Applications of QM (contd.):2D and finite box, HO

Note Title 21-10-2009

Recap

Background: Blackbody radiation

Postulates: Wavefunction, operators, measurement, time development

Applications: Particle in a 1D box, tunneling

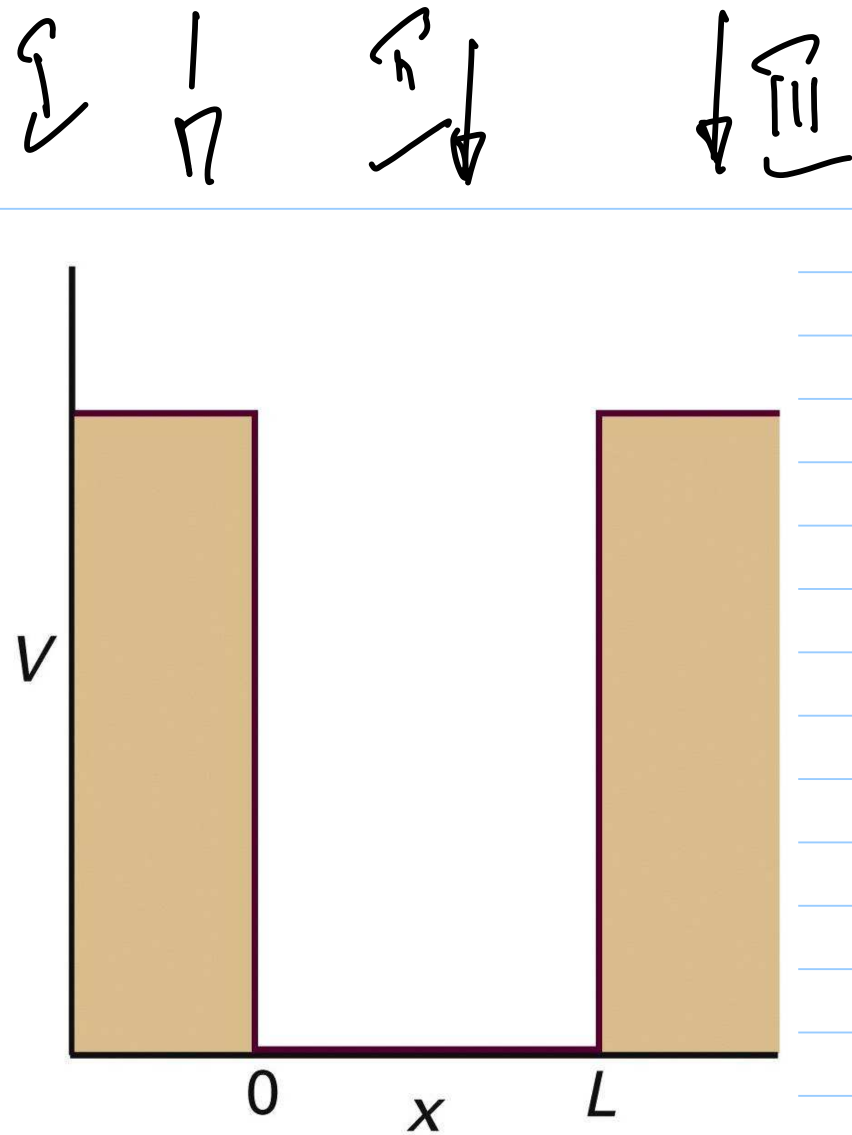


Figure 9-14
Atkins Physical Chemistry, Eighth Edition

Regions I & II

S.E

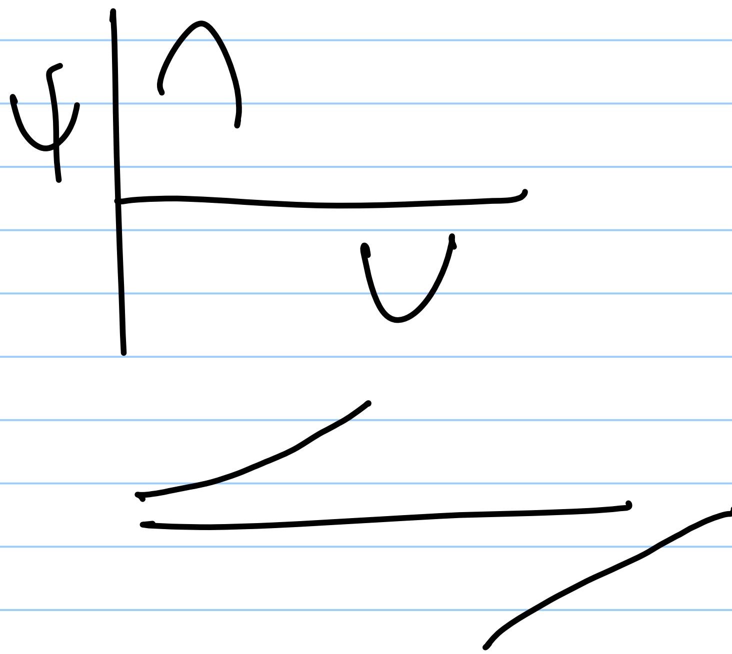
$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V\right)\psi=E\psi$$

II

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

Inside the well:

Solutions - oscillatory



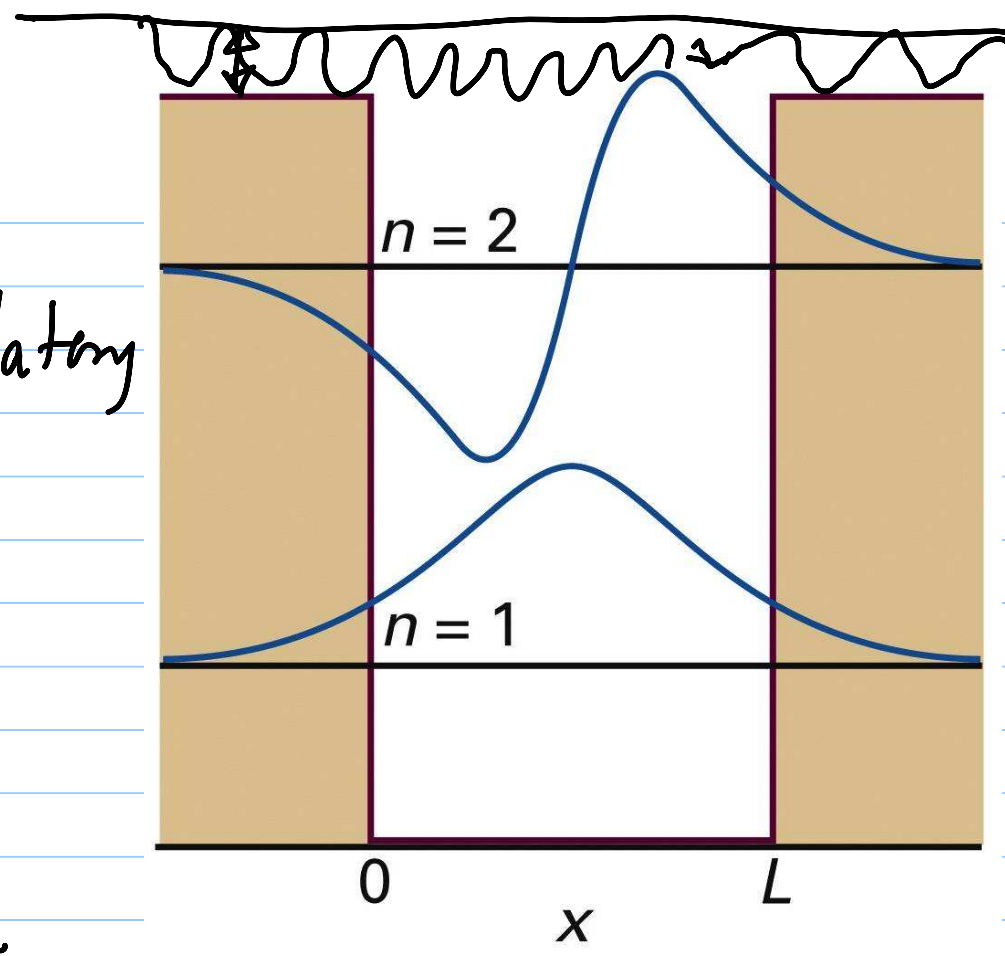


Figure 9-15
Atkins Physical Chemistry, Eighth Edition

Schrödinger equation

$V = 0$

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

$\psi(x, y)$

Separation of Variables

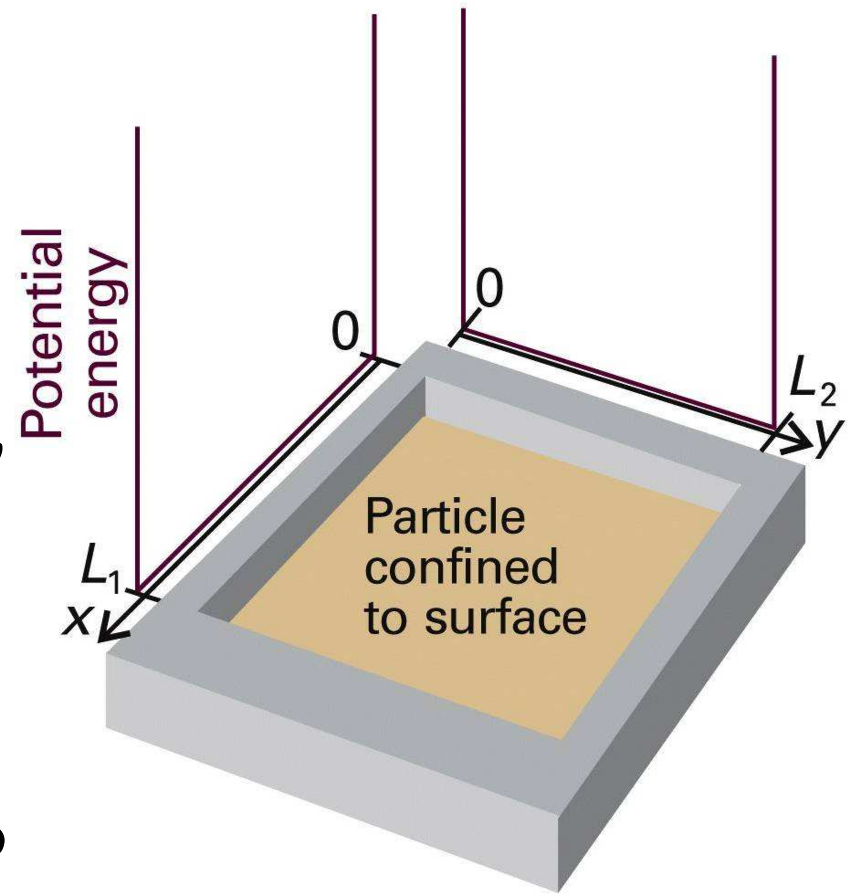


Figure 9-6
Atkins Physical Chemistry, Eighth Edition

$$\hat{H} = \hat{H}_x + \hat{H}_y \qquad kxy$$

$$\psi(x, y) = f(x)\, g(y)$$

$$H = H_1 + H_2 + \cdots H_n$$

$$\psi = \psi_1 \psi_2 \psi_3 \cdots \psi_n$$

$$E = E_x + E_y$$

$$E = \frac{h^2}{8ma^2}\left(n_x^2 + n_y^2\right)$$

$$n_x = 1, 2, \ldots$$

$$n_y = 1, 2, \ldots$$

$$\psi = \frac{2}{a} \underline{\sin\left(\frac{n_x \pi x}{a}\right)} \sin\left(\frac{n_y \pi y}{a}\right)$$

$n_x = 1, n_y = 1$ $\qquad$ $n_x = 2, n_y = 1$ $\qquad$ $n_x = 1, n_y = 2$ $\qquad$ $n_x = 2, n_y = 2$

$\frac{2}{a} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi y}{a}\right)$

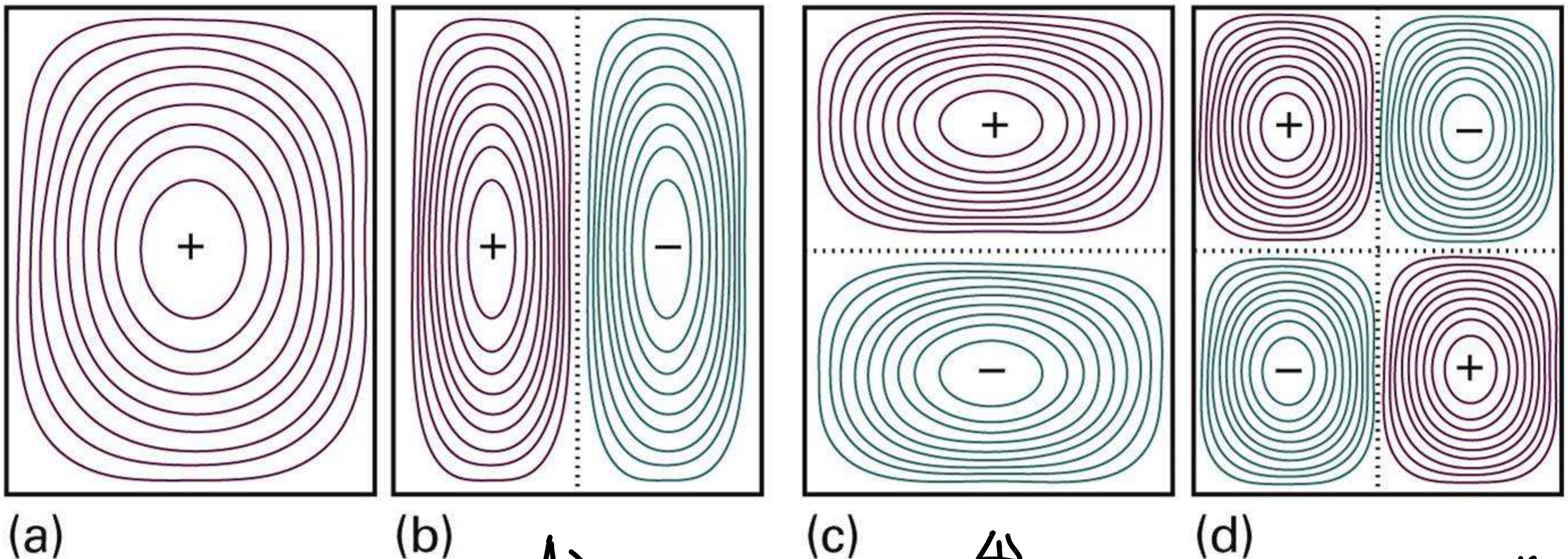


Figure 9-7
Atkins Physical Chemistry, Eighth Edition

"degeneracy"

$$\psi = \frac{2}{a} \sin\left(\frac{2\pi x}{a}\right) \sin\left(\frac{\pi y}{a}\right)$$

Porphyrin

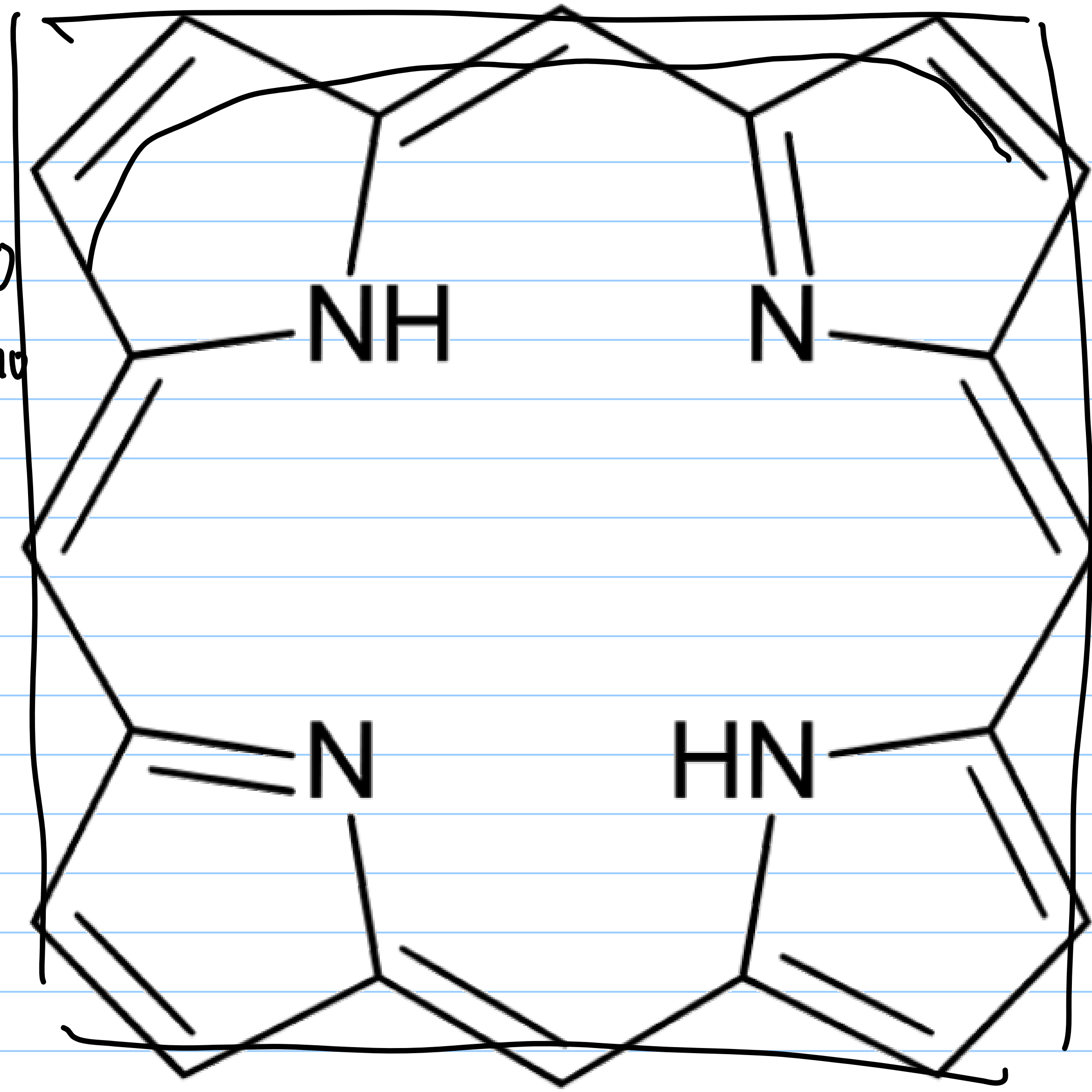
LUMO

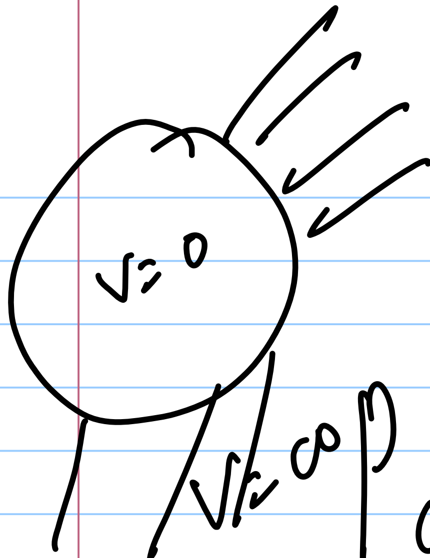
HOMO

$\frac{8h^2}{8ma^2}$ 2,2

$\frac{5h^2}{8ma^2}$ 1,2 2,1

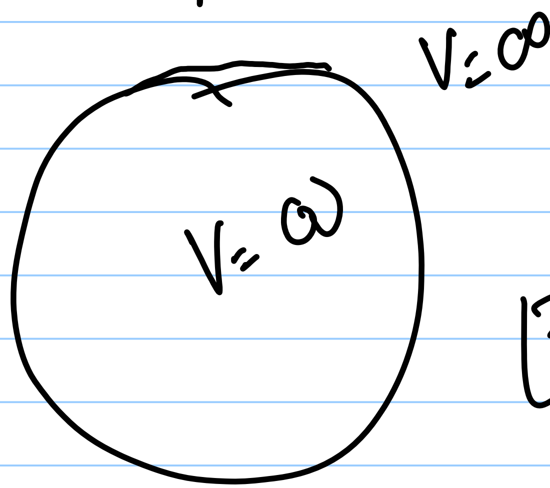
$\frac{2h^2}{8ma^2}$ 1,1





$$\Delta E = E_{LUMO} - E_{HOMO} = h\nu_{light}$$

Particle in a 3D box



$$(n_x, n_y, n_z)$$

$$E = E_x + E_y + E_z$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = E \psi$$

spherical coordinates

Harmonic oscillator

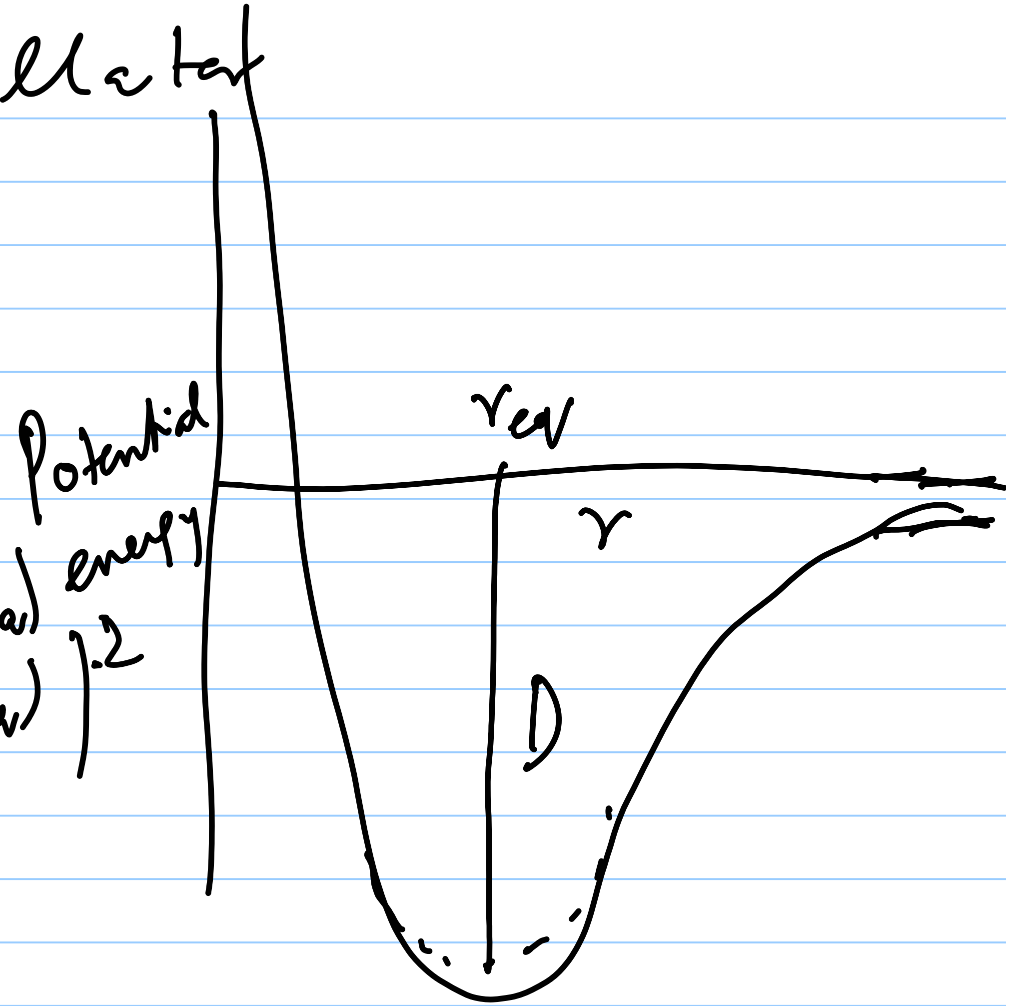
HCl

r

$$V = \underbrace{D(1 - e^{-\beta r})^2}_{\text{Morse}}$$

$(r - r_{eq})$

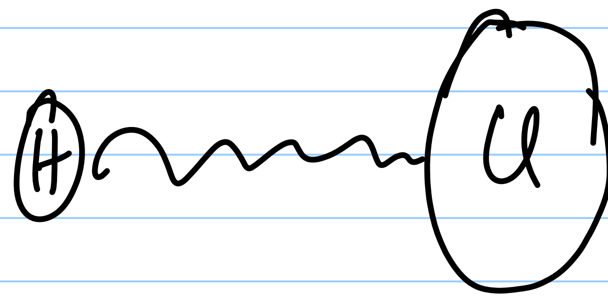
$$D(1 - e^{-\beta(r - r_{eq})})^2$$



$F = -kx$

"Hooke's law)

$\frac{1}{2} k x^2$



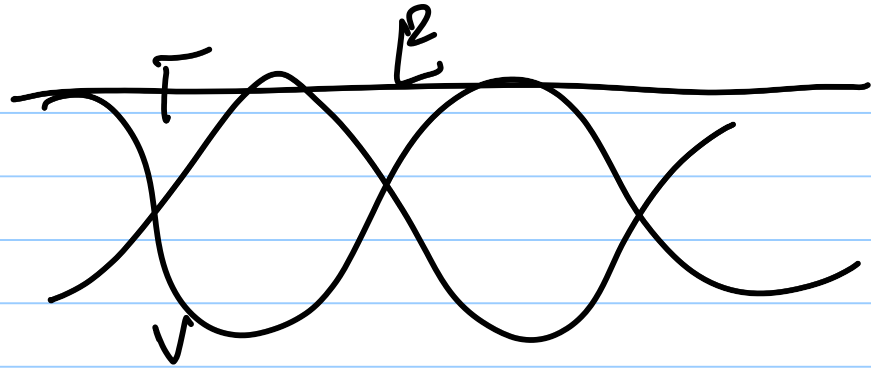
$$F = -kx$$

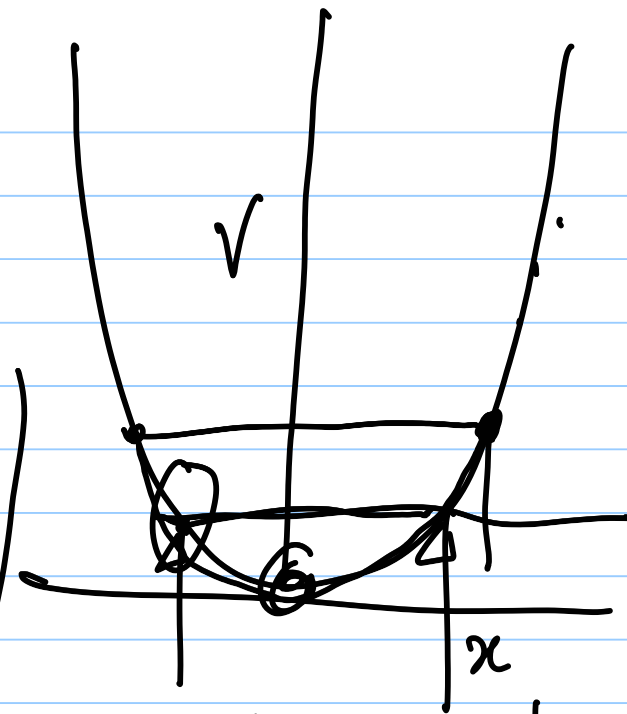
$$m\frac{d^2x}{dt^2} + kx = 0$$

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

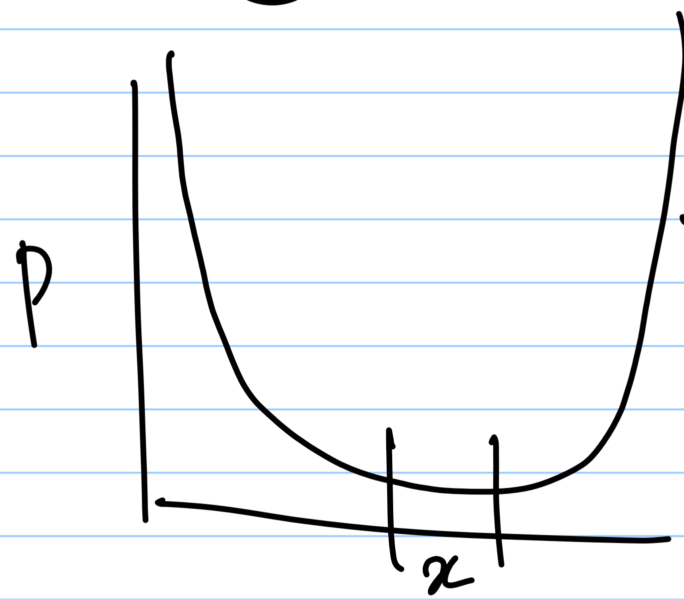
$x(t)$

$$E = T + V$$





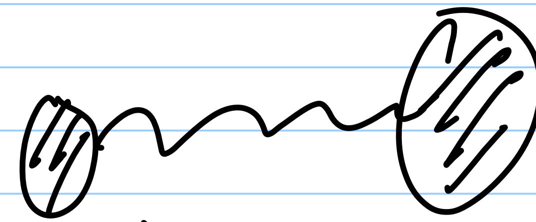
classical turning points



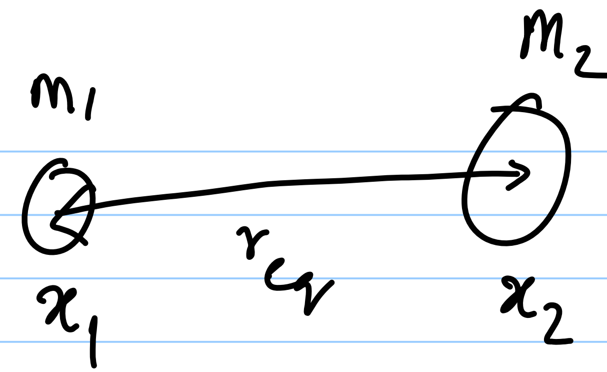
Schrödinger equation $\qquad F = -kx$

$m \qquad V = \frac{1}{2}kx^2$

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



$$m = \mu \qquad \frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2}$$



① $m_1 \dfrac{d^2 x_1}{dt} = -k(x_2 - x_1 - r_{eq})$

② $M_2 \dfrac{d^2 x_2}{dt} = +k(x_2 - x_1 - r_{eq})$

$$M \frac{d^2 X}{dt^2} = 0$$

$$\mu \frac{d^2(x_1 - x_2)}{dt^2} + k(x_1 - x_2) = 0$$

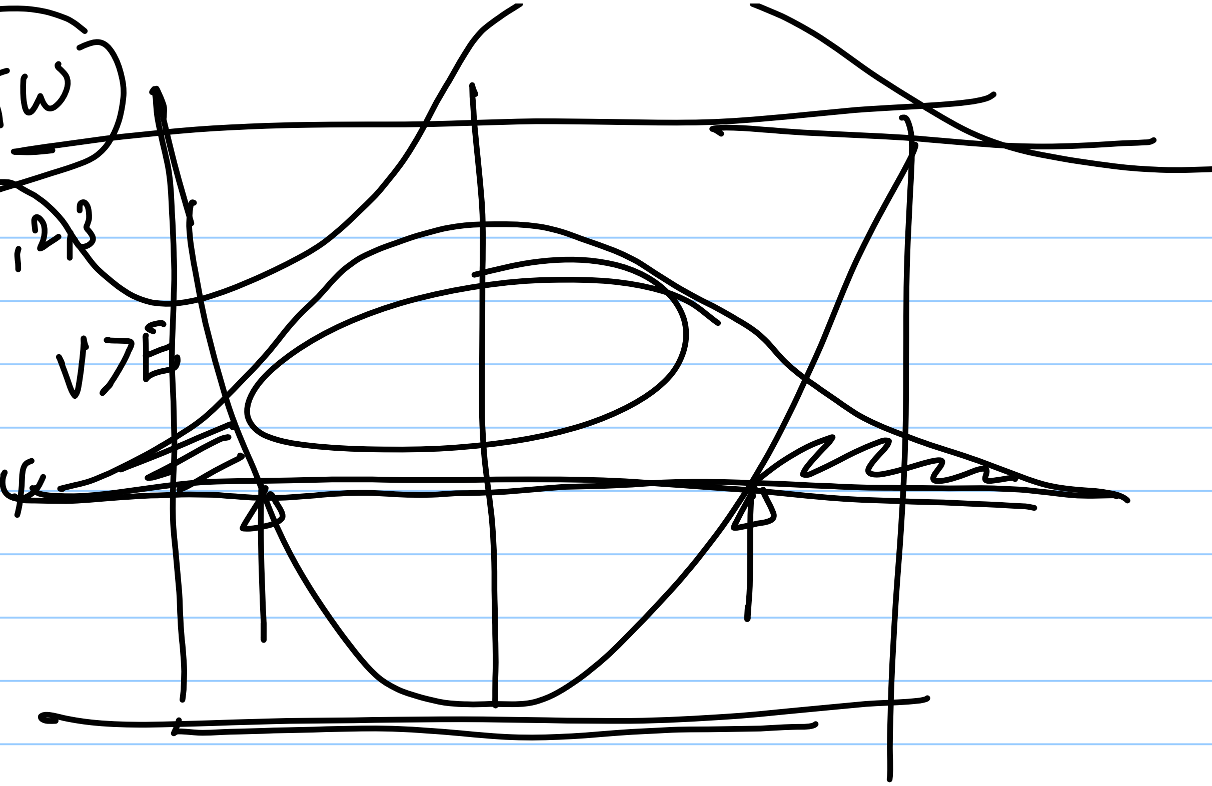
$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

$n\hbar\omega$

$n = 1, 2, 3$

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

$V > E$



$$\frac{d^2x}{dt^2}$$

$E > V$