

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

$$\omega \equiv \sqrt{\frac{k}{m}} \tag{2.42}$$

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

$$V(x) = \frac{1}{2}kx^2; \tag{2.43}$$

its graph is a parabola.

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:

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

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

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

which describes simple harmonic oscillation (about the point x_0), with an effective spring constant $k = V''(x_0)$. 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.²²

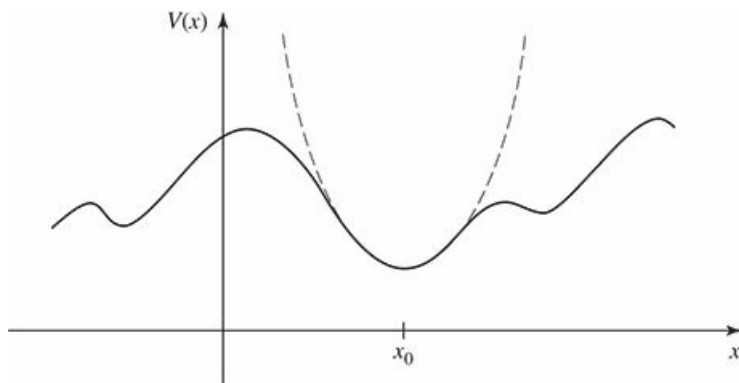


Figure 2.4: Parabolic approximation (dashed curve) to an arbitrary potential, in the neighborhood of a local minimum.

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

$$V(x) = \frac{1}{2}m\omega^2x^2 \quad (2.44)$$

(it is customary to eliminate the spring constant in favor of the classical frequency, using Equation 2.42). As we have seen, it suffices to solve the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi. \quad (2.45)$$

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 hydrogen atom). 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);²³ 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 2.45 in a more suggestive form:

$$\frac{1}{2m} \left[\hat{p}^2 + (m\omega x)^2 \right] \psi = E\psi, \quad (2.46)$$

where $\hat{p} \equiv -i\hbar d/dx$ is the momentum operator.²⁴ The basic idea is to *factor* the Hamiltonian,

$$\hat{H} = \frac{1}{2m} \left[\hat{p}^2 + (m\omega x)^2 \right]. \quad (2.47)$$

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 $\hat{p}$ and x are *operators*, and operators do not, in general, **commute** ($x\hat{p}$ is not the same as $\hat{p}x$, as we'll see in a moment—though you might want to stop right now and think it through for yourself). Still, this does motivate us to examine the quantities

$$\hat{a}_{\pm} \equiv \frac{1}{\sqrt{2\hbar m\omega}} (\mp i\hat{p} + m\omega x) \quad (2.48)$$

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

Well, what *is* the product $\hat{a}_-\hat{a}_+$?

$$\begin{aligned} \hat{a}_-\hat{a}_+ &= \frac{1}{2\hbar m\omega} (i\hat{p} + m\omega x)(-i\hat{p} + m\omega x) \\ &= \frac{1}{2\hbar m\omega} \left[\hat{p}^2 + (m\omega x)^2 - im\omega (x\hat{p} - \hat{p}x) \right]. \end{aligned}$$

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

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}. \quad (2.49)$$

In this notation,

$$\hat{a}_-\hat{a}_+ = \frac{1}{2\hbar m\omega} \left[\hat{p}^2 + (m\omega x)^2 \right] - \frac{i}{2\hbar} [x, \hat{p}]. \quad (2.50)$$

We need to figure out the commutator of x and $\hat{p}$. *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:

$$\begin{aligned} [x, \hat{p}] f(x) &= \left[x(-i\hbar) \frac{d}{dx}(f) - (-i\hbar) \frac{d}{dx}(xf) \right] = -i\hbar \left(x \frac{df}{dx} - x \frac{df}{dx} - f \right) \\ &= i\hbar f(x). \end{aligned} \quad (2.51)$$

Dropping the test function, which has served its purpose,

$$\boxed{[x, \hat{p}] = i\hbar.} \quad (2.52)$$

This lovely and ubiquitous formula is known as the **canonical commutation relation**.²⁵

With this, Equation 2.50 becomes

$$\hat{a}_- \hat{a}_+ = \frac{1}{\hbar\omega} \hat{H} + \frac{1}{2}, \quad (2.53)$$

or

$$\hat{H} = \hbar\omega \left(\hat{a}_- \hat{a}_+ - \frac{1}{2} \right). \quad (2.54)$$

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

$$\hat{a}_+ \hat{a}_- = \frac{1}{\hbar\omega} \hat{H} - \frac{1}{2}. \quad (2.55)$$

In particular,

$$[\hat{a}_-, \hat{a}_+] = 1. \quad (2.56)$$

Meanwhile, the Hamiltonian can equally well be written

$$\hat{H} = \hbar\omega \left(\hat{a}_+ \hat{a}_- + \frac{1}{2} \right). \quad (2.57)$$

In terms of $\hat{a}_\pm$, then, the Schrödinger equation²⁶ for the harmonic oscillator takes the form

$$\hbar\omega \left(\hat{a}_\pm \hat{a}_\mp \pm \frac{1}{2} \right) \psi = E \psi \quad (2.58)$$

(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: $\hat{H}\psi = E\psi$), then $\hat{a}_+\psi$ satisfies the Schrödinger equation with energy $(E + \hbar\omega)$: $\hat{H}(\hat{a}_+\psi) = (E + \hbar\omega)(\hat{a}_+\psi)$.

Proof:

$$\begin{aligned} \hat{H}(\hat{a}_+\psi) &= \hbar\omega \left(\hat{a}_+ \hat{a}_- + \frac{1}{2} \right) (\hat{a}_+\psi) = \hbar\omega \left(\hat{a}_+ \hat{a}_- \hat{a}_+ + \frac{1}{2} \hat{a}_+ \right) \psi \\ &= \hbar\omega \hat{a}_+ \left(\hat{a}_- \hat{a}_+ + \frac{1}{2} \right) \psi = \hat{a}_+ \left[\hbar\omega \left(\hat{a}_+ \hat{a}_- + 1 + \frac{1}{2} \right) \psi \right] \\ &= \hat{a}_+ \left(\hat{H} + \hbar\omega \right) \psi = \hat{a}_+ (E + \hbar\omega) \psi = (E + \hbar\omega) (\hat{a}_+\psi). \quad \text{QED} \end{aligned}$$

(I used Equation 2.56 to replace $\hat{a}_- \hat{a}_+$ by $(\hat{a}_+ \hat{a}_- + 1)$ in the second line. Notice that whereas the ordering of $\hat{a}_+$ and $\hat{a}_-$ *does* matter, the ordering of $\hat{a}_\pm$ and any *constants*—such as $\hbar$, ω , and E —does *not*; an operator commutes with any constant.)

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

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

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 $\hat{a}_\pm$ **ladder operators**, because they allow us to climb up and down in energy; $\hat{a}_+$ is the **raising operator**, and $\hat{a}_-$ the **lowering operator**. The “ladder” of states is illustrated in Figure 2.5.

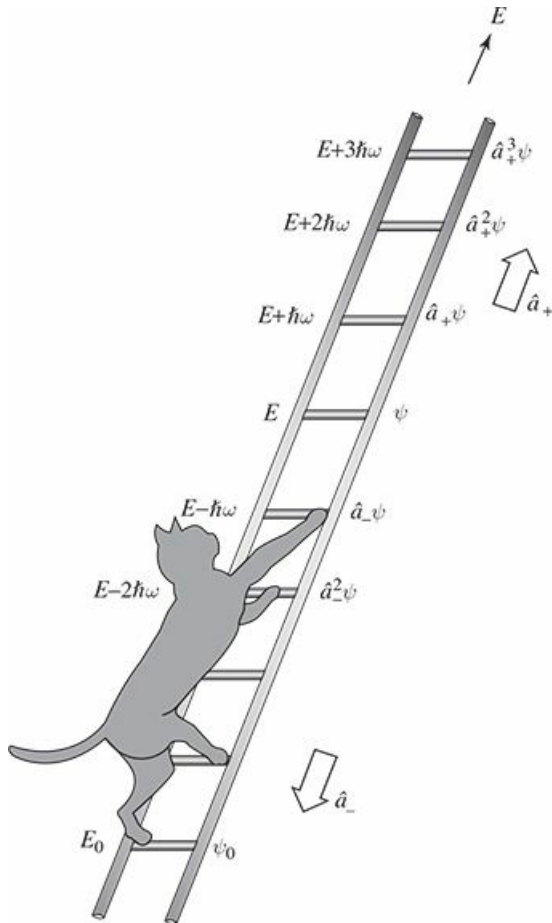


Figure 2.5: The “ladder” of states for the harmonic oscillator.

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 2.3) does not exist! At some point the machine must fail. How can that happen? We know that $\hat{a}_- \psi$ 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

$$\hat{a}_- \psi_0 = 0. \quad (2.59)$$

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:

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

so

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

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

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi \hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar} x^2}.} \quad (2.60)$$

To determine the energy of this state we plug it into the Schrödinger equation (in the form of Equation 2.58), $\hbar\omega (\hat{a}_+ \hat{a}_- + 1/2) \psi_0 = E_0 \psi_0$, and exploit the fact that $\hat{a}_- \psi_0 = 0$:

$$E_0 = \frac{1}{2} \hbar\omega. \quad (2.61)$$

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,²⁷ increasing the energy by $\hbar\omega$ with each step:

$$\boxed{\psi_n(x) = A_n (\hat{a}_+)^n \psi_0(x), \quad \text{with} \quad E_n = \left(n + \frac{1}{2}\right) \hbar\omega,} \quad (2.62)$$

where A_n is the normalization constant. By applying the raising operator (repeatedly) to ψ_0 , then, we can (in principle) construct all²⁸ the stationary states of 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 2.62,

$$\begin{aligned}\psi_1(x) &= A_1 \hat{a}_+ \psi_0 = \frac{A_1}{\sqrt{2\hbar m\omega}} \left(-\hbar \frac{d}{dx} + m\omega x \right) \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega}{2\hbar} x^2} \\ &= A_1 \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}} x e^{-\frac{m\omega}{2\hbar} x^2}.\end{aligned}\tag{2.63}$$

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 2.62 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 $\hat{a}_{\pm} \psi_n$ is *proportional* to $\psi_{n\pm 1}$,

$$\hat{a}_+ \psi_n = c_n \psi_{n+1}, \quad \hat{a}_- \psi_n = d_n \psi_{n-1}\tag{2.64}$$

but what are the proportionality factors, c_n and d_n ? First note that for “any”²⁹ functions $f(x)$ and $g(x)$,

$$\int_{-\infty}^{\infty} f^* (\hat{a}_{\pm} g) dx = \int_{-\infty}^{\infty} (\hat{a}_{\mp} f)^* g dx.\tag{2.65}$$

In the language of linear algebra, $\hat{a}_{\mp}$ is the **hermitian conjugate** (or **adjoint**) of $\hat{a}_{\pm}$.

Proof:

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

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 29), so

$$\begin{aligned}\int_{-\infty}^{\infty} f^* (\hat{a}_{\pm} g) dx &= \frac{1}{\sqrt{2\hbar m\omega}} \int_{-\infty}^{\infty} \left[\left(\pm \hbar \frac{d}{dx} + m\omega x \right) f \right]^* g dx \\ &= \int_{-\infty}^{\infty} (\hat{a}_{\pm} f)^* g dx. \quad \text{QED}\end{aligned}$$

In particular,

$$\int_{-\infty}^{\infty} (\hat{a}_{\pm} \psi_n)^* (\hat{a}_{\pm} \psi_n) dx = \int_{-\infty}^{\infty} (\hat{a}_{\mp} \hat{a}_{\pm} \psi_n)^* \psi_n dx.$$

But (invoking Equations 2.58 and 2.62)

$$\hat{a}_+ \hat{a}_- \psi_n = n \psi_n, \quad \hat{a}_- \hat{a}_+ \psi_n = (n+1) \psi_n, \quad (2.66)$$

so

$$\begin{aligned} \int_{-\infty}^{\infty} (\hat{a}_+ \psi_n)^* (\hat{a}_+ \psi_n) dx &= |c_n|^2 \int_{-\infty}^{\infty} |\psi_{n+1}|^2 dx = (n+1) \int_{-\infty}^{\infty} |\psi_n|^2 dx, \\ \int_{-\infty}^{\infty} (\hat{a}_- \psi_n)^* (\hat{a}_- \psi_n) dx &= |d_n|^2 \int_{-\infty}^{\infty} |\psi_{n-1}|^2 dx = n \int_{-\infty}^{\infty} |\psi_n|^2 dx. \end{aligned}$$

But since ψ_n and $\psi_{n\pm 1}$ are normalized, it follows that $|c_n|^2 = n+1$ and $|d_n|^2 = n$ and hence³⁰

$$\boxed{\hat{a}_+ \psi_n = \sqrt{n+1} \psi_{n+1}, \quad \hat{a}_- \psi_n = \sqrt{n} \psi_{n-1}.} \quad (2.67)$$

Thus

$$\begin{aligned} \psi_1 &= \hat{a}_+ \psi_0, \quad \psi_2 = \frac{1}{\sqrt{2}} \hat{a}_+ \psi_1 = \frac{1}{\sqrt{2}} (\hat{a}_+)^2 \psi_0, \\ \psi_3 &= \frac{1}{\sqrt{3}} \hat{a}_+ \psi_2 = \frac{1}{\sqrt{3 \cdot 2}} (\hat{a}_+)^3 \psi_0, \quad \psi_4 = \frac{1}{\sqrt{4}} \hat{a}_+ \psi_3 = \frac{1}{\sqrt{4 \cdot 3 \cdot 2}} (\hat{a}_+)^4 \psi_0, \end{aligned}$$

and so on. Clearly

$$\boxed{\psi_n = \frac{1}{\sqrt{n!}} (\hat{a}_+)^n \psi_0,} \quad (2.68)$$

which is to say that the normalization factor in Equation 2.62 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:

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n dx = \delta_{mn}. \quad (2.69)$$

This can be proved using Equation 2.66, and Equation 2.65 twice—first moving $\hat{a}_+$ and then moving $\hat{a}_-$:

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

Unless $m = n$, then, $\int \psi_m^* \psi_n dx$ must be zero. Orthonormality means that we can again use Fourier's trick (Equation 2.37) to evaluate the coefficients c_n , when we expand $\Psi(x, 0)$ as a linear combination of stationary states (Equation 2.16). As always, $|c_n|^2$ is 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 n th stationary 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 $\hat{p}$): Use the definition (Equation 2.48) to express x and $\hat{p}$ in terms of the raising and lowering operators:

$$x = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}_+ + \hat{a}_-); \quad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}} (\hat{a}_+ - \hat{a}_-). \quad (2.70)$$

In this example we are interested in x^2 :

$$x^2 = \frac{\hbar}{2m\omega} [(\hat{a}_+)^2 + (\hat{a}_+ \hat{a}_-) + (\hat{a}_- \hat{a}_+) + (\hat{a}_-)^2].$$

So

$$\langle V \rangle = \frac{\hbar\omega}{4} \int_{-\infty}^{\infty} \psi_n^* [(\hat{a}_+)^2 + (\hat{a}_+ \hat{a}_-) + (\hat{a}_- \hat{a}_+) + (\hat{a}_-)^2] \psi_n dx.$$

But $(\hat{a}_+)^2 \psi_n$ is (apart from normalization) ψ_{n+2} , which is orthogonal to ψ_n , and the same goes for $(\hat{a}_-)^2 \psi_n$, which is proportional to ψ_{n-2} . So those terms drop out, and we can use Equation 2.66 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 3.37).

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Problem 2.10

- Construct $\psi_2(x)$.
- Sketch ψ_0 , ψ_1 , and ψ_2 .
- 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.

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Problem 2.11

- Compute $\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$, and $\langle p^2 \rangle$, for the states ψ_0 (Equation 2.60) and ψ_1 (Equation 2.63), 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 $\langle T \rangle$ and $\langle V \rangle$ 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 n th 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 $|\Psi(x, t)|^2$. Don't get too excited if $|\Psi(x, t)|^2$ oscillates at exactly the classical frequency; what would it have been had I specified $\psi_2(x)$, instead of $\psi_1(x)$?³¹
- (c) Find $\langle x \rangle$ and $\langle p \rangle$. 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?

2.3.2 Analytic Method

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

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi = E\psi, \quad (2.71)$$

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

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}} x; \quad (2.72)$$

in terms of ξ the Schrödinger equation reads

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - K) \psi, \quad (2.73)$$

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

$$K \equiv \frac{2E}{\hbar\omega}. \quad (2.74)$$

Our problem is to solve Equation 2.73, 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

$$\frac{d^2\psi}{d\xi^2} \approx \xi^2 \psi, \quad (2.75)$$

which has the approximate solution (check it!)

$$\psi(\xi) \approx Ae^{-\xi^2/2} + Be^{+\xi^2/2}. \quad (2.76)$$

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

$$\psi(\xi) \rightarrow () e^{-\xi^2/2}, \quad \text{at large } \xi. \quad (2.77)$$

This suggests that we “peel off” the exponential part,

$$\psi(\xi) = h(\xi) e^{-\xi^2/2}, \quad (2.78)$$

in hopes that what remains, $h(\xi)$, has a simpler functional form than $\psi(\xi)$ itself.³² Differentiating Equation 2.78,

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

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 2.73) becomes

$$\frac{d^2h}{d\xi^2} - 2\xi \frac{dh}{d\xi} + (K - 1)h = 0. \quad (2.79)$$

I propose to look for solutions to Equation 2.79 in the form of *power series* in ξ :³³

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \dots = \sum_{j=0}^{\infty} a_j \xi^j. \quad (2.80)$$

Differentiating the series term by term,

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

and

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

Putting these into Equation 2.80, we find

$$\sum_{j=0}^{\infty} [(j+1)(j+2) a_{j+2} - 2j a_j + (K-1) a_j] \xi^j = 0. \quad (2.81)$$

It follows (from the uniqueness of power series expansions³⁴) that the coefficient of *each power* of ξ must vanish,

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

and hence that

$$a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)} a_j. \quad (2.82)$$

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

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

and starting with a_1 , it generates the odd coefficients:

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

We write the complete solution as

$$h(\xi) = h_{\text{even}}(\xi) + h_{\text{odd}}(\xi), \quad (2.83)$$

where

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

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

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

is an odd function, built on a_1 . Thus Equation 2.82 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)

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

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 2.78), which is precisely the asymptotic behavior we *didn’t* want.³⁵ 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 2.82 requires that

$$K = 2n + 1,$$

for some positive integer n , which is to say (referring to Equation 2.74) that the *energy* must be

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega, \quad \text{for } n = 0, 1, 2, \dots \quad (2.84)$$

Thus we recover, by a completely different method, the fundamental quantization condition we found algebraically in Equation 2.62.

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 2.71 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). Now try an E slightly *larger* (say, $0.51\hbar\omega$); the “tail” now blows up in the *other* direction (Figure 2.6(b)). As you tweak the parameter in tiny increments from 0.49 to 0.51, the graph

“flips over” at precisely the value 0.5—only here does the solution escape the exponential asymptotic growth that renders it physically unacceptable.³⁶

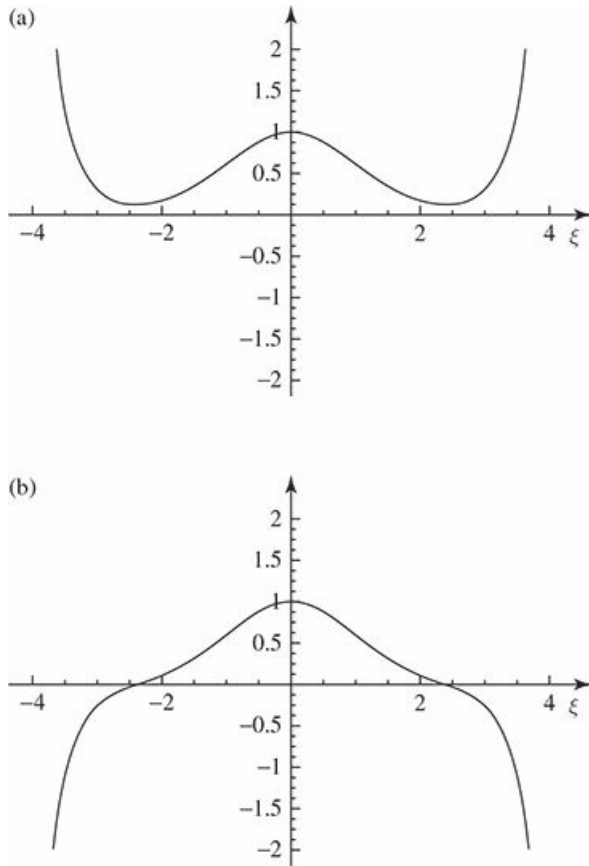


Figure 2.6: Solutions to the Schrödinger equation for (a) $E = 0.49\hbar\omega$, and (b) $E = 0.51\hbar\omega$.

For the allowed values of K , the recursion formula reads

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)}a_j. \quad (2.85)$$

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 2.85 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 2.60). For $n = 1$ we take $a_0 = 0$,³⁷ and Equation 2.85 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 2.63). 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**, $H_n(\xi)$.³⁸ 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 normalized³⁹ stationary states for the harmonic oscillator are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}. \quad (2.86)$$

They are identical (of course) to the ones we obtained algebraically in Equation 2.68.

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

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

In Figure 2.7(a) I have plotted $\psi_n(x)$ for the first few ns . 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 2.14), 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 (Problem 1.11) on the quantum one (for $n = 60$); if you smoothed out the bumps, the two would fit pretty well.

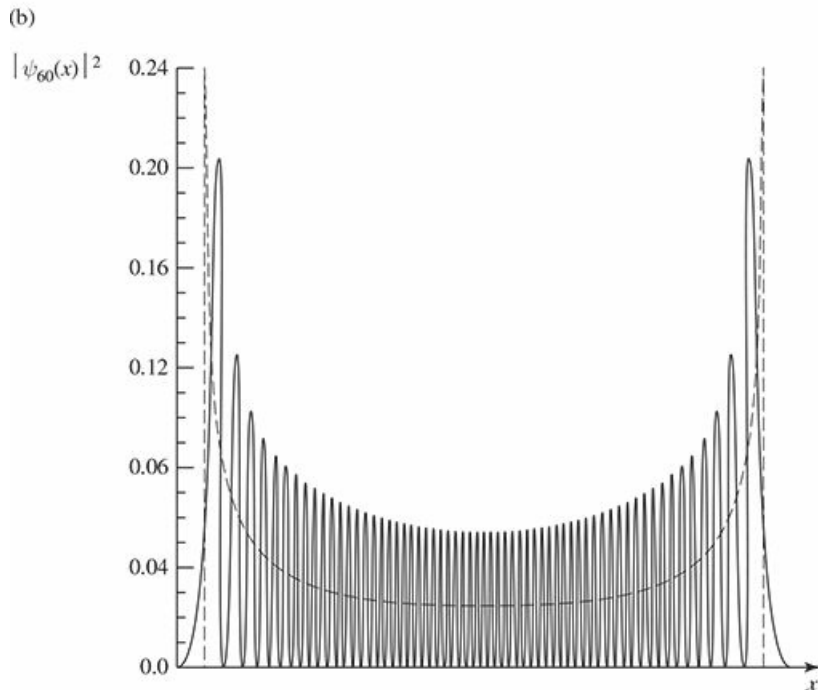
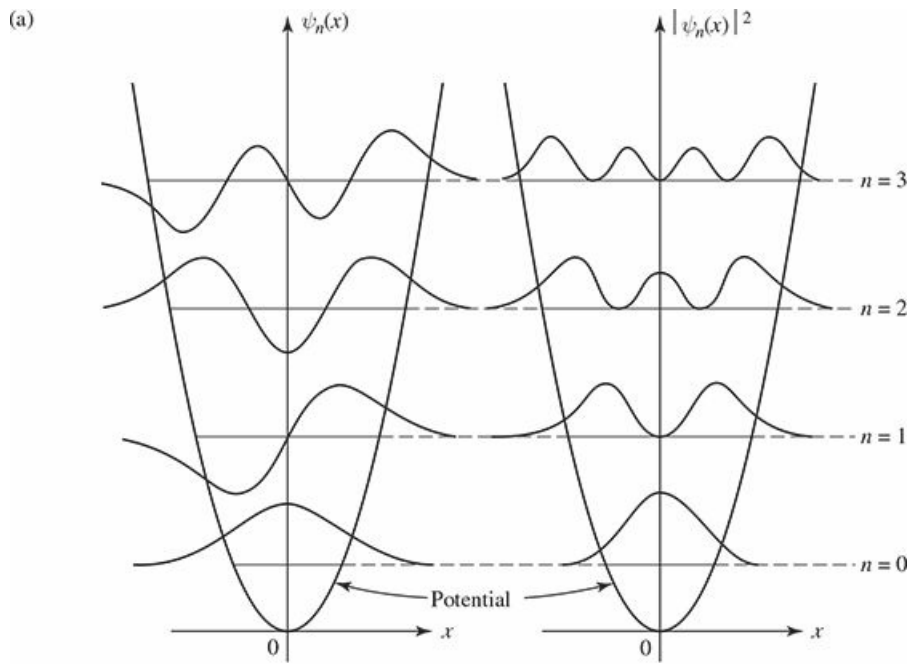


Figure 2.7: (a) The first four stationary states of the harmonic oscillator. (b) Graph of $|\psi_{60}|^2$, with the classical distribution (dashed curve) superimposed.

Problem 2.14 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, or evaluate it by computer.

Problem 2.15 Use the recursion formula (Equation 2.85) 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 2.16 In this problem we explore some of the more useful theorems (stated without proof) involving Hermite polynomials.

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

$$H_n(\xi) = (-1)^n e^{\xi^2} \left(\frac{d}{d\xi} \right)^n e^{-\xi^2}. \quad (2.87)$$

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:

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2n H_{n-1}(\xi). \quad (2.88)$$

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

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

$$\frac{dH_n}{d\xi} = 2n H_{n-1}(\xi). \quad (2.89)$$

Check this, by differentiating H_5 and H_6 .

(d) $H_n(\xi)$ is the n th 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:

$$e^{-z^2+2z\xi} = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(\xi). \quad (2.90)$$

Use this to obtain H_1 , H_2 , and H_3 .

According to the generalized statistical interpretation, the probability that a measurement of momentum would yield a result in the range dp is

$$|\Phi(p, t)|^2 dp. \quad (3.56)$$

Example 3.4

A particle of mass m is bound in the delta function well $V(x) = -\alpha\delta(x)$. What is the probability that a measurement of its momentum would yield a value greater than $p_0 = m\alpha/\hbar$?

Solution: The (position space) wave function is (Equation 2.132)

$$\Psi(x, t) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} e^{-iEt/\hbar}$$

(where $E = -m\alpha^2/2\hbar^2$). The momentum space wave function is therefore

$$\Phi(p, t) = \frac{1}{\sqrt{2\pi\hbar}} \frac{\sqrt{m\alpha}}{\hbar} e^{-iEt/\hbar} \int_{-\infty}^{\infty} e^{-ipx/\hbar} e^{-m\alpha|x|/\hbar^2} dx = \sqrt{\frac{2}{\pi}} \frac{p_0^{3/2} e^{-iEt/\hbar}}{p^2 + p_0^2}$$

(I looked up the integral). The probability, then, is

$$\frac{2}{\pi} p_0^3 \int_{p_0}^{\infty} \frac{1}{(p^2 + p_0^2)^2} dp = \frac{1}{\pi} \left[\frac{pp_0}{p^2 + p_0^2} + \tan^{-1} \left(\frac{p}{p_0} \right) \right] \Big|_{p_0}^{\infty} = \frac{1}{4} - \frac{1}{2\pi} = 0.0908$$

(again, I looked up the integral).

Problem 3.11 Find the momentum-space wave function, $\Phi(p, t)$, for a particle in the ground state of the harmonic oscillator. What is the probability (to two significant digits) that a measurement of p on a particle in this state would yield a value outside the classical range (for the same energy)? *Hint:* Look in a math table under “Normal Distribution” or “Error Function” for the numerical part—or use Mathematica.

Problem 3.12 Find $\Phi(p, t)$ for the free particle in terms of the function $\phi(k)$ introduced in Equation 2.101. Show that for the free particle $|\Phi(p, t)|^2$ is independent of time. *Comment:* the time independence of $|\Phi(p, t)|^2$ for the free particle is a manifestation of momentum conservation in this system.

* **Problem 3.13** Show that

$$\langle x \rangle = \int \Phi^* \left(i\hbar \frac{\partial}{\partial p} \right) \Phi dp. \quad (3.57)$$

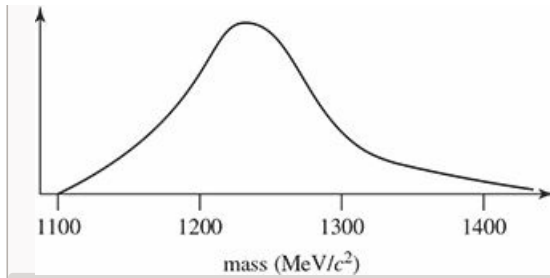


Figure 3.2: Measurements of the Δ mass (Example 3.7).

Notice the variety of specific meanings attaching to the term Δt in these examples: In Example 3.5 it's a period of oscillation; in Example 3.6 it's the time it takes a particle to pass a point; in Example 3.7 it's the lifetime of an unstable particle. In every case, however, Δt is the time it takes for the system to undergo “substantial” change.

It is often said that the uncertainty principle means energy is not strictly conserved in quantum mechanics—that you're allowed to “borrow” energy ΔE , as long as you “pay it back” in a time $\Delta t \approx \hbar / (2\Delta E)$; the greater the violation, the briefer the period over which it can occur. Now, there are many legitimate readings of the energy-time uncertainty principle, but this is not one of them. Nowhere does quantum mechanics license violation of energy conservation, and certainly no such authorization entered into the derivation of Equation 3.76. But the uncertainty principle is extraordinarily robust: It can be misused without leading to seriously incorrect results, and as a consequence physicists are in the habit of applying it rather carelessly.

* **Problem 3.18** Apply Equation 3.73 to the following special cases: (a) $Q = 1$; (b) $Q = H$; (c) $Q = x$; (d) $Q = p$. In each case, comment on the result, with particular reference to Equations 1.27, 1.33, 1.38, and conservation of energy (see remarks following Equation 2.21).

Problem 3.19 Use Equation 3.73 (or Problem 3.18 (c) and (d)) to show that:

- (a) For any (normalized) wave packet representing a free particle ($V(x) = 0$), $\langle x \rangle$ moves at constant velocity (this is the quantum analog to Newton's first law). *Note:* You showed this for a *gaussian* wave packet in Problem 2.42, but it is completely general.
- (b) For any (normalized) wave packet representing a particle in the harmonic oscillator potential ($V(x) = \frac{1}{2}m\omega^2 x^2$), $\langle x \rangle$ oscillates at the classical frequency. *Note:* You showed this for a particular *gaussian* wave packet in Problem 2.49, but it is completely general.

Problem 3.20 Test the energy-time uncertainty principle for the wave function in Problem 2.5 and the observable x , by calculating σ_H , σ_x , and $d\langle x \rangle / dt$ exactly.