Physics 6320
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Simple Harmonic Oscillator
Part IV: Sample Problems

1 Review.

Last time we derived wavefunctions for the first few SHO states:

$$\begin{aligned}
\phi_0(x) = \langle\, x \mid 0 \,\rangle &= \sqrt{\frac{1}{x_0\sqrt{\pi}}}\, e^{-x^2/2x_0^2} \\
\phi_1(x) = \langle\, x \mid 1 \,\rangle &= \frac{\sqrt{2}}{x_0}\, x\phi_0(x) \\
\phi_2(x) = \langle\, x \mid 2 \,\rangle &= \frac{1}{\sqrt{2}x_0^2}(2x^2 - x_0^2)\phi_0(x) \\
&\cdots \\
&\cdots
\end{aligned} \tag{1}$$

We can verify that these satisfy

$$\int_{-\infty}^{\infty} \phi_n(x)^* \phi_m(x) dx \;=\; \delta_{mn} \tag{2}$$

as they must, by using the integral formula

$$\int_{-\infty}^{\infty} x^{2n} e^{-x^2}\, dx \;=\; \Gamma(n + 1/2)$$

and the gamma function properties

$$\Gamma(n+1) \;=\; n\Gamma(n) \qquad \text{and} \qquad \Gamma(1/2) \;=\; \sqrt{\pi}\,.$$

2 Parity of oscillator wavefunctions.

Since the SHO potential $V = \frac{1}{2}\omega^2 x^2$ is invariant under the transformation $x \to -x$, all the energy eigenstates $\phi_n(x)$ have definite parity. In fact, $\phi_n(-x) = (-1)^n \phi_n(x)$. Formally we say that the parity operator commutes with the hamiltonian, and therefore the energy and the parity are compatible: we can have simultaneous eigenstates. This does not mean that we cannot have states of mixed parity, but they will not be energy eigenstates. We consider such an example next.

3 Example 1.

Suppose at time $t = 0$ we prepare the oscillator in state $\mid \psi(0)\,\rangle$ described by the wavefunction

$$\langle\, x \mid \psi(0)\,\rangle \;=\; \psi(x,0) \;=\; C\,(1 + x/x_0)\, e^{-x^2/2x_0^2}\,. \tag{3}$$

How will this state develop with time?

First let's get the normalization, using $\xi = x/x_0$ as usual:

$$\begin{aligned}
\int_{-\infty}^{\infty} |\psi(x,0)|^2\, dx &= C^2 x_0 \int_{-\infty}^{\infty} (1+\xi)^2 e^{-\xi^2} d\xi \;=\; C^2 x_0 \,\{\Gamma(1/2) + 0 + \Gamma(3/2)\} \\
&= \frac{3}{2}\sqrt{\pi} x_0 C^2 \;=\; 1\,. \\
\text{So } C^2 &= \frac{2}{3x_0\sqrt{\pi}}\,.
\end{aligned}$$

Now let's try to express our given $\psi(x,0)$ in terms of energy eigenfunctions so we can get the time dependence. It looks like a linear combination of ϕ_0 and ϕ_1. Let's try that: from (1) we have

$$(1+\xi)\phi_0 \;=\; \phi_0 \;+\; \sqrt{\frac{1}{2}}\phi_1\,. \tag{4}$$

But we are given

$$\psi(x,0) \;=\; C\,(1+\xi)\,e^{-\xi^2/2} \;=\; C\sqrt{x_0\sqrt{\pi}}\,(1+\xi)\,\phi_0 \tag{5}$$

So

$$\begin{aligned}
\psi(x,0) \;&=\; C\sqrt{x_0\sqrt{\pi}}\,(1+\xi)\,\phi_0 \;=\; \sqrt{\frac{2}{3x_0\sqrt{\pi}}}\sqrt{x_0\sqrt{\pi}}\,(1+\xi)\,\phi_0 \\
&=\; \sqrt{\frac{2}{3}}\,(1+\xi)\,\phi_0 \;=\; \sqrt{\frac{2}{3}}\phi_0 \;+\; \sqrt{\frac{1}{3}}\phi_1\,.
\end{aligned} \tag{6}$$

So now the time dependence is obvious,

$$\psi(x,t) \;=\; \sqrt{\frac{2}{3}}\phi_0(x)\,e^{-i\omega_0 t} \;+\; \sqrt{\frac{1}{3}}\phi_1(x)\,e^{-i\omega_1 t} \tag{7}$$

Here of course the eigenfrequencies are

$$\omega_n \;=\; \frac{E_n}{\hbar} \;=\; (n+1/2)\omega \qquad \text{where} \qquad \omega \;=\; \sqrt{k/m} \;=\; \text{classical frequency} \tag{8}$$

Where will we find this particle? Of course when the system is in an energy eigenstate, $|\phi(-x)|^2 \;=\; |\phi(x)|^2$ so that $\langle\, phi_n \mid x \mid \phi_n \,\rangle \;=\; 0$. But our state $\psi(x,t)$ is neither even nor odd, it is a mixture, so $\langle\, x \,\rangle$ need not be zero. Let's calculate it:

$$\begin{aligned}
\psi(x,t) \;&=\; \sqrt{\frac{2}{3}}\phi_0(x)\,e^{-i\omega t/2} \;+\; \sqrt{\frac{1}{3}}\phi_1(x)\,e^{-3i\omega t/2} \\
&=\; \sqrt{\frac{2}{3}}e^{-i\omega t/2}\left(1 \;+\; \xi\,e^{-i\omega t}\right)\phi_0(x) \\
\langle\, \psi \mid x \mid \psi \,\rangle \;&=\; \int_{-\infty}^{\infty} \psi^*(x,t)\,x\,\psi(x,t)dx \\
&=\; \frac{2}{3}x_0^2\int_{-\infty}^{\infty}\left|1 \;+\; \xi\,e^{-i\omega t}\right|^2 |\phi_0(x)|^2\,\xi\,d\xi \\
&=\; \frac{4}{3}x_0^2\,\cos(\omega t)\,\int_{-\infty}^{\infty} |\phi_0(x)|^2\,\xi^2\,d\xi \\
&=\; \frac{4x_0}{3\sqrt{\pi}}\,\cos(\omega t)\,\int_{-\infty}^{\infty}\xi^2\,e^{-\xi^2}\,d\xi \;=\; \frac{2}{3}x_0\cos(\omega t)
\end{aligned}$$

So in this state, the mean value of the particle's position oscillates about zero, with the classical frequency, and with amplitude $2x_0/3$. This is an example of Ehrenfest's theorem, which says that expectation values follow classical equations of motion. In fact, no matter what initial state we prepare, if it has a non-zero value of $\langle\, x \,\rangle$, then that value will oscillate with the classical frequency.

4 Oscillation of a gaussian packet.

Encouraged by our previous example, let us try to prepare our oscillator in a minimum-uncertainty state, sharply peaked about some point $x = y$. That is, we pick

$$\psi(x,0) \;=\; \sqrt{\frac{1}{w\sqrt{\pi}}}\, e^{-(x-y)^2/2w^2} \tag{9}$$

As we already know, this gives a normalized probability function, peaked at y, with width w. ***Now can we expand this in terms of oscillator eigenfunctions?***

It turns out to be quite messy for an arbitrarily chosen value of the width w. But it works out very nicely if we pick $w = x_0$. In other words, suppose we start with the ground state wavefunction ϕ_0, but displaced to be centered around $x = y$ instead of $x = 0$.

We want

$$c_n \;=\; \langle\, \phi_n \mid \psi(0) \,\rangle \qquad \text{so that} \qquad |\, \psi(t) \,\rangle \;=\; \sum_n c_n e^{-i\omega_n t} \mid \phi_n \,\rangle \tag{10}$$

So we need the integral

$$c_n \;=\; \langle\, \phi_n \mid \psi(0) \,\rangle \;=\; \sqrt{\frac{1}{w\sqrt{\pi}}} \int_{-\infty}^{\infty} \phi_n(x)\, e^{-(x-y)^2/2a_0^2} dx \tag{11}$$

This can be done readily if we take advantage of some facts about Hermite polynomials. First of course there is the orthonormality relation,

$$\int_{-\infty}^{\infty} H_n(x) H_m(x)\, e^{-x^2} dx \;=\; \delta_{nm} \sqrt{\pi}\, n!\, 2^n\,. \tag{12}$$

(Note that there is a typo in Sakurai (A.4.5) which gives $2^n!$ instead of $2^n \cdot n!$.)

There is a very useful function called the ***generating function*** for Hermite polynomials. (We will see this kind of thing in other cases, such as Legendre polynomials.) The generating function for Hermite polynomials is

$$F(x,s) \;=\; e^{-s^2 \,+\, 2xs} \;=\; \sum_{n=0}^{\infty} H_n(x) \frac{s^n}{n!}\,. \tag{13}$$

In fact we can ***define*** the Hermite polynomials as the coefficients in the power series of $F(x,s)$. From this we can get two useful formulas. First, consider the integral

$$\int_{-\infty}^{\infty} F(x,s)\, e^{-x^2} H_n(x) dx \;=\; \int_{-\infty}^{\infty} e^{-(x-s)^2} H_n(x) dx \;=\; \sum_{m=0}^{\infty} \frac{s^m}{m!} \int_{-\infty}^{\infty} H_n(x) H_m(x)\, e^{-x^2} dx \tag{14}$$

Now use of (12) gives

$$\int_{-\infty}^{\infty} e^{-(x-s)^2} H_n(x) dx \;=\; \sqrt{\pi}\, (2s)^n \tag{15}$$

This result allows us to do the integral in (11) to get

$$c_n \;=\; \langle\, \phi_n \mid \psi(0) \,\rangle \;=\; \sqrt{\frac{1}{n! 2^n}}\, (z/x_0)^n\, e^{-z^2/4x_0^2} \tag{16}$$

Note this means our initial function has amplitudes for infinitely large energies. Now we can use the generating function ***again*** to do the sum in (10)! The result is a little bit messy, but to get the time-dependent probability distribution we need its modulus squared, which turns out to be just

$$|\psi(x,t)|^2 \;=\; \frac{1}{x_0\sqrt{\pi}}\, e^{-(x - z\cos\omega t)^2/x_0^2} \tag{17}$$

In other words we have reconstructed the ground-state function $\phi_0(x)$, but now as a function of $x(t) \;=\; z\cos(\omega t)$, where again ω is the classical frequency.