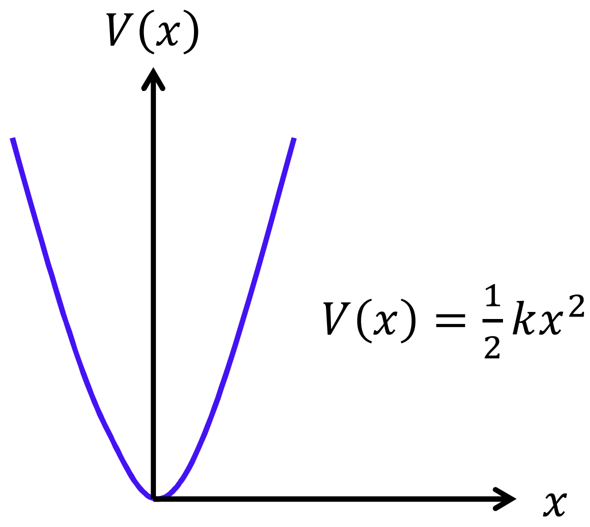
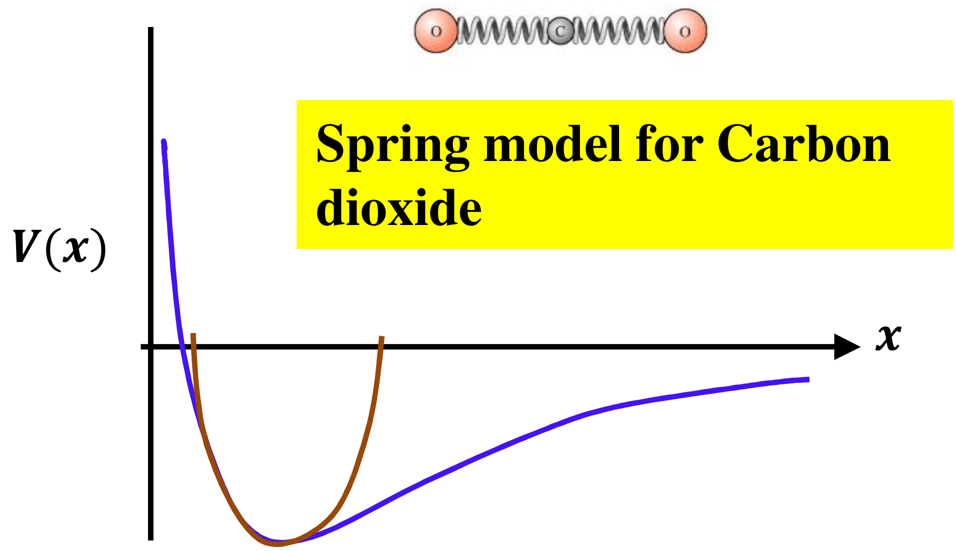
PH101: PHYSICS1

Lecture 4

Harmonic approximation of potential energy



Pure harmonic potential



Harmonic approximation of the potential

- ❑ Potential energy for atom and many other practical systems are close to harmonic around equilibrium point but deviates at larger distance from equilibrium
- ❑ Exact potential is hard to solve.

Harmonic approximation

Taylor series/expansion

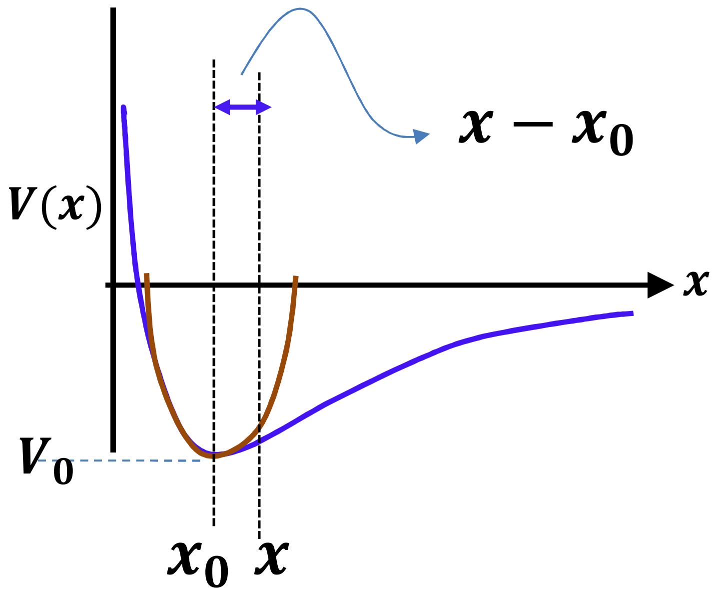
$$V(x) = V(x_0) + V'(x_0)(x - x_0) + \frac{1}{2!}V''(x_0)(x - x_0)^2 + O(3)$$

Here $V'(x) = \frac{dV}{dx}$ and $V''(x) = \frac{d^2V}{dx^2}$

- Here we are taking the expansion around the equilibrium distance x_0.

Hence $V'(x_0) = 0$ since the force is zero (potential has an extremum).

- Let us assume that $V(x_0) = 0$, the potential at the equilibrium (reference) is zero.



Taylor series/expansion Examples:

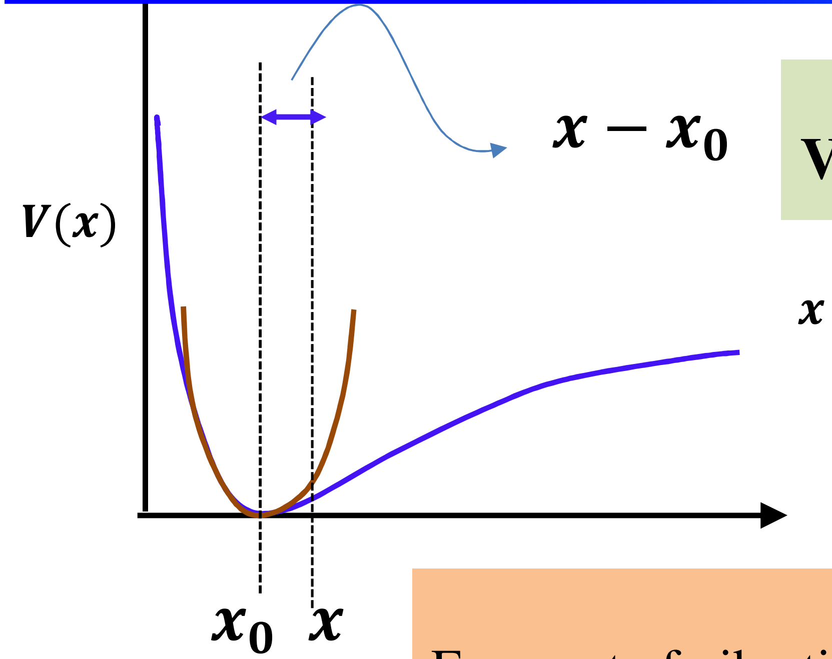
$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots$$

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \ldots$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \ldots$$

$$\ln(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \ldots \quad for\,|x| < 1$$

Harmonic approximation continue..



$$V(x) = \frac{1}{2!}V''(x_0)(x - x_0)^2 = \frac{1}{2}k(x - x_0)^2$$

Spring constant
$k = V''(x_0)$

Frequent of vibration about the equilibrium, $\boldsymbol{\omega} = \sqrt{\frac{k}{m}}$,

For two particle system (molecule),

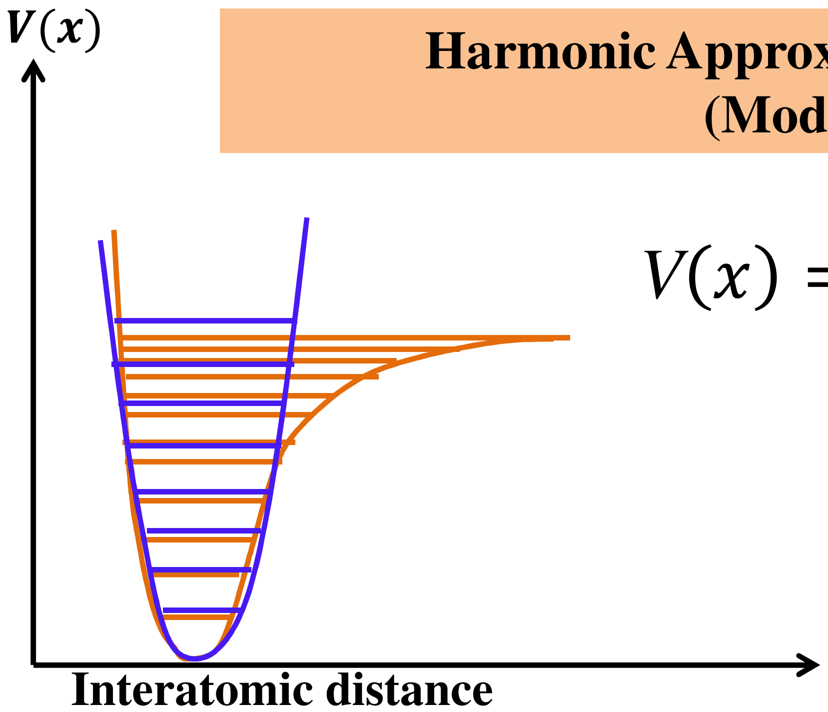
frequency of vibration $\omega = \sqrt{\frac{k}{\mu}}$

Where, *Reduced mass*(μ) *of oscillitator*

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

Harmonic approximation: Example

Harmonic Approximation to Morse Potential
(Model for a diatomic molecule!)



$$V(x) = D(1 - e^{-\alpha(x-x_0)})^2$$

$$V(x_0) = 0$$
$$V(\propto) = D$$

To break the molecule one has to supply energy D. This is a convenient model for diatomic molecules.

Harmonic approximation: Morse Potential

First find the equilibrium

$$V'(x) = 2D\alpha\left(1 - e^{-\alpha(x-x_0)}\right)\ \ e^{-\alpha(x-x_0)} = 0$$

Solving, at equilibrium $x = x_0$

Now $V''(x) = 2D\alpha\left(-\alpha e^{-\alpha(x-x_0)} + 2\alpha e^{-2\alpha(x-x_0)}\right)$

At equilibrium $V''(x_0) = 2D\alpha^2 \approx k$

$$\boldsymbol{\omega = \sqrt{\frac{k}{\mu}} = \alpha\sqrt{2D/\mu}}$$

Work and potential energy in 3D

1D motion: Displacement and force are along the same line
Work done by force

$$\boldsymbol{dW = F\,dx = -dV}$$

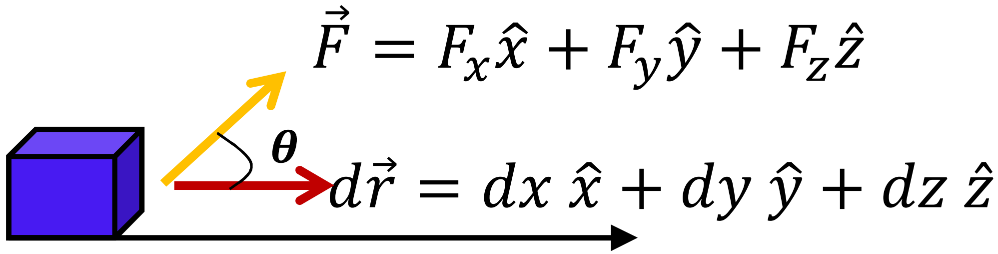
Thus, $\boldsymbol{F = -\frac{dV}{dx}}$

3D motion: Displacement and force are in different directions

$$\boldsymbol{dW = F\cos\theta\,dr}$$

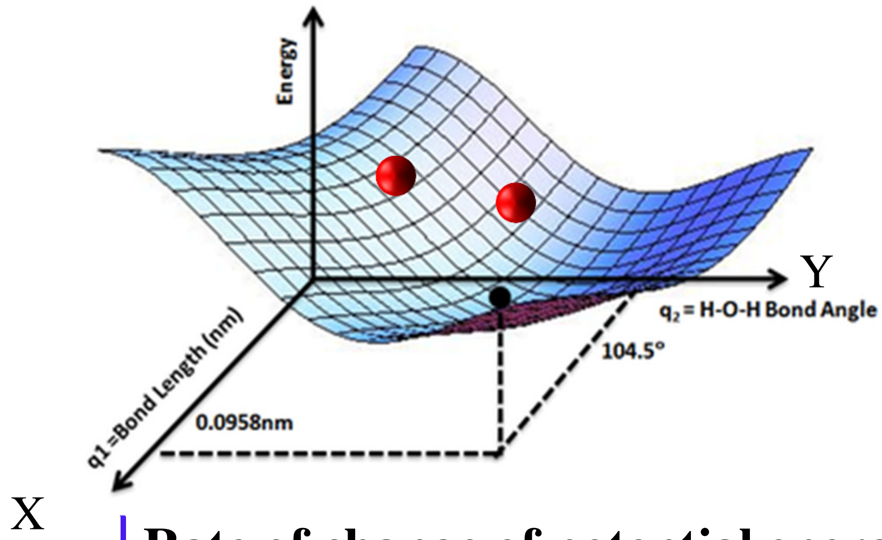
$$\boldsymbol{dW = \vec{F}\cdot d\vec{r} = F_x dx + F_y dy + F_z dz}$$
$$\boldsymbol{= -dV}$$

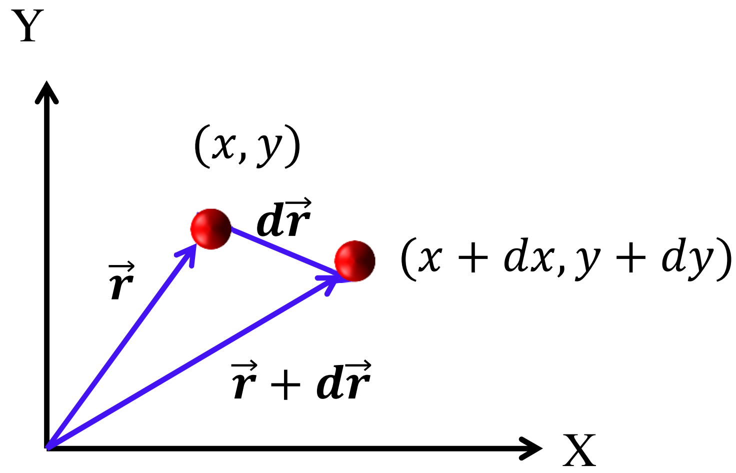
$$\boldsymbol{\vec{F} = ?}$$



$$\boldsymbol{dV = -\vec{F}\cdot d\vec{r} = -(F_x dx + F_y dy + F_z dz)}$$

dV in 2D and 3D?





Rate of change of potential energy is different in different directions

Total change in potential energy due to change of x by dx and y by dy

$$dV = \frac{\partial V}{\partial x}dx + \frac{\partial V}{\partial y}dy$$

3D: Since, $V(x, y, z)$

$$dV = \frac{\partial V}{\partial x}dx + \frac{\partial V}{\partial y}dy + \frac{\partial V}{\partial z}dz$$

Potential energy in 3D

We can write

$$dV = \frac{\partial V}{\partial x}dx + \frac{\partial V}{\partial y}dy + \frac{\partial V}{\partial z}dz$$

$$= \left(\frac{\partial V}{\partial x}\hat{x} + \frac{\partial V}{\partial y}\hat{y} + \frac{\partial V}{\partial z}\hat{z}\right) \cdot (\hat{x}dx + \hat{y}dy + \hat{z}dz)$$

$$dV = \left(\frac{\partial}{\partial x}\hat{x} + \frac{\partial}{\partial y}\hat{y} + \frac{\partial}{\partial z}\hat{z}\right)V \cdot (\hat{x}dx + \hat{y}dy + \hat{z}dz)$$

$$dV = \vec{\nabla}V \cdot d\vec{r}$$

$\vec{\nabla}$ symbols stands for an operator $\vec{\nabla} = \frac{\partial}{\partial x}\hat{x} + \frac{\partial}{\partial y}\hat{y} + \frac{\partial}{\partial z}\hat{z}$

$\vec{\nabla}V$ -this operation is know as gradient of V

Since, $dV = -\vec{F} \cdot d\vec{r}$

$$\vec{F} = -\vec{\nabla}V$$

$$F_x = -\frac{\partial V}{\partial x} \qquad F_y = -\frac{\partial V}{\partial y} \qquad F_z = -\frac{\partial V}{\partial z}$$

Gradient in plane polar!

Let we have, $V(r, \theta)$

$$dV = \frac{\partial V}{\partial r} dr + \frac{\partial V}{\partial \theta} d\theta \qquad \text{(by rule!)}$$

But, $$dV = -\vec{F} \cdot d\vec{r} = -\left(F_r \hat{r} + F_\theta \hat{\theta}\right) \cdot \left(dr\,\hat{r} + r d\theta\,\hat{\theta}\right)$$

$$= -\left(F_r dr + F_\theta r d\theta\right)$$

$$F_r = -\frac{\partial V}{\partial r} \qquad \& \qquad F_\theta = -\frac{1}{r}\frac{\partial V}{\partial \theta}$$

Or, $$dV = \vec{\nabla} V \cdot d\vec{r} = -\left(F_r \hat{r} + F_\theta \hat{\theta}\right)$$

$$\Rightarrow \qquad \vec{\nabla} = \frac{\partial(\ )}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial(\ )}{\partial \theta}\hat{\theta} \qquad \text{(in plane polar)}$$

Note: Conservative vs non-conservative forces

$\vec{\boldsymbol{F}} = -\vec{\boldsymbol{\nabla}}\boldsymbol{V}$ (true only for conservative forces ?)

Let's review how we have arrived to this relation:
We have assumed that
Work done by the force is entirely stored in the system as potential energy,
$-\,dW = dV$

Work done by all type of forces do not converted to potential energy stored in the system, it may lost by dissipation in the form of heat, sound etc. Those forces are dissipative force/non-conservative force, **Example: Friction**

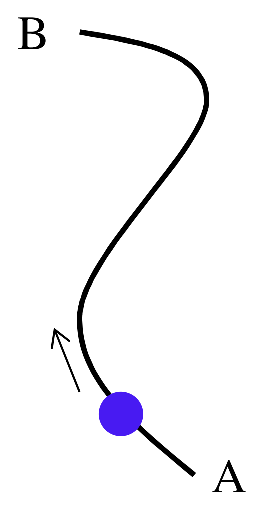
Work done by dissipative force dW $= \vec{f}\cdot d\vec{r} \neq dV,$
$Energy\ is\ not\ stored\ as\ potential\ energy.$

Hence $\vec{f} \neq -\vec{\nabla}V$
$T + V \neq constant$ when a particle is under dissipative forces. Thus they are non-conservative force.

Note: Conservative force

Is the force always derivable from scalar potential $\vec{F} = -\vec{\nabla}V$?
Answer is no, all forces are not derivable from scalar potential.

Those forces which are derivable from scalar potential ($\vec{F} = -\vec{\nabla}V$) are known as **conservative force**.



Work done due to motion from A to B

$$dW = \vec{F}\cdot d\vec{r} = -\vec{\nabla}V\cdot d\vec{r} = -dV\ ;\ thus\ W = -\int_A^B dV = V_A - V_B$$

$$Agian, dW = \vec{F}\cdot d\vec{r} = m\frac{d\vec{v}}{dt}.d\vec{r} = m\frac{d\vec{v}}{dt}\cdot\vec{v}dt = \frac{1}{2}md(\vec{v}\cdot\vec{v}) = \frac{1}{2}m\,d(v^2)$$

$$\boldsymbol{W = \int_A^B \frac{1}{2}m\,d(v^2) = \frac{1}{2}m{v_B}^2 - \frac{1}{2}m{v_A}^2\ (= Change\ in\ K.E.)}$$

Thus, $V_A - V_B = \frac{1}{2}\boldsymbol{m{v_B}^2} - \frac{1}{2}\boldsymbol{m{v_A}^2} \Rightarrow V_A + \frac{1}{2}\boldsymbol{m{v_A}^2} = V_B + \frac{1}{2}\boldsymbol{m{v_B}^2}$

Energy conserved (True for conservative force)

Conservative forces

For a conservative force $\vec{F} = -\vec{\nabla}V$, where $\vec{\boldsymbol{\nabla}} = \frac{\partial}{\partial x}\hat{\boldsymbol{x}} + \frac{\partial}{\partial y}\hat{\boldsymbol{y}} + \frac{\partial}{\partial z}\hat{\boldsymbol{z}}$

For a conservative force what will be the value of $\vec{\nabla} \times \vec{F}$?

Let's remember that: $\vec{A} \times \vec{B} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ A_x & A_y & A_z \\ B_x & B_y & \boldsymbol{F}_z \end{vmatrix}$

❑ "**Curl**" of a vector in Cartesian

$$\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{F}} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F_x & F_y & F_z \end{vmatrix} = \hat{x}\left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z}\right) + \hat{y}\left(\frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x}\right) + \hat{z}\left(\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y}\right)$$

$$\frac{\partial \boldsymbol{F_z}}{\partial \boldsymbol{y}} = \frac{\partial(-\frac{\partial V}{\partial z})}{\partial y} = -\frac{\partial^2 V}{\partial y \partial z} \;\; \& \;\; \frac{\partial \boldsymbol{F_y}}{\partial \boldsymbol{z}} = \frac{\partial(\frac{-\partial V}{\partial y})}{\partial z} = -\frac{\partial^2 V}{\partial z \partial y}$$

But, $\dfrac{\partial^2 V}{\partial x \partial y} = \dfrac{\partial^2 V}{\partial y \partial x}$

(***order is immeterial by rule***!)

For a conservative force: $\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{F}} = \boldsymbol{0}$

Summery

- **Taylor series expansion of a potential in 1D**

$$\mathbf{V}(\boldsymbol{x}) = \boldsymbol{V}(\boldsymbol{x_0}) + \boldsymbol{V'}(\boldsymbol{x_0})(\boldsymbol{x}-\boldsymbol{x_0}) + \frac{1}{2!}\boldsymbol{V''}(\boldsymbol{x_0})(\boldsymbol{x}-\boldsymbol{x_0})^2 + \boldsymbol{O}(3)$$

Here $\boldsymbol{V'}(\mathbf{x}) = \frac{\boldsymbol{dU}}{\boldsymbol{dx}}$ **and** $\mathbf{V''}(\mathbf{x}) = \frac{\boldsymbol{d^2V}}{\boldsymbol{dx^2}}$

Harmonic approximation consider only upto square term

Frequency of oscillation $\omega = \sqrt{\frac{k}{\mu}}$, $\quad k = \boldsymbol{U''}(\boldsymbol{x_0})$, and μ is the reduced mass.

So, **if**

$$\vec{\boldsymbol{F}} = -\vec{\boldsymbol{\nabla}}\boldsymbol{V} \qquad \text{(“gradient” of V)}$$

“Curl” of F, $\quad \vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{F}} = \mathbf{0} \quad$ (always!)

Curl of gradient is always zero $\left(\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{\nabla}}\boldsymbol{f} = \mathbf{0}\right)$ **(for any scalar function)**

Questions ?