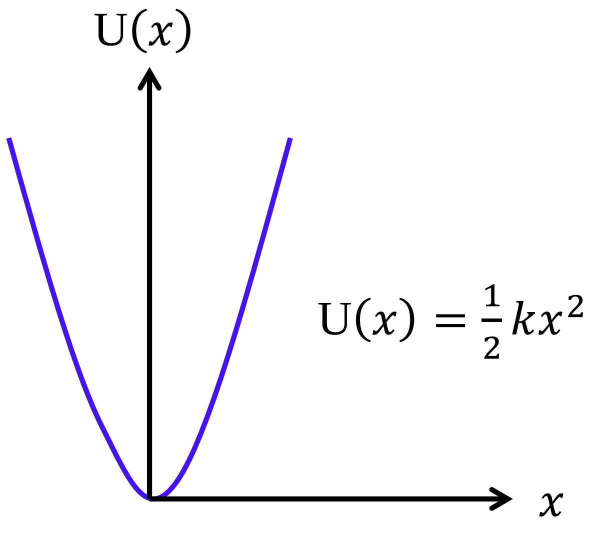
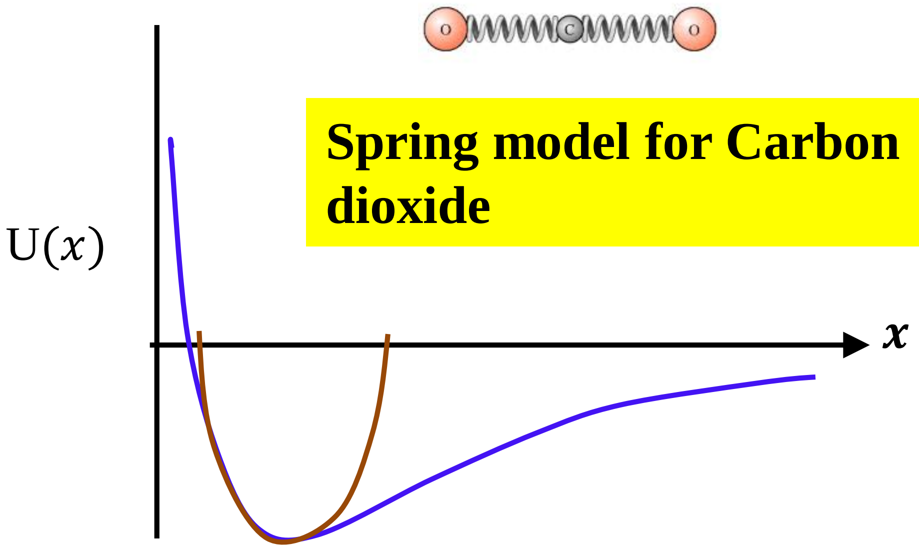
PH101: PHYSICS 1

Lecture 4

Harmonic approximation of potential energy





Spring model for Carbon dioxide

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 effectively hard to solve.

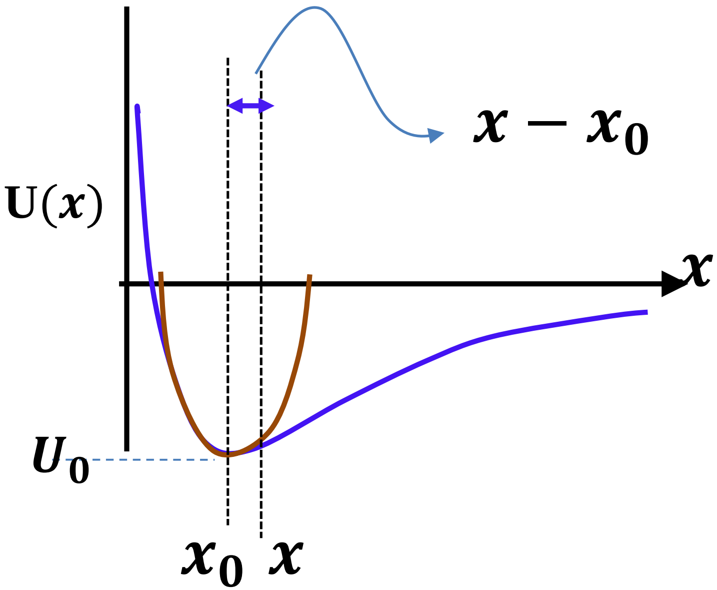
Harmonic approximation

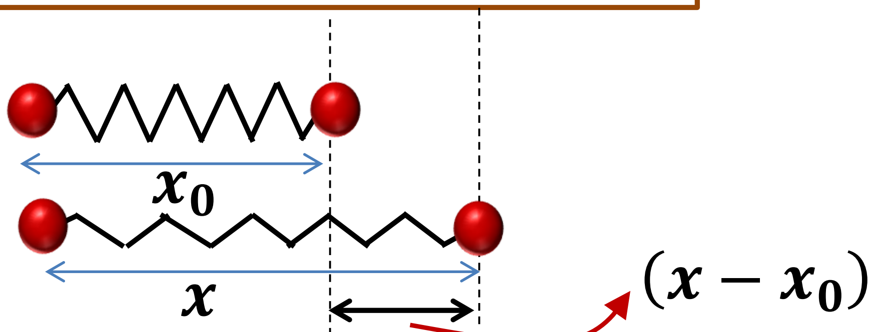
Taylor series expansion

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

We use $\boldsymbol{U'}(\mathbf{x}) = \frac{d\boldsymbol{U}}{d\boldsymbol{x}}$ and $\mathrm{U''}(\mathbf{x}) = \frac{d^2\boldsymbol{U}}{d\boldsymbol{x}^2}$

- Here we are taking the expansion around the equilibrium distance x_0. Hence $U'(x_0) = 0$, since the force is zero (potential has an extremum).
- Let us assume that $U(x_0) = 0$; potential at equilibrium (reference) is zero.





Taylor series/expansion Examples:

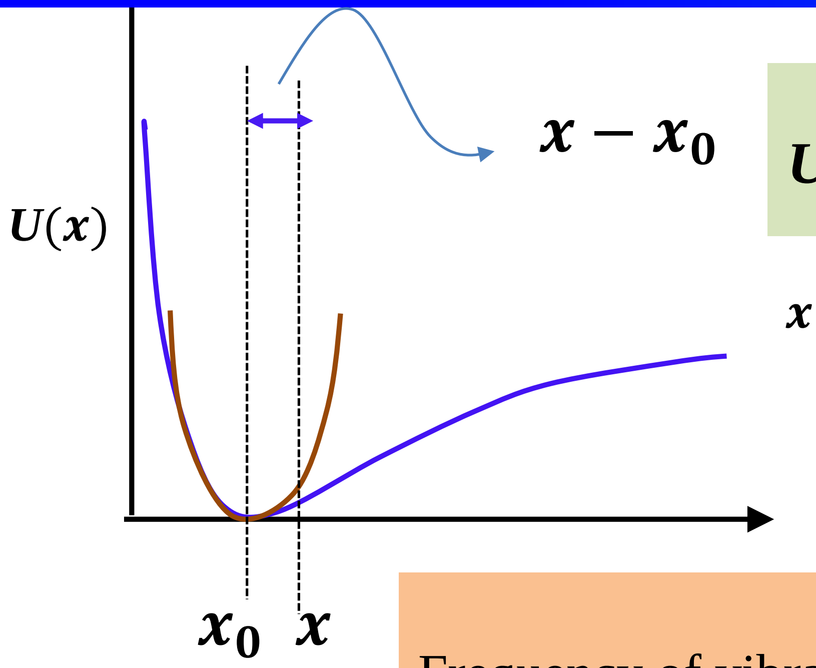
$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots$$

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

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

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

Harmonic approximation continue..



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

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

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

For two particle system (molecule),

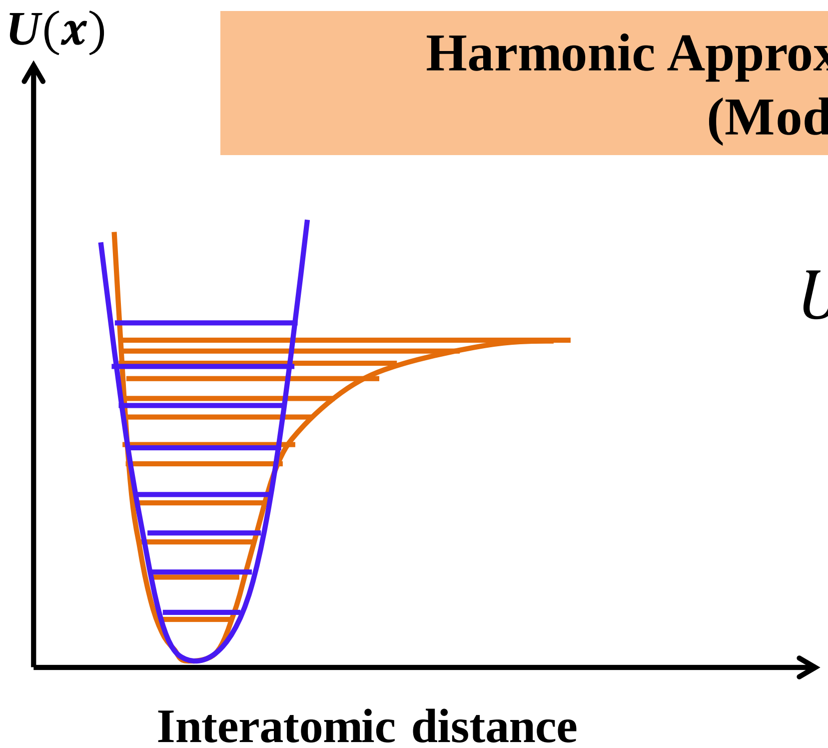
$$\text{Frequency of vibration} \;\; \omega = \sqrt{\frac{k}{\mu}}$$

where r*educed mass* (μ) *of oscillitator* is

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

Harmonic approximation: Example

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



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

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

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

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

Solving at equilibrium $x = x_0$

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

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

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

Work and potential energy in 3D

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

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

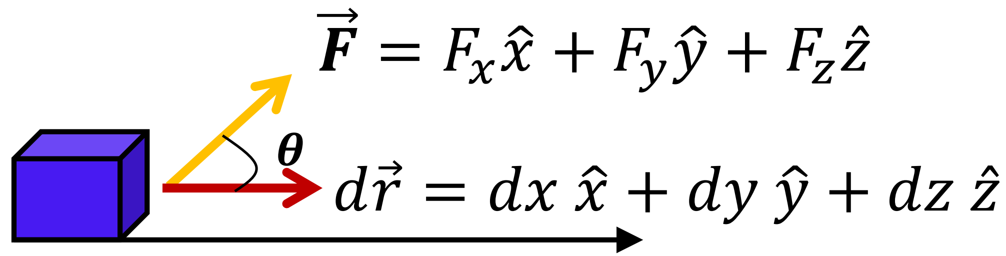
Thus, $\boldsymbol{F = -\frac{dU}{dx}}$

3D motion: Displacement and force are in different directions

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

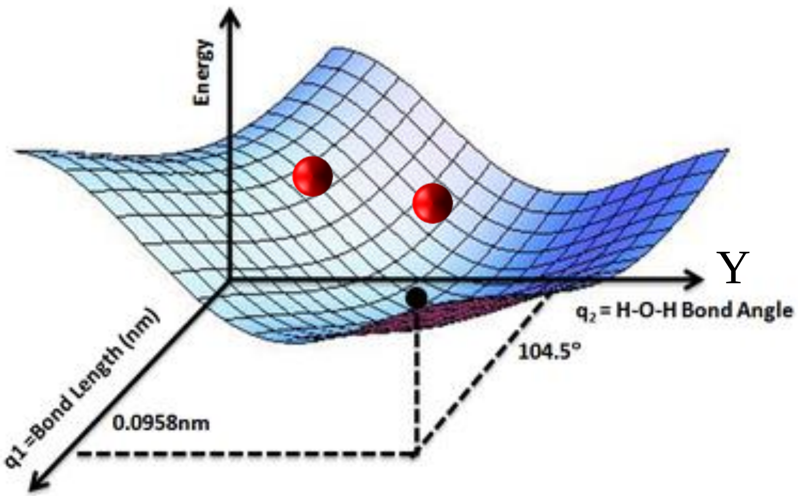
$$\boldsymbol{dW = \vec{F}\cdot d\vec{r} = F_x dx + F_y dy + F_z dz}$$
$$\boldsymbol{= -dU}$$

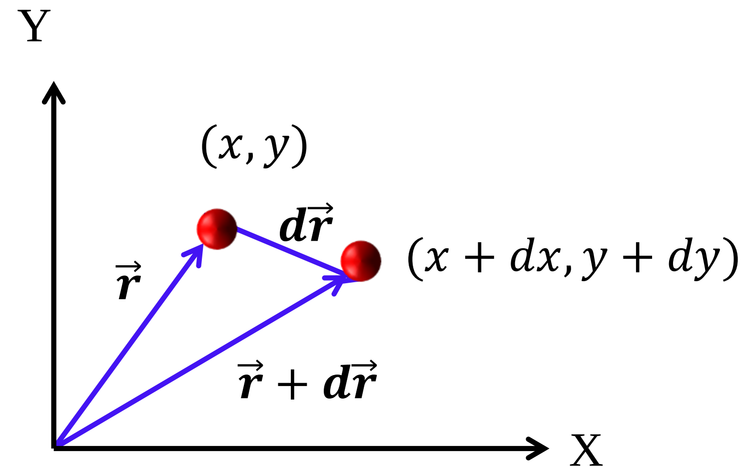
$$\vec{\boldsymbol{F}} = ?$$



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

dU 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

$$\boldsymbol{dU = \frac{\partial U}{\partial x} dx + \frac{\partial U}{\partial y} dy}$$

3D: Since, $\boldsymbol{U(x, y, z)}$

$$\boldsymbol{dU = \frac{\partial U}{\partial x} dx + \frac{\partial U}{\partial y} dy + \frac{\partial U}{\partial z} dz}$$

Potential energy in 3D

We can write

$$dU = \frac{\partial U}{\partial x}dx + \frac{\partial U}{\partial y}dy + \frac{\partial U}{\partial z}dz$$

$$= \left(\frac{\partial U}{\partial x}\hat{x} + \frac{\partial U}{\partial y}\hat{y} + \frac{\partial U}{\partial z}\hat{z}\right)\cdot(\hat{x}dx + \hat{y}d\mathrm{y} + \hat{z}dz)$$

$$dU = \left(\frac{\partial}{\partial x}\hat{x} + \frac{\partial}{\partial y}\hat{y} + \frac{\partial}{\partial z}\hat{z}\right)U\cdot(\hat{x}dx + \hat{y}d\mathrm{y} + \hat{z}dz)$$

$$dU = \vec{\nabla}U\cdot d\vec{r}$$

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

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

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

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

$$F_{\mathrm{x}} = -\frac{\partial U}{\partial x} \qquad F_{\mathrm{y}} = -\frac{\partial U}{\partial y} \qquad F_{\mathrm{z}} = -\frac{\partial U}{\partial z}$$

Gradient in plane polar

Suppose we have, $U(r, \theta)$

$$dU = \frac{\partial U}{\partial r} dr + \frac{\partial U}{\partial \theta} d\theta$$ (by rule!)

$$\vec{\nabla} U = \frac{\partial U}{\partial r} \hat{r} + \frac{1}{r} \frac{\partial U}{\partial \theta} \hat{\theta}$$

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

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

$$F_r = -\frac{\partial U}{\partial r}$$

$$F_\theta = -\frac{1}{r} \frac{\partial U}{\partial \theta}$$

Gradient in Cylindrical

Suppose we have, $U(r, \theta, z)$

$$dU = \frac{\partial U}{\partial r} dr + \frac{\partial U}{\partial \theta} d\theta + \frac{\partial U}{\partial z} dz \qquad \text{(by rule!)}$$

$$\vec{\nabla} U = \frac{\partial U}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial U}{\partial \theta}\hat{\theta} + \frac{\partial U}{\partial z}\hat{z}$$

$$dU = -\vec{F}\cdot d\vec{r} = -\left(F_r\hat{r} + F_\theta\hat{\theta} + F_z\hat{z}\right)\cdot\left(dr\,\hat{r} + r\,d\theta\,\hat{\theta} + dz\,\hat{z}\right)$$

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

$$F_r = -\frac{\partial U}{\partial r}, \quad F_\theta = -\frac{1}{r}\frac{\partial U}{\partial \theta}, \quad F_z = -\frac{\partial U}{\partial z}$$

Gradient in Sperical Polar

Suppose we have, $U(r, \theta, \varphi)$

$$dU = \frac{\partial U}{\partial r} dr + \frac{\partial U}{\partial \theta} d\theta + \frac{\partial U}{\partial \varphi} d\varphi$$ (by rule!)

$$\vec{\nabla} U = \frac{\partial U}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial U}{\partial \theta}\hat{\theta} + \frac{1}{r sin\theta}\frac{\partial U}{\partial \varphi}\hat{\varphi}$$

$$dU = -\vec{F} \cdot d\vec{r}$$

$$= -\left(F_r\hat{r} + F_\theta\hat{\theta} + F_\varphi\hat{\varphi}\right) \cdot (dr\,\hat{r} + r d\theta\hat{\theta} + r\, sin\theta\, d\varphi\, \hat{\varphi})$$

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

$$F_r = -\frac{\partial U}{\partial r}, F_\theta = -\frac{1}{r}\frac{\partial U}{\partial \theta}, F_\varphi = -\frac{1}{r\, sin\theta}\frac{\partial U}{\partial \varphi}$$

Note: Conservative vs non-conservative forces

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

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

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

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

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

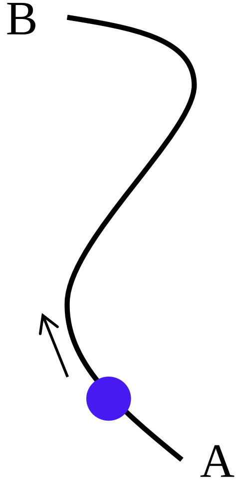
Note: Conservative force

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

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

Work done due to motion from A to B

$$dW = \vec{F} \cdot d\vec{r} = -\vec{\nabla}U \cdot d\vec{r} = -dU \text{ ; thus } W = -\int_A^B dU = U_A - U_B$$



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

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

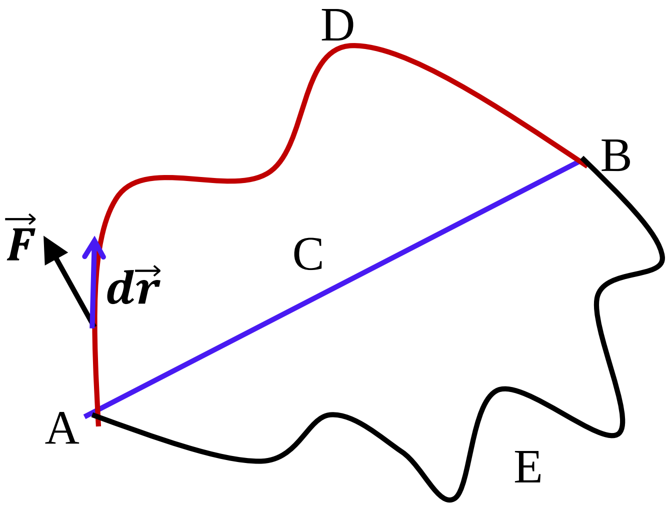
Thus, $U_A - U_B = \boldsymbol{\frac{1}{2} m{v_B}^2 - \frac{1}{2} m{v_A}^2} \Rightarrow U_A + \boldsymbol{\frac{1}{2} m{v_A}^2} = U_B + \boldsymbol{\frac{1}{2} m{v_B}^2}$

***Energy conserved** (**True for conservative force**)*

Conservative force: Work done is independent of path

Total work done, when a particle moves from A to B along ADB

$$W_{ADB} = \int_A^B \vec{F} \cdot d\vec{r} = \int_A^B -\vec{\nabla} U \cdot d\vec{r} = \int_A^B -dU$$
$$= U_A - U_B$$



Important: Work done only depends on potential at the end points A and B if the force is conservative.

$$W_{ADB} = W_{ACB} = W_{AEB}$$

Conservative forces

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

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

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

❑ **"Curl"** of a vector in Cartesian

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

$$\frac{\boldsymbol{\partial F_z}}{\boldsymbol{\partial y}} = \frac{\boldsymbol{\partial}\left(\frac{\boldsymbol{\partial U}}{\boldsymbol{\partial z}}\right)}{\boldsymbol{\partial y}} = \frac{\boldsymbol{\partial^2 U}}{\boldsymbol{\partial y \partial z}} \quad \& \quad \frac{\boldsymbol{\partial F_y}}{\boldsymbol{\partial z}} = \frac{\boldsymbol{\partial}\left(\frac{\boldsymbol{\partial U}}{\boldsymbol{\partial y}}\right)}{\boldsymbol{\partial z}} = \frac{\boldsymbol{\partial^2 U}}{\boldsymbol{\partial z \partial y}}$$

But, $\frac{\boldsymbol{\partial^2 U}}{\boldsymbol{\partial x \partial y}} = \frac{\boldsymbol{\partial^2 U}}{\boldsymbol{\partial y \partial x}}$

(***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**

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

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

Harmonic approximation consider only upto square term

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

- **Work done by a force**

$$W = \int \vec{F} \cdot d\vec{r}\,;$$ **if the force is conservative**

$$\vec{\boldsymbol{F}} = -\vec{\boldsymbol{\nabla}}\boldsymbol{U}$$ (“**gradient**” of U)

“Curl” of F, $$\vec{\boldsymbol{\nabla}} \times \vec{\boldsymbol{F}} = \mathbf{0}$$

Questions ?