

8. The Simple Harmonic Oscillator

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It's time to study another example of solving the Schrödinger equation for a particular potential energy function $V(x)$. This example is the *simple harmonic oscillator*, for which $V(x)$ is quadratic:

$$V(x) = \frac{1}{2}k_s x^2 = \frac{1}{2}m\omega_c^2 x^2, \quad (1)$$

where k_s is some “spring constant” and $\omega_c = \sqrt{k_s/m}$ is the *classical oscillation frequency*, that is, the angular frequency of oscillation of a classical mass m attached to a rigid wall by a spring with constant k_s .

The quantum harmonic oscillator is important for two reasons.

First, it's a quantitatively useful model of almost anything small that wiggles, such as vibrating molecules and acoustic vibrations (“phonons”) in solids. The simple harmonic oscillator even serves as the basis for modeling the oscillations of the electromagnetic field and the other fundamental quantum fields of nature.

Second, the simple harmonic oscillator is another example of a one-dimensional quantum problem that can be solved exactly. Its detailed solutions will give us further insight into the behavior of quantum systems in general, helping us understand which features of the infinite square well are or aren't common to all trapped quantum particles. And although we won't do it in this class, we could also use the known harmonic oscillator energy eigenstates as an alternate “basis” for analyzing other quantum systems, as in the matrix diagonalization method described in the previous lesson.

Natural units

The full Hamiltonian for the (nonrelativistic) simple harmonic oscillator is

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega_c^2 x^2. \quad (2)$$

Although this expression contains three constants (\hbar , m , and ω_c), they appear in only two different combinations. Without loss of generality we can choose units in which both of these combinations, \hbar^2/m and $m\omega_c^2$, are equal to 1; then the Hamiltonian becomes simply

$$H = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2. \quad (3)$$

To interpret these units, note that the combination

$$\sqrt{\frac{\hbar}{m\omega_c}} = \left(\frac{\hbar^2/m}{m\omega_c^2} \right)^{1/4} = 1 \quad (4)$$

has units of distance, while the combination

$$\hbar\omega_c = \sqrt{(\hbar^2/m)(m\omega_c^2)} = 1 \quad (5)$$

has units of energy. All distances and energies will therefore be measured in multiples of these quantities.

Numerical solutions

It's completely straightforward to solve the time-independent Schrödinger equation, for the simple harmonic oscillator, using either of the numerical methods described in the previous lesson.

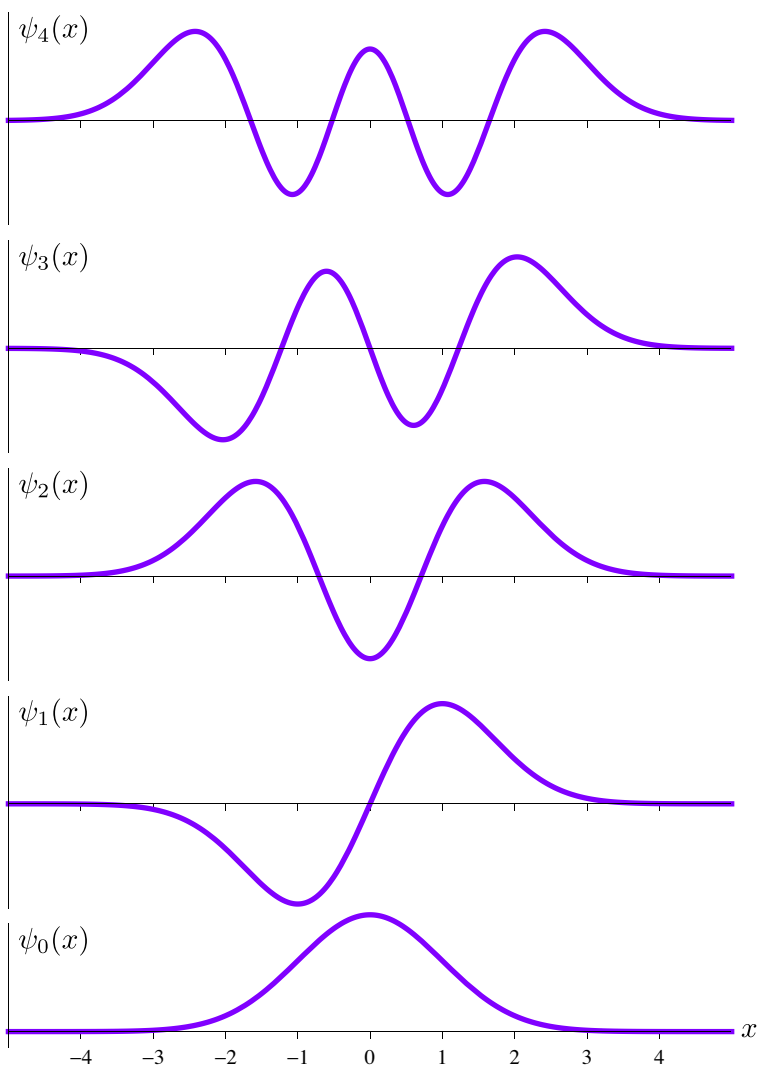
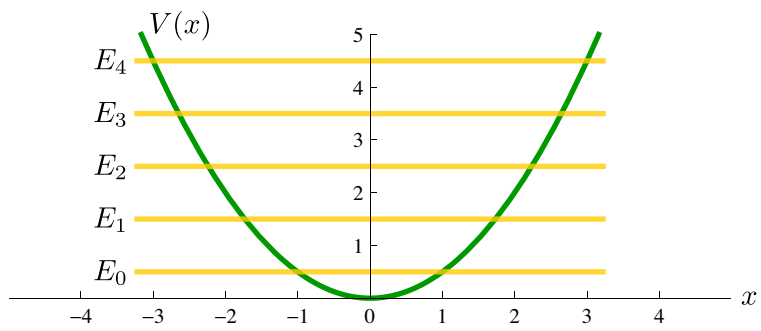
If you use the shooting method, you can exploit the fact that $V(x)$ is an even function and therefore assume that the solutions $\psi(x)$ are either even or odd, supplying boundary conditions $\psi(0) = 1$ and $\psi'(0) = 0$ for the even solutions and $\psi(0) = 0$ and $\psi'(0) = 1$ for the odd solutions. The wavefunction plots turn out as described in Lesson 6: oscillating in the classically allowed region, with increasing wavelength and amplitude as one moves outward, and exponentially decaying in the classically forbidden regions to either side. Unlike a generic $V(x)$, however, the harmonic oscillator potential yields an extremely simple set of energy eigenvalues: $1/2, 3/2, 5/2$, and so on, in natural units.

If instead you use the matrix diagonalization method, embedding the oscillator inside an infinite square well, it's just a matter of centering the oscillator inside the infinite well and choosing the well width and number of basis functions to yield as many accurate eigenvalues and eigenfunctions as possible in whatever time you're willing to wait for them. Again, the answers for the eigenvalues are simply $1/2, 3/2, 5/2$, and so on, and of course you can construct the associated wavefunctions out of the associated eigenvectors.

The illustration on the following page shows the lowest five energy levels superimposed on a graph of the potential energy, with the corresponding wavefunctions plotted below using the same horizontal scale. Distances and energies are labeled in natural units. Notice that the energy levels on this quantum ladder are *evenly spaced*, unlike the infinite square well for which they get farther apart as you go up. It's conventional to number the harmonic oscillator energies and wavefunctions starting with 0 rather than 1, so the number indicates how many "units" of energy the system has, relative to the ground state. This convention is a departure from the one that we use for essentially all other one-dimensional quantum systems.

The natural unit of energy is $\hbar\omega_c$, so in conventional units, the harmonic oscillator energy levels can be summarized in the formula

$$E_n = (n + \frac{1}{2})\hbar\omega_c, \quad \text{for } n = 0, 1, 2, \dots \quad (6)$$



Exact solutions

When you solve a problem numerically and get an unexpectedly simple answer, that's probably a clue that you could have solved the problem analytically. There are at least three approaches to analytically solving the TISE for the simple harmonic oscillator:

1. **Guess the answers.** Look at the ground-state wavefunction on the previous page, and notice that it looks an awful lot like a Gaussian, e^{-ax^2} for some constant a . Plug this formula into the TISE and you'll see that it works as long as $a = 1/2$ and $E = 1/2$. One down. For the next solution, a look at the graph might lead you to the guess the formula xe^{-ax^2} , and if you plug this in you'll find that it works for the same $a = 1/2$, but with $E = 3/2$. That's two. At this point you might guess (correctly) that all the solutions are polynomial functions multiplied by the same Gaussian, $e^{-x^2/2}$. Each polynomial has only even or odd terms (to give the correct symmetry for the wavefunctions), and you can find the coefficients by requiring that the TISE be satisfied in each case. It gets laborious after the first few, but if you fiddle with the equations long enough you might notice some patterns and discover some general procedures for finding the coefficients.
2. **Power series.** This is the most traditional approach, and it's presented in all the traditional textbooks (e.g., Griffiths, 2nd ed., pp. 51–56). By this method you can prove that the allowed energies are $n + 1/2$ for *any* nonnegative integer n , and that *all* of the associated wavefunctions are $e^{-x^2/2}$ times an n th-order polynomial. You end up with “recursion formulas” that let you calculate the coefficients of the polynomials in a straightforward way, but again it gets laborious to work out more than a handful of them.
3. **Ladder operators.** This is by far the most elegant method, although it's also the most abstract, and it's hard to see how anyone would have thought of it, and it's still laborious to work out more than a handful of the wavefunction formulas. We'll cover this method in detail in a few weeks, as we gear up to use a similar method to understand angular momentum in quantum mechanics. Feel free to look ahead if you're curious!

Whatever the method used to obtain them, the harmonic oscillator energy eigenfunctions are n th-order polynomials multiplied by the Gaussian $e^{-x^2/2}$. There's no general formula for the polynomials themselves—just algorithms for calculating their coefficients. But they do have a name: they're called *Hermite polynomials*, abbreviated $H_n(x)$, with the normalization convention that the coefficient on x^n (the highest power that appears in H_n) is 2^n . Then all the other coefficients turn

out to be integers; here's a table of the first few:

$$\begin{aligned}H_0(x) &= 1 \\H_1(x) &= 2x \\H_2(x) &= 4x^2 - 2 \\H_3(x) &= 8x^3 - 12x \\H_4(x) &= 16x^4 - 48x^2 + 12 \\H_5(x) &= 32x^5 - 160x^3 + 120x\end{aligned}\tag{7}$$

With the polynomials normalized in this way, there's still an n -dependent normalization coefficient that's not especially easy to work out, but at least it has a formula. The final formula for the normalized energy eigenfunctions is

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) e^{-x^2/2}.\tag{8}$$

The Hermite polynomials are built into Mathematica as `HermiteH[n, x]`, so you can easily use that software to work with eigenfunctions up to $n = 100$ or more.

Like those of the infinite square well (and indeed, any other quantum system), the harmonic oscillator eigenfunctions are mutually orthogonal,

$$\int_{-\infty}^{\infty} \psi_m(x) \psi_n(x) dx = \delta_{mn},\tag{9}$$

and they form a complete basis that you can use to expand any other wavefunction:

$$\psi(x) = \sum_{n=0}^{\infty} c_n \psi_n(x),\tag{10}$$

for any wavefunction $\psi(x)$ and some set of complex coefficients $\{c_n\}$. I'll omit the proofs that go with these claims, but you can easily check some special cases.

Once you have the eigenfunctions and eigenvalues, and know that the eigenfunctions form an orthonormal basis, you can do all the usual things with them:

- Integrate $|\psi_n(x)|^2$ to calculate probabilities of finding the particle in various locations, when it's in a particular energy eigenfunction.
- Expand an arbitrary wavefunction in terms of energy eigenfunctions, to predict the probabilities of finding the particle with various energy values.
- Predict the time dependence of an arbitrary wavefunction, by expanding it in terms of energy eigenfunctions and inserting wobble factors. (The Harmonic Oscillator web app, linked from our course web page, can animate the behavior of any linear combination of ψ_0 through ψ_7 .)
- Use the harmonic oscillator eigenfunctions as basis vectors for analyzing other one-dimensional quantum systems.