What is this equation?

E =Tot. energy, V=potential energy

$$\frac{\frac{\partial^2 \Psi}{\partial x^2}}{\Psi} = \frac{2m_e}{\hbar^2}(V - E)$$

what is this equation?

$$-\frac{\hbar^2}{2m_e}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi = E\Psi$$

Both are exactly the
1 D Schroedinger Eq.

The FIRST way talks to you:
What does it say?
It says: The ***fractional curvature*** is proportional to V – E = **-T**

Rewrite in "**Atomic Units**"

$$\text{In atomic units and } \frac{\partial^2 \Psi}{\partial x^2} \equiv \nabla^2 \Psi \equiv \Psi''$$

$$\frac{\Psi''}{\Psi} = 2(V - E)$$

Atomic Units

Fundamental

$h/2\pi$ = **hbar = 1** = $1.054571726(47)\times10^{-34}$ J·s

mass = mass of electron = **m_e = 1** = $9.10938291(40)\times10^{-31}$ kg

charge = charge of proton= **e = 1** =$1.602176565(35)\times10^{-19}$ C

electric constant^{-1} **k =1** = $(4\pi\varepsilon_0)^{-1}$ = $8.9875517873681\times10^{9}$ $kg\cdot m^3\cdot s^{-2}\cdot C^{-2}$

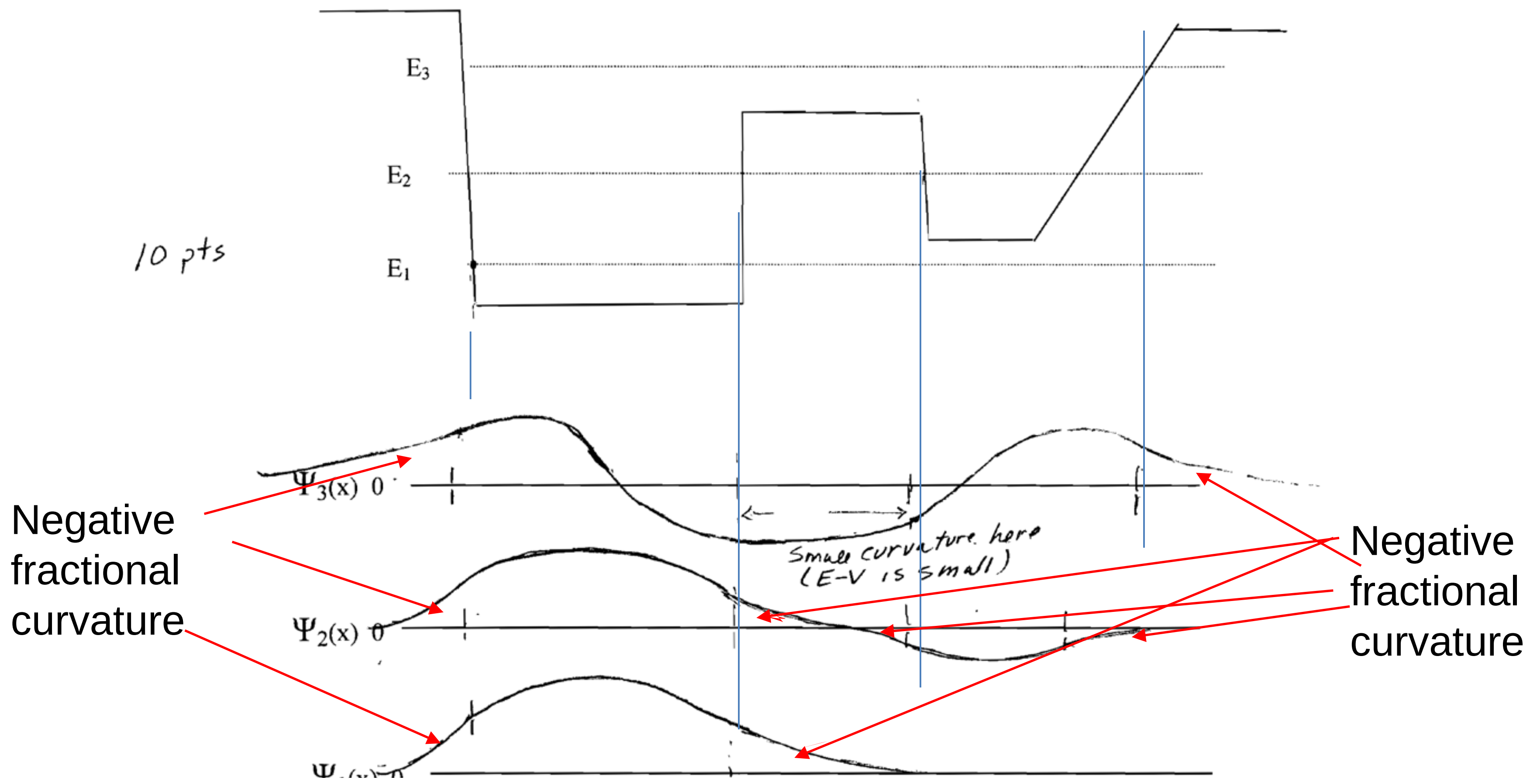
Derived and often used:

length = bohr radius = **a_0 = 1** = $5.2917721092(17)\times10^{-11}$ m

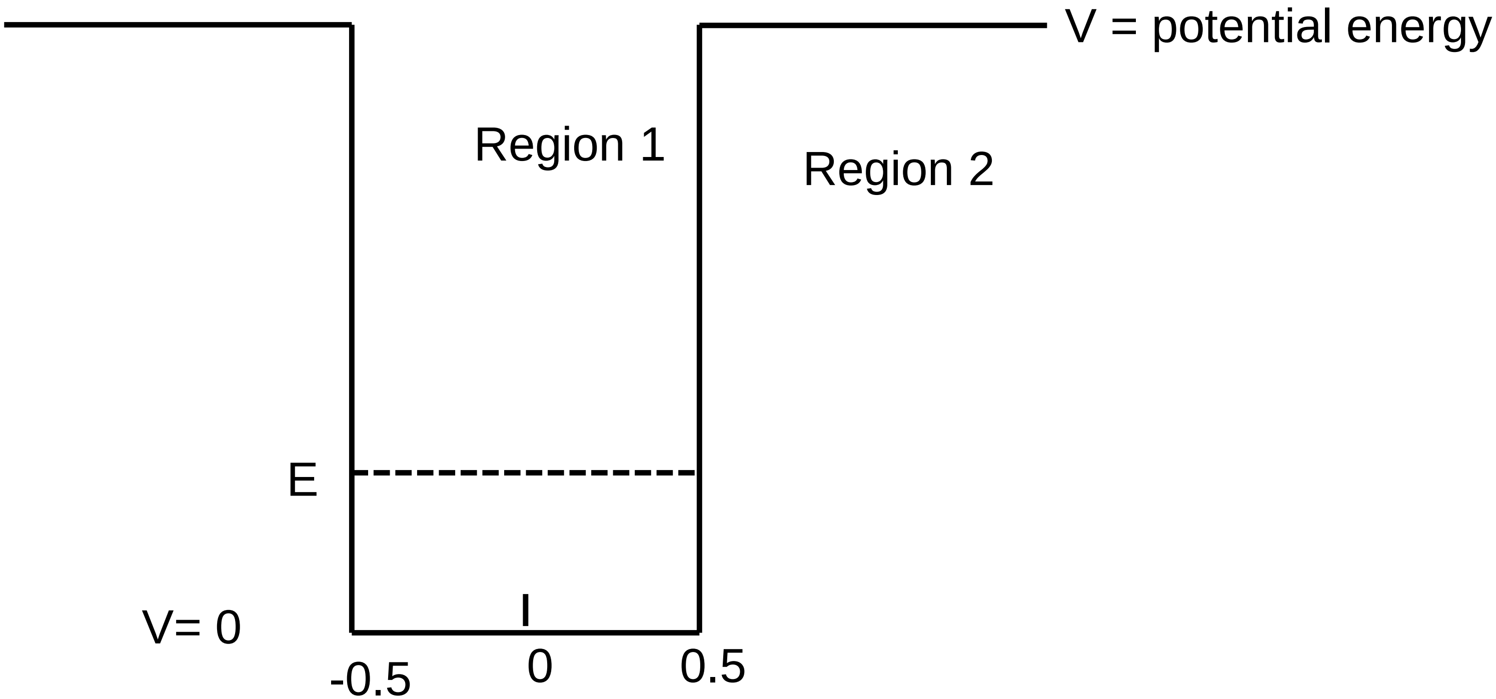
energy = e^2/a_0 = **1 hartree** = 1.602176565E-19^2/ 5.2917721092E−11
= 4.35974E-18 J/molecule =2.625499E+03 kJ/mol = 627.509 $kcal\cdot mol^{-1}$

Typical Exam problem in this course:

1. For the one-dimensional potential for a certain particle below, draw qualitatively the 3 lowest energy well-behaved energy eigenfunctions separately on the abscissas provided below. **For full credit, the sign of the curvature must be correct at all points**, as prescribed by the respective energy eigenvalues of these states shown by the dotted lines. In addition, other general aspects associated with the lowest 3 energy eigenfunctions of any system should be apparent in your drawing.



electron in a finite square well = 1 bohr radius



$$-\frac{\hbar^2}{2m_e}\Psi''+V\Psi=E\Psi$$

$$-\frac{1}{2}\Psi''+V\Psi=E\Psi \text{ in atomic units}$$

$$-\frac{1}{2}\frac{\Psi''}{\Psi}=E-V=T=\text{Kinetic Energy}$$

What is the Kinetic Energy sign in region 2 where V > E

Obviously negative KE wh

This is called tunneling

region 1: V(x)= 0 so V – E = -E

$$\Psi_1'' = -2E\Psi =$$

$$\Psi_1(x) = ae^{-ik_1 x} + be^{ik_1 x}$$

$$\text{we choose } \Psi_1(x) = \cos(k_1 x) \text{ or } \sin(k_1 x)$$

$$\mathrm{k}_1 = \sqrt{2E}$$

region 2: V(x)= V and V> E

$$\Psi_2'' = 2(V-E)\Psi, \ \mathrm{V} > \mathrm{E}$$

$$\Psi_2(x) = ce^{-k_2(x-0.5)} + de^{k_2(x-0.5)}$$

$$\mathrm{k}_2 = \sqrt{2(V-E})$$

$$\Psi_2(x) = ce^{-\sqrt{2(V-E)}(x-0.5)} + de^{\sqrt{2(V-E)}(x-0.5)}$$

Boundary Conditions for even case

1. Equal amplitudes at x =0.5 :

$$\cos(k_1 0.5) = ce^{-k_2(0.5-0.5)} + de^{k_2(0.5-0.5)}$$

$$= \cos(k_1 0.5) = c + d \qquad (Eq.1)$$

k_2 times Eq. 1: $$k_2 \cos(k_1 0.5) = k_2 c + k_2 d$$

2. Equal slopes at x =0.5 :

$$-k_1 \sin(k_1 0.5) = -k_2 ce^{-k_2(0.5-0.5)} + k_2 de^{k_2(0.5-0.5)}$$

$$-k_1 \sin(k_1 0.5) = -k_2 c + k_2 d \quad (Eq.2)$$

$$\mathrm{k}_1 = \sqrt{(2E)} \qquad \mathrm{k}_2 = \sqrt{2(V-E)}$$

2 equations and 2 unknowns, c and d

Subtract Eq. 2 from k_2 times Eq. 1 , solve for c

$$c = 1/2\left[\cos(k_1 0.5) + \frac{k_1}{k_2}\sin(k_1 0.5\right]$$

Add Eq. 2 to k_2 times Eq. 1 , solve for d

$$d = 1/2\left[\cos(k_1 0.5) - \frac{k_1}{k_2}\sin(k_1 0.5\right]$$

Boundary Conditions for odd case (sin)

1. Equal amplitudes at x =0.5 : $\sin(k_1 0.5) = ae^{-k_2(0.5-0.5)} \quad + \quad be^{k_2(0.5-0.5)}$

$$= \sin(k_1 0.5) = a \quad + \quad b \qquad (Eq.1)$$

$$k_2 \sin(k_1 0.5) = k_2 a \quad + \quad k_2 b$$ (k_2 times Eq. 1)

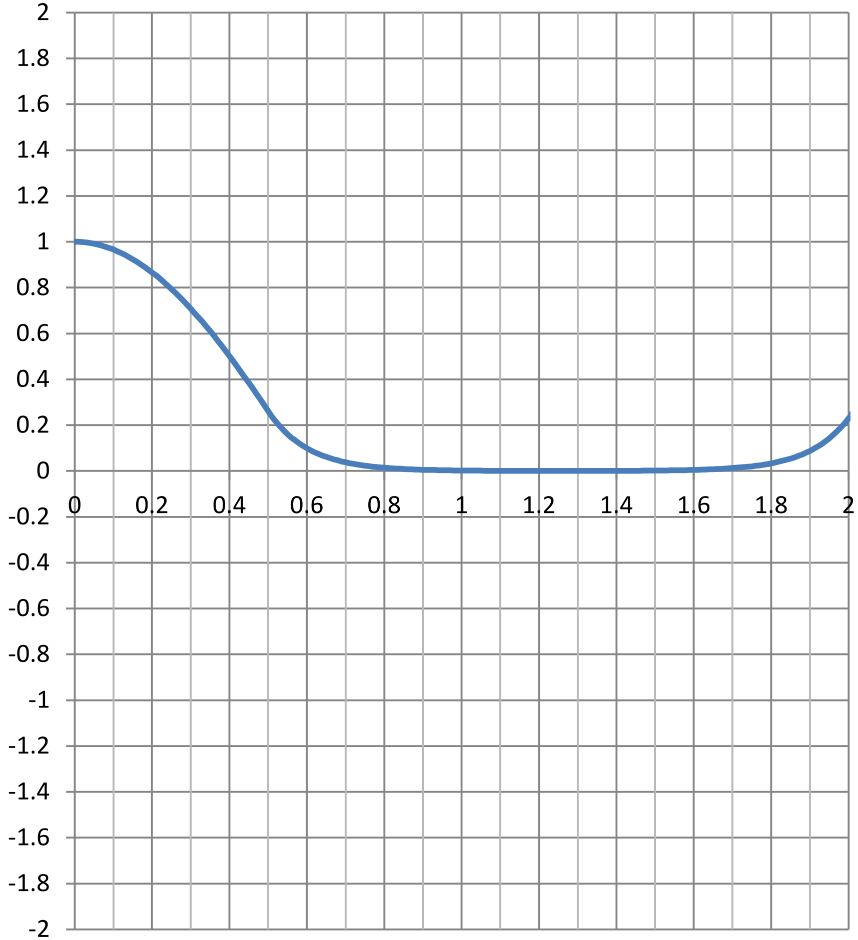
2. Equal slopes at x =0.5 :

2 equations and 2 unknowns, a and b $\quad \mathrm{k}_1 = \sqrt{(2E)} \qquad \mathrm{k}_2 = \sqrt{2(V-E)}$

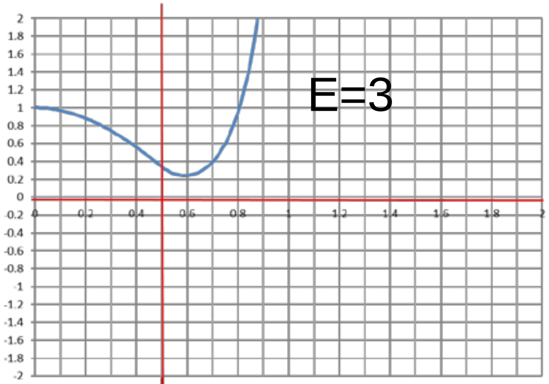
Subtract Eq. 2 from k_2 times Eq. 1 , solve for a $\quad a = 1/2\left[\cos(k_1 0.5) + \frac{k_1}{k_2}\sin(k_1 0.5\right]$

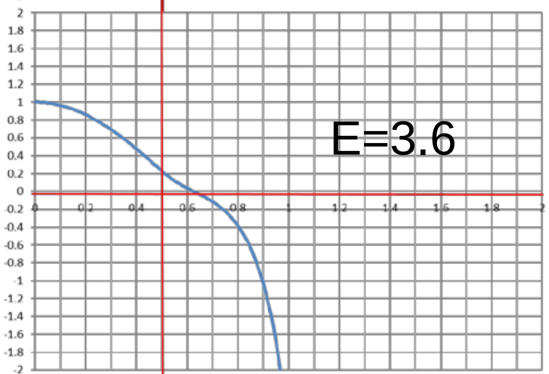
Add Eq. 2 to k_2 times Eq. 1 , solve for b $\quad b = 1/2\left[\cos(k_1 0.5) - \frac{k_1}{k_2}\sin(k_1 0.5\right]$

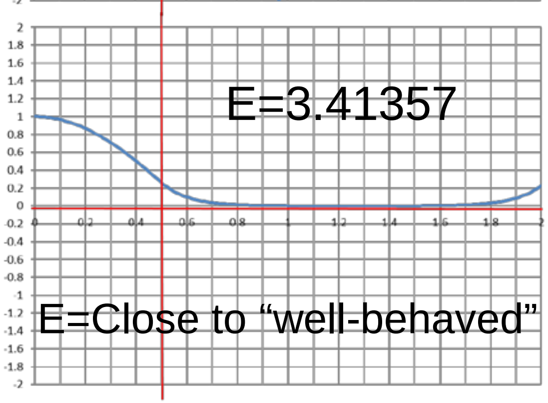
Numerical Solution for ground state using excel spreadsheet, which you can download from our website.

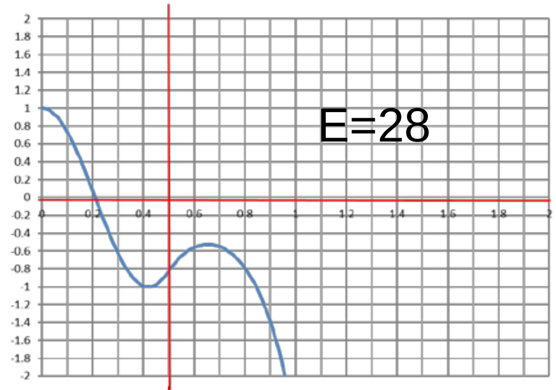


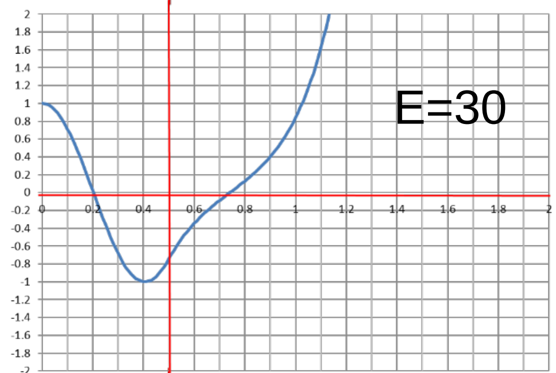
All have V=50

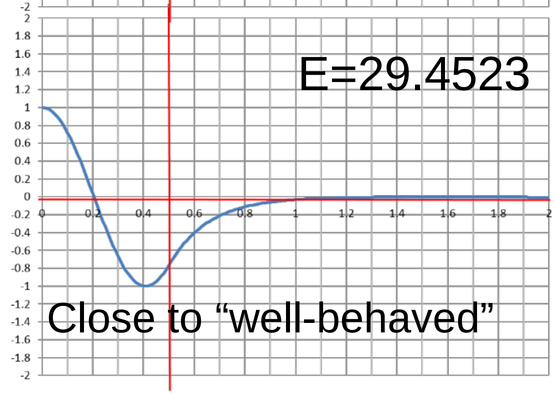












All are solutions,
and are eigenstates,
but only certain energies
give acceptable
wavefunctions.

Figures created with an
excel spreadsheet.

2.4 Particle in a Rectangular Well

Consider a particle in a one-dimensional box with walls of finite height (**Fig. 2.5a**). The potential-energy function is $V = V_0$ for $x < 0$, $V = 0$ for $0 \le x \le l$, and $V = V_0$ for $x > l$. There are two cases to examine, depending on whether the particle's energy E is less than or greater than V_0.

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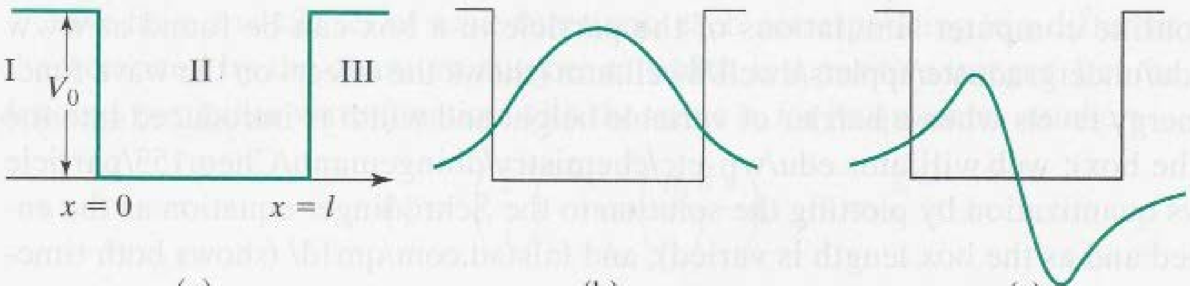

(a) (b) (c)

Comments? Is this curve correct in all details?

HARMONIC OSCILLATOR REVIEW

According to (4.22), the classical harmonic oscillator vibrates back and forth between $x = A$ and $x = -A$. These two points are the turning points for the motion. The particle has zero speed at these points, and the speed increases to a maximum at $x = 0$, where the potential energy is zero and the energy is all kinetic energy. The classical harmonic oscillator spends more time in each of the regions near $x = A$ and $x = -A$ (where it is moving the slowest) than it does in the region near $x = 0$. Problem 4.18 works out the probability density for finding the classical harmonic oscillator at various locations. (Interestingly, this probability density becomes infinite at the turning points.)

Quantum-Mechanical Treatment

The harmonic-oscillator Hamiltonian operator is [Eqs. (3.27) and (4.27)]

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + 2\pi^2\nu^2 mx^2 = -\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2} - \alpha^2x^2\right) \quad (4.30)$$

where, to save time in writing, α was defined as

$$\alpha \equiv 2\pi\nu m/\hbar \quad (4.31)$$

The Schrödinger equation $\hat{H}\psi = E\psi$ reads, after multiplication by $2m/\hbar^2$,

$$\frac{d^2\psi}{dx^2} + (2mE\hbar^{-2} - \alpha^2x^2)\psi = 0 \quad (4.32)$$

We might now attempt a power-series solution of (4.32). If we do now try a power series for ψ of the form (4.4), we will find that it leads to a three-term recursion relation, which is harder to deal with than a two-term recursion relation like Eq. (4.14). We therefore modify the form of (4.32) so as to get a two-term recursion relation when we try a series solution. A substitution that will achieve this purpose is (see Prob. 4.22) $f(x) \equiv e^{\alpha x^2/2}\psi(x)$. Thus

$$\psi = e^{-\alpha x^2/2}f(x) \quad (4.33)$$

This equation is simply the definition of a new function $f(x)$ that replaces $\psi(x)$ as the unknown function to be solved for. (We can make any substitution we please in a differential equation.) Differentiating (4.33) twice, we have

$$\psi'' = e^{-\alpha x^2/2}(f'' - 2\alpha xf' - \alpha f + \alpha^2x^2f) \quad (4.34)$$

Substituting (4.33) and (4.34) into (4.32), we find

$$f''(x) - 2\alpha xf'(x) + (2mE\hbar^{-2} - \alpha)f(x) = 0 \quad (4.35)$$

Now we try a series solution for $f(x)$:

$$f(x) = \sum_{n=0}^{\infty} c_n x^n \quad (4.36)$$

Assuming the validity of term-by-term differentiation of (4.36), we get

$$f'(x) = \sum_{n=1}^{\infty} nc_n x^{n-1} = \sum_{n=0}^{\infty} nc_n x^{n-1} \quad (4.37)$$

[The first term in the second sum in (4.37) is zero.] Also,

$$f''(x) = \sum_{n=2}^{\infty} n(n-1)c_n x^{n-2} = \sum_{j=0}^{\infty}(j+2)(j+1)c_{j+2}x^j = \sum_{n=0}^{\infty}(n+2)(n+1)c_{n+2}x^n$$

Quantum-Mechanical Treatment

The harmonic-oscillator Hamiltonian operator is [Eqs. (3.27) and (4.27)]

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + 2\pi^2\nu^2 m x^2 = -\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2} - \alpha^2 x^2\right) \quad (4.30)$$

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$$\psi = e^{-\alpha x^2/2} f(x) \quad (4.33)$$

More obvious from this equation.

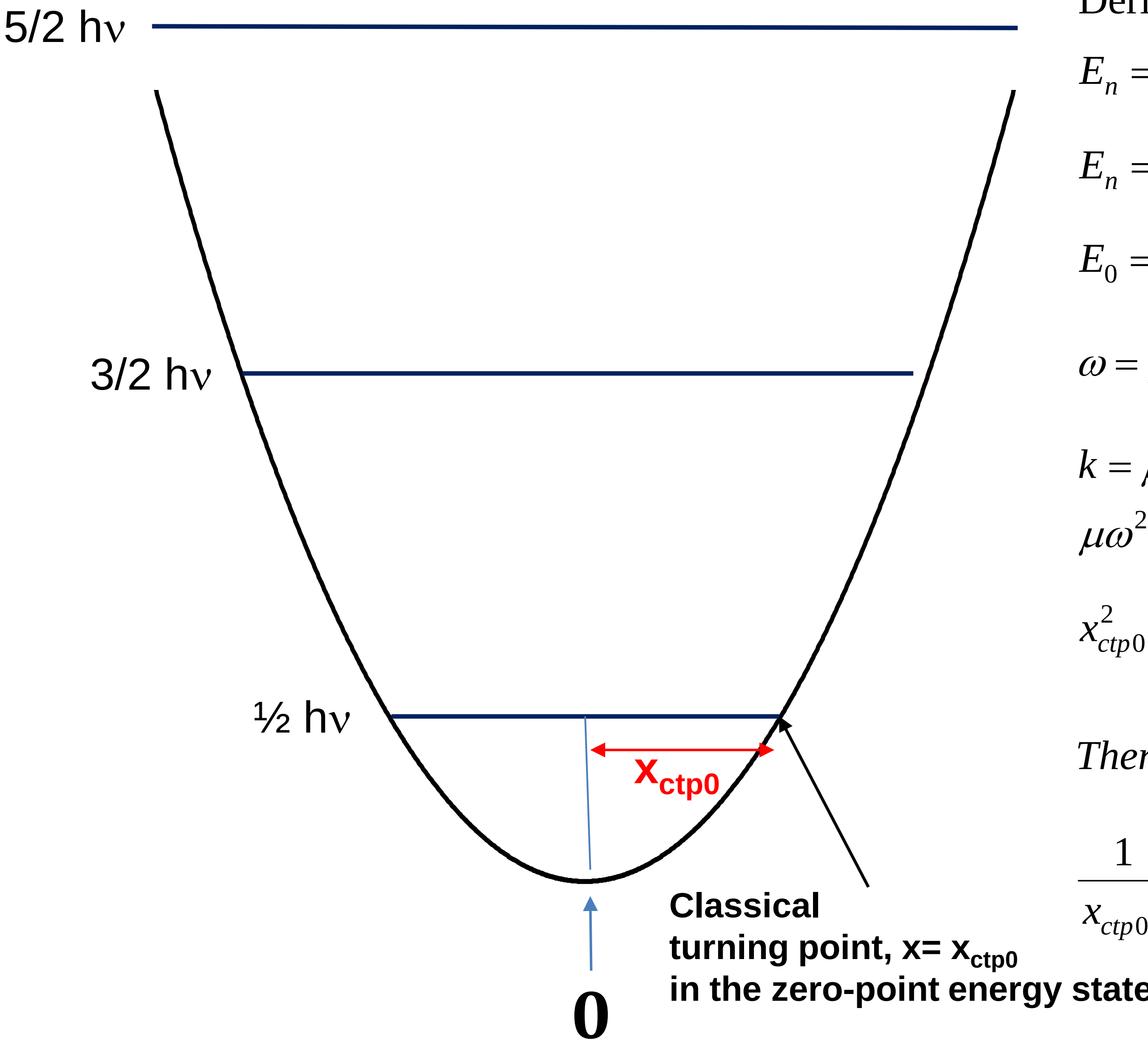
What are the units of α ?

Units of α = **length^{-2}**

Next, show that $\alpha^{-1/2}$ is the "Bohr radius of the harmonic oscillator"

Levine:

$$\alpha = \frac{\omega\mu}{\hbar}$$



Derivation:

$$E_n = (n + \tfrac{1}{2})h\nu$$

$$E_n = (n + \tfrac{1}{2})\frac{h}{2\pi}\ \ 2\pi\nu = (n + \tfrac{1}{2})\hbar\omega$$

$$E_0 = \tfrac{1}{2}\hbar\omega = \tfrac{1}{2}kx_{ctp0}^2 = \tfrac{1}{2}\mu\omega^2 x_{xtp}^{2}{}^{2}$$

$$\omega = \sqrt{\frac{k}{\mu}}$$

$$k = \mu\omega^2$$

$$\mu\omega^2 x_{ctp0}^2 = \hbar\omega$$

$$x_{ctp0}^2 = \frac{\hbar\omega}{\mu\omega^2} = \frac{\hbar}{\mu\omega}$$

$$Therefore: \quad x_{ctp0} = \sqrt{\frac{\hbar}{\mu\omega}}$$

$$\frac{1}{x_{ctp0}{}^2} = \frac{\mu\omega}{\hbar} = \alpha$$