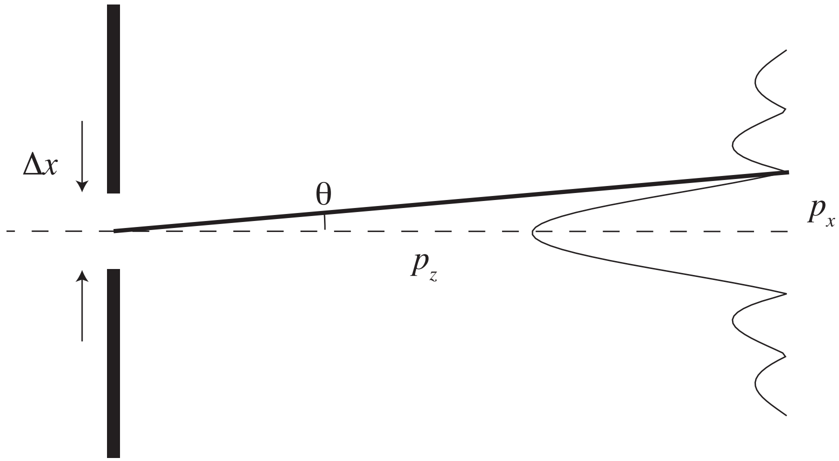
Uncertainty and slits

- Consider the act of trying to measure the $\hat{x}$ momentum of a particle passing through a defined position Δx:



- Because the particle is wavelike in its properties, it will be diffracted by the slit with a semi-angle θ of $\sin\theta = \lambda/\Delta x$.
- If the particle had a velocity v_z, we will now have an uncertainty in the $\hat{x}$ velocity of

$$\Delta p_x = p_z \sin\theta = \frac{h}{\lambda}\frac{\lambda}{\Delta x} = \frac{h}{\Delta x}$$

giving $\Delta p_x \, \Delta x = h$.

Heisenberg uncertainty relationship

- Our relationship $\Delta p_x \, \Delta x = h$ was for the full slit width and the semi-opening angle. We can usually estimate the centroid a bit more accurately, but we can't be too exact about the fuzziness so there is a bit of wiggle room in the prefactor used! Heisenberg concluded (*cf.* Serway Eq. 5.31):

  (1) $$\Delta x \, \Delta p_x \simeq \frac{h}{4\pi} = \frac{\hbar}{2}$$

  in a paper in *Zeitschrift für Physik* **43**, 172–198 (1927).

- So particles in quantum mechanics are like many politicians, or overweight wrestlers: the more you try to pin them down, the squishier they get.

- The act of limiting a particle to a certain position inevitably means that you cannot predict its momentum exactly, and vice versa.

The energy-time uncertainty relationship

- Let's count wave crests that go by in a time interval Δt.
- If the wave has a period T, we can only count $N = \Delta t/T$ waves.
- Therefore we can really only specify the period to plus or minus a wave, or $\Delta T \simeq T/N$.
- The product is $\Delta T\,\Delta t \simeq (T/N)(NT) \simeq T^2$.
- Substituting $\omega = 2\pi/T$ gives $\Delta\omega = 2\pi/T^2\,\Delta T$ or

$$\begin{aligned} \Delta T\,\Delta t &\simeq T^2 \\ \Delta\omega \frac{T^2}{2\pi}\,\Delta t &\simeq T^2 \\ \Delta\omega\Delta t \simeq 2\pi \end{aligned}$$

- Since $\Delta E = \hbar\,\Delta\omega$ we then get $\Delta E\,\Delta t \simeq h$. Again we can pin the centroid down a bit more so the convention is to say $\Delta E\,\Delta t \simeq \hbar/2$ (*cf.* Serway Eq. 5.34).

Confusion over uncertainty

- It will not fly if you write the following as your total solution to an exam problem: “According to Heisenberg, the answer is uncertain.”
- The Heisenberg uncertainty relationship is widely abused. Some postmodernists say it means we can’t know anything for certain in life, so all points of view are equally valid. This is a rather sweeping overgeneralization of the observation that matter behaves like de Broglie waves!
- Another overinterpretation is to say that this marks the death of classical physics, in the following argument:
  - → With Newtonian mechanics, if we could measure the position and momentum of all particles in the universe, we could predict the future with perfect accuracy.
  - → The Heisenberg uncertainty relationship means we can’t know both, so we’ve lost the ability to predict the future (unless, of course, we are astrologers).
- In fact we can’t even do it in classical mechanics. There are a great number of situations where a small change in initial conditions produces nonlinear changes in outcomes. These situations are *chaotic*, and they exist in classical mechanics.

Clarity over uncertainty

- So let's limit ourselves to things we can do experiments on, such as electron transitions in atoms. If an excited state has a lifetime of Δt, we can define the energy of its transition only as well as $\Delta E = \hbar/\Delta t$. Short-lifetime states have broad energy/wavelength distributions; long-lifetime states have well-defined energy/wavelength distributions. We can measure this in spectroscopy experiments!
- Another example we'll consider is the confinement of protons and neutrons to the nucleus, where we can gain insight into their momenta p and thus energy from their confinement distance Δx.

The Schrödinger perscription (again)

- Find the potential U. Think of boundary conditions.
- Try a guess of the wave function ψ, by taking its second derivative and seeing if it satisfies

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right)+U\psi=E\psi.$$

- This will often give you the energies of the solutions.
- Enforcing $\int\psi^*\psi=1$ will give you the normalization.
- Then ψ gives you the probability amplitude, and $|\psi^*\psi|$ gives you the probability.

The harmonic oscillator

- Recall that we talked about restoring forces. We can represent any force by a Taylor series expansion about the zero-force point which we'll assume is at $x = 0$:

  $$F(x) \simeq a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + \ldots$$

  We must have $a_0 = 0$ at the no-force point.

  We must have $a_1 = -|a_1|$ and $a_3 = -|a_3|$ to have a restoring force.

  We must have $a_2 \simeq 0$ and $a_4 \simeq 0$ to have a symmetric restoring force.

  So at small displacement, *any* restoring force can be approximated as $F(x) \simeq -kx$.

- Therefore if we can solve the harmonic oscillator (Serway Sec. 6.6), we can gain insight into *many* physical situations!

The harmonic oscillator again

- The restoring force is of the form $F = -kx$, representing the dominant term of the Taylor series expansion of *any* restoring force.
- By the way, you will learn in Physics 306 that you can solve many problems in quantum mechanics using first order perturbation theory. This involves treating the potential as something you can solve exactly plus the first order deviation (like the next term in a Taylor's series), in which case you can calculate the first order correction to the exact wave function and energy solutions. The harmonic oscillator can be used as a starting point in many perturbation theory solutions.
- Back to the regular old harmonic oscillator: the potential is $U = (1/2)kx^2$.
- The maximum classical excursion from equilibrium is when all the energy E is in the potential energy U, or

$$\begin{aligned} \frac{1}{2}kx^2_{\text{extremum}} &= E \\ x_{\text{extremum}} &= \pm\sqrt{\frac{2E}{k}}. \end{aligned}$$

Harmonic oscillator I

- Potential is $U = \frac{1}{2}kx^2$. Solution must approach zero as $x \to \pm\infty$, so let's try $\psi(x) = A\exp[-ax^2]$ as a first, most basic solution (see Serway Eq. 6.26).
- We'll need the second derivative of ψ:

$$\begin{aligned}
\frac{d}{dx}\left(\frac{d}{dx}(A\exp[-ax^2])\right) &= \frac{d}{dx}\left(-2ax\,(A\exp[-ax^2])\right) \\
&= -2a\,(A\exp[-ax^2]) + (-2ax)(-2ax)(A\exp[-ax^2]) \\
&= (4a^2x^2 - 2a)(A\exp[-ax^2]) = (4a^2x^2 - 2a)\,\psi(x).
\end{aligned}$$

- Therfore Schrödinger says

$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U\psi &= E\psi \\
-\frac{\hbar^2}{2m}(4a^2x^2 - 2a)\,\psi(x) + \frac{1}{2}kx^2\,\psi(x) &= E\,\psi(x) \\
\frac{a\hbar^2}{m} + \left(\frac{1}{2}k - \frac{2a^2\hbar^2}{m}\right)x^2 &= E
\end{aligned}$$

Harmonic oscillator II

Again,

$$E = \frac{a\hbar^2}{m} + \left(\frac{1}{2}k - \frac{2a^2\hbar^2}{m}\right)x^2$$

This must be valid for *any* x. The only way we can do that is to have $\left(\frac{1}{2}k - \frac{2a^2\hbar^2}{m}\right) = 0$ giving

$$a = \frac{\sqrt{km}}{2\hbar}$$

for the x^2 term. With the x^2 term always zeroed out, we have

$$E = \frac{a\hbar^2}{m} = \frac{\sqrt{km}\hbar^2}{2\hbar m} = \frac{1}{2}\hbar\sqrt{\frac{k}{m}}$$

after using the x^2 term solution for a. If we define $\omega \equiv \sqrt{k/m}$ as in the classical solution, we have

$$E = \frac{1}{2}\hbar\omega. \qquad \text{(Serway Eq. 6.28)}$$

Harmonic oscillator III

- Again, classically the maximum excursion from equilibrium is $x_{\text{extremum}} = \pm\sqrt{2E/k}$. Plug in our energy solution of $E = \frac{1}{2}\hbar\sqrt{\frac{k}{m}}$:

$$x_{\text{classical extremum}} = \pm\sqrt{\frac{\hbar\sqrt{\frac{k}{m}}}{k}} = \pm\sqrt{\frac{\hbar}{\sqrt{km}}}$$

In other words, the classical result confines the particle within a definite boundary. The quantum mechanical solution

$$\psi = A\exp[-\frac{\sqrt{km}}{2\hbar}x^2]$$

does not! In fact, if we plug in classical extremum we have

$$\frac{\psi(x_{\text{classical extremum}})}{\psi(x=0)} = \frac{A\exp[-\frac{\sqrt{km}}{2\hbar}\ \frac{\hbar}{\sqrt{km}}]}{A} = \exp[-1/2]$$

so the probability is down by $|\psi|^2 = \exp[-1] = 0.37$ relative to the probability of being in the center.

Harmonic oscillator IV

There are other solutions beyond

$$\psi = A \exp[-\frac{\sqrt{km}}{2\hbar} x^2].$$

If we write the Schrödinger equation as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}kx^2\psi = E\psi,$$

we can make some substitutions: $\beta \equiv \sqrt{m\omega/\hbar}$, $\xi \equiv \beta x$, $\eta(\xi) \equiv \psi(x)$, and $\epsilon \equiv 2E/(\hbar\omega)$. With these substitutions, the derivative becomes

$$\frac{d}{dx}\left(\frac{d}{dx}\psi(x)\right) = \left(\frac{d\xi}{dx}\right)^2 \frac{d}{d\xi}\left(\frac{d}{d\xi}\eta(\xi)\right) = \beta^2 \frac{d^2\eta(\xi)}{d\xi^2}$$

and the Schrödinger equation becomes

$$-\frac{d^2\eta(\xi)}{d\xi^2} + \xi^2\eta(\xi) = \epsilon\,\eta(\xi)$$

zeta: ζ, xi=ξ, eta=η, beta=β

Harmonic oscillator V

- The equation

$$-\frac{d^2\eta(\xi)}{d\xi^2} + \xi^2\eta(\xi) = \epsilon\,\eta(\xi)$$

is known in the differential equations literature as Weber's equation. The solutions that satisfy $|\psi| \to 0$ as $x \to \pm\infty$ are $\eta(\xi) = H(\xi)\exp[-\xi^2/2]$ with $H(\xi)$ being polynomials, as you will learn in PHY 306.

- The first few polynomial solutions are

$$H_0 = 1, \qquad H_1 = 2\xi, \qquad H_2 = 4\xi^2 - 2, \qquad H_3 = 8\xi^3 - 12\xi,$$

- The H_0 result is $\eta(\xi) = 1\exp[-\xi^2/2]$ which becomes

$$\psi(x) = \exp[-\frac{m\omega\,x^2}{2\hbar}] = \exp[-\frac{m\sqrt{k}\,x^2}{2\hbar\sqrt{m}}] = \exp[-\frac{\sqrt{km}\,x^2}{2\hbar}]$$

which is what we already found!

Harmonic oscillator solutions

Krane Fig. 5.11:

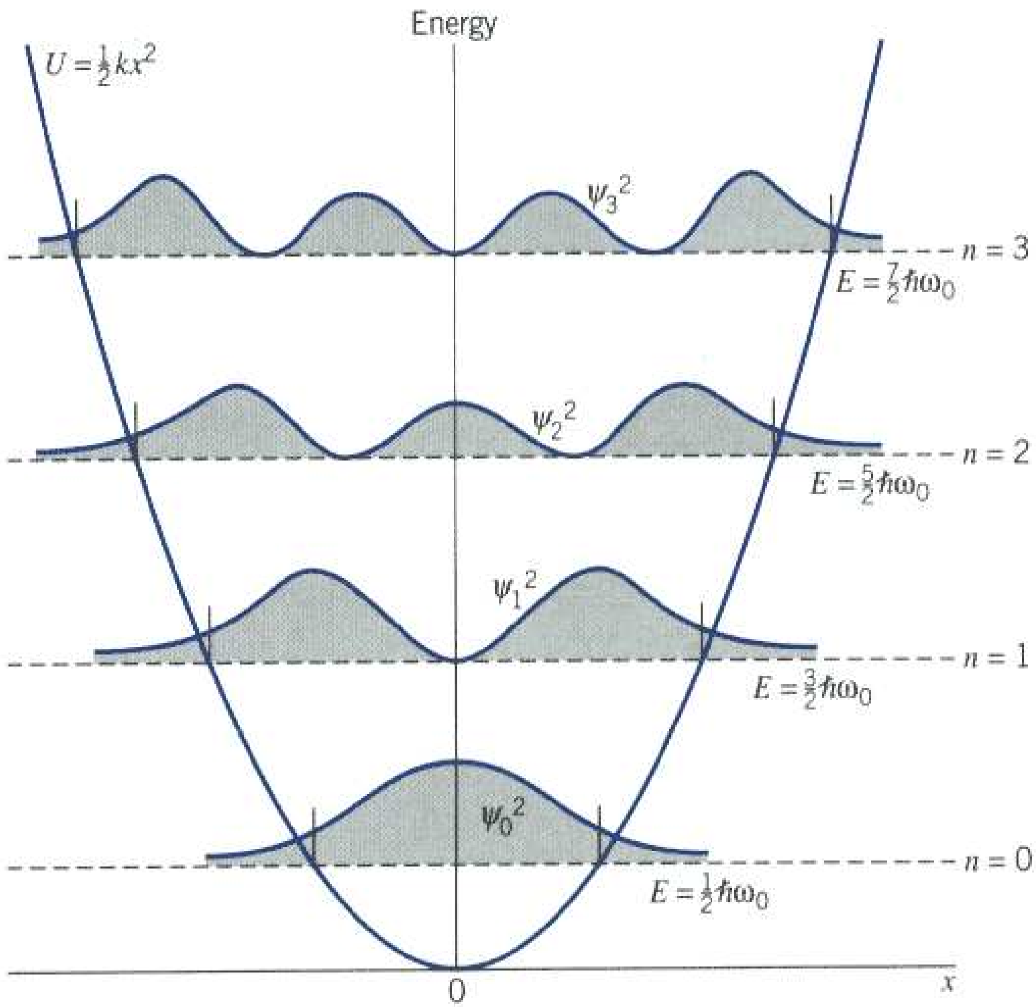


FIGURE 5.11 The lowest few energy levels and corresponding probability densities of the harmonic oscillator. The short vertical lines mark the classical turning points.

Harmonic oscillator energy solutions

- If we were to plug the various solutions of $\eta(\xi) = H(\xi)\exp[-\xi^2/2]$ back into the Schrödinger equation, we would find energy solutions of

$$E = \hbar\omega(n + \frac{1}{2}) \qquad \text{with} \qquad n = 0, 1, 2, \ldots \qquad \text{(Serway 6.29)}$$

- Remember that the harmonic oscillator problem is a good first approximation to *any* ground state problem.
- What does this say about motion at zero temperature?

Motion at zero temperature

- Zero temperature does *not* mean that all molecular motion has ceased!
- It just means that all atoms are in their ground state. But if the electric field of the crystal lattice defines an equilibrium position for each atom, then there is (to first approximation) a harmonic oscillator potential associated with this restoring force!
- The lowest energy state of a harmonic oscillator is not zero, but $E = \hbar\omega/2$!