Lecture 18 Relevant sections in text: §2.3

Oscillator 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)

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

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)

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

Stationary states and classical mechanics

Here we use the oscillator to illustrate a very key point about the relation between classical and quantum mechanics.

The stationary states we just studied do not provide any explicitly dynamical behavior. This is not a specific feature of the oscillator, but a general feature of stationary states in quantum mechanics. This is, at first sight, a little weird compared to classical mechanics. Think about it: the probability distributions for position and momentum are time independent in any state of definite energy. In classical mechanics the position and momentum (and the energy) can, at each moment of time, be determined with certainty; the values for the position and momentum oscillate in time in every state but the ground state.* In light of the incompatibility of the position, momentum and energy observables in the quantum description, one cannot directly compare the classical and quantum predictions in the excited states. The quantum predictions are purely statistical, involving repeated state preparations – states specified only by their energy – and measurements of various observables. If we want to compare the quantum and classical descriptions we need to ask the right questions of classical mechanics — this means statistical questions. Let us pause for a moment to expand on this.

^k In the ground state, the classical motion is of course trivial — the position (relative to the equilibrium position) and the momentum vanish. In the quantum ground state the position and momentum have Gaussian probability distributions centered at the vanishing values. For macroscopic values of m and ω the widths of these distributions are negligible.

In classical mechanics every solution of the equations of motion is a state of definite energy (assuming energy is conserved). Fix an energy E. Let us ask the same question that we ask in quantum theory: Given the energy what is the probability for finding the particle at various locations? To answer this question we define the probability for finding the classical particle to be in the interval [x, x + dx] to be proportional to the time spent in that region. (The proportionality constant is used to normalize the probability distribution.) For a classical oscillator at the point x, a displacement dx takes place in the time dt where (exercise)

$$dt = \frac{dx}{\sqrt{\frac{2E}{m} - \omega^2 x^2}}$$

Here it is understood that x lies between the two classical turning points, where

$$E = \frac{1}{2}m\omega^2 x^2.$$

Up to a constant normalization factor, this defines the probability density P(x) for the classical oscillator:

$$P(x) = (const.)\frac{1}{\sqrt{\frac{2E}{m} - \omega^2 x^2}}.$$

(The probability density vanishes outside the turning points.) For $E \neq 0$, the resulting probability density is strongly peaked near the classical turning points of the motion and relatively small and flat near the equilibrium position. This just reflects the fact that, because the oscillator moves slowly near the turning points and rapidly at the equilibrium position, it is more likely to find the particle near the turning points. In general, a quantum oscillator does not have anything like this classical probability distribution. First of all, it oscillates in a non-trivial way because of the Hermite polynomials. Furthermore, while the probability density is exponentially damped outside of the turning points, the probability distribution is not identically zero there. However, it can be shown that the quantum probability distribution does approximate the classical distribution in the limit of "large energy". Here, "large" means sufficiently "macroscopic", *i.e.*, $E_n >> \hbar \omega$ so that n >> 1. To see this one simply computes $|u_n|^2$ for a large n. The result is a very rapidly oscillating wavefunction; the oscillations occur about an average curve which approaches the classical probability distribution as n gets larger and larger. For any finite interval of x, a large enough n will result in a probability for finding the particle in that interval to agree with the classical prediction to any desired accuracy. To see this quickly, simply ask your favorite computer math software to plot the graphs!

We have seen that the probability distribution for position predicted by quantum mechanics approaches that predicted by classical *statistical mechanics* in the limit of "large quantum numbers". This result is satisfying, but is far from the complete story of the

relation of the classical and quantum features of the oscillator. A much better way to model the classical oscillator does not use stationary states but instead minimum uncertainty "coherent states" (see the exercises at the end of chapter 2). Recall that the excited states are not minimum uncertainty states in position and momentum. The coherent states are minimum uncertainty states; for macroscopic mass and frequency the oscillator has a small enough uncertainty in energy, position and momentum and a suitable time dependence to model a classical oscillator. In particular, because the coherent states aren't stationary (except for the ground state), the position and momentum probability distributions can mimic their classical counterparts – sinusoidal oscillations. We will not explore the coherent states here. We do note that the ground state of the oscillator is one such state. For macroscopic values of m and ω the width of the ground state Gaussian position probability distribution – controlled by $x_0 = \frac{\hbar}{m\omega}$ is truly negligible compared to macroscopic length scales, so you can see at least in this state that classical behavior is recovered.