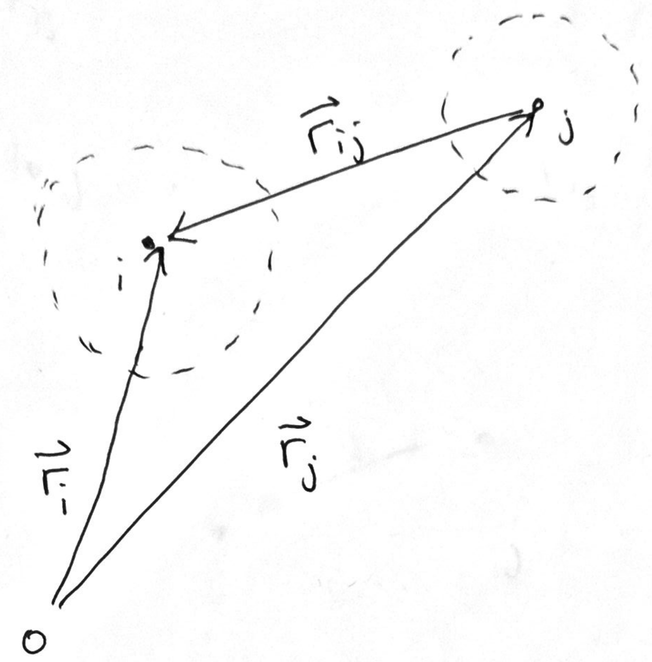
Pair Potentials



$$\vec{r}_i = \vec{r}_j + \vec{r}_{ij}$$

$$\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$$

$$= (x_i - x_j)\,\hat{x} + (y_i - y_j)\,\hat{y}$$

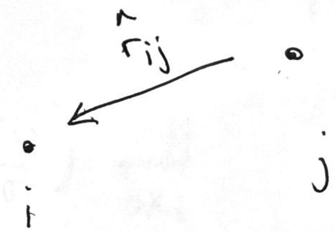
points from j to i

Central Forces

$$\vec{F}_{ij} = (\ )\,\hat{r}_{ij} \qquad \hat{r}_{ij} = \frac{\vec{r}_{ij}}{r_{ij}} = \frac{x_{ij}\,\hat{x} + y_{ij}\,\hat{y}}{r_{ij}}$$

F_{ij}

force on i due to j $\qquad \hat{r}_{ij} \cdot \hat{r}_{ij} = 1$



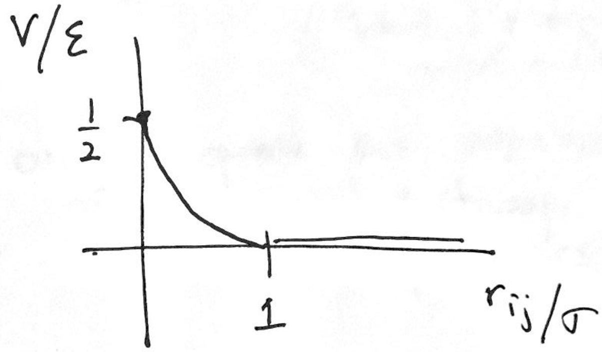
repulsive force if $\vec{F}_{ij} \propto \hat{r}_{ij}$, i.e. $F_{ij} > 0$

attractive force if $\vec{F}_{ij} \propto -\hat{r}_{ij}$, ie $F_{ij} < 0$

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

$$= -\begin{pmatrix} \frac{\partial V}{\partial x_i} \\ \frac{\partial V}{\partial y_i} \end{pmatrix}$$

$$V = \frac{\varepsilon}{2}\left(1 - \frac{r_{ij}}{\sigma}\right)^2 \theta\left(\sigma - r_{ij}\right)$$



$$\frac{\partial V}{\partial x_i} = -\frac{\varepsilon}{\sigma}\left(1 - \frac{r_{ij}}{\sigma}\right)\frac{\partial r_{ij}}{\partial x_i}$$

$$r_{ij} = \sqrt{x_{ij}^2 + y_{ij}^2}$$

$$= \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$$

$$\frac{\partial r_{ij}}{\partial x_i} = \frac{1}{2}\cdot 2\,\frac{x_{ij}}{r_{ij}} = \frac{x_{ij}}{r_{ij}}$$

$$\frac{\partial V}{\partial x_i} = -\frac{\varepsilon}{\sigma}\left(1 - \frac{r_{ij}}{\sigma}\right)\frac{x_{ij}}{r_{ij}}$$

$$\frac{\partial V}{\partial y_i} = -\varepsilon\left(1 - \frac{r_{ij}}{\sigma}\right)\frac{y_{ij}}{r_{ij}}$$

$$\vec{F}_i = +\frac{\varepsilon}{\sigma}\begin{pmatrix} \frac{x_{ij}}{r_{ij}} \\ \frac{y_{ij}}{r_{ij}} \end{pmatrix}\left(1 - \frac{r_{ij}}{\sigma}\right)$$

$$\hat{r}_{ij} = \frac{\vec{r}_{ij}}{r_{ij}} \qquad \vec{r}_{ij} = \begin{pmatrix} x_{ij} \\ y_{ij} \end{pmatrix}$$

$$\vec{F}_i = \frac{\varepsilon}{\sigma}\left(1 - \frac{r_{ij}}{\sigma}\right)\hat{r}_{ij}$$

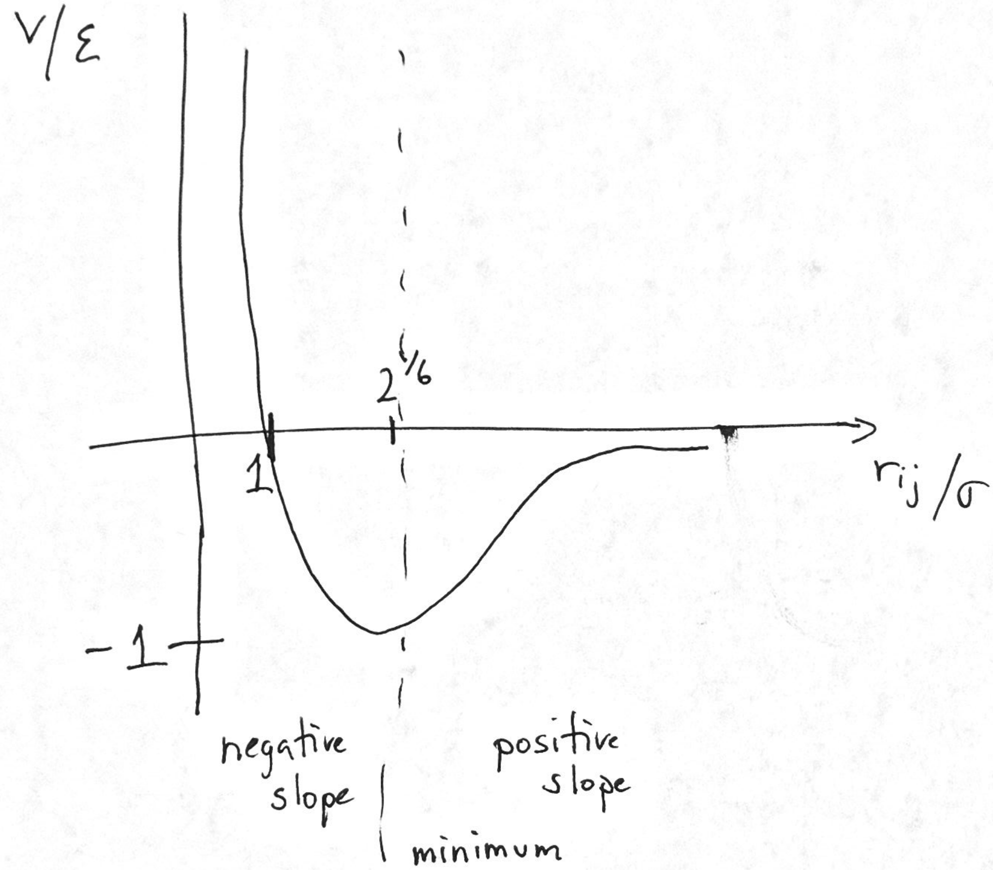
purely repulsive spring force is repulsive, (Potential always has negative slope)

For central potentials, only depend on separation between particles i an j

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

$$= -\frac{\partial V}{\partial r_{ij}}\hat{r}_{ij}$$

$$V(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$



$$\vec{F}_{ij}(r_{ij}) = -4\varepsilon\left[-12\frac{\sigma^{12}}{r_{ij}^{13}} - (-6)\frac{\sigma^{6}}{r_{ij}^{7}}\right]$$

$$= 24\frac{\varepsilon}{r_{ij}}\left[2\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] > 0$$

for $r_{ij} > 2^{1/6}\sigma$