Physics 371, Lecture 20

Harmonic oscillator wavefunctio[ns]

Corresponding to the quantized energy level $E_n = \hbar\omega(n + 1/2)$ is a wavefunction

$$\psi_n(\xi) = A_n H_n(\xi)\, e^{-\xi^2/2},$$

where H_n is a polynomial of order n known as a <u>Hermite polynomial</u>, and A_n is a normalization constant.

To illustrate how the Hermite polynomials can be obtained from the recursion relation, consider $H_3(\xi)$.

$$\epsilon = 2n + 1 = 7$$

$$\frac{a_{k+2}}{a_k} = -\frac{\epsilon - 1 - 2k}{(k+1)(k+2)}$$

$$\frac{a_3}{a_1} = -\frac{7-1-2}{2 \cdot 3} = -\frac{2}{3}$$

$$H_3(\xi) = a_1\left(\xi - \frac{2}{3}\xi^3\right)$$

The value of a_1 is arbitrary, and can be absorbed in the normalization constant.

- However, a convenient convention is to choose a_1 (or a_0) such that the coefficient of the term of highest order is 2^n. In this example, $a_1 = -12$.
- A few of the Hermite polynomials so normalized are:

$$H_0(\xi) = 1$$
$$H_1(\xi) = 2\xi$$
$$H_2(\xi) = 4\xi^2 - 2$$
$$H_3(\xi) = 8\xi^3 - 12\xi$$
$$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12$$

A general formula for the Hermite polynomials is

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2}.$$

$$H_0(\xi) = \underline{1}$$

$$H_1(\xi) = 2\xi$$

$$H_2(\xi) = e^{\xi^2} \frac{d^2}{d\xi^2} e^{-\xi^2} = e^{\xi^2} \frac{d}{d\xi}\left(-2\xi e^{-\xi^2}\right)$$

$$= -2 + 4\xi^2$$

$\vdots$

Orthonormality

$$\psi_n(\xi) = A_n H_n(\xi) e^{-\xi^2/2}$$

$$\langle n|n'\rangle = \int_{-\infty}^{\infty} d\xi \, \psi_n^*(\xi) \psi_{n'}(\xi)$$

$$= A_n^* A_{n'} \int_{-\infty}^{\infty} d\xi \, e^{-\xi^2} H_n(\xi) H_{n'}(\xi)$$

$$= (-1)^{n'} A_n^* A_{n'} \int_{-\infty}^{\infty} d\xi \, H_n(\xi) \frac{d^{n'}}{d\xi^{n'}} e^{-\xi^2}$$

$$= (-1)^{n'-n} 2^n n! \, A_n^* A_{n'} \int_{-\infty}^{\infty} d\xi \, \frac{d^{n'-n}}{d\xi^{n'-n}} e^{-\xi^2}$$

(integrating by parts n times, assuming $n' > n$). Here we used the fact that $e^{-\xi^2}$ and all its derivatives vanish at

$|\xi| = \infty$. Clearly $\langle n|n'\rangle = 0$ if $n \neq n'$.

$$\langle n|n\rangle = |A_n|^2\, 2^n\, n!\int_{-\infty}^{\infty} d\xi\, e^{-\xi^2}$$

$$= |A_n|^2\, 2^n\, n!\,\sqrt{\pi} = 1$$

$$\Rightarrow \quad A_n = \sqrt{\frac{1}{2^n\, n!\,\sqrt{\pi}}}$$

The normalized harmonic oscillator wavefunctions are thus

$$\psi_n(\xi) = \left(2^n\, n!\,\sqrt{\pi}\right)^{-1/2} e^{-\xi^2/2}\, H_n(\xi).$$

It is sometimes useful to use the normalization over x, rather than over the dimensionless variable ξ. In this case, the normalized wavefunction becomes

$$\psi_n(x) = \left(\frac{\sqrt{m\omega/\hbar}}{2^n n! \sqrt{\pi}} \right)^{1/2} e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right).$$

A few of the normalized harmonic oscillator wave functions are

$$\psi_0(\xi) = \left(\frac{1}{\sqrt{\pi}}\right)^{1/2} e^{-\xi^2/2}$$

$$\psi_1(\xi) = \left(\frac{2}{\sqrt{\pi}}\right)^{1/2} \xi\, e^{-\xi^2/2}$$

$$\psi_2(\xi) = \left(\frac{1}{2\sqrt{\pi}}\right)^{1/2} (2\xi^2 - 1)\, e^{-\xi^2/2}$$

$$\psi_3(\xi) = \left(\frac{1}{3\sqrt{\pi}}\right)^{1/2} (2\xi^3 - 3\xi)\, e^{-\xi^2/2}$$

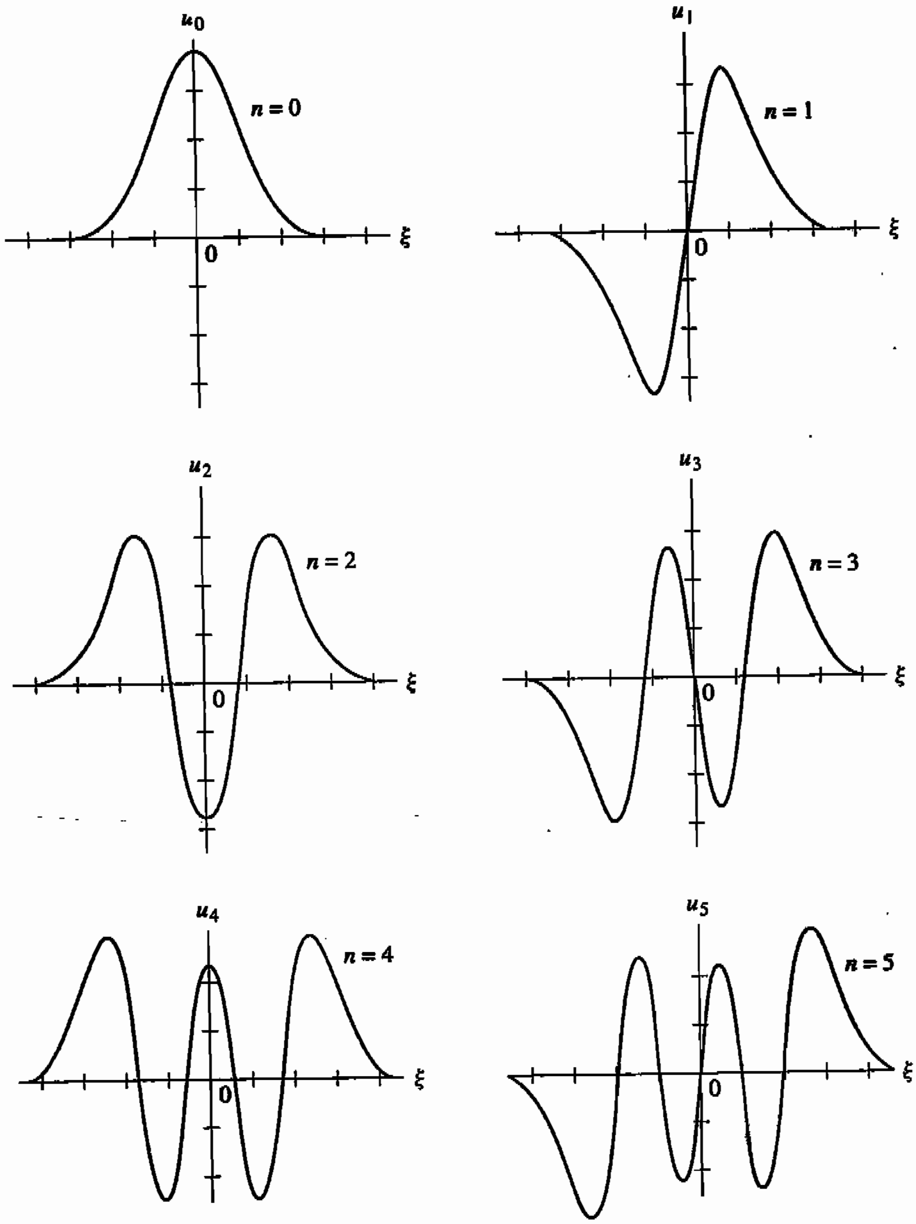
$\Rightarrow$ show transparency

Note that since the harmonic oscillator wavefunctions form a complete set of orthonormal functions, any function $f(\xi)$ can be expanded as a series

Changing variables to ξ, we get

$$\langle x \rangle = |C_n|^2(\hbar/m\omega)\int_{-\infty}^{\infty} d\xi\, e^{-\xi^2} H_n(\xi)\xi H_n(\xi)$$

FIGURE 7.4
The first five harmonic oscillator eigenfunctions.



$$f(\xi) = \sum_{n=0}^{\infty} c_n \psi_n(\xi).$$

This is similar to a Fourier series. It is mainly useful if $f(\xi)$ is well localized about $\xi = 0$, so that only a few terms are needed in the series.

Probability density

Quantum mechanically,

$$P(x)\,dx = |\psi(x)|^2 \, dx.$$

Q: How does this compare to the probability distribution for a classical oscillator?

Classically, the probability $P_{cl}(x)\,dx$ to find the particle between x and $x+dx$ is equal to the time the particle spends in this interval divided by the period of motion $T = \frac{2\pi}{\omega}$.

$$P_{cl}(x)\,dx = \frac{dt}{T} = \frac{1}{T}\,\frac{2\,dx}{V(x)} = \frac{\omega}{\pi}\,\frac{dx}{V(x)}$$

where $V(x) = \sqrt{\frac{2E}{m} - \omega^2 x^2}$ is the speed of a particle of energy E moving in the oscillator potential. [11]

$$P_{cl}(x) = \frac{1/\pi}{\sqrt{\frac{2E}{m\omega^2} - x^2}}$$

$P_{cl}(x)$ diverges at the classical turning points

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

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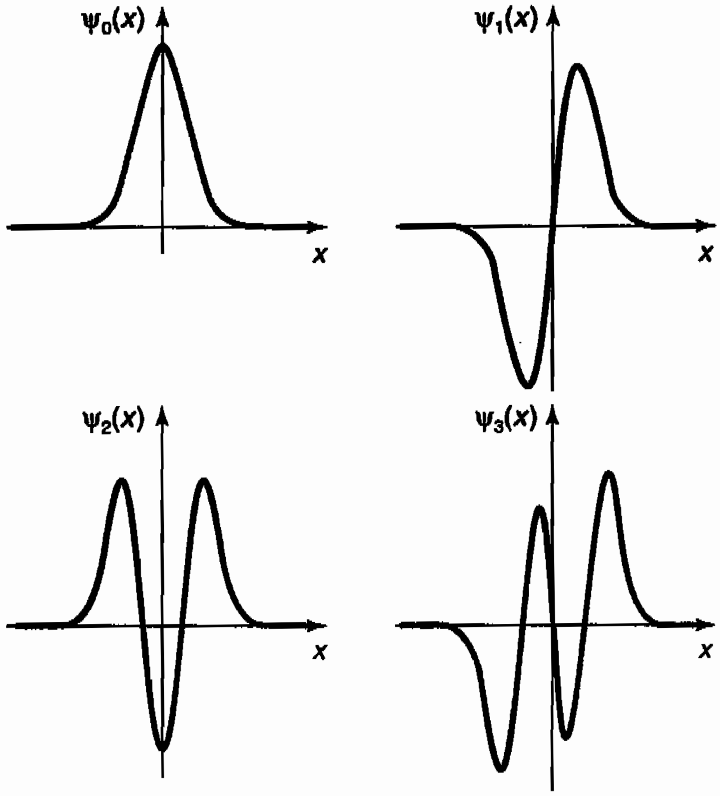
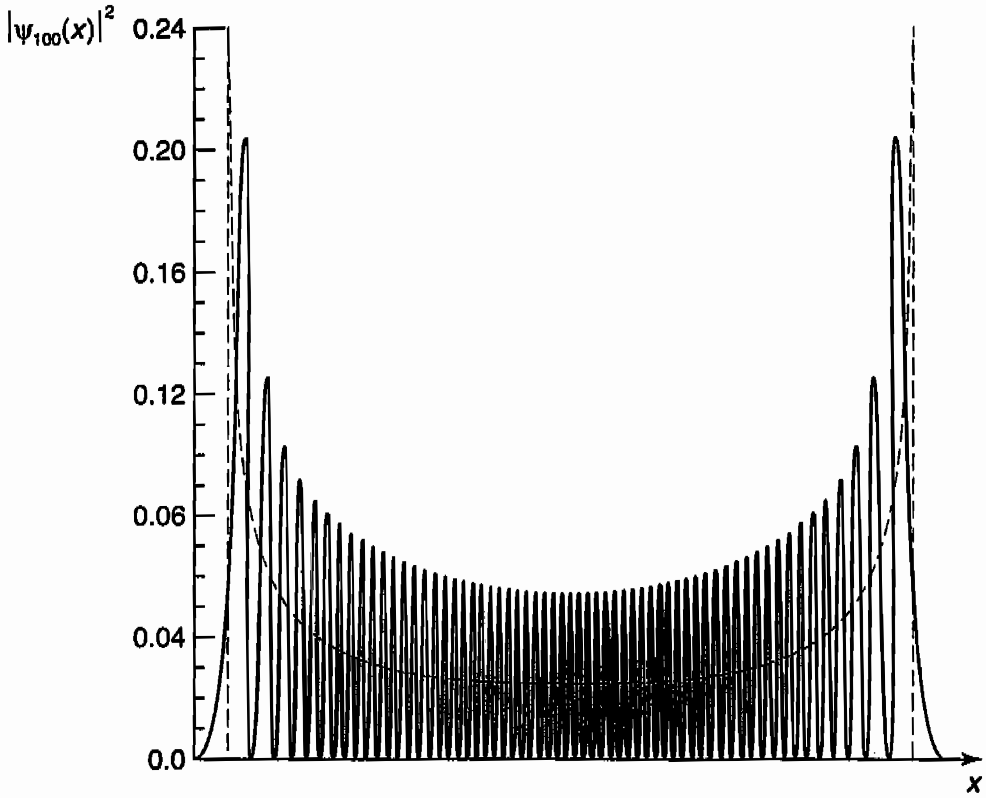


(a)



(b)

Figure 2.5: (a) The first four stationary states of the harmonic oscillator. (b) Graph of $|\psi_{100}|^2$, with the classical distribution (dashed curve) superimposed.