(c) What is the probability that a measurement of the energy would yield the value E_1?

(d) Find the expectation value of the energy.

Problem 2.8 A particle of mass m in the infinite square well (of width a) starts out in the left half of the well, and is (at $t = 0$) equally likely to be found at any point in that region.

(a) What is its initial wave function, $\Psi(x, 0)$? (Assume it is real. Don't forget to normalize it.)

(b) What is the probability that a measurement of the energy would yield the value $\pi^2\hbar^2/2ma^2$?

Problem 2.9 For the wave function in Example 2.2, find the expectation value of H, at time $t = 0$, the "old fashioned" way:

$$\langle H\rangle = \int \Psi(x,0)^* \hat{H}\Psi(x,0)\,dx.$$

Compare the result obtained in Example 2.3, using Equation 2.39. *Note:* because $\langle H\rangle$ is independent of time, there is no loss of generality in using $t = 0$.

2.3 THE HARMONIC OSCILLATOR

The paradigm for a classical harmonic oscillator is a mass m attached to a spring of force constant k. The motion is governed by **Hooke's law**,

$$F = -kx = m\frac{d^2x}{dt^2}$$

(ignoring friction), and the solution is

$$x(t) = A\sin(\omega t) + B\cos(\omega t),$$

where

$$\omega \equiv \sqrt{\frac{k}{m}} \qquad [2.41]$$

is the (angular) frequency of oscillation. The potential energy is

$$V(x) = \frac{1}{2}kx^2; \qquad [2.42]$$

its graph is a parabola.

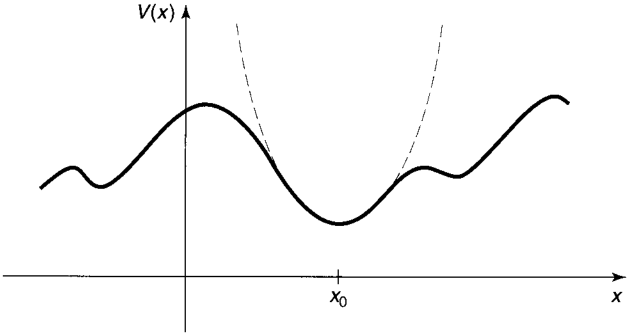

FIGURE 2.4: Parabolic approximation (dashed curve) to an arbitrary potential, in the neighborhood of a local minimum.

Of course, there's no such thing as a *perfect* harmonic oscillator—if you stretch it too far the spring is going to break, and typically Hooke's law fails long before that point is reached. But practically any potential is *approximately* parabolic, in the neighborhood of a local minimum (Figure 2.4). Formally, if we expand $V(x)$ in a **Taylor series** about the minimum:

$$V(x) = V(x_0) + V'(x_0)(x - x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 + \cdots,$$

subtract $V(x_0)$ (you can add a constant to $V(x)$ with impunity, since that doesn't change the force), recognize that $V'(x_0) = 0$ (since x_0 is a minimum), and drop the higher-order terms (which are negligible as long as $(x - x_0)$ stays small), we get

$$V(x) \cong \frac{1}{2}V''(x_0)(x - x_0)^2,$$

which describes simple harmonic oscillation (about the point x_0), with an effective spring constant $k = V''(x_0)$.[16] That's why the simple harmonic oscillator is so important: Virtually *any* oscillatory motion is approximately simple harmonic, as long as the amplitude is small.

The *quantum* problem is to solve the Schrödinger equation for the potential

$$V(x) = \frac{1}{2}m\omega^2x^2 \qquad [2.43]$$

(it is customary to eliminate the spring constant in favor of the classical frequency, using Equation 2.41). As we have seen, it suffices to solve the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi. \qquad [2.44]$$

---

[16] Note that $V''(x_0) \geq 0$, since by assumption x_0 is a *minimum*. Only in the rare case $V''(x_0) = 0$ is the oscillation not even approximately simple harmonic.

In the literature you will find two entirely different approaches to this problem. The first is a straightforward "brute force" solution to the differential equation, using the **power series method**; it has the virtue that the same strategy can be applied to many other potentials (in fact, we'll use it in Chapter 4 to treat the Coulomb potential). The second is a diabolically clever algebraic technique, using so-called **ladder operators**. I'll show you the algebraic method first, because it is quicker and simpler (and a lot more fun);[17] if you want to skip the power series method for now, that's fine, but you should certainly plan to study it at some stage.

2.3.1 Algebraic Method

To begin with, let's rewrite Equation 2.44 in a more suggestive form:

$$\frac{1}{2m}[p^2 + (m\omega x)^2]\psi = E\psi, \qquad [2.45]$$

where $p \equiv (\hbar/i)d/dx$ is, of course, the momentum operator. The basic idea is to *factor* the Hamiltonian,

$$H = \frac{1}{2m}[p^2 + (m\omega x)^2]. \qquad [2.46]$$

If these were *numbers*, it would be easy:

$$u^2 + v^2 = (iu + v)(-iu + v).$$

Here, however, it's not quite so simple, because p and x are *operators*, and operators do not, in general, **commute** (xp is not the same as px). Still, this does motivate us to examine the quantities

$$\boxed{a_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x)} \qquad [2.47]$$

(the factor in front is just there to make the final results look nicer).

Well, what *is* the product a_-a_+?

$$\begin{aligned} a_-a_+ &= \frac{1}{2\hbar m\omega}(ip + m\omega x)(-ip + m\omega x) \\ &= \frac{1}{2\hbar m\omega}[p^2 + (m\omega x)^2 - im\omega(xp - px)]. \end{aligned}$$

---

[17] We'll encounter some of the same strategies in the theory of angular momentum (Chapter 4), and the technique generalizes to a broad class of potentials in **super-symmetric quantum mechanics** (see, for example, Richard W. Robinett, *Quantum Mechanics*, (Oxford U.P., New York, 1997), Section 14.4).

As anticipated, there's an extra term, involving $(xp - px)$. We call this the **commutator** of x and p; it is a measure of how badly they *fail* to commute. In general, the commutator of operators A and B (written with square brackets) is

$$[A, B] \equiv AB - BA. \qquad [2.48]$$

In this notation,

$$a_-a_+ = \frac{1}{2\hbar m\omega}[p^2 + (m\omega x)^2] - \frac{i}{2\hbar}[x, p]. \qquad [2.49]$$

We need to figure out the commutator of x and p. *Warning:* Operators are notoriously slippery to work with in the abstract, and you are bound to make mistakes unless you give them a "test function," $f(x)$, to act on. At the end you can throw away the test function, and you'll be left with an equation involving the operators alone. In the present case we have:

$$[x, p]f(x) = \left[x\frac{\hbar}{i}\frac{d}{dx}(f) - \frac{\hbar}{i}\frac{d}{dx}(xf)\right] = \frac{\hbar}{i}\left(x\frac{df}{dx} - x\frac{df}{dx} - f\right) = i\hbar f(x). \qquad [2.50]$$

Dropping the test function, which has served its purpose,

$$\boxed{[x, p] = i\hbar.} \qquad [2.51]$$

This lovely and ubiquitous result is known as the **canonical commutation relation.**[18]

With this, Equation 2.49 becomes

$$a_-a_+ = \frac{1}{\hbar\omega}H + \frac{1}{2}, \qquad [2.52]$$

or

$$H = \hbar\omega\left(a_-a_+ - \frac{1}{2}\right). \qquad [2.53]$$

Evidently the Hamiltonian does *not* factor perfectly—there's that extra $-1/2$ on the right. Notice that the ordering of a_+ and a_- is important here; the same argument, with a_+ on the left, yields

$$a_+a_- = \frac{1}{\hbar\omega}H - \frac{1}{2}. \qquad [2.54]$$

In particular,

$$[a_-, a_+] = 1. \qquad [2.55]$$

---

[18] In a deep sense all of the mysteries of quantum mechanics can be traced to the fact that position and momentum do not commute. Indeed, some authors take the canonical commutation relation as an *axiom* of the theory, and use it to *derive* $p = (\hbar/i)d/dx$.

So the Hamiltonian can equally well be written

$$H = \hbar\omega\left(a_+a_- + \frac{1}{2}\right). \qquad [2.56]$$

In terms of $a_\pm$, then, the Schrödinger equation[19] for the harmonic oscillator takes the form

$$\hbar\omega\left(a_\pm a_\mp \pm \frac{1}{2}\right)\psi = E\psi \qquad [2.57]$$

(in equations like this you read the upper signs all the way across, or else the lower signs).

Now, here comes the crucial step: I claim that *if ψ satisfies the Schrödinger equation with energy E,* (that is: $H\psi = E\psi$), *then $a_+\psi$ satisfies the Schrödinger equation with energy $(E + \hbar\omega)$*: $H(a_+\psi) = (E + \hbar\omega)(a_+\psi)$. *Proof:*

$$\begin{aligned} H(a_+\psi) &= \hbar\omega\left(a_+a_- + \frac{1}{2}\right)(a_+\psi) = \hbar\omega\left(a_+a_-a_+ + \frac{1}{2}a_+\right)\psi \\ &= \hbar\omega a_+\left(a_-a_+ + \frac{1}{2}\right)\psi = a_+\left[\hbar\omega\left(a_+a_- + 1 + \frac{1}{2}\right)\psi\right] \\ &= a_+(H + \hbar\omega)\psi = a_+(E + \hbar\omega)\psi = (E + \hbar\omega)(a_+\psi). \end{aligned}$$

(I used Equation 2.55 to replace a_-a_+ by $a_+a_- + 1$, in the second line. Notice that whereas the ordering of a_+ and a_- *does* matter, the ordering of $a_\pm$ and any *constants*—such as $\hbar$, ω, and E—does *not*; an operator commutes with any constant.)

By the same token, $a_-\psi$ is a solution with energy $(E - \hbar\omega)$:

$$\begin{aligned} H(a_-\psi) &= \hbar\omega\left(a_-a_+ - \frac{1}{2}\right)(a_-\psi) = \hbar\omega a_-\left(a_+a_- - \frac{1}{2}\right)\psi \\ &= a_-\left[\hbar\omega\left(a_-a_+ - 1 - \frac{1}{2}\right)\psi\right] = a_-(H - \hbar\omega)\psi = a_-(E - \hbar\omega)\psi \\ &= (E - \hbar\omega)(a_-\psi). \end{aligned}$$

Here, then, is a wonderful machine for generating new solutions, with higher and lower energies—if we could just find *one* solution, to get started! We call $a_\pm$ **ladder operators**, because they allow us to climb up and down in energy; a_+ is the **raising operator**, and a_- the **lowering operator**. The "ladder" of states is illustrated in Figure 2.5.

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[19] I'm getting tired of writing "time-independent Schrödinger equation," so when it's clear from the context which one I mean, I'll just call it the "Schrödinger equation."

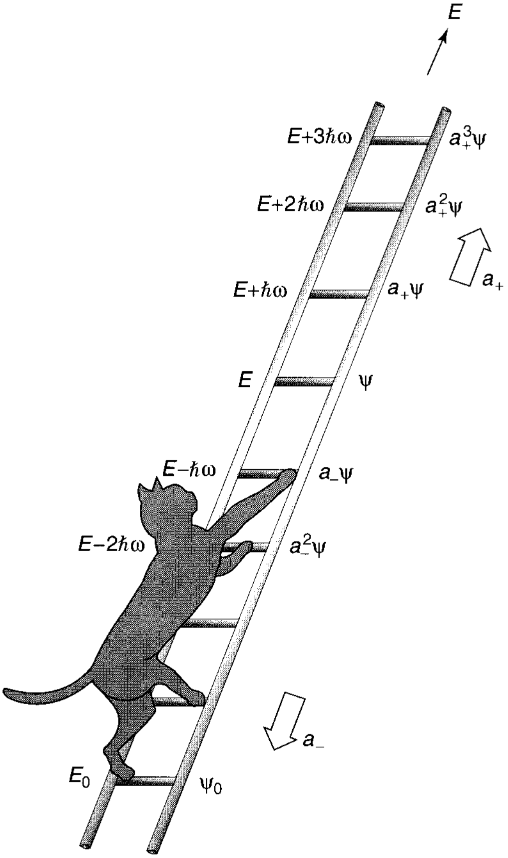

FIGURE 2.5: The "ladder" of states for the harmonic oscillator.

But wait! What if I apply the lowering operator repeatedly? Eventually I'm going to reach a state with energy less than zero, which (according to the general theorem in Problem 2.2) does not exist! At some point the machine must fail. How can that happen? We know that $a_-\psi$ is a new solution to the Schrödinger equation, but *there is no guarantee that it will be normalizable*—it might be zero, or its square-integral might be infinite. In practice it is the former: There occurs a "lowest rung" (call it ψ_0) such that

$$a_-\psi_0 = 0. \qquad [2.58]$$

We can use this to determine $\psi_0(x)$:

$$\frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0 = 0,$$

or

$$\frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar} x\psi_0.$$

This differential equation is easy to solve:

$$\int \frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar}\int x\,dx \quad \Rightarrow \quad \ln\psi_0 = -\frac{m\omega}{2\hbar}x^2 + \text{constant},$$

so

$$\psi_0(x) = Ae^{-\frac{m\omega}{2\hbar}x^2}.$$

We might as well normalize it right away:

$$1 = |A|^2 \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar}\,dx = |A|^2\sqrt{\frac{\pi\hbar}{m\omega}},$$

so $A^2 = \sqrt{m\omega/\pi\hbar}$, and hence

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}.} \qquad [2.59]$$

To determine the energy of this state we plug it into the Schrödinger equation (in the form of Equation 2.57), $\hbar\omega(a_+a_- + 1/2)\psi_0 = E_0\psi_0$, and exploit the fact that $a_-\psi_0 = 0$:

$$E_0 = \frac{1}{2}\hbar\omega. \qquad [2.60]$$

With our foot now securely planted on the bottom rung (the ground state of the quantum oscillator), we simply apply the raising operator (repeatedly) to generate the excited states,[20] increasing the energy by $\hbar\omega$ with each step:

$$\boxed{\psi_n(x) = A_n(a_+)^n\psi_0(x), \quad \text{with } E_n = \left(n + \frac{1}{2}\right)\hbar\omega,} \qquad [2.61]$$

where A_n is the normalization constant. By applying the raising operator (repeatedly) to ψ_0, then, we can (in principle) construct all[21] the stationary states of

---

[20] In the case of the harmonic oscillator it is customary, for some reason, to depart from the usual practice, and number the states starting with $n = 0$, instead of $n = 1$. Obviously, the lower limit on the sum in a formula such as Equation 2.17 should be altered accordingly.

[21] Note that we obtain *all* the (normalizable) solutions by this procedure. For if there were some *other* solution, we could generate from it a second ladder, by repeated application of the raising and lowering operators. But the bottom rung of this new ladder would have to satisfy Equation 2.58, and since that leads inexorably to Equation 2.59, the bottom rungs would be the same, and hence the two ladders would in fact be identical.

the harmonic oscillator. Meanwhile, without ever doing that explicitly, we have determined the allowed energies.

Example 2.4 Find the first excited state of the harmonic oscillator.

Solution: Using Equation 2.61,

$$\begin{aligned}\psi_1(x) = A_1 a_+ \psi_0 &= \frac{A_1}{\sqrt{2\hbar m\omega}}\left(-\hbar\frac{d}{dx} + m\omega x\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \\ &= A_1\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}\,x e^{-\frac{m\omega}{2\hbar}x^2}.\end{aligned} \qquad [2.62]$$

We can normalize it "by hand":

$$\int |\psi_1|^2\,dx = |A_1|^2\sqrt{\frac{m\omega}{\pi\hbar}}\left(\frac{2m\omega}{\hbar}\right)\int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega}{\hbar}x^2}\,dx = |A_1|^2,$$

so, as it happens, $A_1 = 1$.

I wouldn't want to calculate ψ_{50} this way (applying the raising operator fifty times!), but never mind: In *principle* Equation 2.61 does the job—except for the normalization.

You can even get the normalization algebraically, but it takes some fancy footwork, so watch closely. We know that $a_\pm \psi_n$ is *proportional* to $\psi_{n\pm 1}$,

$$a_+\psi_n = c_n\psi_{n+1}, \quad a_-\psi_n = d_n\psi_{n-1} \qquad [2.63]$$

but what are the proportionality factors, c_n and d_n? First note that for "any"[22] functions $f(x)$ and $g(x)$,

$$\int_{-\infty}^{\infty} f^*(a_\pm g)\,dx = \int_{-\infty}^{\infty} (a_\mp f)^* g\,dx. \qquad [2.64]$$

(In the language of linear algebra, $a_\mp$ is the **hermitian conjugate** of $a_\pm$.)

Proof:

$$\int_{-\infty}^{\infty} f^*(a_\pm g)\,dx = \frac{1}{\sqrt{2\hbar m\omega}}\int_{-\infty}^{\infty} f^*\left(\mp\hbar\frac{d}{dx} + m\omega x\right) g\,dx,$$

---

[22] Of course, the integrals must *exist*, and this means that $f(x)$ and $g(x)$ must go to zero at $\pm\infty$.

and integration by parts takes $\int f^*(dg/dx)\,dx$ to $-\int (df/dx)^* g\,dx$ (the boundary terms vanish, for the reason indicated in footnote 22), so

$$\int_{-\infty}^{\infty} f^*(a_\pm g)\,dx = \frac{1}{\sqrt{2\hbar m\omega}}\int_{-\infty}^{\infty}\left[\left(\pm\hbar\frac{d}{dx}+m\omega x\right)f\right]^* g\,dx = \int_{-\infty}^{\infty}(a_\mp f)^* g\,dx.$$

QED

In particular,

$$\int_{-\infty}^{\infty}(a_\pm\psi_n)^*(a_\pm\psi_n)\,dx = \int_{-\infty}^{\infty}(a_\mp a_\pm\psi_n)^*\psi_n\,dx.$$

But (invoking Equations 2.57 and 2.61)

$$a_+a_-\psi_n = n\psi_n, \quad a_-a_+\psi_n = (n+1)\psi_n, \tag{2.65}$$

so

$$\int_{-\infty}^{\infty}(a_+\psi_n)^*(a_+\psi_n)\,dx = |c_n|^2\int_{-\infty}^{\infty}|\psi_{n+1}|^2\,dx = (n+1)\int_{-\infty}^{\infty}|\psi_n|^2\,dx,$$

$$\int_{-\infty}^{\infty}(a_-\psi_n)^*(a_-\psi_n)\,dx = |d_n|^2\int_{-\infty}^{\infty}|\psi_{n-1}|^2\,dx = n\int_{-\infty}^{\infty}|\psi_n|^2\,dx.$$

But since ψ_n and $\psi_{n\pm1}$ are normalized, it follows that $|c_n|^2 = n+1$ and $|d_n|^2 = n$, and hence

$$\boxed{a_+\psi_n = \sqrt{n+1}\,\psi_{n+1}, \quad a_-\psi_n = \sqrt{n}\,\psi_{n-1}.} \tag{2.66}$$

Thus

$$\psi_1 = a_+\psi_0, \quad \psi_2 = \frac{1}{\sqrt{2}}a_+\psi_1 = \frac{1}{\sqrt{2}}(a_+)^2\psi_0,$$

$$\psi_3 = \frac{1}{\sqrt{3}}a_+\psi_2 = \frac{1}{\sqrt{3\cdot2}}(a_+)^3\psi_0, \quad \psi_4 = \frac{1}{\sqrt{4}}a_+\psi_3 = \frac{1}{\sqrt{4\cdot3\cdot2}}(a_+)^4\psi_0,$$

and so on. Clearly

$$\boxed{\psi_n = \frac{1}{\sqrt{n!}}(a_+)^n\psi_0,} \tag{2.67}$$

which is to say that the normalization factor in Equation 2.61 is $A_n = 1/\sqrt{n!}$ (in particular, $A_1 = 1$, confirming our result in Example 2.4).

As in the case of the infinite square well, the stationary states of the harmonic oscillator are orthogonal:

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx = \delta_{mn}. \qquad [2.68]$$

This can be proved using Equation 2.65, and Equation 2.64 twice—first moving a_+ and then moving a_-:

$$\begin{aligned}\int_{-\infty}^{\infty} \psi_m^* (a_+ a_-) \psi_n \, dx &= n \int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx \\ &= \int_{-\infty}^{\infty} (a_- \psi_m)^* (a_- \psi_n) \, dx = \int_{-\infty}^{\infty} (a_+ a_- \psi_m)^* \psi_n \, dx \\ &= m \int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx.\end{aligned}$$

Unless $m = n$, then, $\int \psi_m^* \psi_n \, dx$ must be zero. Orthonormality means that we can again use Fourier's trick (Equation 2.34) to evaluate the coefficients, when we expand $\Psi(x, 0)$ as a linear combination of stationary states (Equation 2.16), and $|c_n|^2$ is again the probability that a measurement of the energy would yield the value E_n.

Example 2.5 Find the expectation value of the potential energy in the nth state of the harmonic oscillator.

Solution:

$$\langle V \rangle = \left\langle \frac{1}{2} m \omega^2 x^2 \right\rangle = \frac{1}{2} m \omega^2 \int_{-\infty}^{\infty} \psi_n^* x^2 \psi_n \, dx.$$

There's a beautiful device for evaluating integrals of this kind (involving powers of x or p): Use the definition (Equation 2.47) to express x and p in terms of the raising and lowering operators:

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a_+ + a_-); \qquad p = i \sqrt{\frac{\hbar m \omega}{2}} (a_+ - a_-). \qquad [2.69]$$

In this example we are interested in x^2:

$$x^2 = \frac{\hbar}{2m\omega} \left[(a_+)^2 + (a_+ a_-) + (a_- a_+) + (a_-)^2 \right].$$

So

$$\langle V \rangle = \frac{\hbar \omega}{4} \int \psi_n^* \left[(a_+)^2 + (a_+ a_-) + (a_- a_+) + (a_-)^2 \right] \psi_n \, dx.$$

But $(a_+)^2\psi_n$ is (apart from normalization) ψ_{n+2}, which is orthogonal to ψ_n, and the same goes for $(a_-)^2\psi_n$, which is proportional to ψ_{n-2}. So those terms drop out, and we can use Equation 2.65 to evaluate the remaining two:

$$\langle V\rangle = \frac{\hbar\omega}{4}(n+n+1) = \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right).$$

As it happens, the expectation value of the potential energy is exactly *half* the total (the other half, of course, is kinetic). This is a peculiarity of the harmonic oscillator, as we'll see later on.

***Problem 2.10**

(a) Construct $\psi_2(x)$.

(b) Sketch ψ_0, ψ_1, and ψ_2.

(c) Check the orthogonality of ψ_0, ψ_1, and ψ_2, by explicit integration. *Hint:* If you exploit the even-ness and odd-ness of the functions, there is really only one integral left to do.

***Problem 2.11**

(a) Compute $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$, and $\langle p^2\rangle$, for the states ψ_0 (Equation 2.59) and ψ_1 (Equation 2.62), by explicit integration. *Comment:* In this and other problems involving the harmonic oscillator it simplifies matters if you introduce the variable $\xi \equiv \sqrt{m\omega/\hbar}\,x$ and the constant $\alpha \equiv (m\omega/\pi\hbar)^{1/4}$.

(b) Check the uncertainty principle for these states.

(c) Compute $\langle T\rangle$ (the average kinetic energy) and $\langle V\rangle$ (the average potential energy) for these states. (No new integration allowed!) Is their sum what you would expect?

***Problem 2.12** Find $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$, $\langle p^2\rangle$, and $\langle T\rangle$, for the nth stationary state of the harmonic oscillator, using the method of Example 2.5. Check that the uncertainty principle is satisfied.

Problem 2.13 A particle in the harmonic oscillator potential starts out in the state

$$\Psi(x,0) = A[3\psi_0(x) + 4\psi_1(x)].$$

(a) Find A.

(b) Construct $\Psi(x,t)$ and $|\Psi(x,t)|^2$.

(c) Find $\langle x\rangle$ and $\langle p\rangle$. Don't get too excited if they oscillate at the classical frequency; what would it have been had I specified $\psi_2(x)$, instead of $\psi_1(x)$? Check that Ehrenfest's theorem (Equation 1.38) holds for this wave function.

(d) If you measured the energy of this particle, what values might you get, and with what probabilities?

Problem 2.14 A particle is in the ground state of the harmonic oscillator with classical frequency ω, when suddenly the spring constant quadruples, so $\omega' = 2\omega$, without initially changing the wave function (of course, Ψ will now *evolve* differently, because the Hamiltonian has changed). What is the probability that a measurement of the energy would still return the value $\hbar\omega/2$? What is the probability of getting $\hbar\omega$? [*Answer:* 0.943.]

2.3.2 Analytic Method

We return now to the Schrödinger equation for the harmonic oscillator,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi, \qquad [2.70]$$

and solve it directly, by the series method. Things look a little cleaner if we introduce the dimensionless variable

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x; \qquad [2.71]$$

in terms of ξ the Schrödinger equation reads

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi, \qquad [2.72]$$

where K is the energy, in units of $(1/2)\hbar\omega$:

$$K \equiv \frac{2E}{\hbar\omega}. \qquad [2.73]$$

Our problem is to solve Equation 2.72, and in the process obtain the "allowed" values of K (and hence of E).

To begin with, note that at very large ξ (which is to say, at very large x), ξ^2 completely dominates over the constant K, so in this regime

$$\frac{d^2\psi}{d\xi^2} \approx \xi^2\psi, \qquad [2.74]$$

which has the approximate solution (check it!)

$$\psi(\xi) \approx Ae^{-\xi^2/2} + Be^{+\xi^2/2}. \qquad [2.75]$$

The B term is clearly not normalizable (it blows up as $|x| \to \infty$); the physically acceptable solutions, then, have the asymptotic form

$$\psi(\xi) \to (\quad) e^{-\xi^2/2}, \quad \text{at large } \xi. \qquad [2.76]$$

This suggests that we "peel off" the exponential part,

$$\psi(\xi) = h(\xi) e^{-\xi^2/2}, \qquad [2.77]$$

in hopes that what remains, $h(\xi)$, has a simpler functional form than $\psi(\xi)$ itself.[23] Differentiating Equation 2.77,

$$\frac{d\psi}{d\xi} = \left(\frac{dh}{d\xi} - \xi h\right) e^{-\xi^2/2},$$

and

$$\frac{d^2\psi}{d\xi^2} = \left(\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\xi^2 - 1)h\right) e^{-\xi^2/2},$$

so the Schrödinger equation (Equation 2.72) becomes

$$\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K - 1)h = 0. \qquad [2.78]$$

I propose to look for solutions to Equation 2.78 in the form of *power series* in ξ:[24]

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \cdots = \sum_{j=0}^{\infty} a_j \xi^j. \qquad [2.79]$$

Differentiating the series term by term,

$$\frac{dh}{d\xi} = a_1 + 2a_2\xi + 3a_3\xi^2 + \cdots = \sum_{j=0}^{\infty} j a_j \xi^{j-1},$$

and

$$\frac{d^2h}{d\xi^2} = 2a_2 + 2\cdot 3a_3\xi + 3\cdot 4a_4\xi^2 + \cdots = \sum_{j=0}^{\infty}(j+1)(j+2)a_{j+2}\xi^j.$$

---

[23] Note that although we invoked some approximations to *motivate* Equation 2.77, what follows is *exact*. The device of stripping off the asymptotic behavior is the standard first step in the power series method for solving differential equations—see, for example, Boas (footnote 11), Chapter 12.

[24] This is known as the **Frobenius method** for solving a differential equation. According to Taylor's theorem, *any* reasonably well-behaved function can be expressed as a power series, so Equation 2.79 ordinarily involves no loss of generality. For conditions on the applicability of the method, see Boas (footnote 11) or George B. Arfken and Hans-Jurgen Weber, *Mathematical Methods for Physicists*, 5th ed., Academic Press, Orlando (2000), Section 8.5.

Putting these into Equation 2.78, we find

$$\sum_{j=0}^{\infty}\left[(j+1)(j+2)a_{j+2}-2ja_j+(K-1)a_j\right]\xi^j=0. \qquad [2.80]$$

It follows (from the uniqueness of power series expansions[25]) that the coefficient of *each power* of ξ must vanish,

$$(j+1)(j+2)a_{j+2}-2ja_j+(K-1)a_j=0,$$

and hence that

$$a_{j+2}=\frac{(2j+1-K)}{(j+1)(j+2)}a_j. \qquad [2.81]$$

This **recursion formula** is entirely equivalent to the Schrödinger equation. Starting with a_0, it generates all the even-numbered coefficients:

$$a_2=\frac{(1-K)}{2}a_0, \quad a_4=\frac{(5-K)}{12}a_2=\frac{(5-K)(1-K)}{24}a_0, \quad \cdots,$$

and starting with a_1, it generates the odd coefficients:

$$a_3=\frac{(3-K)}{6}a_1, \quad a_5=\frac{(7-K)}{20}a_3=\frac{(7-K)(3-K)}{120}a_1, \quad \cdots.$$

We write the complete solution as

$$h(\xi)=h_{\text{even}}(\xi)+h_{\text{odd}}(\xi), \qquad [2.82]$$

where

$$h_{\text{even}}(\xi)\equiv a_0+a_2\xi^2+a_4\xi^4+\cdots$$

is an even function of ξ, built on a_0, and

$$h_{\text{odd}}(\xi)\equiv a_1\xi+a_3\xi^3+a_5\xi^5+\cdots$$

is an odd function, built on a_1. Thus Equation 2.81 determines $h(\xi)$ in terms of two arbitrary constants (a_0 and a_1)—which is just what we would expect, for a second-order differential equation.

However, not all the solutions so obtained are *normalizable*. For at very large j, the recursion formula becomes (approximately)

$$a_{j+2}\approx\frac{2}{j}a_j,$$

---

[25] See, for example, Arfken (footnote 24), Section 5.7.

with the (approximate) solution

$$a_j \approx \frac{C}{(j/2)!},$$

for some constant C, and this yields (at large ξ, where the higher powers dominate)

$$h(\xi) \approx C \sum \frac{1}{(j/2)!} \xi^j \approx C \sum \frac{1}{j!} \xi^{2j} \approx C e^{\xi^2}.$$

Now, if h goes like $\exp(\xi^2)$, then ψ (remember ψ?—that's what we're trying to calculate) goes like $\exp(\xi^2/2)$ (Equation 2.77), which is precisely the asymptotic behavior we *didn't* want.[26] There is only one way to wiggle out of this: For normalizable solutions *the power series must terminate.* There must occur some "highest" j (call it n), such that the recursion formula spits out $a_{n+2} = 0$ (this will truncate *either* the series h_{even} *or* the series h_{odd}; the *other* one must be zero from the start: $a_1 = 0$ if n is even, and $a_0 = 0$ if n is odd). For physically acceptable solutions, then, Equation 2.81 requires that

$$K = 2n + 1,$$

for some non-negative integer n, which is to say (referring to Equation 2.73) that the *energy* must be

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad \text{for } n = 0, 1, 2, \ldots. \qquad [2.83]$$

Thus we recover, by a completely different method, the fundamental quantization condition we found algebraically in Equation 2.61.

It seems at first rather surprising that the quantization of energy should emerge from a technical detail in the power series solution to the Schrödinger equation, but let's look at it from a different perspective. Equation 2.70 has solutions, of course, for *any* value of E (in fact, it has *two* linearly independent solutions for every E). But almost all of these solutions blow up exponentially at large x, and hence are not normalizable. Imagine, for example, using an E that is slightly *less* than one of the allowed values (say, $0.49\hbar\omega$), and plotting the solution (Figure 2.6(a)); the "tails" fly off to infinity. Now try an E slightly *larger* (say, $0.51\hbar\omega$); the "tails" now blow up in the *other* direction (Figure 2.6(b)). As you tweak the parameter in tiny increments from 0.49 to 0.51, the tails flip over when you pass through 0.5—only at *precisely* 0.5 do the tails go to zero, leaving a normalizable solution.[27]

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[26] It's no surprise that the ill-behaved solutions are still contained in Equation 2.81; this recursion relation is equivalent to the Schrödinger equation, so it's *got* to include both the asymptotic forms we found in Equation 2.75.

[27] It is possible to set this up on a computer, and discover the allowed energies "experimentally." You might call it the **wag the dog** method: When the tail wags, you know you've just passed over an allowed value. See Problems 2.54–2.56.

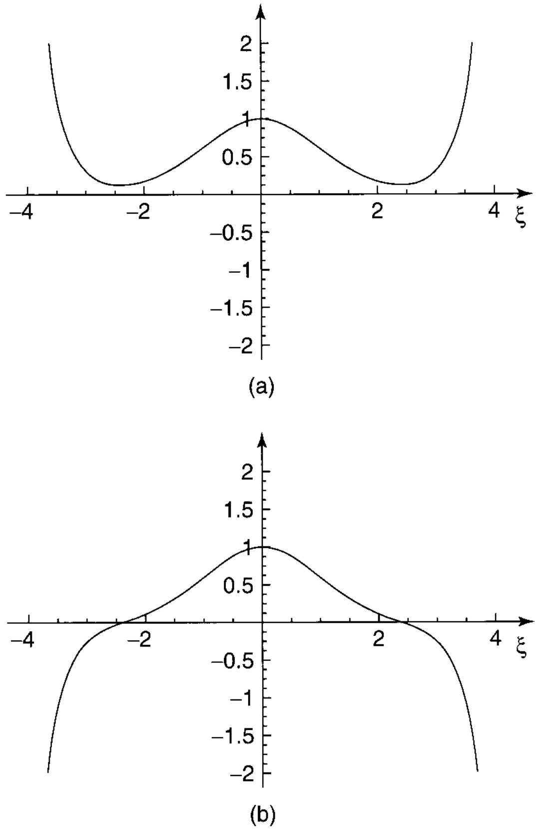

FIGURE 2.6: Solutions to the Schrödinger equation for (a) $E = 0.49\,\hbar\omega$, and (b) $E = 0.51\,\hbar\omega$.

For the allowed values of K, the recursion formula reads

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)} a_j. \qquad [2.84]$$

If $n = 0$, there is only one term in the series (we must pick $a_1 = 0$ to kill h_{odd}, and $j = 0$ in Equation 2.84 yields $a_2 = 0$):

$$h_0(\xi) = a_0,$$

and hence

$$\psi_0(\xi) = a_0 e^{-\xi^2/2}$$

(which, apart from the normalization, reproduces Equation 2.59). For $n = 1$ we take $a_0 = 0$,[28] and Equation 2.84 with $j = 1$ yields $a_3 = 0$, so

$$h_1(\xi) = a_1\xi,$$

and hence

$$\psi_1(\xi) = a_1\xi e^{-\xi^2/2}$$

(confirming Equation 2.62). For $n = 2$, $j = 0$ yields $a_2 = -2a_0$, and $j = 2$ gives $a_4 = 0$, so

$$h_2(\xi) = a_0(1 - 2\xi^2),$$

and

$$\psi_2(\xi) = a_0(1 - 2\xi^2)e^{-\xi^2/2},$$

and so on. (Compare Problem 2.10, where this last result was obtained by algebraic means.)

In general, $h_n(\xi)$ will be a polynomial of degree n in ξ, involving even powers only, if n is an even integer, and odd powers only, if n is an odd integer. Apart from the overall factor (a_0 or a_1) they are the so-called **Hermite polynomials**, $H_n(\xi)$.[29] The first few of them are listed in Table 2.1. By tradition, the arbitrary multiplicative factor is chosen so that the coefficient of the highest power of ξ is 2^n. With this convention, the normalized[30] stationary states for the harmonic oscillator are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi)e^{-\xi^2/2}. \qquad [2.85]$$

They are identical (of course) to the ones we obtained algebraically in Equation 2.67.

TABLE 2.1: The first few Hermite polynomials, $H_n(\xi)$.

$H_0 = 1,$
$H_1 = 2\xi,$
$H_2 = 4\xi^2 - 2,$
$H_3 = 8\xi^3 - 12\xi,$
$H_4 = 16\xi^4 - 48\xi^2 + 12,$
$H_5 = 32\xi^5 - 160\xi^3 + 120\xi.$

---

[28] Note that there is a completely different set of coefficients a_j for each value of n.

[29] The Hermite polynomials have been studied extensively in the mathematical literature, and there are many tools and tricks for working with them. A few of these are explored in Problem 2.17.

[30] I shall not work out the normalization constant here; if you are interested in knowing how it is done, see for example Leonard Schiff, *Quantum Mechanics*, 3rd ed., McGraw-Hill, New York (1968), Section 13.

In Figure 2.7(a) I have plotted $\psi_n(x)$ for the first few n's. The quantum oscillator is strikingly different from its classical counterpart—not only are the energies quantized, but the position distributions have some bizarre features. For instance, the probability of finding the particle outside the classically allowed range (that is, with x greater than the classical amplitude for the energy in question) is *not* zero (see Problem 2.15), and in all odd states the probability of finding the particle at the center is zero. Only at large n do we begin to see some resemblance to the classical case. In Figure 2.7(b) I have superimposed the classical position distribution on the quantum one (for $n = 100$); if you smoothed out the bumps, the two would fit pretty well (however, in the classical case we are talking about the distribution of positions over *time* for *one* oscillator, whereas in the quantum case we are talking about the distribution over an *ensemble* of identically prepared systems).[31]

Problem 2.15 In the ground state of the harmonic oscillator, what is the probability (correct to three significant digits) of finding the particle outside the classically allowed region? *Hint:* Classically, the energy of an oscillator is $E = (1/2)ka^2 = (1/2)m\omega^2a^2$, where a is the amplitude. So the "classically allowed region" for an oscillator of energy E extends from $-\sqrt{2E/m\omega^2}$ to $+\sqrt{2E/m\omega^2}$. Look in a math table under "Normal Distribution" or "Error Function" for the numerical value of the integral.

Problem 2.16 Use the recursion formula (Equation 2.84) to work out $H_5(\xi)$ and $H_6(\xi)$. Invoke the convention that the coefficient of the highest power of ξ is 2^n to fix the overall constant.

****Problem 2.17** In this problem we explore some of the more useful theorems (stated without proof) involving Hermite polynomials.

(a) The **Rodrigues formula** says that

$$H_n(\xi) = (-1)^n e^{\xi^2}\left(\frac{d}{d\xi}\right)^n e^{-\xi^2}. \qquad [2.86]$$

Use it to derive H_3 and H_4.

(b) The following recursion relation gives you H_{n+1} in terms of the two preceding Hermite polynomials:

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi). \qquad [2.87]$$

Use it, together with your answer in (a), to obtain H_5 and H_6.

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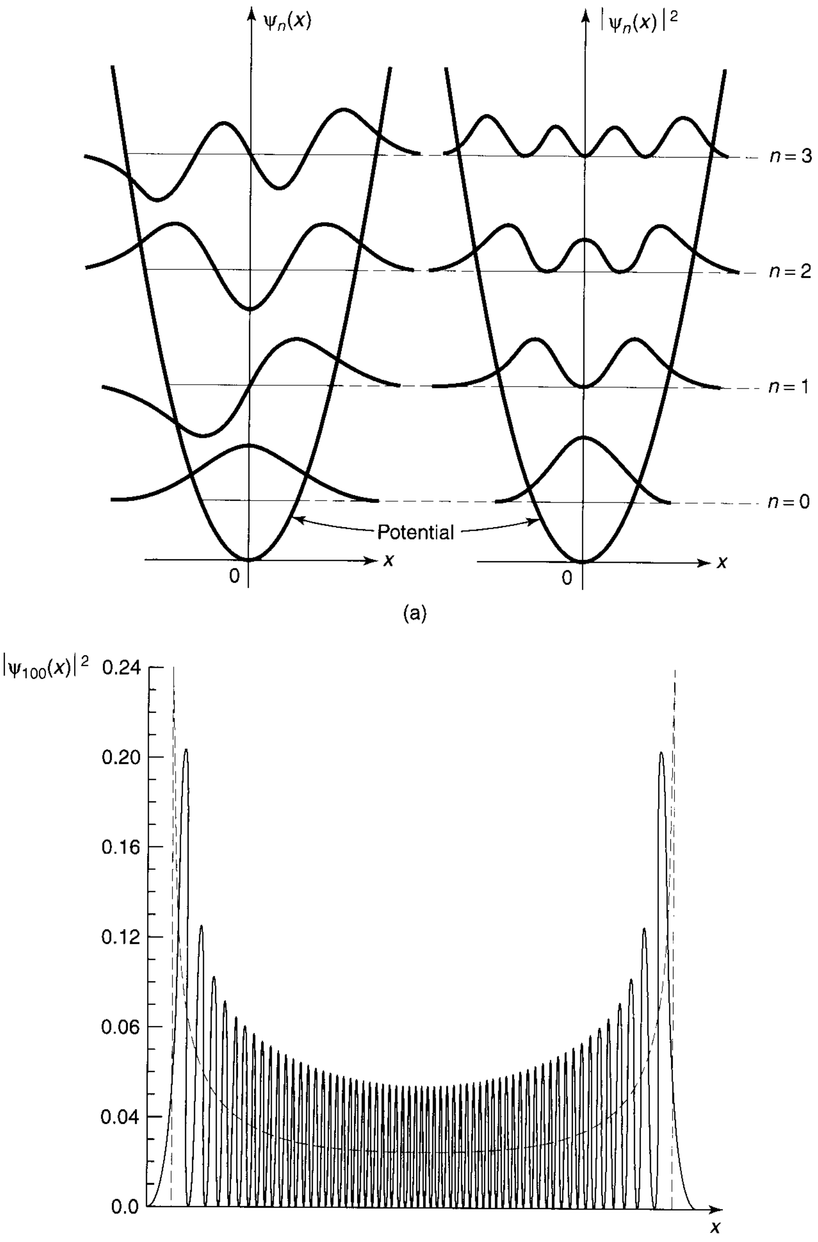
[31] The parallel is perhaps more direct if you interpret the classical distribution as an ensemble of oscillators all with the same energy, but with random starting times.



(a)

(b)

FIGURE 2.7: (a) The first four stationary states of the harmonic oscillator. This material is used by permission of John Wiley & Sons, Inc.; Stephen Gasiorowicz, *Quantum Physics*, John Wiley & Sons, Inc., 1974. (b) Graph of $|\psi_{100}|^2$, with the classical distribution (dashed curve) superimposed.

(c) If you differentiate an nth-order polynomial, you get a polynomial of order $(n-1)$. For the Hermite polynomials, in fact,

$$\frac{dH_n}{d\xi} = 2nH_{n-1}(\xi). \qquad [2.88]$$

Check this, by differentiating H_5 and H_6.

(d) $H_n(\xi)$ is the nth z-derivative, at $z = 0$, of the **generating function** $\exp(-z^2 + 2z\xi)$; or, to put it another way, it is the coefficient of $z^n/n!$ in the Taylor series expansion for this function:

$$e^{-z^2+2z\xi} = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(\xi). \qquad [2.89]$$

Use this to rederive H_0, H_1, and H_2.

2.4 THE FREE PARTICLE

We turn next to what *should* have been the simplest case of all: the free particle ($V(x) = 0$ everywhere). Classically this would just mean motion at constant velocity, but in quantum mechanics the problem is surprisingly subtle and tricky. The time-independent Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \qquad [2.90]$$

or

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}. \qquad [2.91]$$

So far, it's the same as inside the infinite square well (Equation 2.21), where the potential is also zero; this time, however, I prefer to write the general solution in exponential form (instead of sines and cosines), for reasons that will appear in due course:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}. \qquad [2.92]$$

Unlike the infinite square well, there are no boundary conditions to restrict the possible values of k (and hence of E); the free particle can carry *any* (positive) energy. Tacking on the standard time dependence, $\exp(-iEt/\hbar)$,

$$\Psi(x,t) = Ae^{ik(x-\frac{\hbar k}{2m}t)} + Be^{-ik(x+\frac{\hbar k}{2m}t)}. \qquad [2.93]$$

Now, *any* function of x and t that depends on these variables in the special combination $(x \pm vt)$ (for some constant v) represents a wave of fixed profile, traveling in the $\mp x$-direction, at speed v. A fixed point on the waveform (for