like?

(viii) The classical solution for the harmonic oscillator is $x = A \sin \omega t$. Deduce the classical $p(t)$ and E in terms of A. Consider the superposition state

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\Big(\exp(-i\omega_- t)|n-1\rangle + \exp(-i\omega_+ t)|n\rangle\Big).$$

What must ω_- and ω_+ be for this state to satisfy the TDSE? Find $\langle E\rangle$, $\langle x(t)\rangle$ and $\langle p(t)\rangle$. (Can you work out how to do this with matrices? It will save a lot of thinking!) Compare with the classical results. (You could consider quite a range of comparisons: $x(t)$; $p(t)$; the relationship between x and p; x and E; p and E; E, x^2 and p^2 for example.)

(ix) You should have found a major discrepancy between the amplitude and the energy above. Consider a much larger superposition, of $2N+1$ states from $n-N$ to $n+N$. In the limit of large N and even larger n you should find a more classical picture emerging. You could also look at $\langle x^2\rangle$ and $\langle p^2\rangle$ for these two states for a further insight into the reason for the discrepancy in the state $|\psi\rangle$. (Matrix method is the only rational approach here. It's OK to use an equal superposition with coefficients $1/\sqrt{2N+1}$, and it's helpful to look at n so large compared with N that $n - N \approx n$ for all practical purposes, e.g. $n = 10^{30}$ and $N = 10^{15}$.)