Highlights of the course

1. Co-ordinate Systems
2. Introduction to Vector Operators
3. Work , Energy and Conservation laws
4. Rigid body in motion
5. Oscillations and Waves
6. Quantum Physics

Chapter-3:Work , Energy and Conservation laws

Concept of equilibrium

Duffing Oscillator (Georg Duffing, German engineer)

$$V(x) = \frac{1}{2}\beta x^2 + \frac{1}{4}\alpha x^4, \quad \beta < 0$$

Plot V(x) v/s x

How to Plot the graph?

1. Find Maxima and Minima

2. Find the zero crossing points

3. Imagine the function for smaller and larger values of x

1. Maxima and Minima

Condition for maxima and minima of a function

A function V(x) is maximum when $\frac{dV(x)}{dx} = 0$ and $\frac{d^2V(x)}{dx^2} < 0$

A function V(x) is minimum when $\frac{dV(x)}{dx} = 0$ and $\frac{d^2V(x)}{dx^2} > 0$

1. Maxima and Minima

$$V(x) = \frac{1}{2}\beta x^2 + \frac{1}{4}\alpha x^4$$

To find maxima and minima:

$$\frac{dV(x)}{dx} = 0$$

$$\beta x + \alpha x^3 = 0$$

$$\Rightarrow \quad x(\beta + \alpha x^2) = 0$$

$$\Rightarrow \quad x = 0 \text{ and } x = \pm\sqrt{\frac{-\beta}{\alpha}}$$

1. Maxima and Minima

$$\frac{d^2V(x)}{dx^2} = \beta + 3\alpha x^2$$

$$\text{When x=0, } \frac{d^2V(x)}{dx^2} = \beta < 0 \Rightarrow \text{Maxima}$$

$$\text{When x} = \pm\sqrt{\frac{-\beta}{\alpha}},\ \frac{d^2V(x)}{dx^2} = -2\beta > 0$$

$$(\text{since}\beta < 0) \Rightarrow \text{Minima}$$

2. Zero crossing points

$$V(x) = 0$$

$$\frac{1}{2}\beta x^2 + \frac{1}{4}\alpha x^4 = 0$$

$$\Rightarrow \quad x = \pm\sqrt{\frac{-2\beta}{\alpha}} \text{ and } x=0$$

Plot for small and large values of x

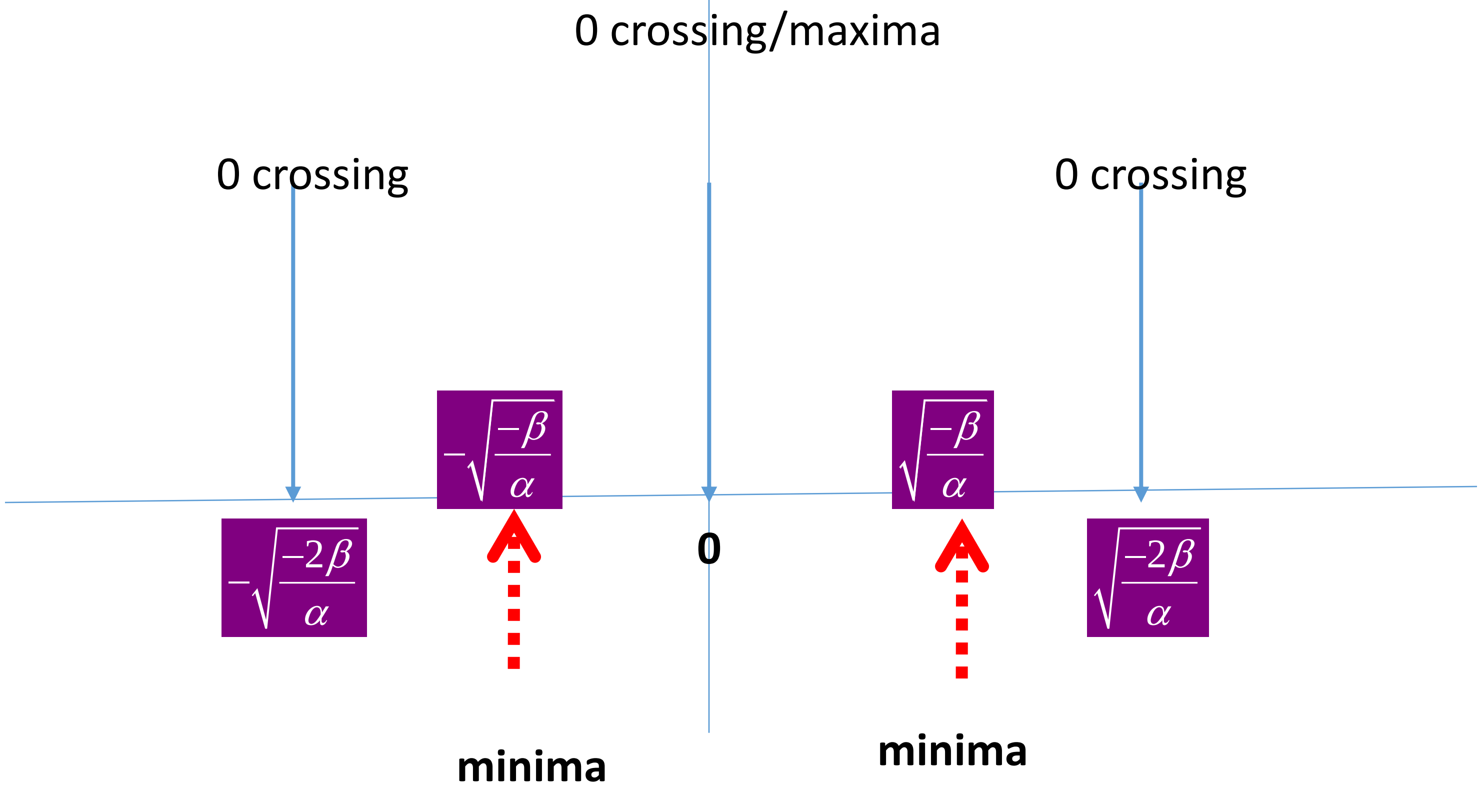
1. Maxima at x =0

Minima at $-\sqrt{\frac{-\beta}{\alpha}}$

and $\sqrt{\frac{-\beta}{\alpha}}$

$$V(x) = \frac{1}{2}\beta x^2 + \frac{1}{4}\alpha x^4$$

2. Zero crossing at 3 points, x = 0, $-\sqrt{\frac{-2\beta}{\alpha}}$ $\sqrt{\frac{-2\beta}{\alpha}}$

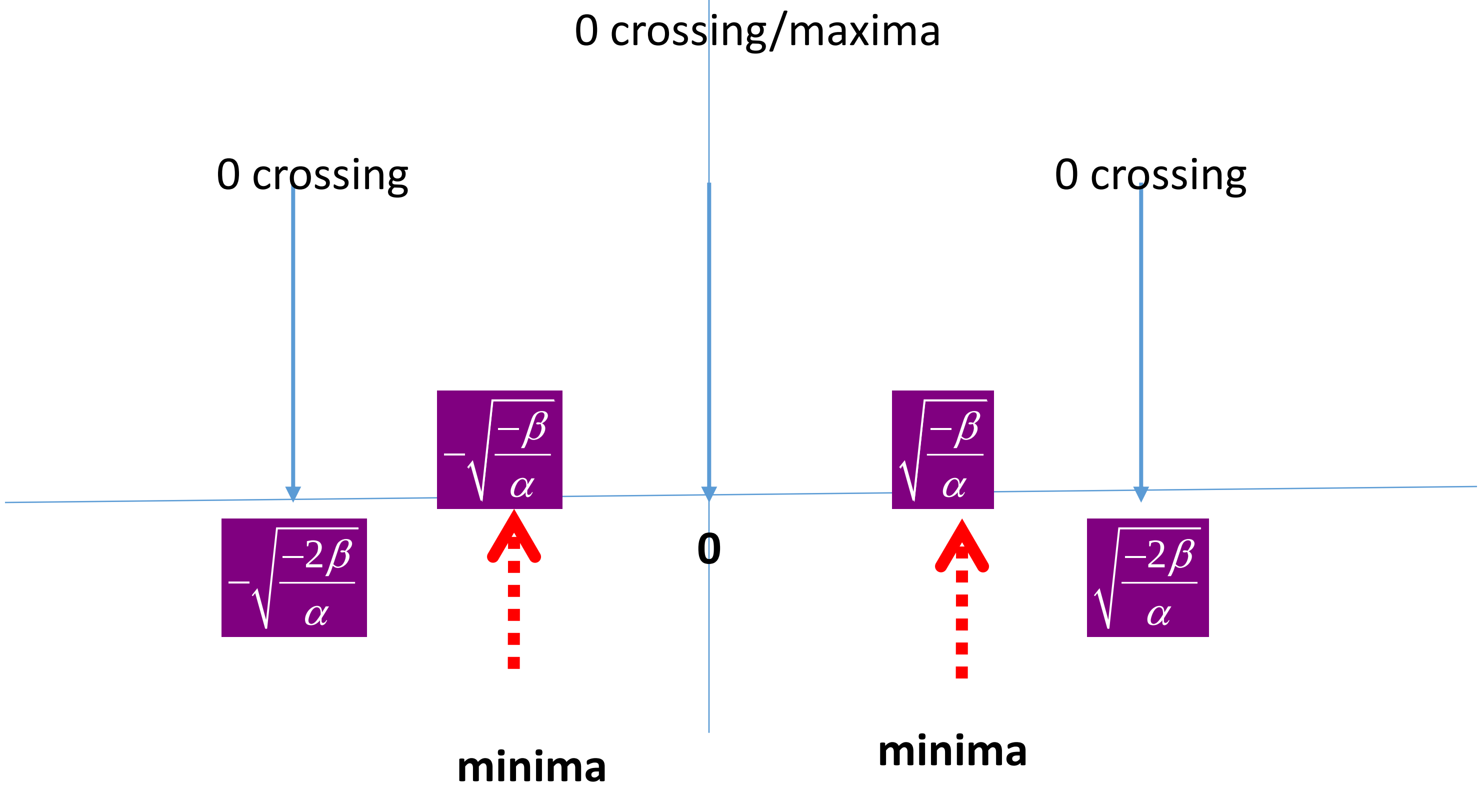


Plot for small and large values of x

$$V(x) = \frac{1}{2}\beta x^2 + \frac{1}{4}\alpha x^4$$

For small values of x , V(x) behaves as x^2

For large values of x , V(x) behaves as x^4

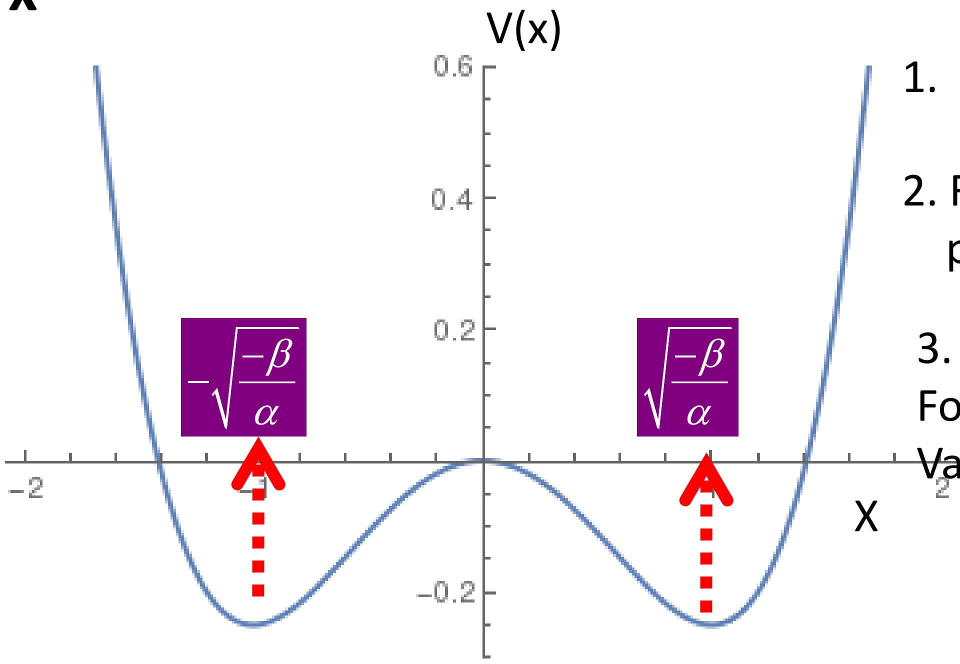


Concept of equilibrium

Duffing Oscillator

$$V(x) = \frac{1}{2}\beta x^2 + \frac{1}{4}\alpha x^4, \quad \beta < 0$$

Plot V(x) v/s x



1. Maxima at x =0

Minima at $-\sqrt{\frac{-\beta}{\alpha}}$

and $\sqrt{\frac{-\beta}{\alpha}}$

2. Zero crossing at 3 points, x = 0, $-\sqrt{\frac{-2\beta}{\alpha}}$, $\sqrt{\frac{-2\beta}{\alpha}}$

To Plot the graph

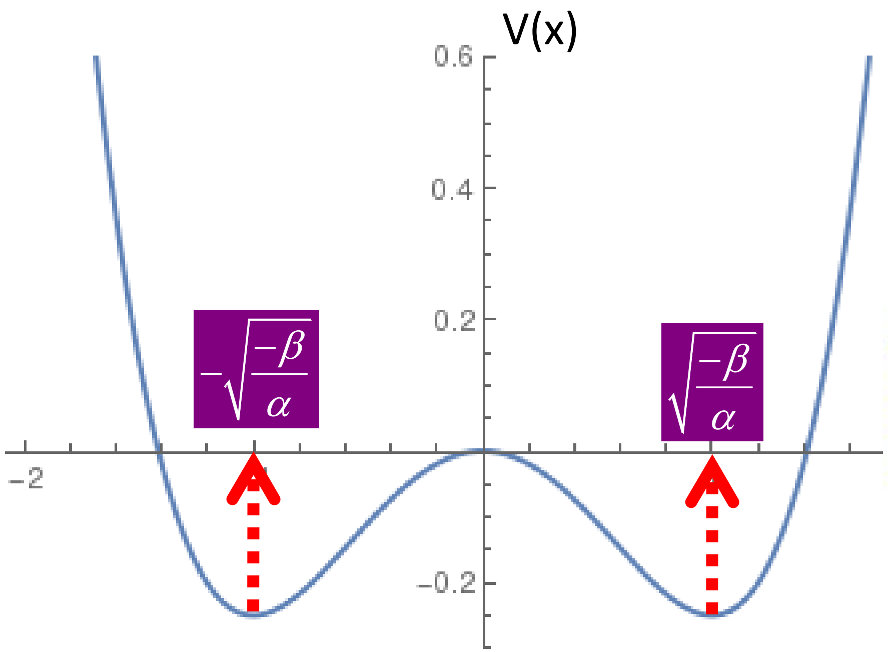
1. Find Maxima and Minima
2. Find the zero crossing points
3. Imagine the function For smaller and larger Values of x

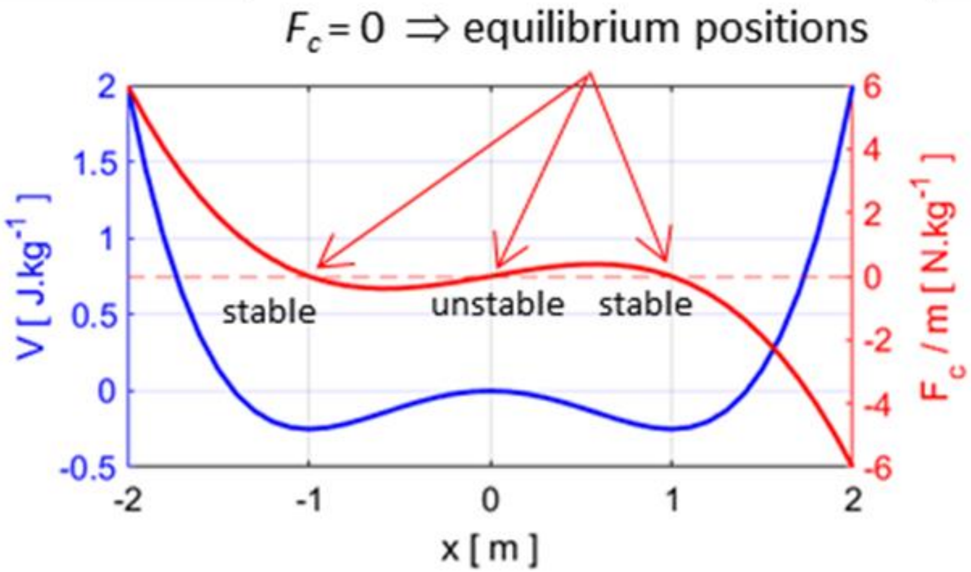
Concept of equilibrium

Duffing Oscillator

$$V(x) = \frac{1}{2}\beta x^2 + \frac{1}{4}\alpha x^4, \quad \beta < 0$$

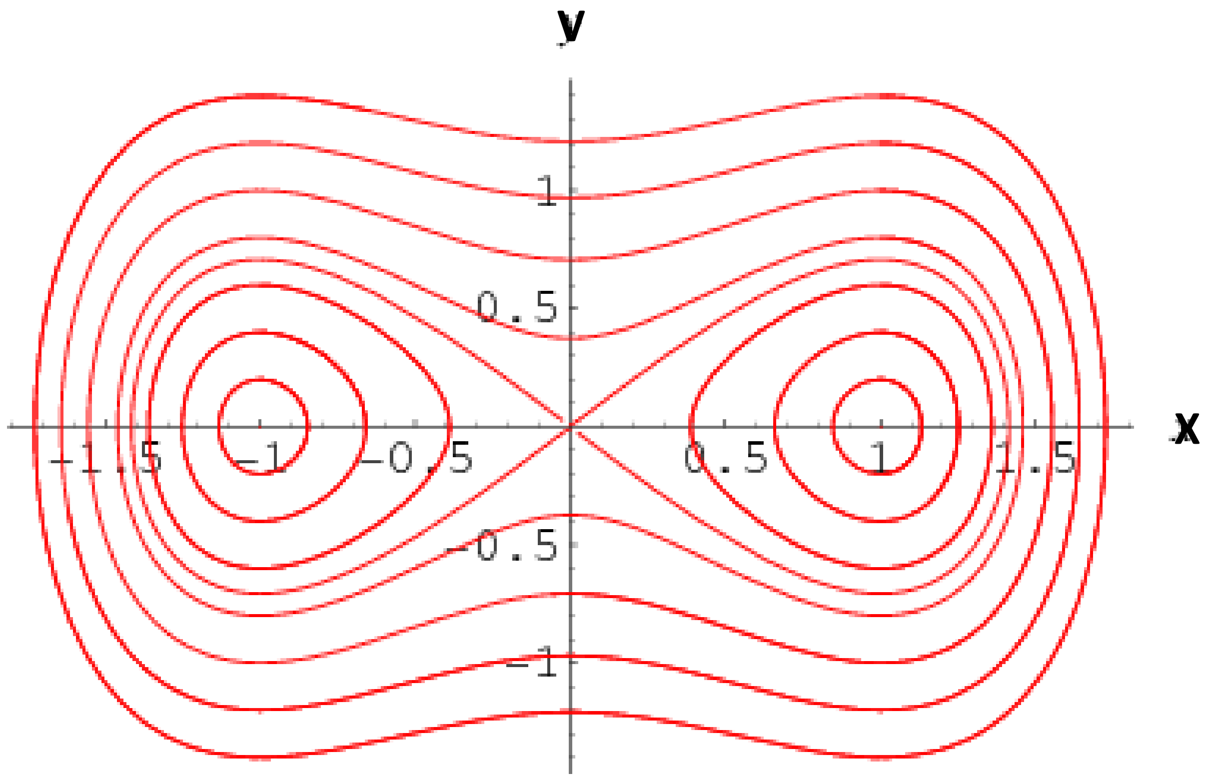
Component of Force $F(x) = -\frac{dV(x)}{dx} = -\beta x - \alpha x^3$



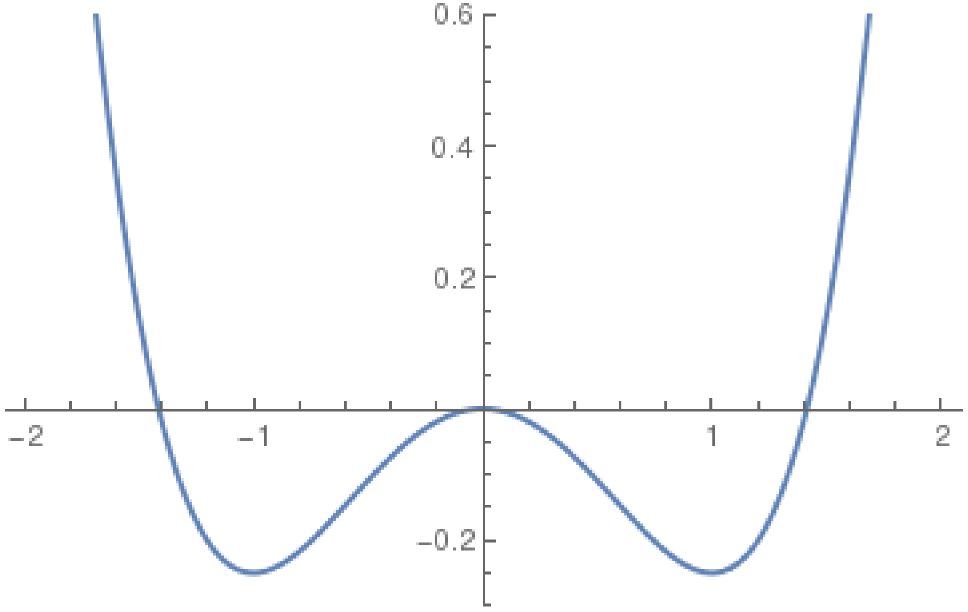


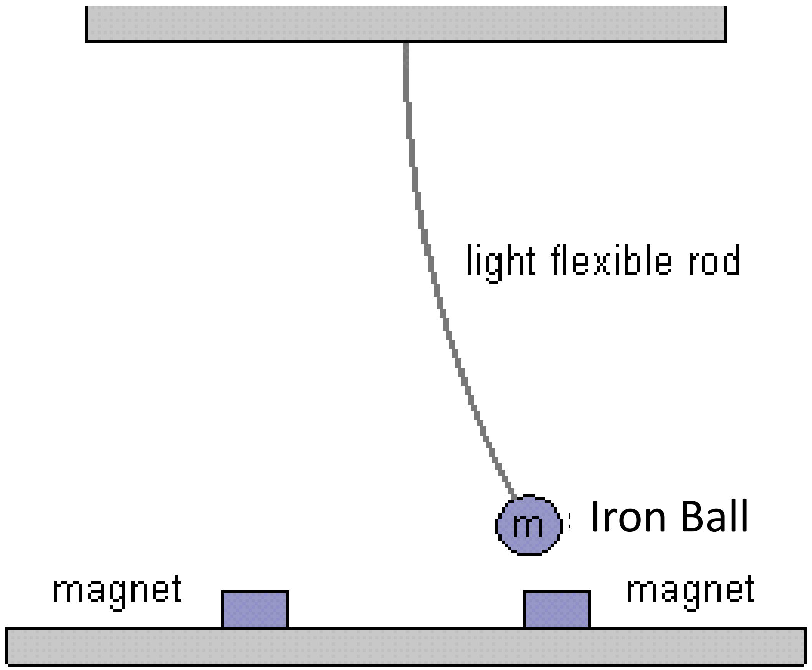
Velocity Vs. Position plot

$$E = \frac{1}{2}\beta x^2 + \frac{1}{4}\alpha x^4 + \frac{1}{2}mv^2$$

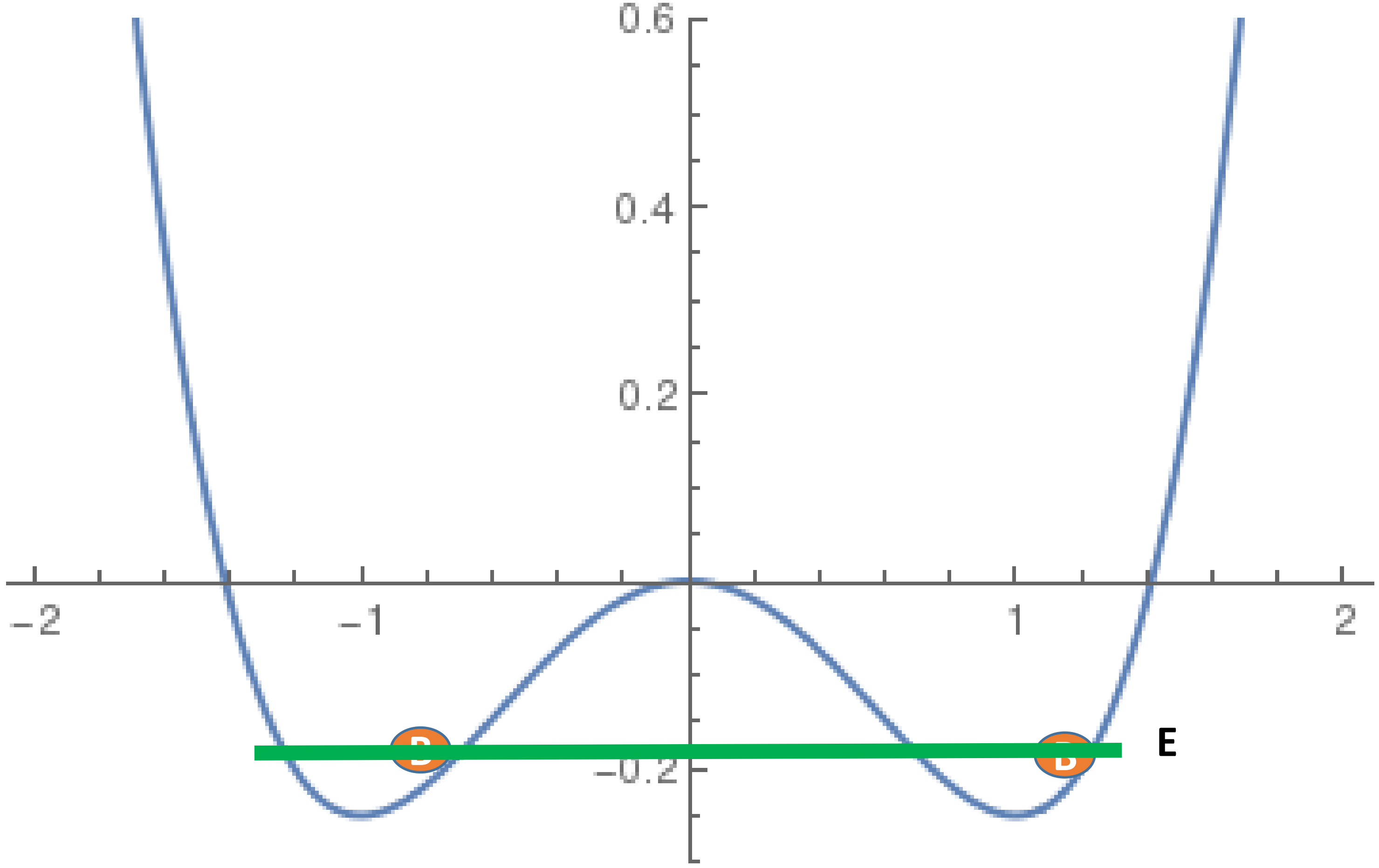


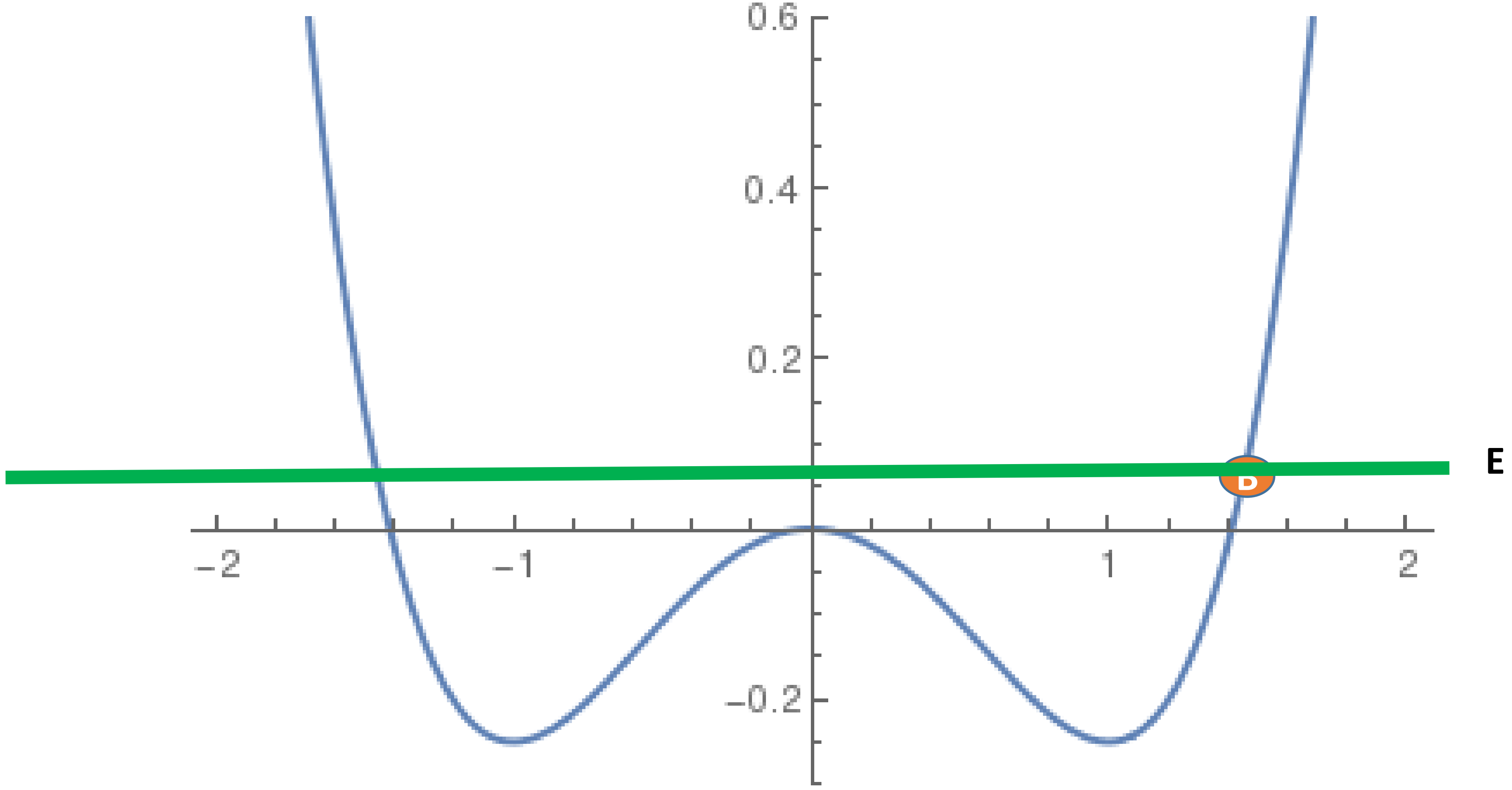
Physical Example of double well



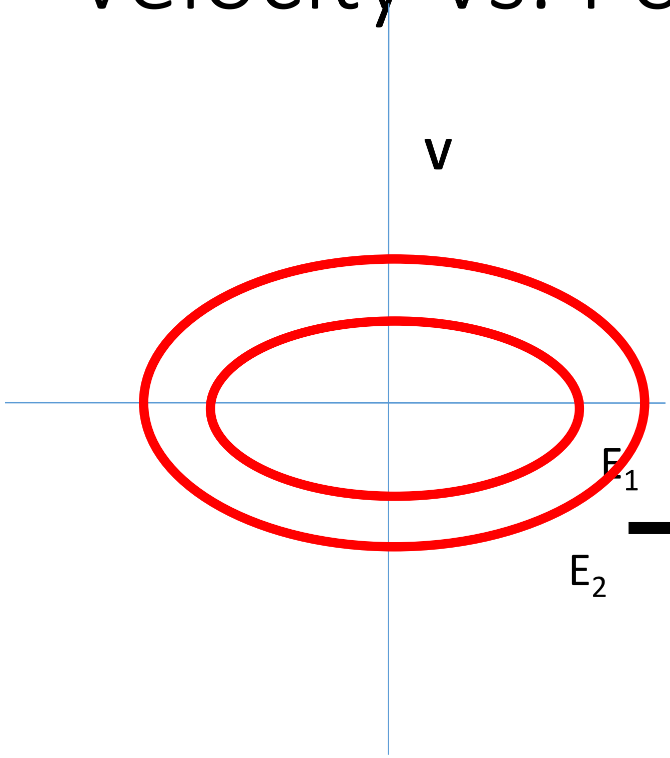


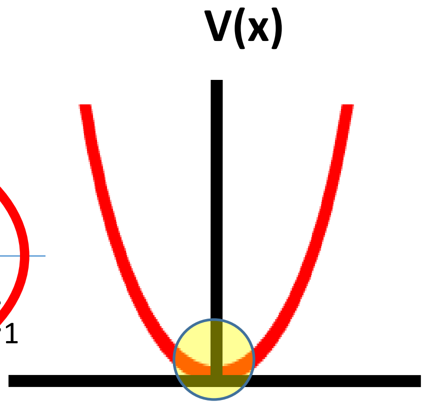
Duffing Oscillator (Georg Duffing, German engineer)

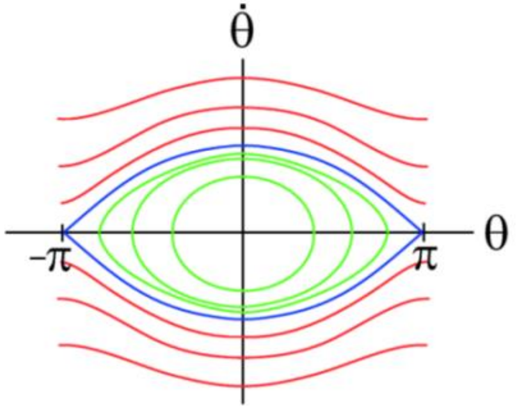


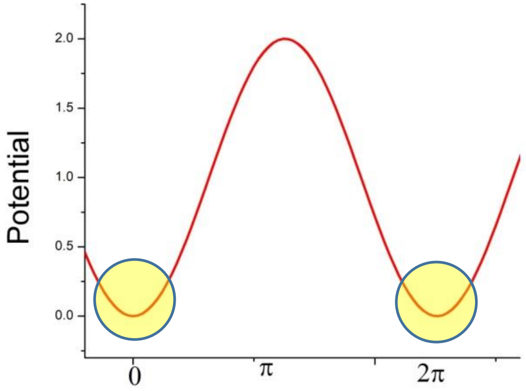

0.6
0.4
0.2
−0.2
−2
−1
1
2
E
B

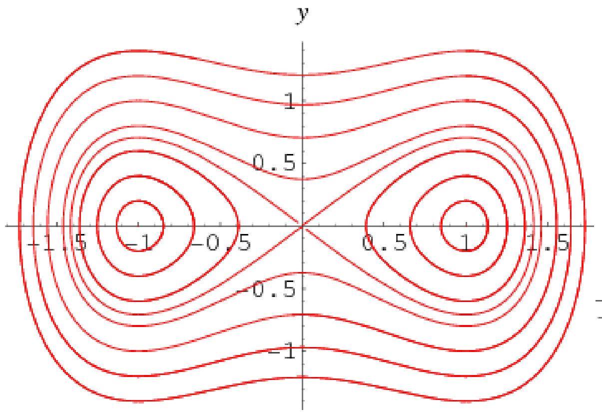
Velocity Vs. Position plot (Summary)

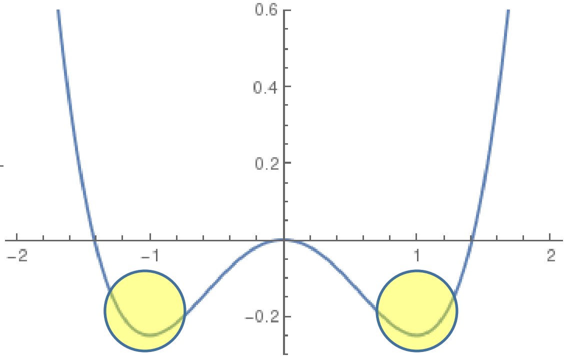












Interatomic Potential: Lennard Jones Potential

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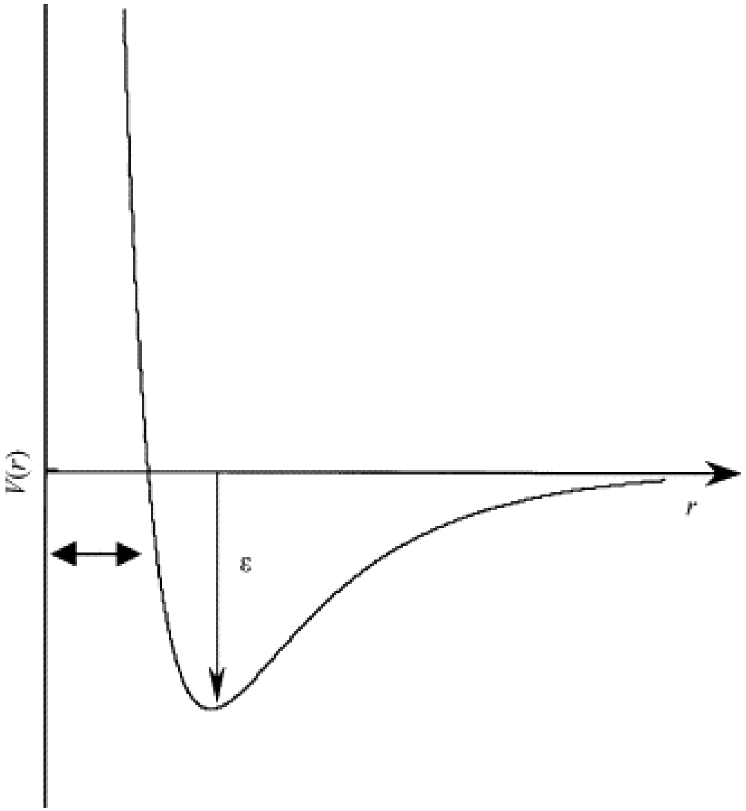
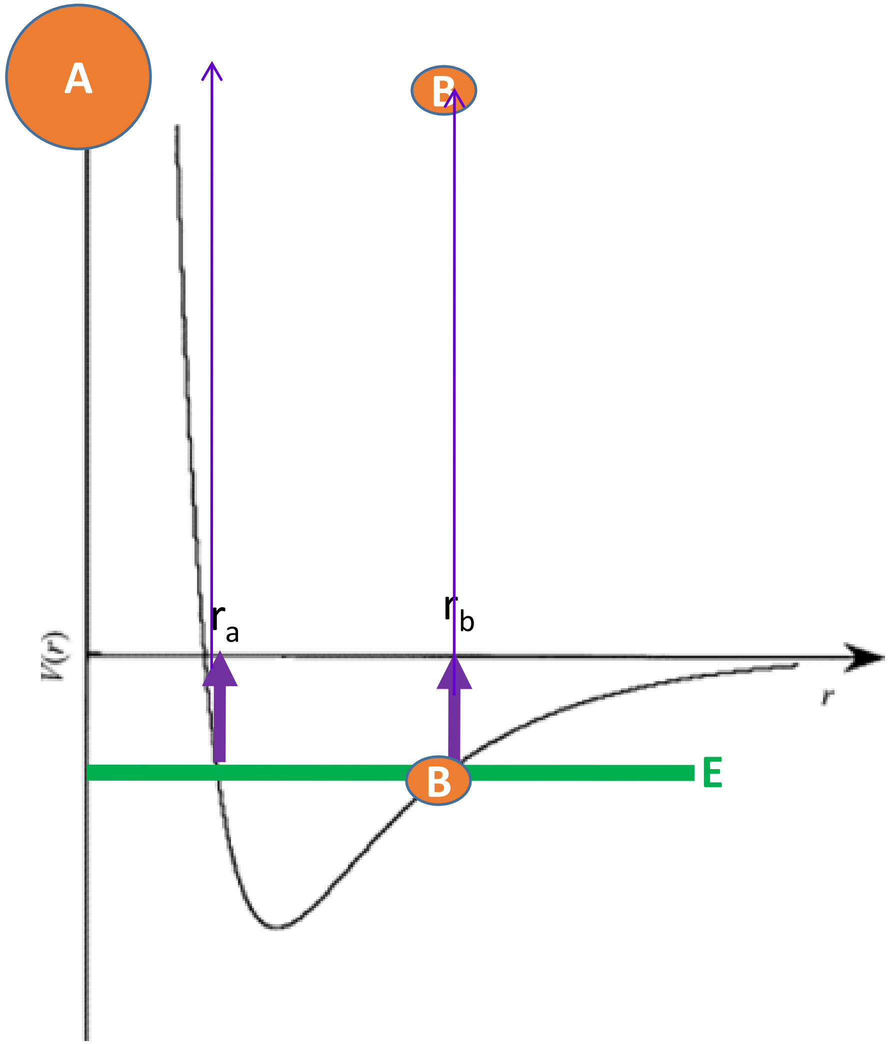


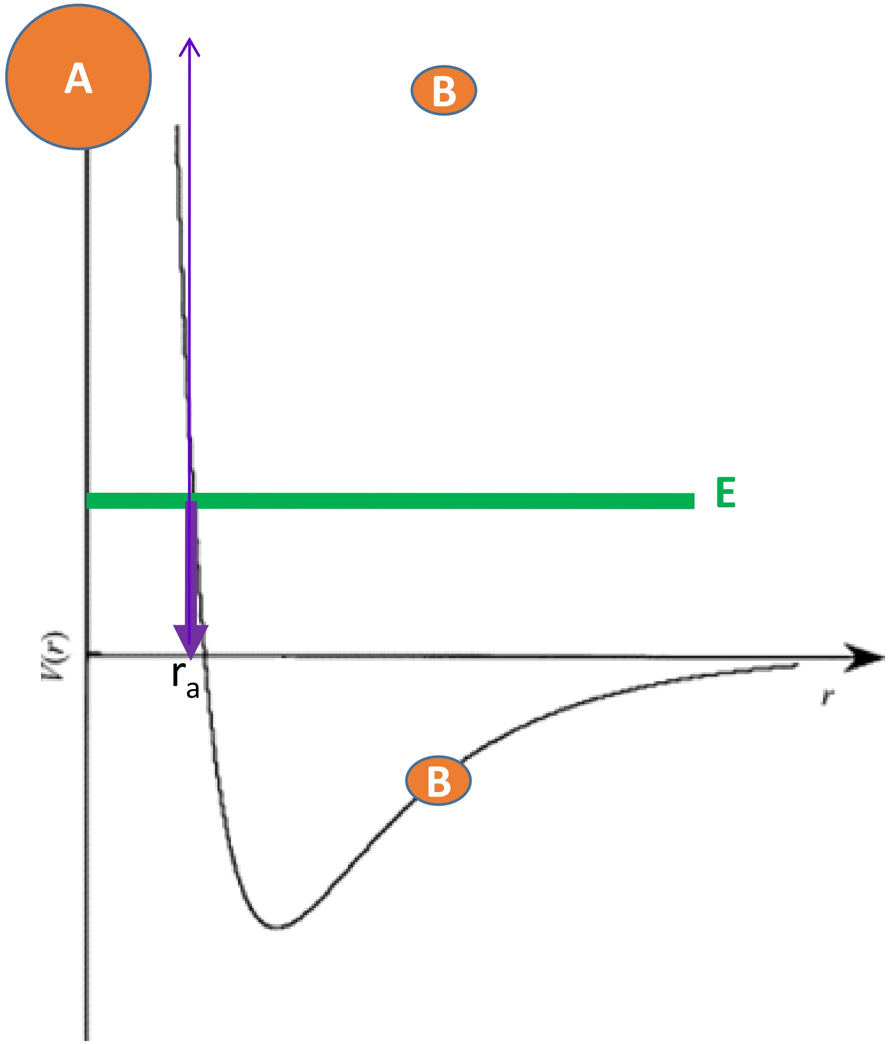
Lennard Jones Potential

$$U_{LJ}(r) = \varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - 2\left(\frac{\sigma}{r}\right)^{6}\right]$$

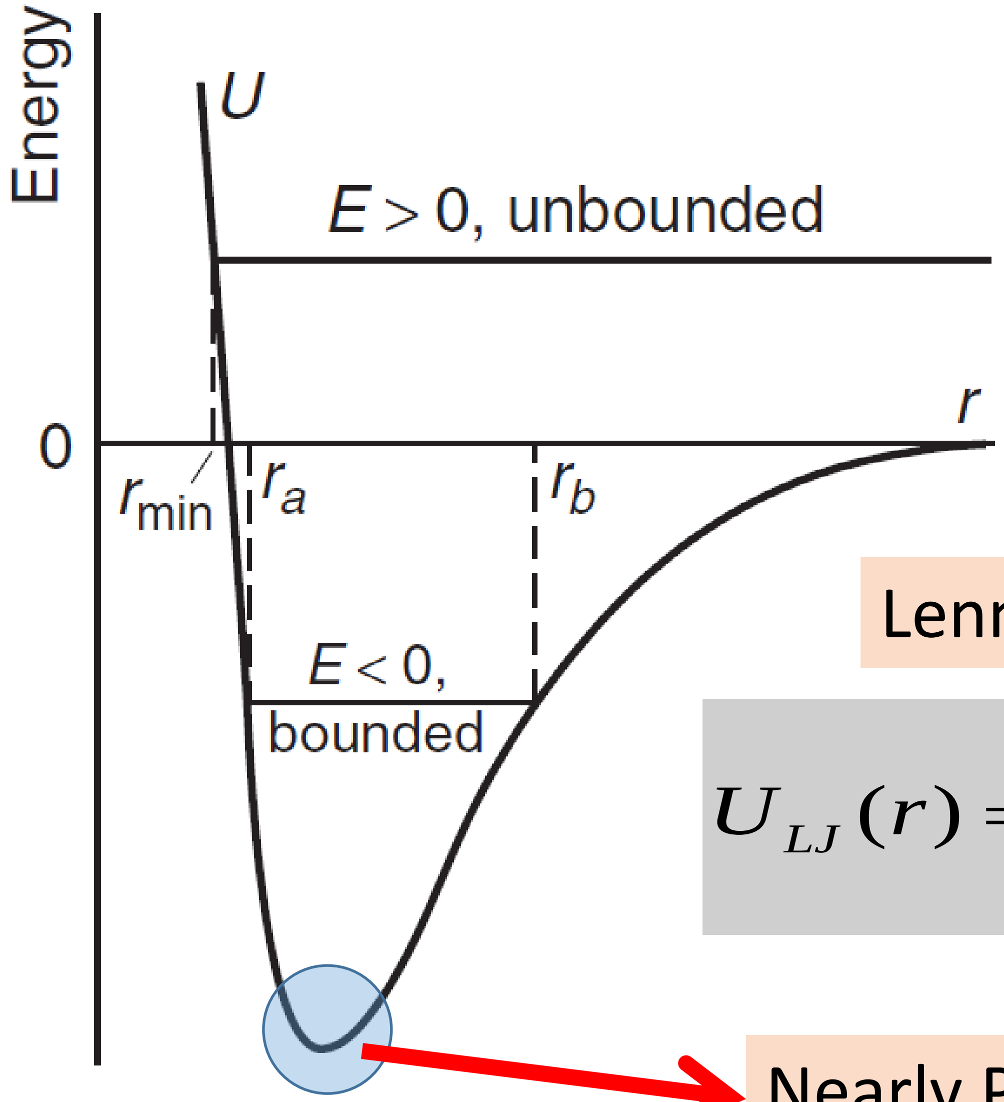
Interatomic potential



Interatomic potential



Interatomic potential

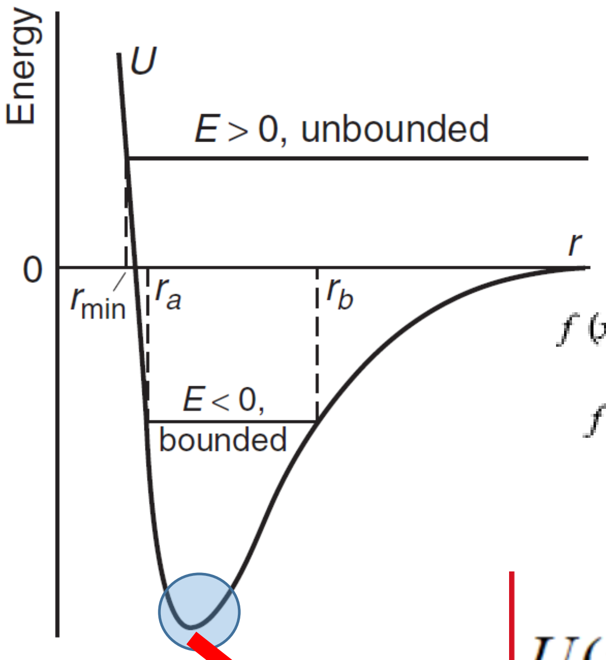


Lennard Jones Potential

$$U_{LJ}(r) = \varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - 2\left(\frac{\sigma}{r}\right)^{6}\right]$$

Nearly Parabolic

Small Oscillations



Taylor series expansion of a function f(x), about
A point x=a is given as

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f^{(3)}(a)}{3!}(x-a)^3 + \ldots + \frac{f^{(n)}(a)}{n!}(x-a)^n + \ldots.$$

$$U(r) = U(r_0) + (r - r_0)\left.\frac{dU}{dr}\right|_{r_0} + \frac{1}{2}(r-r_0)^2 \left.\frac{d^2U}{dr^2}\right|_{r_0} + \ldots$$

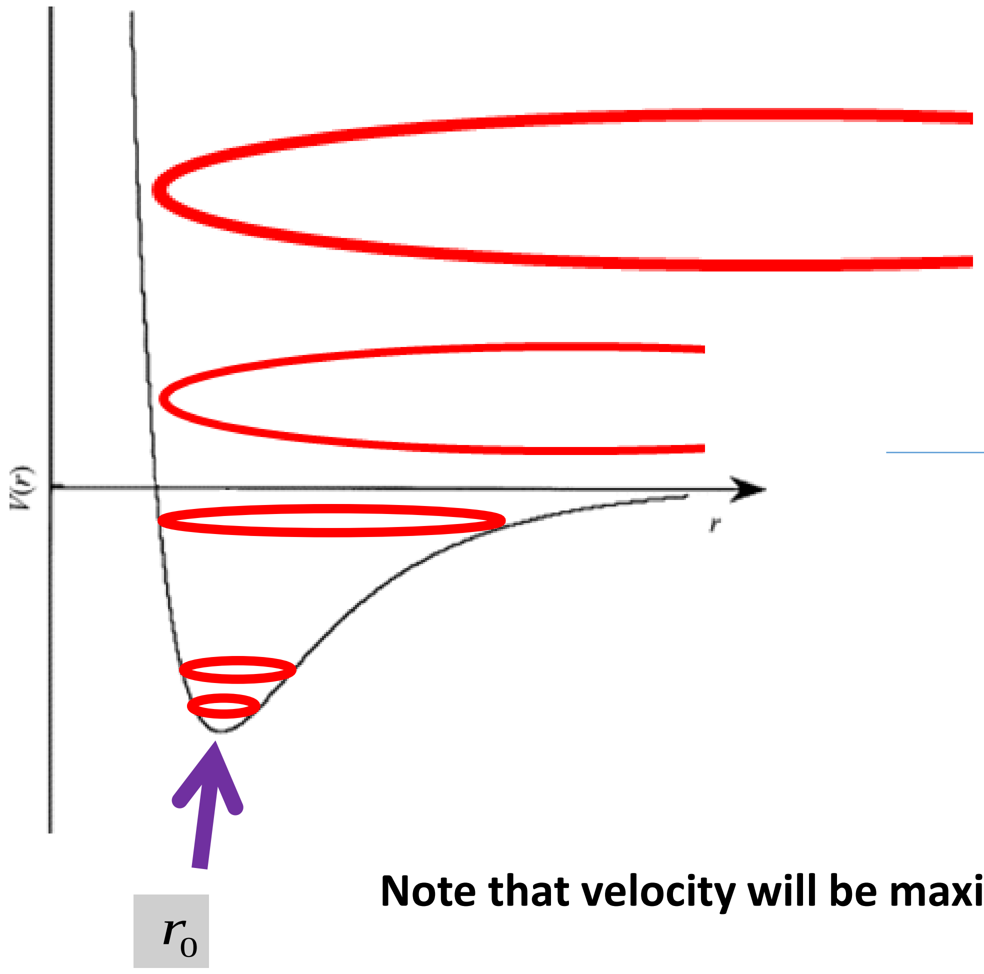
Nearly Parabolic

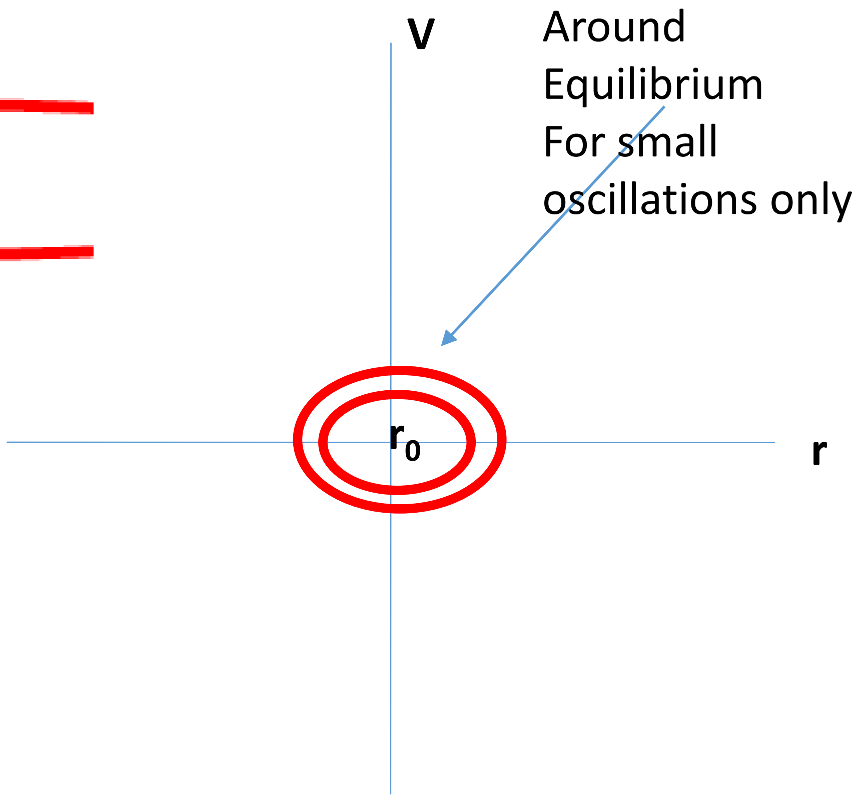
$$U(r) = \text{Constant} + \frac{1}{2}kx^2$$

Harmonic Oscillator

$$k = \omega^2 m = \left.\frac{d^2U}{dr^2}\right|_{r_0}$$

Velocity Vs. Position plot



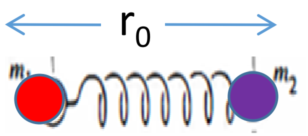


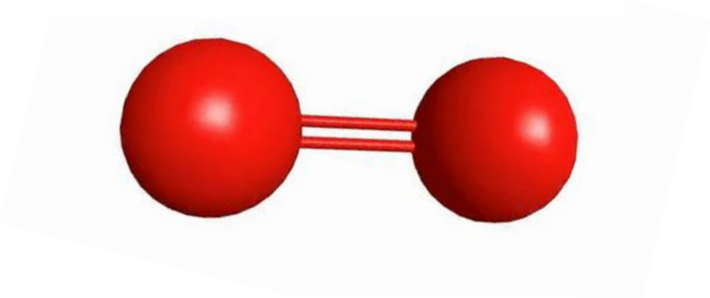
Note that velocity will be maximum at equilibrium point

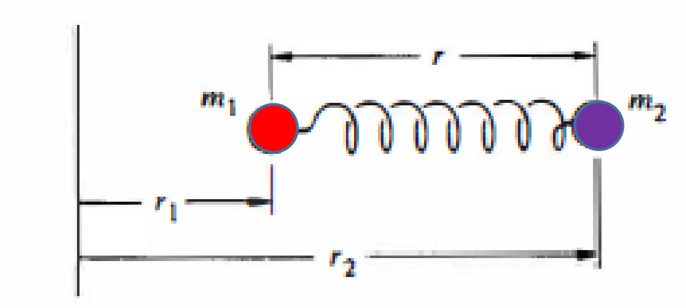
Practice Problems

Molecular vibrations

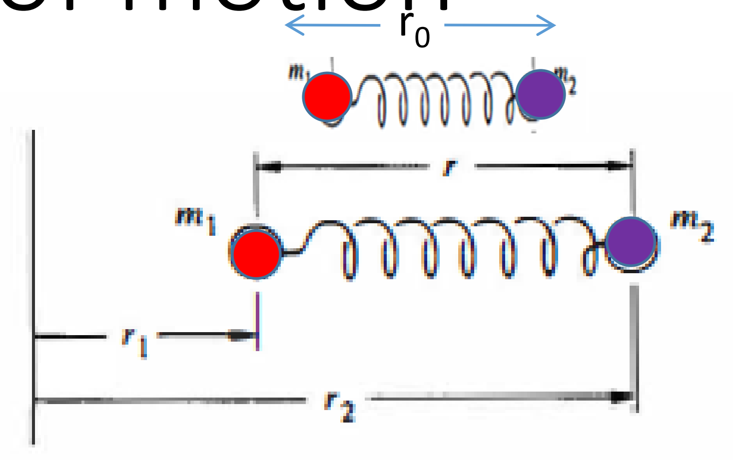
How to find the vibration frequency of diatomic molecule which is bound with very low energy such that their separation is almost close to equilibrium distance r_0?







Equation of motion



Extend spring

Restoring force direction

Provided, r_0 is the equilibrium distance,

$$m_1 \ddot{r}_1 = k(r - r_0)$$

$$m_2 \ddot{r}_2 = -k(r - r_0),$$

$$\ddot{r}_2 - \ddot{r}_1 = \ddot{r} = -k\left(\frac{1}{m_1} + \frac{1}{m_2}\right)(r - r_0)$$

Equation of motion

$$\ddot{r_2} - \ddot{r_1} = \ddot{r} = -k\left(\frac{1}{m_1} + \frac{1}{m_2}\right)(r - r_0)$$

or

$$\ddot{r} = -\frac{k}{\mu}(r - r_0),$$

$$\mu = m_1 m_2/(m_1 + m_2)$$

By Comparing with Small Oscillations of Harmonic Oscillator. We get

$$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\left.\frac{d^2U}{dr^2}\right|_{r_0} \frac{1}{\mu}}.$$

Remember

$$k = \omega^2 m = \left.\frac{d^2U}{dr^2}\right|_{r_0}$$

1. A commonly used potential energy function to describe the interaction between two atoms is the Morse potential

$$V(r) = D\left[1 - e^{-a(r-r_0)}\right]^2 - D,$$

where r_0 is the equilibrium distance, D is the well depth and a controls the width of the potential. For HCl molecule $r_0 = 1.275 \times 10^{-10}$ m, $D = 4.618$ eV, $a = 1.869 \times 10^{10} m^{-1}$.

(a) Sketch the V(r) and Force.

(b) Find the frequency of small oscillations about equilibrium for HCl molecule? (AMU of Cl is 35)

Sketch the V(r) and Force.

$$V(r) = D\left[1 - e^{-a(r-r_0)}\right]^2 - D$$

Zero crossings: $[1 - e^{-a(r-r_0)}]^2 = 1$

$e^{-a(r-r_0)} = 0$

$e^{-a(r-r_0)} = 2$

r = infinity, $r = r_0 - \frac{1}{a} ln2$

Minima/Maxima:

$$\frac{dV}{dr} = 2Da[1 - e^{-a(r-r_0)}] \times e^{-a(r-r_0)} = 0$$

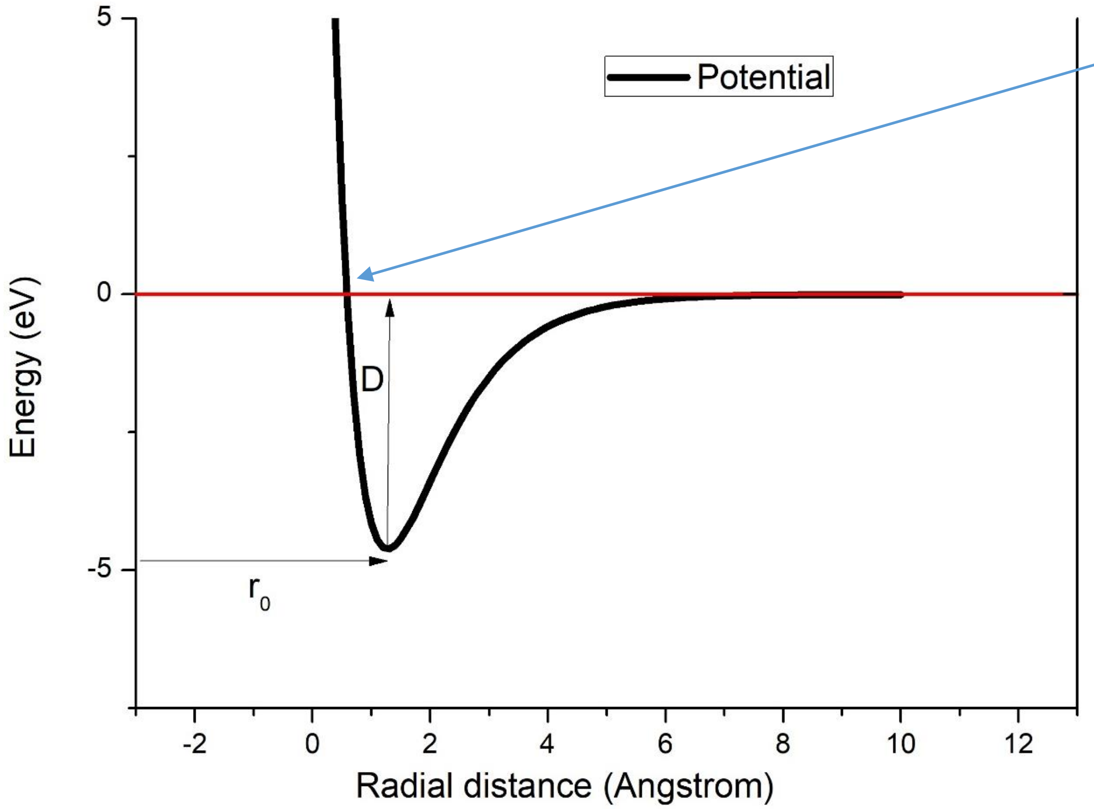
$r = r_0$

$$\frac{d^2V}{dr^2}|_{r=r_0} = 2Da^2$$ Is Positive, Stable equilibrium

$$\frac{d^2V}{dr^2} = 2Da[0 + ae^{-a(r-r_0)}]e^{-a(r-r_0)} - 2Da^2[1 - e^{-a(r-r_0)}] \times e^{-a(r-r_0)}$$

Sketch the V(r)

$$V(r) = D\left[1 - e^{-a(r-r_0)}\right]^2 - D$$



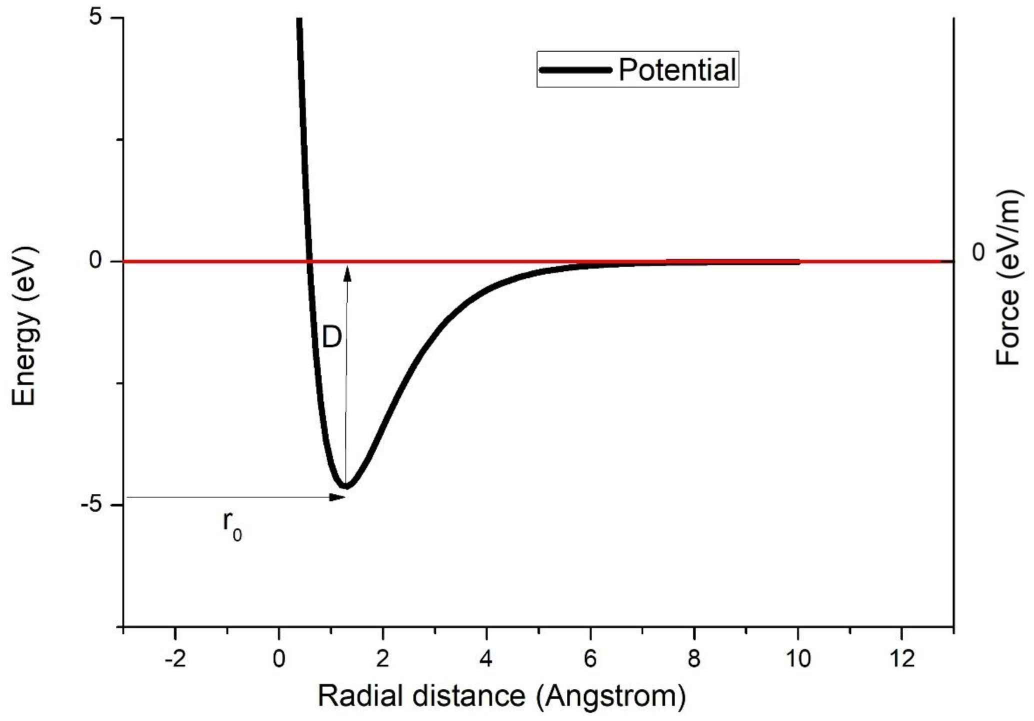
$r = r_0 - \frac{1}{a} ln2$

Sketch the V(r) and Force.

$$F = -\frac{dV}{dr}$$

$$-\frac{dV}{dr} = -2Da[1 - e^{-a(r-r_0)}] \times e^{-a(r-r_0)}$$

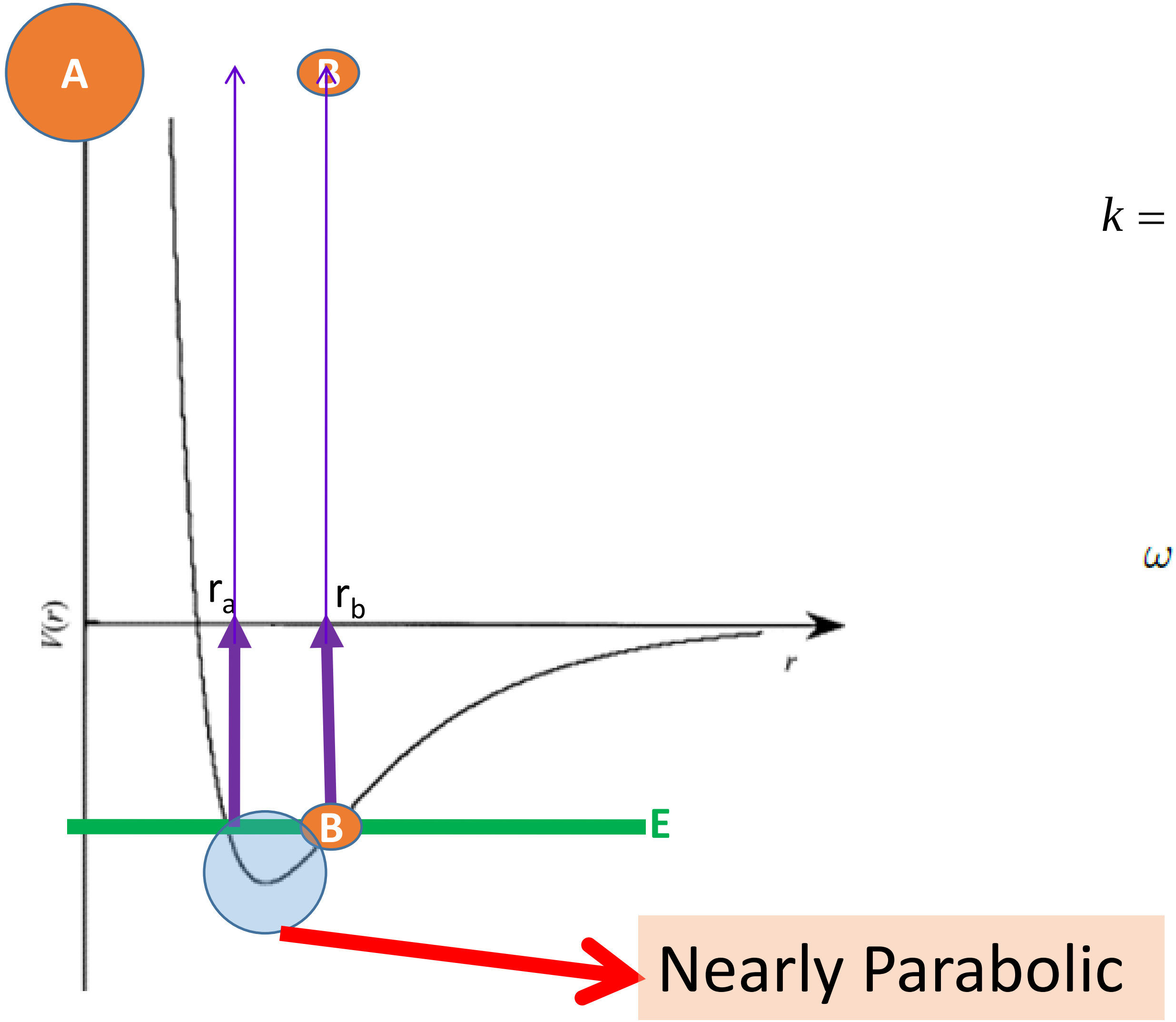
$$= 2Da[e^{-2a(r-r_0)} - e^{-a(r-r_0)}]$$



(b) Find the frequency of small oscillations about equilibrium for HCl molecule? (AMU of Cl is 35)

Potential V(r) is given, how to find the molecular vibrational frequency?

RECOLECT SMALL OSCILLATIONS (LOW ENERGY CASE)



$$k = \omega^2 m = \left.\frac{d^2V}{dr^2}\right|_{r_0}$$

$$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{\frac{d^2V}{dr^2}|_{r=r_0}}{\mu}}$$

(b) Find the frequency of small oscillations about equilibrium for HCl molecule? (AMU of Cl is 35)

$$V(r) = D\left[1 - e^{-a(r-r_0)}\right]^2 - D$$

$$\frac{dV}{dr} = 2Da[1 - e^{-a(r-r_0)}] \times e^{-a(r-r_0)}$$

$$\frac{d^2V}{dr^2} = 2Da[0 + ae^{-a(r-r_0)}]e^{-a(r-r_0)} - 2Da^2[1 - e^{-a(r-r_0)}] \times e^{-a(r-r_0)}$$

$$\frac{d^2V}{dr^2}|_{r=r_0} = 2Da^2$$

(b) Find the frequency of small oscillations about equilibrium for HCl molecule? (AMU of Cl is 35)

$$\omega = \sqrt{\frac{\frac{d^2V}{dr^2}|_{r=r_0}}{\mu}} = \sqrt{\frac{2Da^2}{\mu}} \approx 5.37 \times 10^{14} radians/s.$$

Conversion factors are $1eV = 1.602 \times 10^{-19} J$

$1amu = 1.66 \times 10^{-27}\mathrm{Kg}$