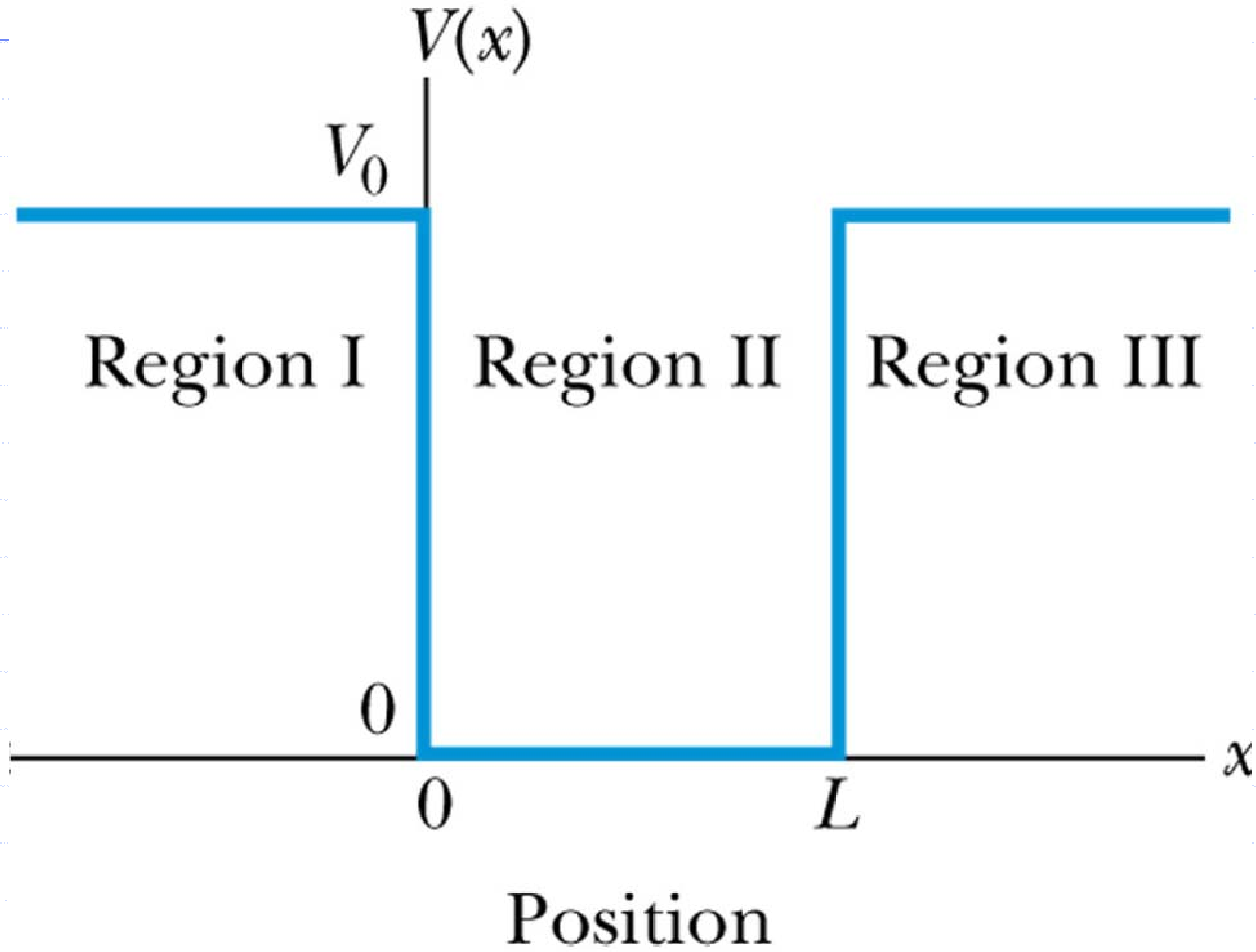
Finite Square Well



Finite Square Well

- In regions I and III

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2}+V\psi_I=E\psi_I$$

$$\frac{d^2\psi_I}{dx^2}-k_I^2\psi_I=0 \text{ where } k_I=k_{III}=\frac{\sqrt{2m(V_0-E)}}{\hbar}$$

- In region II

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2}=E\psi_{II}$$

$$\frac{d^2\psi_{II}}{dx^2}+k_{II}^2\psi_{II}=0 \text{ where } k_{II}=k=\frac{\sqrt{2mE}}{\hbar}$$

Finite Square Well

- Solutions in region I and III

$$Ae^{k_I x} + Be^{-k_I x} \to Ae^{k_I x}$$

$$Ee^{k_{III} x} + Fe^{-k_{III} x} \to Fe^{-k_{III} x}$$

- Solutions in region II

$$Ce^{ikx} + De^{-ikx} \text{ or}$$

$$C\sin kx + D\cos kx$$

Finite Square Well

- The next step is to match boundary conditions inside and out for both ψ and dψ/dx
  - At x=0

$$A = D$$

$$k_I A = kC$$

  - At x=L

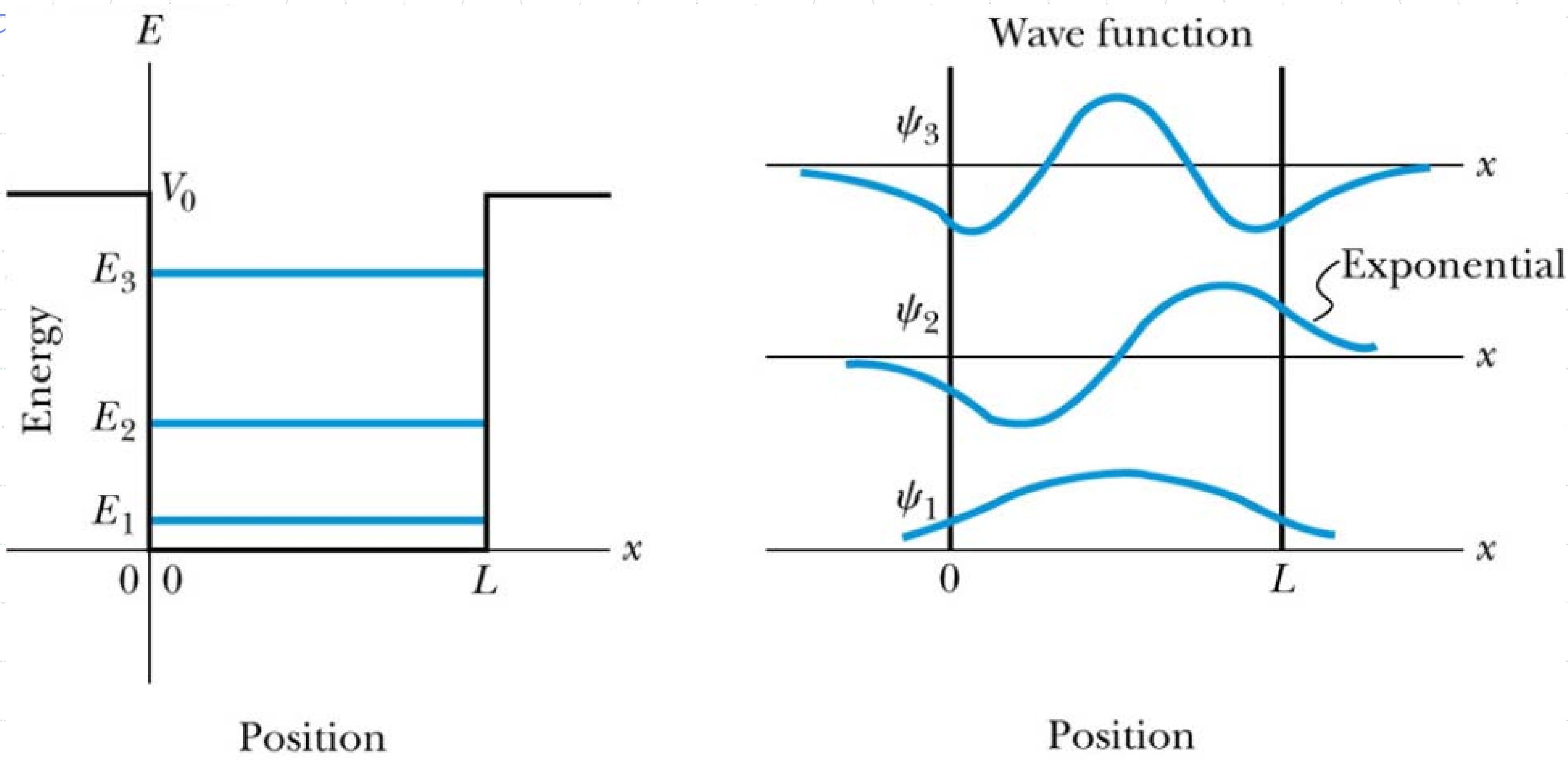
$$Fe^{-k_I L} = C\sin kL + D\cos kL$$

$$-k_I Fe^{-k_I L} = Ck\cos kL - Dk\sin kL$$

Finite Square Well

- Unfortunately we will not go much further
  - As with the infinite well, application of the boundary conditions leads to energy quantization
  - Although there are 4 equations for 4 unknowns the energy levels must be found numerically or graphically
  - As with the infinite well, the n'th eigenfunction will have n-1 nodes

Finite Square Well



Harmonic Oscillator

- The (simple) harmonic oscillator is one of the most important physical systems in physics
  - Any physical system in the neighborhood of a stable equilibrium position can be approximated by a harmonic oscillator (in the limit of small oscillations)
  - Vibrations of atoms in a molecule, oscillations of atoms in a crystal, …

Harmonic Oscillator

- Review from classical physics
  - Mass on a spring

$$F_x = -kx \quad \text{(Hooke's law)}$$

$$V = -W = -\int F dx = \frac{1}{2}kx^2$$

$$m\frac{d^2x}{dt^2} = -kx \text{ has solution } x = A\cos(\omega t - \phi) \text{ where } \omega = \sqrt{\frac{k}{m}}$$

$$E = T + V = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

$$= \frac{m^2A^2\omega^2}{2m}\sin^2(\omega t - \phi) + \frac{1}{2}kA^2\cos^2(\omega t - \phi)$$

$$= \frac{1}{2}m\omega^2A^2$$

Harmonic Oscillator

- Consider the neighborhood of the minimum of an arbitrary potential

Expand $V(x)$ in a Taylor's series about the minimum at $x = x_0$

$$V(x) = a + b(x - x_0) + c(x - x_0)^2 + \ldots$$

where

$$a = V(x_0) \equiv 0$$

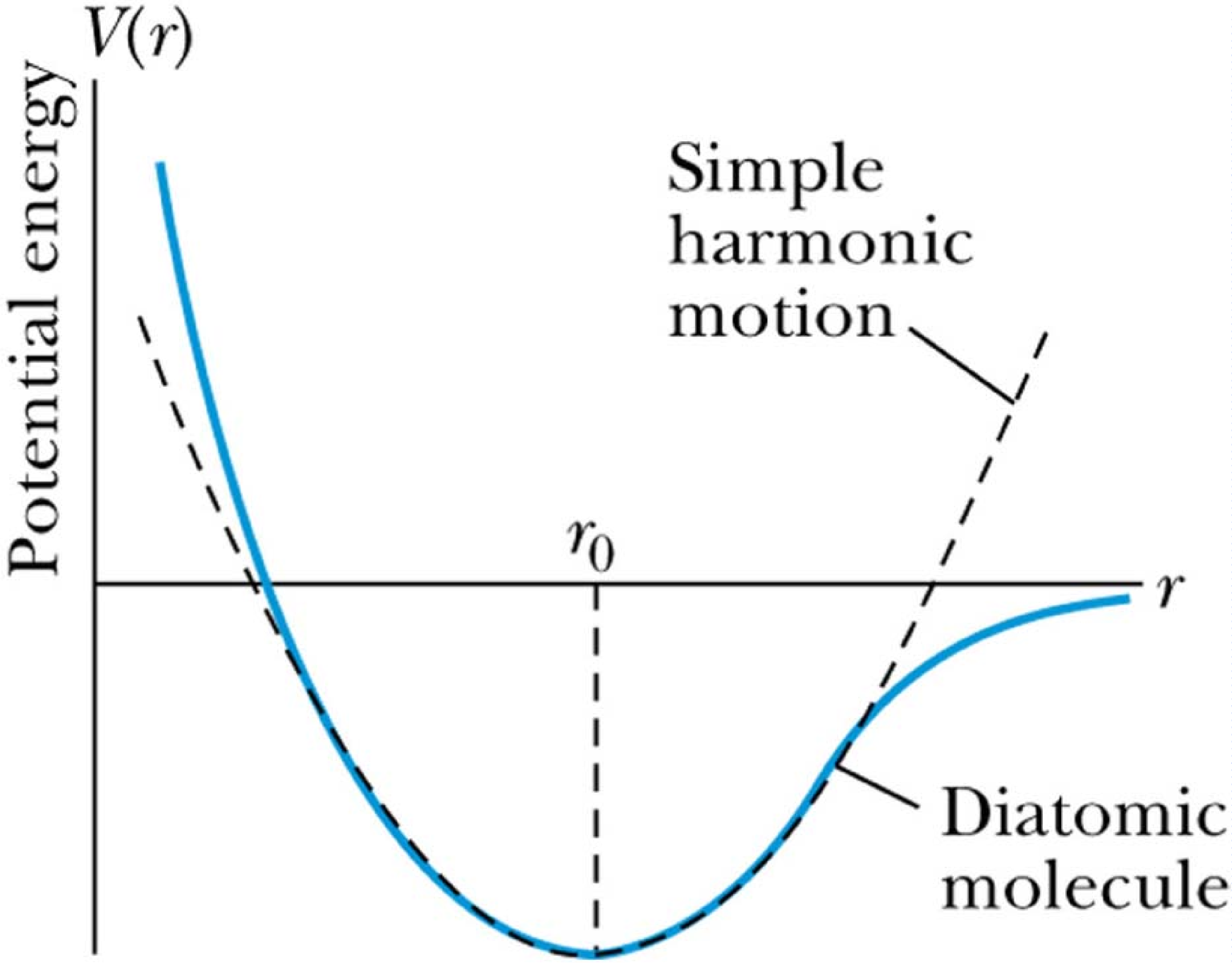
$$b = \frac{dV}{dx}\Big|_{x=x_0} = 0$$

$$c = \frac{1}{2}\left(\frac{d^2V}{dx^2}\right)\Big|_{x=x_0}$$

then

$$V(x) = \frac{1}{2}c(x - x_0)^2$$

Harmonic Oscillator



Harmonic Oscillator

- We want to solve

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

- Unfortunately this is not trivial. And an "easier" method (using ladder operators) is beyond the scope of the class.
- We will obtain the asymptotic solution however

Harmonic Oscillator

- We start with the time independent Schrodinger equation

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

$$\text{let } \omega = \sqrt{\frac{k}{m}}, \varepsilon = \frac{2E}{\hbar\omega}, y = \sqrt{\frac{m\omega}{\hbar}}x$$

$$\text{then } \frac{d^2\psi}{dy^2}+\left(\varepsilon - y^2\right)\psi = 0$$

Harmonic Oscillator

- To find the asymptotic solution, we note that $y^2 \to \infty$ and hence ε can be neglected

$$\frac{d^2\psi_\infty}{dy^2} - y^2\psi_\infty = 0$$

Multiplying by $2\dfrac{d\psi_\infty}{dy}$

$$\frac{d}{dy}\left(\frac{d\psi_\infty}{dy}\right)^2 - y^2\frac{d\psi_\infty^2}{dy} = 0$$

$$\frac{d}{dy}\left[\left(\frac{d\psi_\infty}{dy}\right)^2 - y^2\psi_\infty^2\right] = -2y\psi_\infty^2$$

We can neglect the term on the right side thus

$$\frac{d\psi_\infty}{dy} = \left(C + y^2\psi_\infty^2\right)^{1/2}$$

Harmonic Oscillator

- Since the asymptotic solution and its derivative must vanish at infinity (why?) it must be that C=0

$$\frac{d\psi_\infty}{dy} = \pm y\psi_\infty$$

The solution at infinity is thus

$$\psi_\infty(y) = e^{-\frac{y^2}{2}}$$

- And that was easy compared to the full solution

Harmonic Oscillator

- The (unnormalized) solution for all y is

$$\psi(y) = H_n(y)e^{-\frac{y^2}{2}}$$

where $H_n(y)$ are the Hermite polynomials

The first few are

$$H_0(y) = 1$$

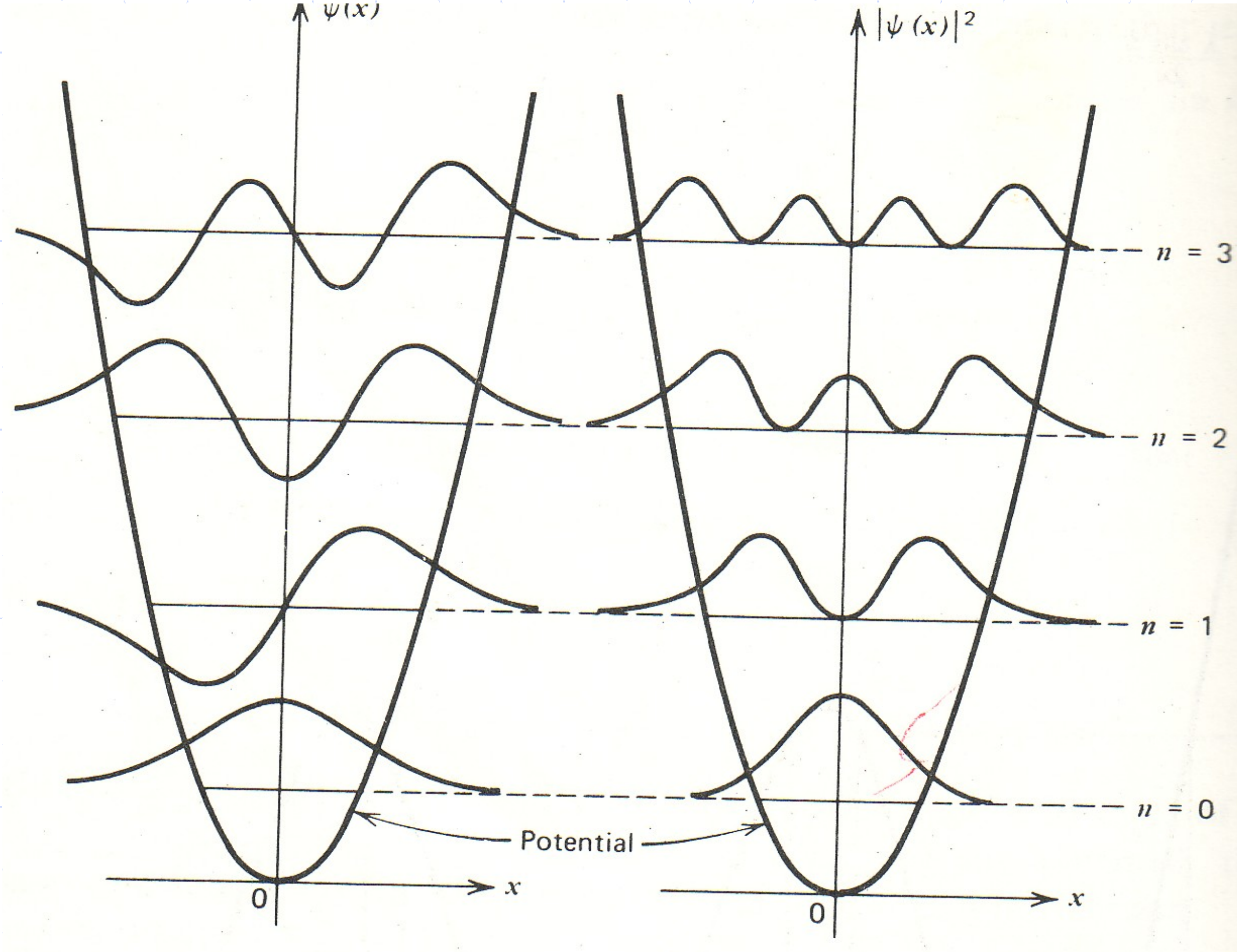
$$H_1(y) = 2y$$

$$H_2(y) = -2 + 4y^2$$

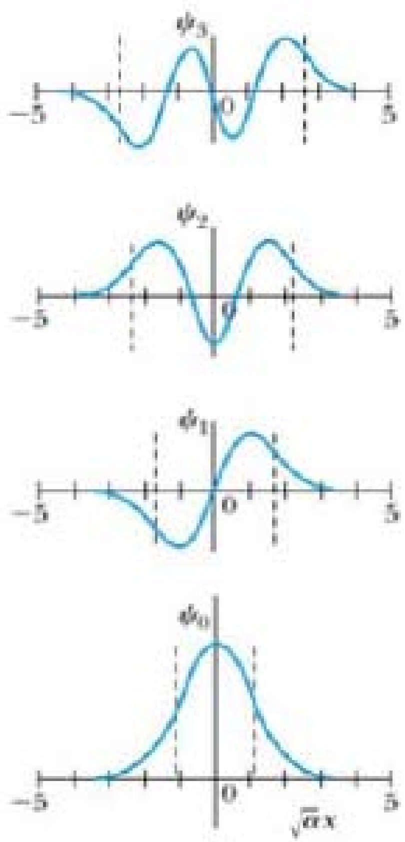
Harmonic Oscillator

- The normalized wave functions = ψ(x) are given in Thornton and Rex (p223) and are not so illuminating
- You should have be able to sketch the first few wave functions based on your experience with the infinite and finite wells and your knowledge of ψ in general

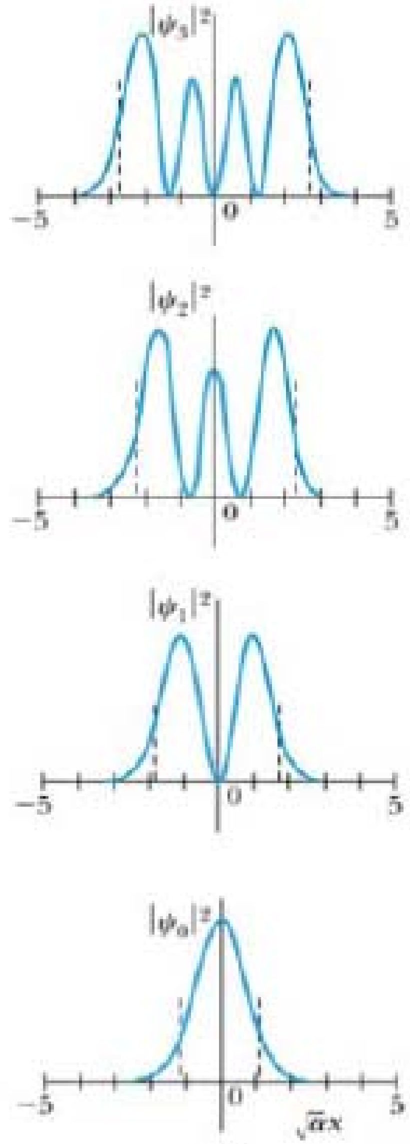
Harmonic Oscillator



Harmonic Oscillator



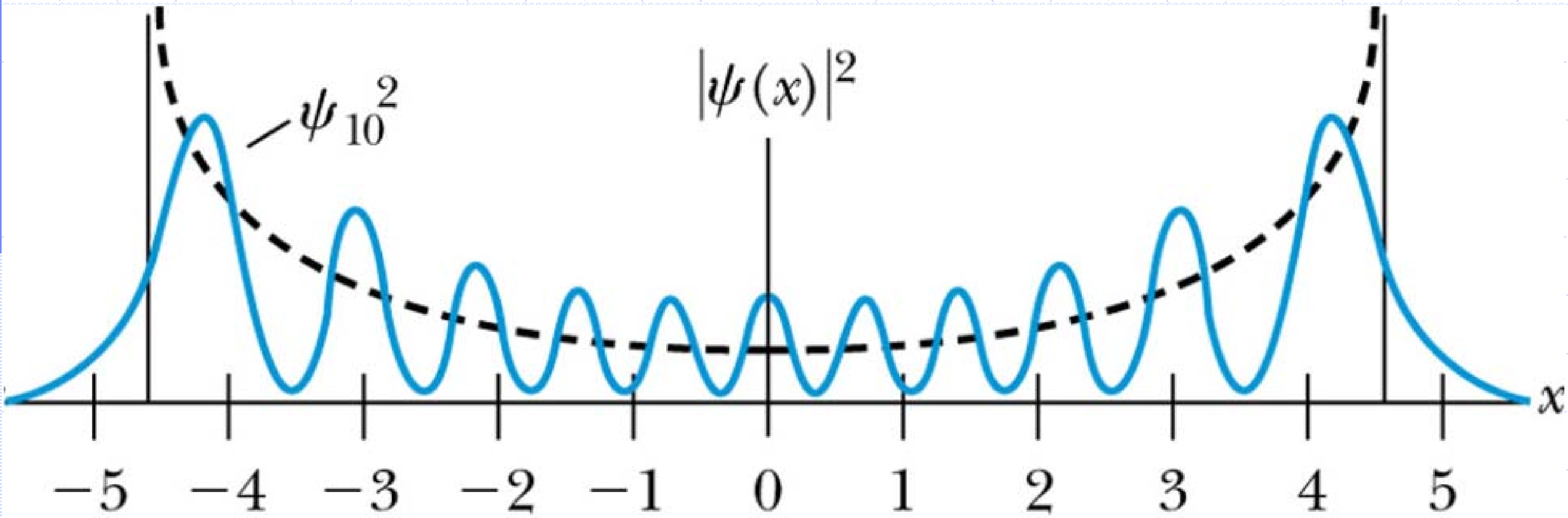
(b)



(c)

Harmonic Oscillator

- What do you expect as n becomes large?



Harmonic Oscillator

- In solving the harmonic oscillator problem for all y, the requirement that the wave function vanish at infinity leads to quantized energy
- The energy levels of the harmonic oscillator are

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

  - The zero point energy is $E_0 = h\omega/2$
  - The energy levels are equally spaced
  - This is similar to the Planck relation for radiation
    - Recall we said that standing EM waves in the blackbody cavity arose from harmonic oscillators in the walls

Harmonic Oscillator

Problem

- Use the Heisenberg uncertainty principle to estimate the ground state energy of the harmonic oscillator

Harmonic Oscillator

- **Problem**
  - Let $\psi(x,0)=A\{\psi_0(x) + \psi_1(x)\}$ for the harmonic oscillator
    - Normalize ψ
    - Find $|\psi(x,t)|^2$

Harmonic Oscillator

Problem

- Consider a potential that has
  - $V(x)=\infty$ for $x < 0$
  - $V(x)=1/2kx^2$ for $x > 0$
- What are the possible energy levels?

Harmonic Oscillator

- Einstein used the quantum solution of the harmonic oscillator to solve the temperature dependence of the specific heats of solids
- Classically

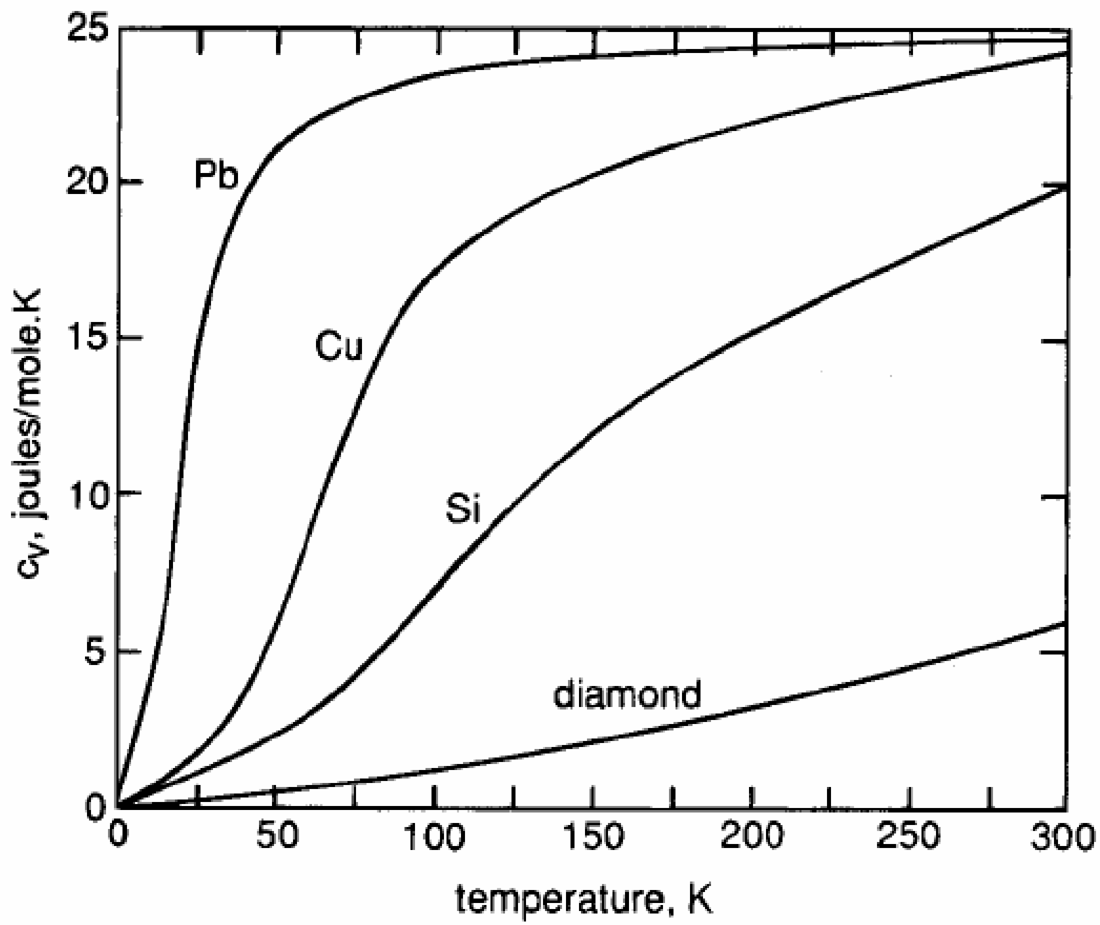
$$E = \frac{f}{2} N k_B T = \frac{f}{2} nRT$$

$$C_V = \frac{1}{n}\frac{dE}{dT} = \frac{f}{2} R$$

$$\text{For solids } C_V = 3R \approx 25 \text{ J/molK}$$

This is called the DuLong - Petit law

Harmonic Oscillator



Harmonic Oscillator

- If atoms are modeled by quantum harmonic oscillators, explain why specific heats drop as $T \rightarrow 0$