

Lecture 17

Relevant sections in text: §2.3

Spectrum of the SHO Hamiltonian (cont.)

It is shown in detail in the text that the eigenvalues of N are non-degenerate and are non-negative integers,

$$\lambda \equiv n = 0, 1, 2, \dots$$

The essence of the proof is to note that the number operator must have a non-negative expectation value:

$$\langle \psi | N | \psi \rangle = \langle \psi | a^\dagger a | \psi \rangle = (\langle \psi | a^\dagger)(a | \psi \rangle) \geq 0,$$

where

$$\langle \psi | N | \psi \rangle = 0 \iff a | \psi \rangle = 0.$$

On the other hand, since a lowers the eigenvalue of N by one unit, there must be a unique (up to normalization) lowest-eigenvalue eigenvector $|0\rangle$ such that

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

One then easily infers that the spectrum of N is non-degenerate, consisting of the non-negative integers:

$$N | n \rangle = n | n \rangle, \quad n = 0, 1, 2, \dots$$

Therefore, the energy spectrum is purely discrete:

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega, \quad n = 0, 1, 2, \dots$$

and the energy eigenvectors are labeled $|n\rangle$. These results arise from the assumption that X and P are self-adjoint operators on a Hilbert space (or, equivalently, that a and a^\dagger are adjoints of each other with respect to the Hilbert space scalar product).

Finally, it is shown in the text that we have

$$a | n \rangle = \sqrt{n} | n - 1 \rangle, \quad a^\dagger | n \rangle = \sqrt{n + 1} | n + 1 \rangle, \quad \langle n | m \rangle = \delta_{nm}.$$

Note that the “ground state” $|0\rangle$ has energy $\frac{1}{2}\hbar\omega$ and satisfies

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

Energy eigenfunctions

We have defined the simple harmonic oscillator and computed the spectrum of its Hamiltonian. Now we explore some properties of the energy eigenvectors, that is, the

stationary states. Of course, each of these vectors $|n\rangle$ represents a state in which the energy is known with certainty to have the value $E_n = (n + \frac{1}{2})\hbar\omega$. These states also define probability distributions for all other observables, in particular the position and momentum. Let us consider the position probability distribution, which is controlled by the position wave functions

$$u_n(x) = \langle x|n\rangle.$$

It is easy enough to compute these functions. For example, consider the ground state wave function u_0 ; it satisfies

$$au_0(x) = \langle x|a|0\rangle = 0.$$

Since

$$au_n(x) = \sqrt{\frac{m\omega}{2\hbar}} \left(X + \frac{i}{m\omega} P \right) u_n(x) = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{\hbar}{m\omega} \frac{d}{dx} \right) u_n(x),$$

we have that

$$\left(x + \frac{\hbar}{m\omega} \frac{d}{dx} \right) u_0(x) = 0.$$

This equation is easily solved and normalized to give a Gaussian (exercise)

$$u_0(x) = \frac{1}{\pi^{1/4} \sqrt{x_0}} e^{-\frac{1}{2} \left(\frac{x}{x_0} \right)^2},$$

where

$$x_0 = \sqrt{\frac{\hbar}{m\omega}}$$

is a length scale set by the problem and, as you can see, it determines the width of the Gaussian.

Here we can see one way in which the quantum and classical mechanics regimes are related. Of course, a classical mechanics description of an oscillator implies that in the ground state the oscillator has position $x = 0$ with certainty. Quantum mechanics provides instead a Gaussian probability distribution about $x = 0$. However, provided that x_0 is “small”, the width of the Gaussian is negligible and the quantum description starts to coalesce with the classical description in this regard. I used quotation marks about the word “small” since x_0 has dimensions of length; whether or not you consider it to be small depends on comparing it to some other length scale. When we speak of “macroscopic phenomena” we usually are interested in length scales on the order of, say, centimeters, masses on the order of grams, and times on the order of seconds. In such a regime x_0 is indeed very, very small. But, of course, in a “microscopic” regime, x_0 can be appreciable.

The “excited states” ($n > 0$) are easily obtained from the identity (exercise)

$$|n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle,$$

so that

$$u_n(x) = \left(\frac{1}{\pi^{1/4} \sqrt{2^n n!} x_0^{n+1/2}} \right) \left(-x_0^2 \frac{d}{dx} + x \right)^n e^{-\frac{1}{2} \left(\frac{x}{x_0} \right)^2}.$$

As you may know, this formula represents (up to the dimensionful constants) one of the standard “generating function” methods for defining the Hermite polynomials. Thus, $u_n(x)$ is a Hermite polynomial times the ground state Gaussian. See your text for detailed formulas.

Expectation values

It is instructive to see how to compute stationary state expectation values and, of course, to see what they look like. To begin, we observe that stationary state expectation values of observables that are linear in position and/or momentum will vanish:

$$\langle n|X|n\rangle = 0 = \langle n|P|n\rangle.$$

To see this, just note that such observables are linear in the ladder operators and we have (by orthogonality)

$$\langle n|a|n\rangle \propto \langle n|n-1\rangle = 0, \quad \langle n|a^\dagger|n\rangle \propto \langle n|n+1\rangle = 0.$$

Another way to see that the expectation values of position and momentum vanish in stationary states is to note that (exercise)

$$X \propto [P, H], \quad P \propto [X, H].$$

From which the result easily follows (exercise).

On the other hand, quadratic functions of position and momentum need not have vanishing expectation values. For example, in the ground state (exercise)

$$\langle 0|X^2|0\rangle = \frac{x_0^2}{2} \langle 0|(a^\dagger + a)^2|0\rangle = \frac{x_0^2}{2}.$$

Which gibes with our earlier comment about the width of the ground state Gaussian position probability distribution. A similar computation for $\langle P^2 \rangle$ shows that (exercise)

$$\langle 0|P^2|0\rangle = \frac{\hbar^2}{2x_0^2}.$$

We see that the dispersions in position and momentum satisfy (in the ground state)

$$\langle \Delta X^2 \rangle \langle \Delta P^2 \rangle = \frac{\hbar^2}{4},$$

which is in accord with the uncertainty principle, but also shows that the ground state is a “minimum uncertainty state”. The excited states are not minimum uncertainty states; a straightforward computation reveals (exercise)

$$\langle \Delta X^2 \rangle \langle \Delta P^2 \rangle = \left(n + \frac{1}{2} \right)^2 \hbar^2.$$