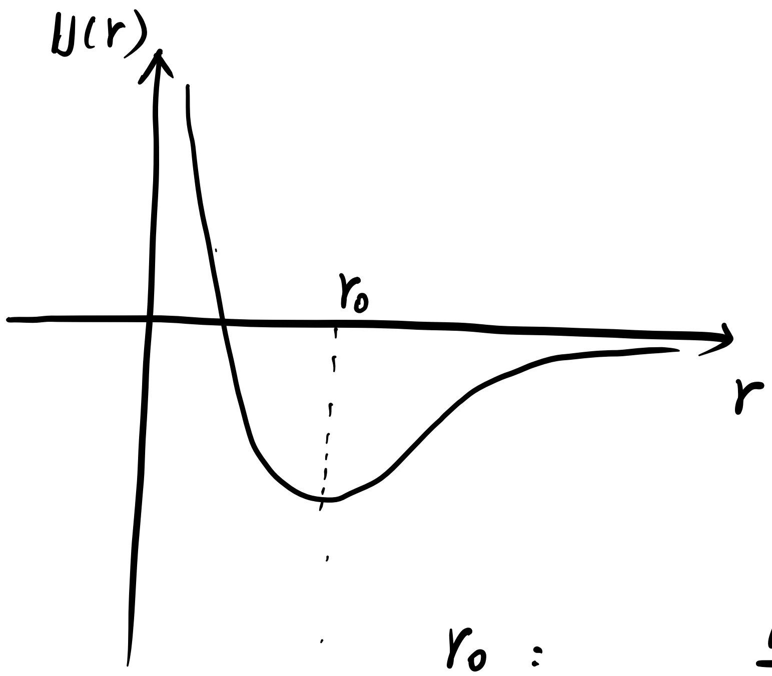
分子力势能曲线



r_0 : $\frac{dU(r)}{dr} = 0$

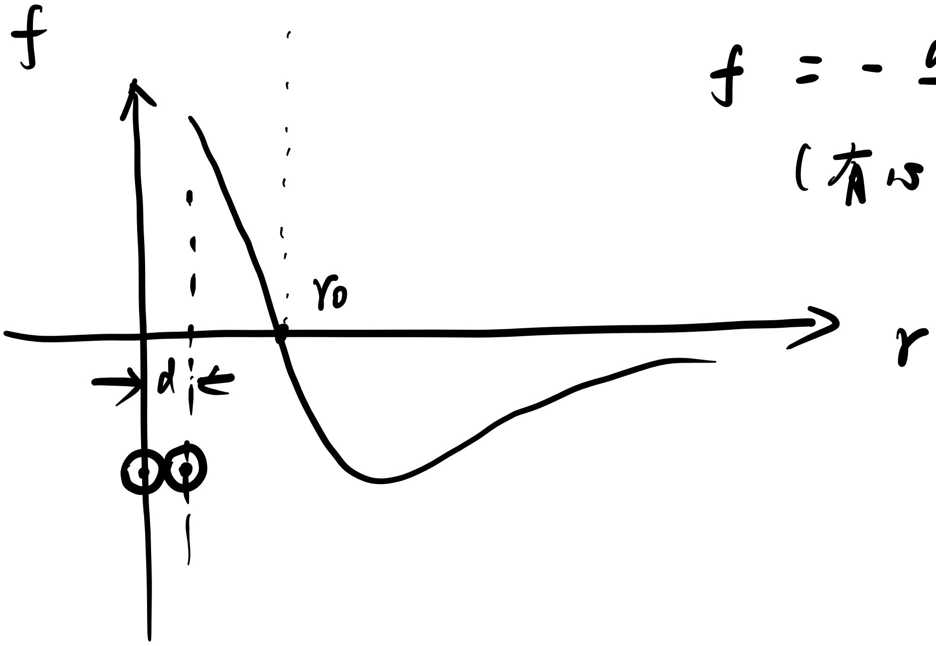
平衡位置

分子力

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

$f = -\frac{dU}{dr}$

(有心力)



问：$\vec{F} = \vec{i}\,x^2y^3 + \vec{j}\,xy^2$

是个保守力吗？

if $\vec{F}$ is a conservative force

$F_x = -\frac{\partial U}{\partial x}$, $F_y = -\frac{\partial U}{\partial y}$

观察 $\vec{i}$ 分量

$U \sim x^3y^3$

观察 $\vec{j}$ 分量

$U \sim xy^3$

no such U to satisfy the two components

$$\frac{\partial U}{\partial y\,\partial x} = -\frac{\partial F_x}{\partial y}$$

$||$

$$\frac{\partial U}{\partial x \, \partial y} = - \frac{F_y}{\partial x} \Rightarrow$$

$$\boxed{\frac{F_x}{\partial y} = \frac{F_y}{\partial x} \quad (\text{判据})}$$

势能函数仅依赖位置

dE_p：在数学上意味着

它是一个全微分

这样的被积函数将与路径无关

积分结果仅与出发点，目的地相关

冲过微分 again ^◡^

Linear approximation

$$F(y) = F(y_0) + F'(y_0)(y-y_0)$$

Taylor expansion:

$$F(y) = F(y_0) + F'(y_0)(y-y_0) + \frac{1}{2} F''(y_0)(y-y_0)^2$$

$$+ \cdots + \frac{1}{n!} F^n(y_0)(y-y_0)^n + \cdots$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} F^{(n)}(y_0)(y-y_0)^n$$

y 在 y_0 邻域，$\Delta y = y - y_0$ (smallness)

$(\Delta y)^n$：高阶(n)小量

$$\nabla \equiv \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$$

$$\frac{\partial f(x,y,z)}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x, y, z) - f(x,y,z)}{\Delta x}$$

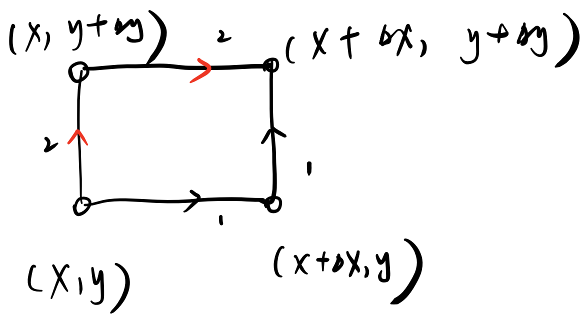
partial derivative

(here, y, z keep invariant)

gradient (∇)：上升最快的方向 (势函数)

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

$\vec{F}$ ：其方向是势的下降最快的方向



路径1： $f(x+\Delta x, y+\Delta y) - f(x,y)$

$$= f(x+\Delta x, y+\Delta y) - f(x+\Delta x, y) + f(x+\Delta x, y) - f(x,y)$$

$$= \underbrace{\left.\frac{\partial f}{\partial y}\right|_{x+\Delta x, y} \Delta y}_{①} + \underbrace{\left.\frac{\partial f}{\partial x}\right|_{x, y} \Delta x}_{②}$$

路径2： $f(x+\Delta x, y+\Delta y) - f(x,y)$

$$= f(x+\Delta x, y+\Delta y) - f(x, y+\Delta y)$$

$$+ f(x, y+\Delta y) - f(x, y))$$

$$= \left.\frac{\partial f}{\partial x}\right|_{x, y+\Delta y} \Delta x + \left.\frac{\partial f}{\partial y}\right|_{x, y} \Delta y$$

$$③ \qquad ④$$

$$① + ② - ③ - ④ = 0$$

$$① - ④ = \frac{\partial}{\partial x}\frac{\partial f}{\partial y} \Delta x \Delta y$$

$$② - ③ = - \frac{\partial}{\partial y}\frac{\partial f}{\partial x} \Delta y \Delta x$$

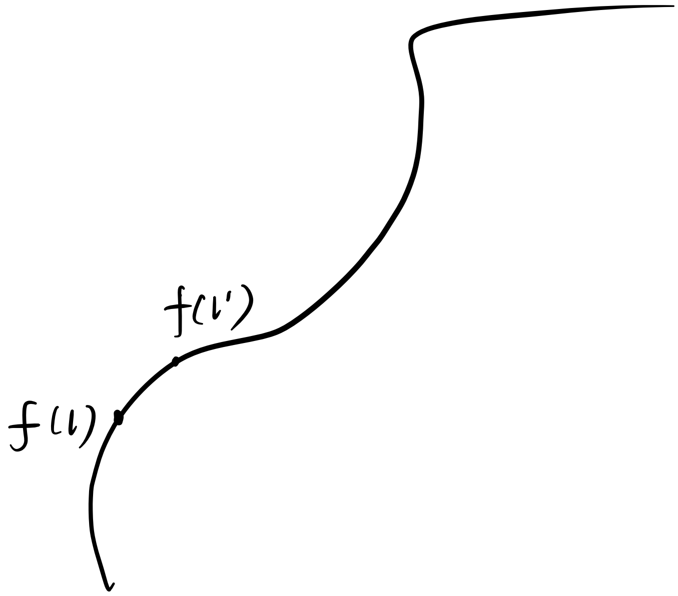
$$\Downarrow$$

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x}$$

$$\frac{\partial f}{\partial x} = - F_x , \qquad \frac{\partial f}{\partial y} = - F_y$$

$$\frac{\partial F_x}{\partial y} = \frac{\partial F_y}{\partial x}$$

方向导数：



$$\frac{df}{d\vec{l}}$$

① $= \lim_{l \to l'} \frac{f(l') - f(l)}{\Delta l} \hat{l}$

② $= (\nabla f \cdot \hat{l})\, \hat{l}$

E.g. $E_k = \frac{1}{2} m v^2 = \frac{1}{2} m \vec{v} \cdot \vec{v}$

计算 $\frac{\partial E_k}{\partial \vec{v}} = \frac{1}{2} m \left(\frac{\partial v^2}{\partial \vec{v}} \right)$

$= \frac{1}{2} m (\nabla v^2 \cdot \hat{v})\, \hat{v}$ （用等号"="②）

$= \frac{1}{2} m \left[(2 v_x \hat{i} + 2 v_y \hat{j} + 2 v_z \hat{k}) \cdot \hat{v} \right] \hat{v}$

$$= m\left[\vec{v}\cdot\hat{v}\right]\hat{v}$$

$$= m v \hat{v} = m\vec{v}$$

或者 $E_k = \frac{1}{2} m v^2$

$$\frac{\partial E_k}{\partial \vec{v}} = \frac{\partial E_k}{\partial v}\hat{v}$$ (用"="①)

根据定义 $= m v \hat{v} = m\vec{v}$

$$\int \vec{F}\cdot d\vec{r} = \int m\vec{a}\cdot d\vec{r}$$

$$= \int m\frac{d\vec{v}}{dt}\cdot d\vec{r}$$

$$= \int m\vec{v}\cdot d\vec{v}$$

$$= \int d\left(\frac{1}{2} m v^2\right) = \Delta E_k$$