More 1D Potential Cases

- Harmonic oscillator
  - Asymptotic approximation trick for solving a differential equation
  - Hermite polynomials

The Schrodinger Equation

$$\hat{H}\psi = \hat{E}\psi$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x,t)\psi = i\hbar\frac{\partial\psi}{\partial t}$$

and if V(x) is constant in time,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + (E - V)\psi(x) = 0$$

The Harmonic Oscillator

- The potential $V(x) = \frac{1}{2}kx^2$ is a useful approximation to many physical systems (including springs).
  - Vibration of molecules

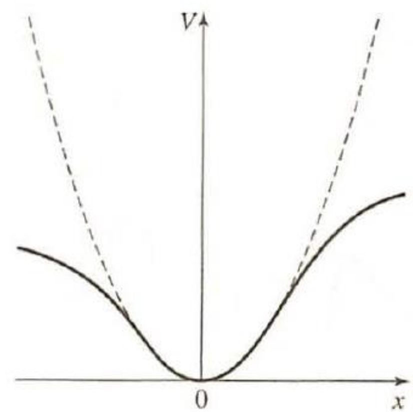


Figure 4.11 In the vicinity of a minimum the potential energy can be approximated as a parabola, namely the potential energy of the simple harmonic oscillator.

- In analogy to the spring, we rewrite the potential in terms of a classical oscillation frequency.

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$$

$$\text{where } \omega = \sqrt{\frac{k}{m}}$$

- So the Schrodinger Equation is:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi$$

- This is a difficult problem. We'll approach it by trying to factor out the behavior of the solution for very large x.

To be consistent with Appendix B1 in Townsend, we change variables to avoid writing constants repeatedly. $(Let\, y = \sqrt{\frac{m\omega}{\hbar}}x, and\ \epsilon = \frac{2E}{\hbar\omega})$

$$\frac{\partial^2\psi}{\partial y^2} = (y^2 - \epsilon)\psi$$

Find the approximate solution for large *y*.

$$\frac{\partial^2\psi}{\partial y^2} \approx y^2\psi$$

Solution:

$$\psi(very\ large\ y) = Ay^n e^{-\frac{y^2}{2}}$$

- Any polynomial in y, times the exponential decay term $e^{-\frac{y^2}{2}}$ will satisfy the large y equation.
- Now we can see what polynomials ($H(y)$) can satisfy the full equation, and what conditions they impose on the energy.

$$\frac{d^2 H(y) e^{-\frac{y^2}{2}}}{dy^2} = (y^2 - \epsilon) H(y) e^{-\frac{y^2}{2}}$$

$$\frac{d\psi}{dy} = -yH(y)e^{-\frac{y^2}{2}} + e^{-\frac{y^2}{2}} \frac{dH}{dy}$$

$$\frac{d^2\psi}{dy^2} = -He^{-\frac{y^2}{2}} - y\frac{dH}{dy}e^{-\frac{y^2}{2}} + e^{-\frac{y^2}{2}}\frac{d^2 H}{dy^2}$$

- Plugging it all back in and factoring out the exponential term yields a differential equation for *H*.

$$\frac{d^2H}{dy^2} - 2y\frac{dH}{dy} + (\epsilon - 1)H = 0$$

This equation is known as the Hermite equation.

The lowest order polynomial we could guess is H=constant=a_0. Let's try it.

$$(\epsilon - 1)a_0 = 0$$

Which is a solution if $\epsilon = 1$!

So $E_0 = \frac{\hbar\omega}{2}$!!

- So the lowest order solution to the harmonic oscillator potential is

$$\psi_0 = a_0 e^{-\frac{m\omega}{\hbar}x^2}$$

And normalizing,

$$a_0^2 \int_{-\infty}^{\infty} e^{-\frac{2m\omega}{\hbar}x^2} dx = 1$$

And looking up the integral,

$$a_0^2 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}}$$

So

$$\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{m\omega}{\hbar}x^2}$$

Higher order polynomials.

Now let's try $H_1 = (ay + b)$

$$\frac{d^2 H_1}{dy^2} - 2y\frac{dH_1}{dy} + (\epsilon - 1)H_1 = 0$$

$\frac{dH_1}{dy} = a$; $\frac{d^2 H_1}{dy^2} = 0$

$$-2ya + (\epsilon - 1)(ay + b) = 0$$

Each set of terms of a particular order in y must sum to zero:

$-2a + \epsilon a - a = 0$ so $\epsilon_1 = 3$ and therefore

$$E_1 = \frac{3}{2}\hbar\omega$$

We also know that $(\epsilon_1 - 1)(+b) = 0$, which yields either $\epsilon_1 = 1$ or $b = 0$.

We choose $b = 0$ because setting a=0 just results in the lowest order polynomial again.

Hence:

$$\psi_1(y) = a_1 y e^{-\frac{y^2}{2}}$$

- Townsend shows a more general approach to solving the Hermite equation in which he assumes that: $H_n(y) = \sum_{k=0}^{n} a_k y^k$
- And finds the following properties:

$\epsilon_n = 2n + 1$ so $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$

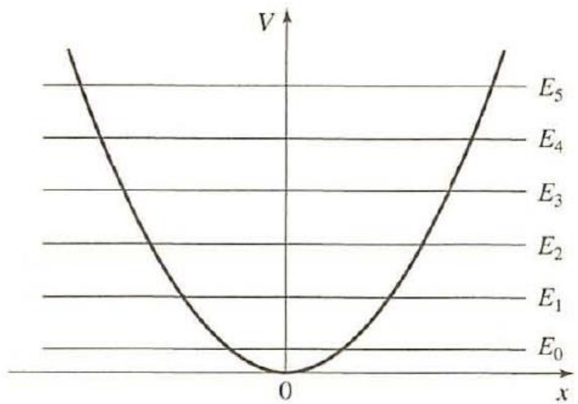
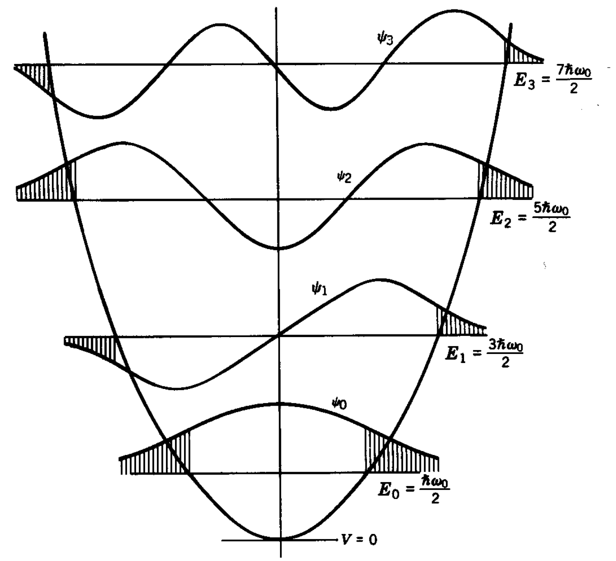


Figure 4.12 The energy spectrum of the harmonic oscillator superimposed on the potential energy $V(x) = m\omega^2 x^2/2$.

Hermite Polynomials

Figure 5-9
Energy levels and eigenfunctions for the first four stationary states of the harmonic oscillator. Shaded areas represent the penetration of the wave function into regions where classical motion is forbidden.



$H_0(y) = 1$ (even)
$H_1(y) = 2y$ (odd)
$H_2(y) = 4y^2 - 2$ (even)
$H_{3(y)} = 8y^3 - 12y$ (odd)

$$H_n(x) = n! \sum_{m=0}^{\left\lfloor \frac{n}{2} \right\rfloor} \frac{(-1)^m}{m!(n-2m)!} (2x)^{n-2m}.$$

Wavefunction solutions

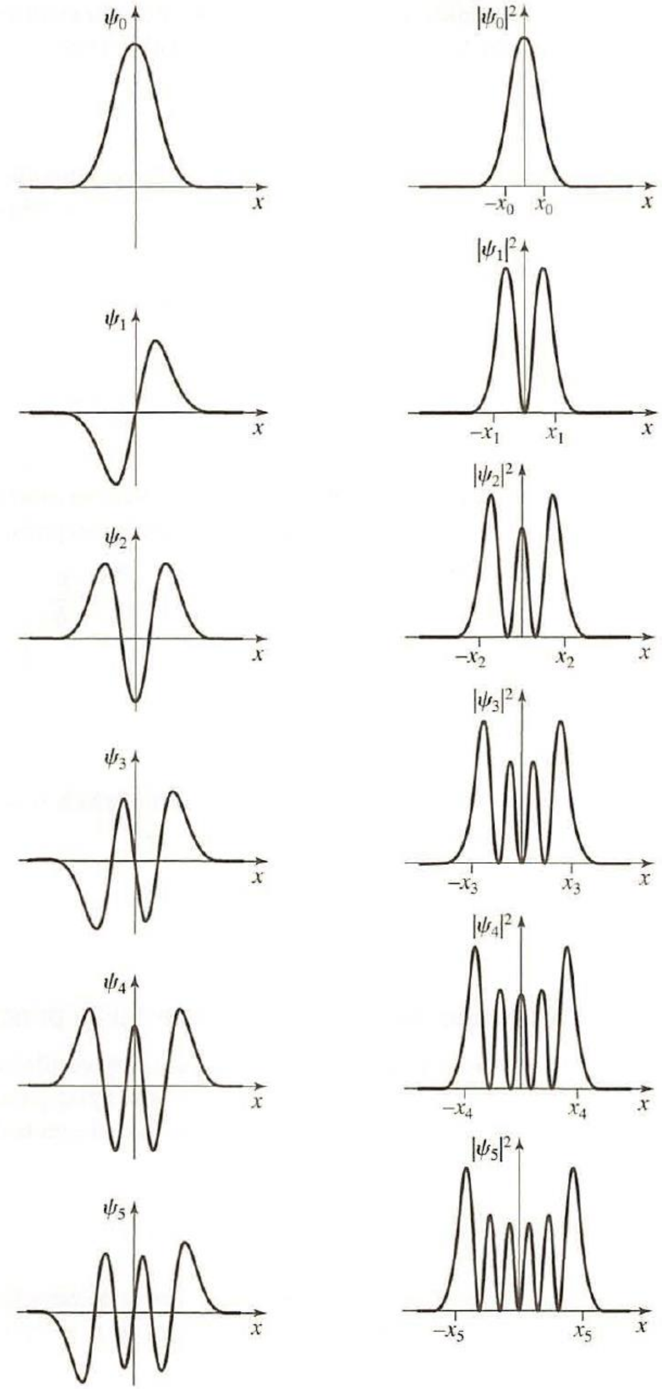
$$\psi_0(y) = A_0 e^{-\frac{y^2}{2}}$$

$$= A_0 \exp\left(-\frac{m\omega x^2}{\hbar}\right)$$

$$\psi_1(y) = A_1 \sqrt{\frac{m\omega}{\hbar}}\, x \exp\left(-\frac{m\omega x^2}{\hbar}\right)$$

$$\psi_2(y) = A_2(4y^2 - 2)e^{-\frac{y^2}{2}}$$

$$\psi_3(y) = A_3(8y^3 - 12y)e^{-\frac{y^2}{2}}$$



Probability density

Figure 5-10
Ground-state probability density as a function of the variable $\xi = (mk/\hbar^2)^{1/4}x$. Classical motion with energy $\hbar\omega_0/2$ is forbidden outside the interval $-1 \leq \xi \leq 1$.

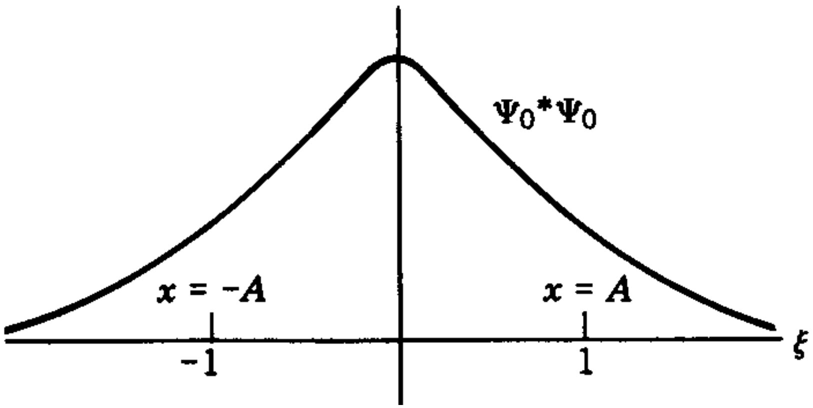
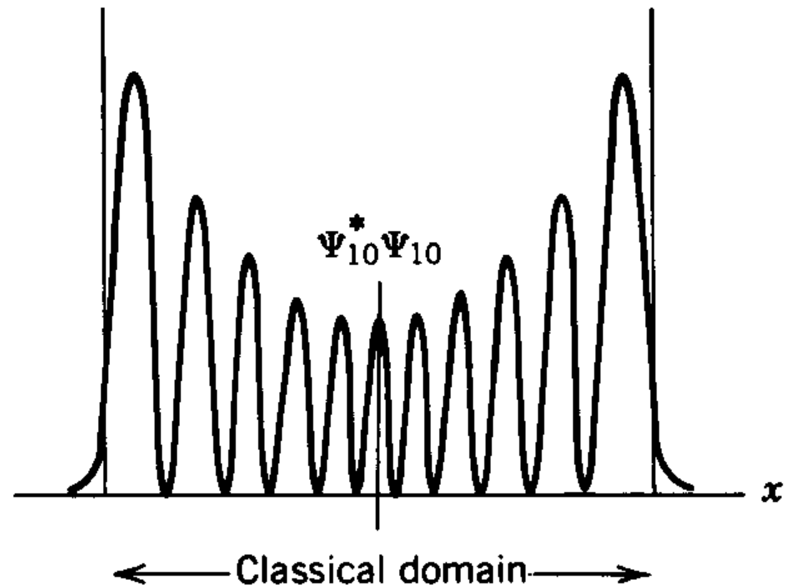


Figure 5-11
Probability density for the $n = 10$ state of the harmonic oscillator. The average of the distribution agrees with the classical probability density in Figure 5-7.



Note that particles in a high energy state spend more time at the edges of the allowed region.

Normalization

The normalization requirement is:

$$1 = \int_{-\infty}^{\infty} \psi_n^* \psi_n dx = |A_0|^2 \int e^{-ax^2} dx$$

The integral of a Gaussian function can be solved using a “cute” trick shown on p 126 of Townsend. We just give the result here:

$$\int e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

And so:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}}$$

Normalization

Other Gaussian integrals for normalization of Harmonic Oscillator eigenfunctions will all be of the form:

$$\int_{-\infty}^{\infty} x^{2n} e^{-ax^2} dx$$

These can be deduced using another trick:

$$\frac{\partial}{\partial a}\int_{-\infty}^{\infty} e^{-ax^2} dx = \frac{\partial}{\partial a}\sqrt{\frac{\pi}{a}}$$

$$\int_{-\infty}^{\infty} -x^2 e^{-ax^2} dx = \frac{1}{2a}\sqrt{\frac{\pi}{a}}$$

Other properties of Harmonic oscillator solutions

- The solutions are even or odd.
  - $\langle x \rangle = \int \psi^* x \psi dx = 0$
- The derivative of an even solution is odd and of an odd solution is even
  - $\langle p_x \rangle = -i\hbar \int \psi^* \frac{\partial}{\partial x} \psi dx = \int odd\ dx = 0$
- The space solutions are real, therefore the probability current is zero.
- Since the ground state is a Gaussian, it will have the minimum value for $\Delta x \Delta p \geq \frac{\hbar}{2}$