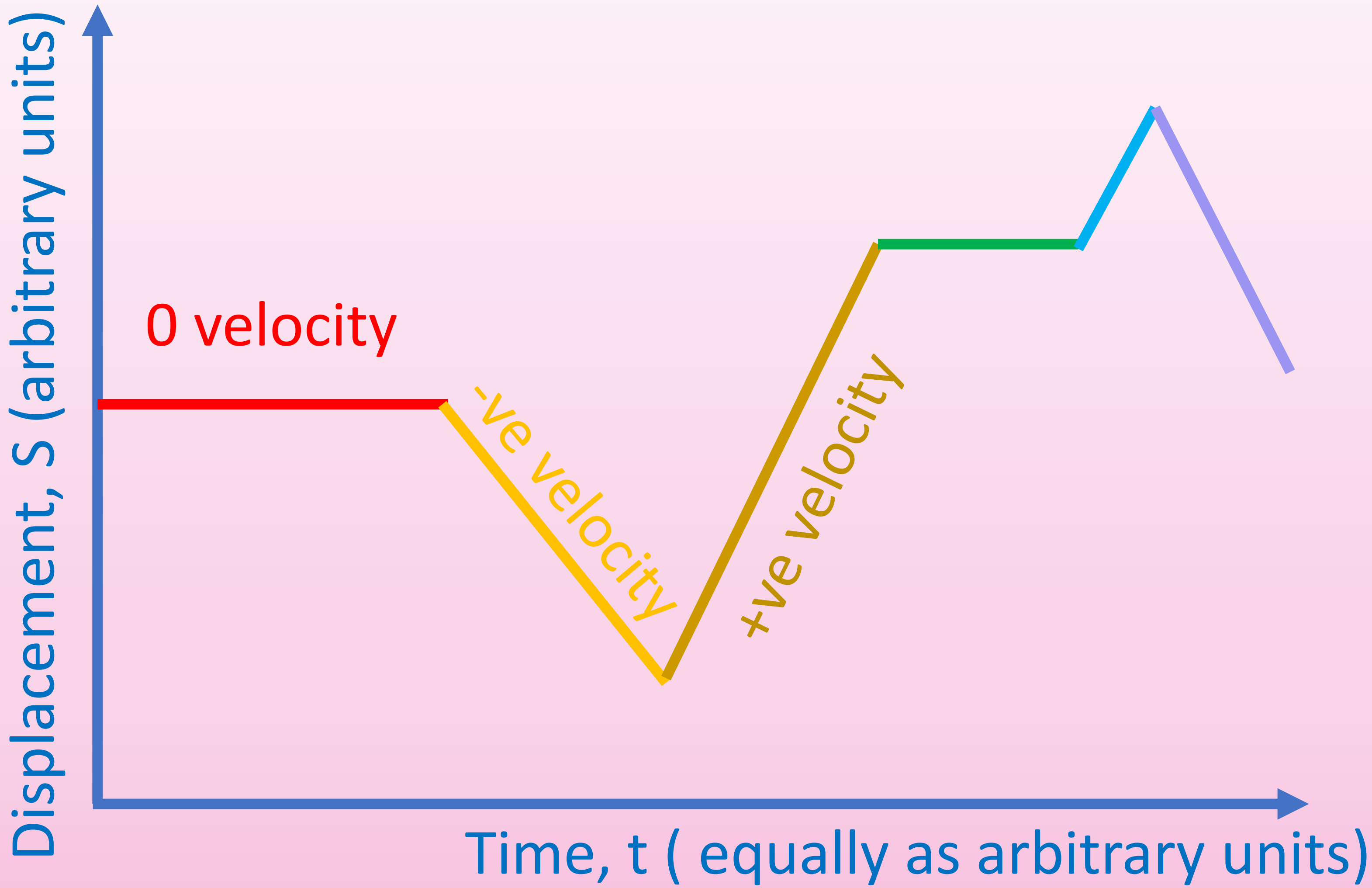
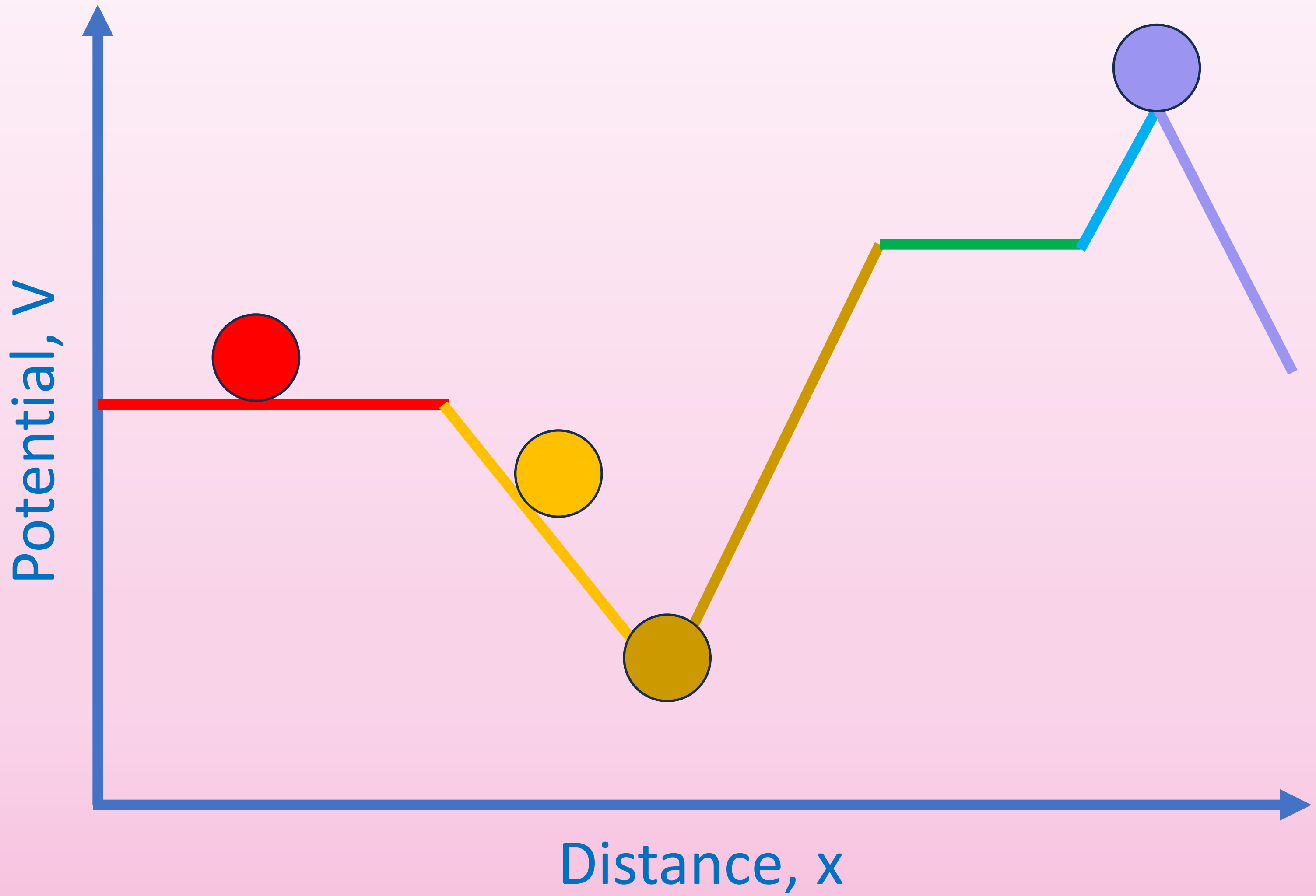
Potential-distance plots



Gradient gives velocity!

$$v = \frac{\mathrm{d}S}{\mathrm{d}t}$$

Potential-distance plots



Gradient gives force!

$$F = -\frac{\mathrm{d}V}{\mathrm{d}x}$$

Which ball(s) feel(s) a force?

Which ball(s) is/are in a stable equilibrium?

Which ball(s) is/are in an unstable equilibrium?

What must be true for our potential/force?

Derivation of A and B

$V_{LJ} = \frac{A}{r^{12}} - \frac{B}{r^6}$ => $F_{LJ} = \frac{12A}{r^{13}} - \frac{6B}{r^7}$

At equilibrium, $F_{LJ} = 0$ and r=r_0

$$\boxed{r_0 = \sqrt[6]{\frac{2A}{B}}}$$

$$A = \varepsilon\, r_0^{12}$$

$$B = 2\varepsilon\, r_0^{6}$$

Potential at equilibrium?

$$\boxed{\varepsilon = \frac{B^2}{4A}}$$

Lennard-Jones potential revisited

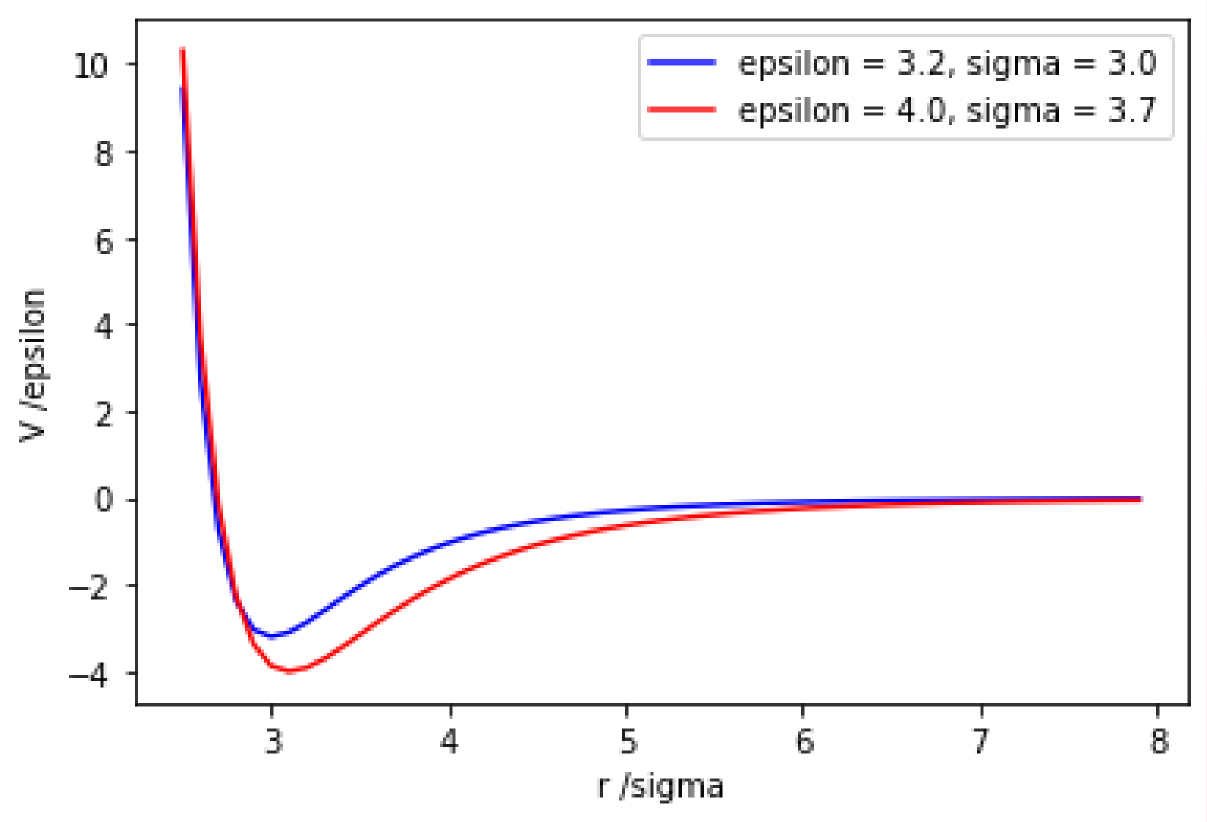
Repulsive

Attractive

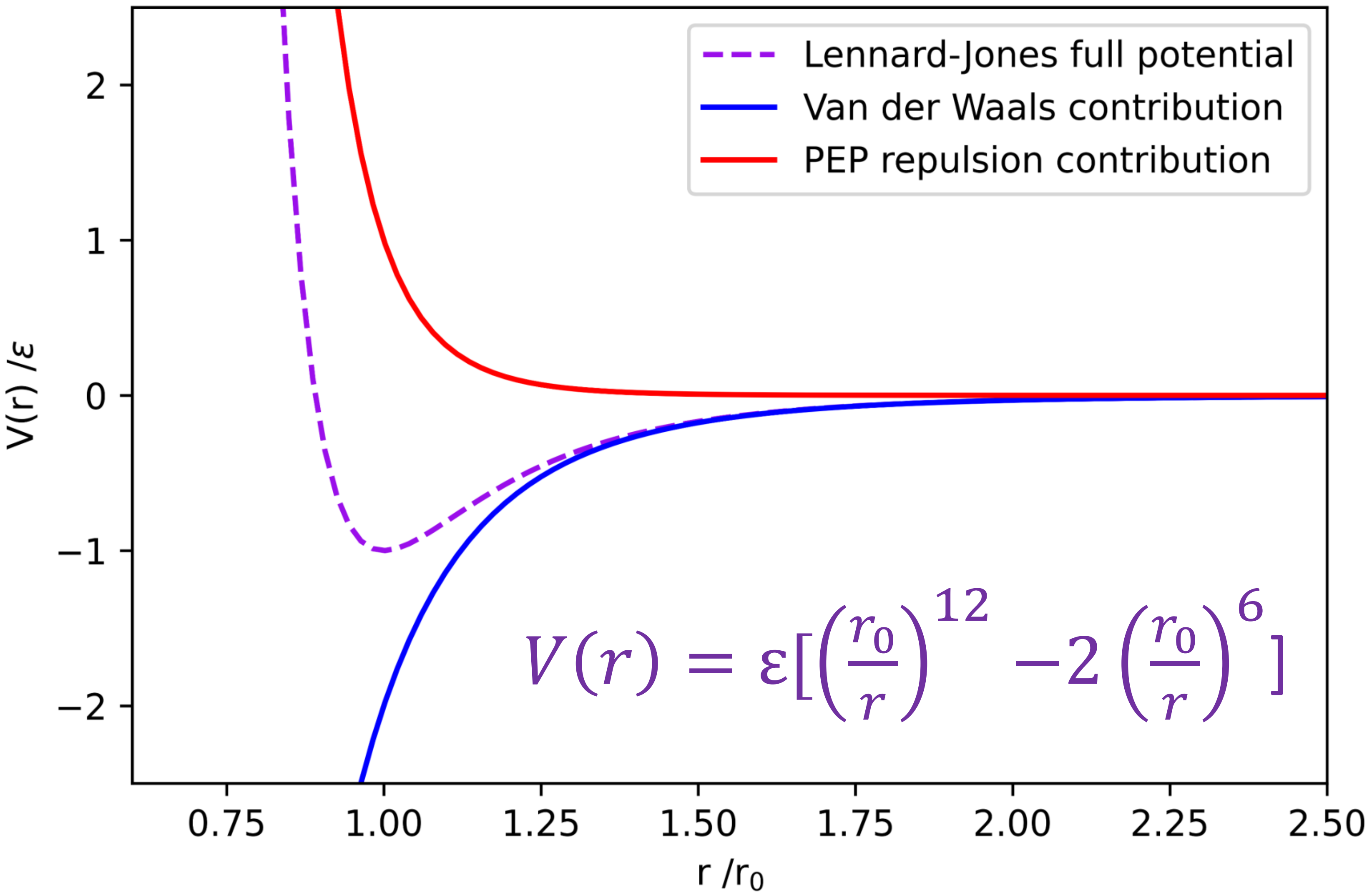
$$V_{LJ} = \frac{A}{r^{12}} - \frac{B}{r^{6}}$$

$$v_{LJ} = \varepsilon\left(\left(\frac{r_0}{r}\right)^{12} - 2\left(\frac{r_0}{r}\right)^{6}\right)$$

$$v_{LJ} = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$



Where ε is the depth of the potential well and r_0 is distance at which V = - ε (equilibrium)

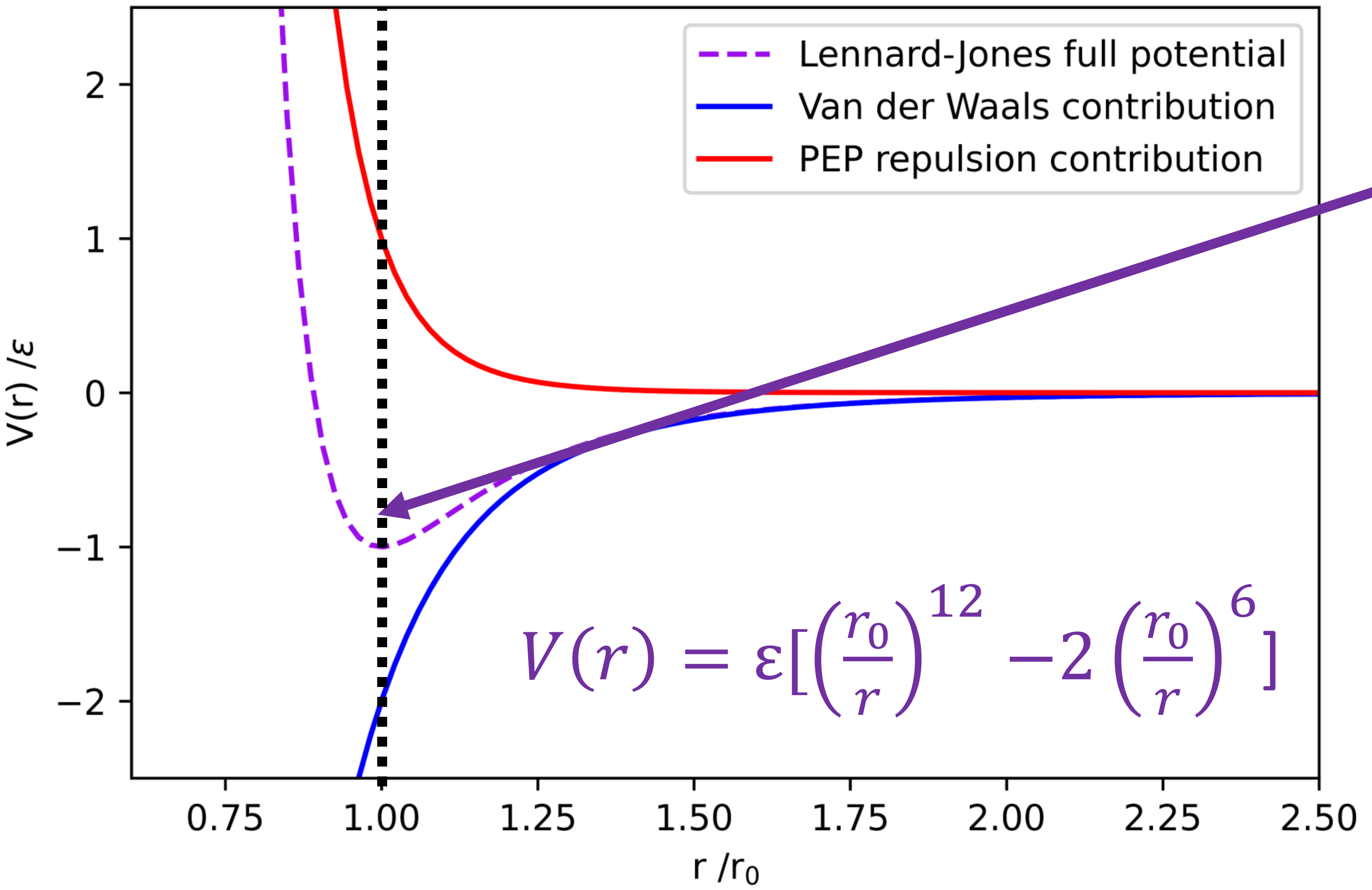


$$V(r) = \varepsilon\left[\left(\frac{r_0}{r}\right)^{12} - 2\left(\frac{r_0}{r}\right)^{6}\right]$$

$$V(r) = -2\varepsilon\left(\frac{r_0}{r}\right)^{6}$$

$$V(r) = \varepsilon\left(\frac{r_0}{r}\right)^{12}$$

Form of these potentials has V(r) = 0 at r -> ∞

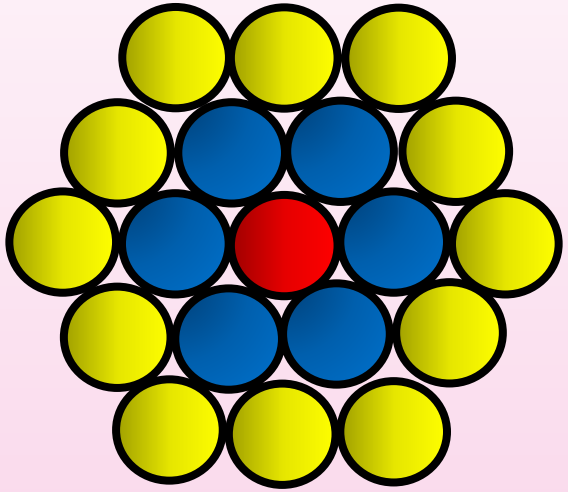


Stable equilibrium at $r = r_0$

r_0 is the spacing between particles

Require energy $-V(r_0) = \varepsilon = U_0$ to rip two atoms apart

Implications of the Lennard-Jones potential



Red – central atom
Blue – nearest neighbours
Yellow – other atoms

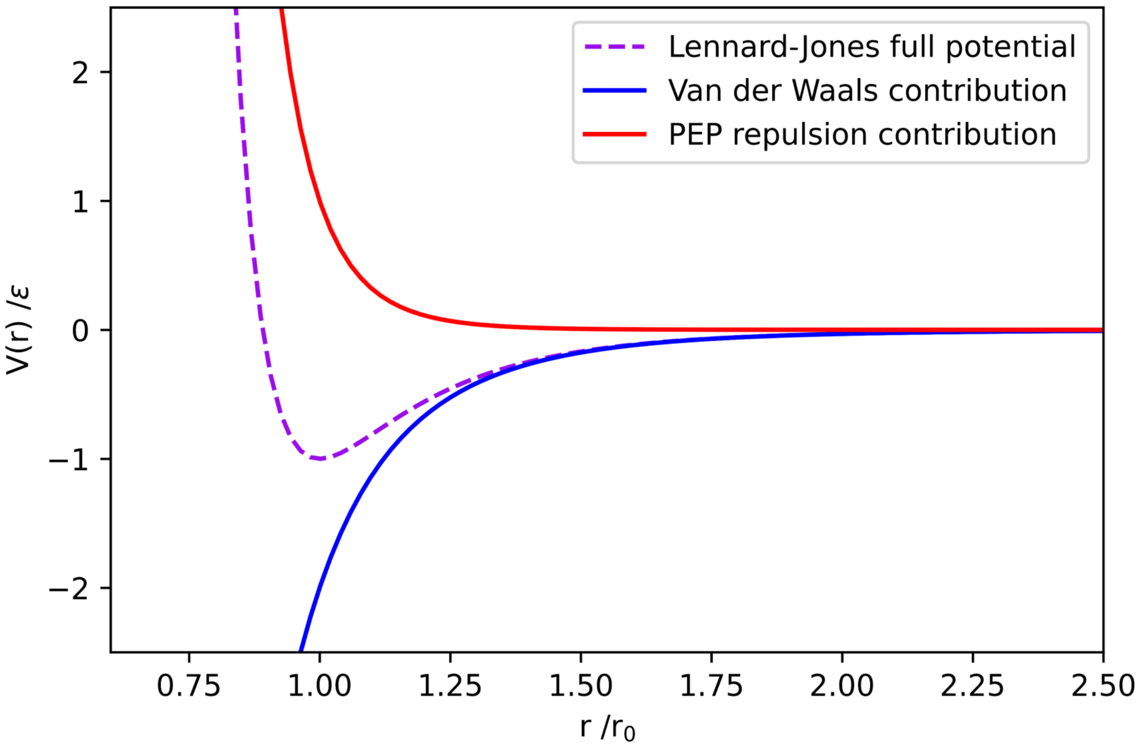
Central atom sits in a potential well of depth = number of nearest neighbours x ε

In equilibrium, atoms are separated from each other by $\mathrm{r} = \mathrm{r}_0$

Other atoms contribute to potential, but much lower (~ ε/30) – 0 to first order

Lennard-Jones force

$$F(r) = -\frac{\mathrm{d}V(r)}{\mathrm{d}r}$$

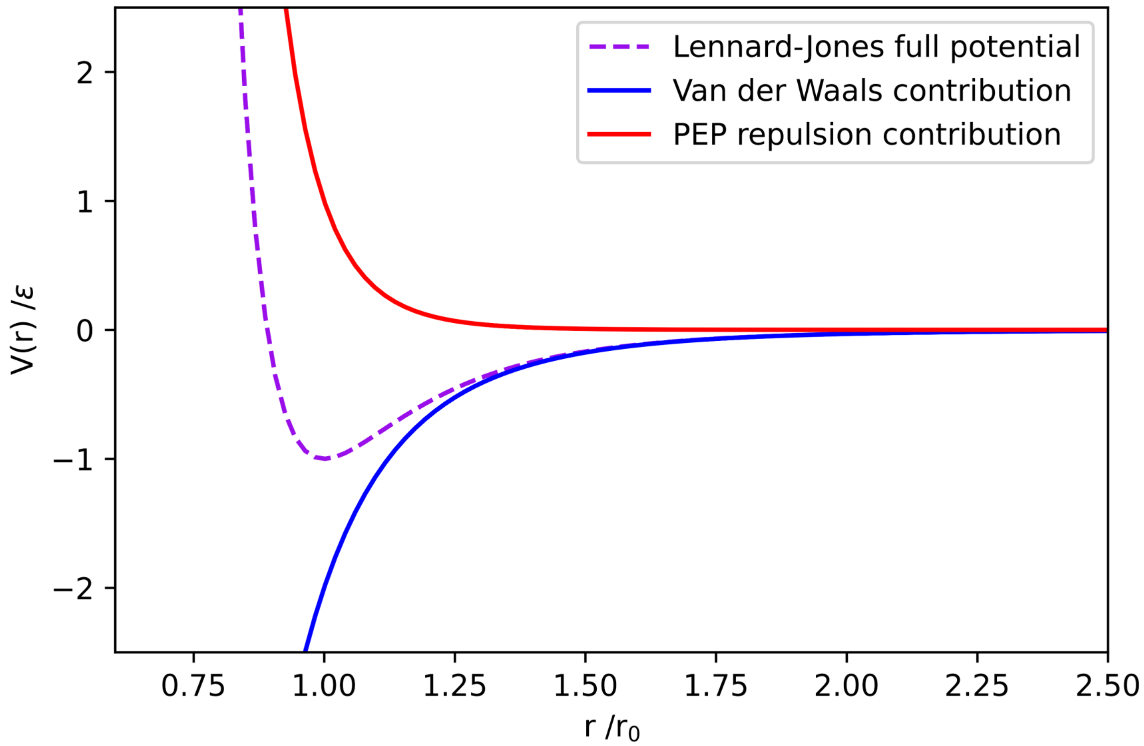


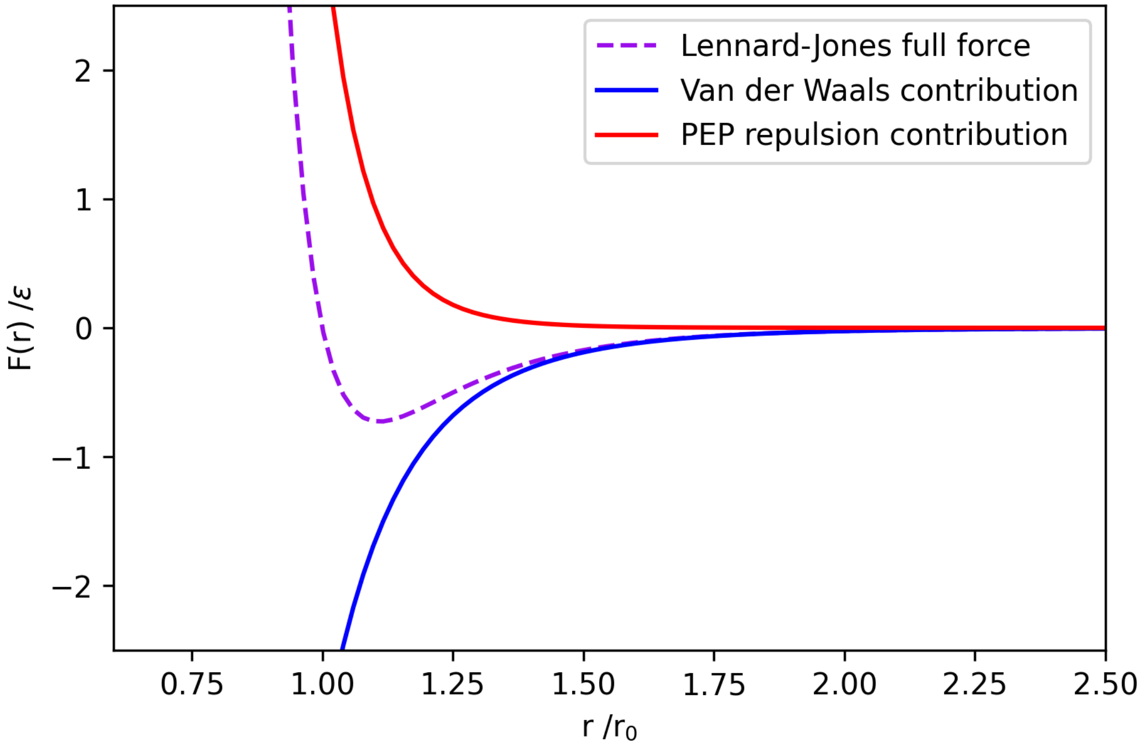
$$V(r) = \varepsilon[\left(\frac{r_0}{r}\right)^{12} - 2\left(\frac{r_0}{r}\right)^{6}]$$

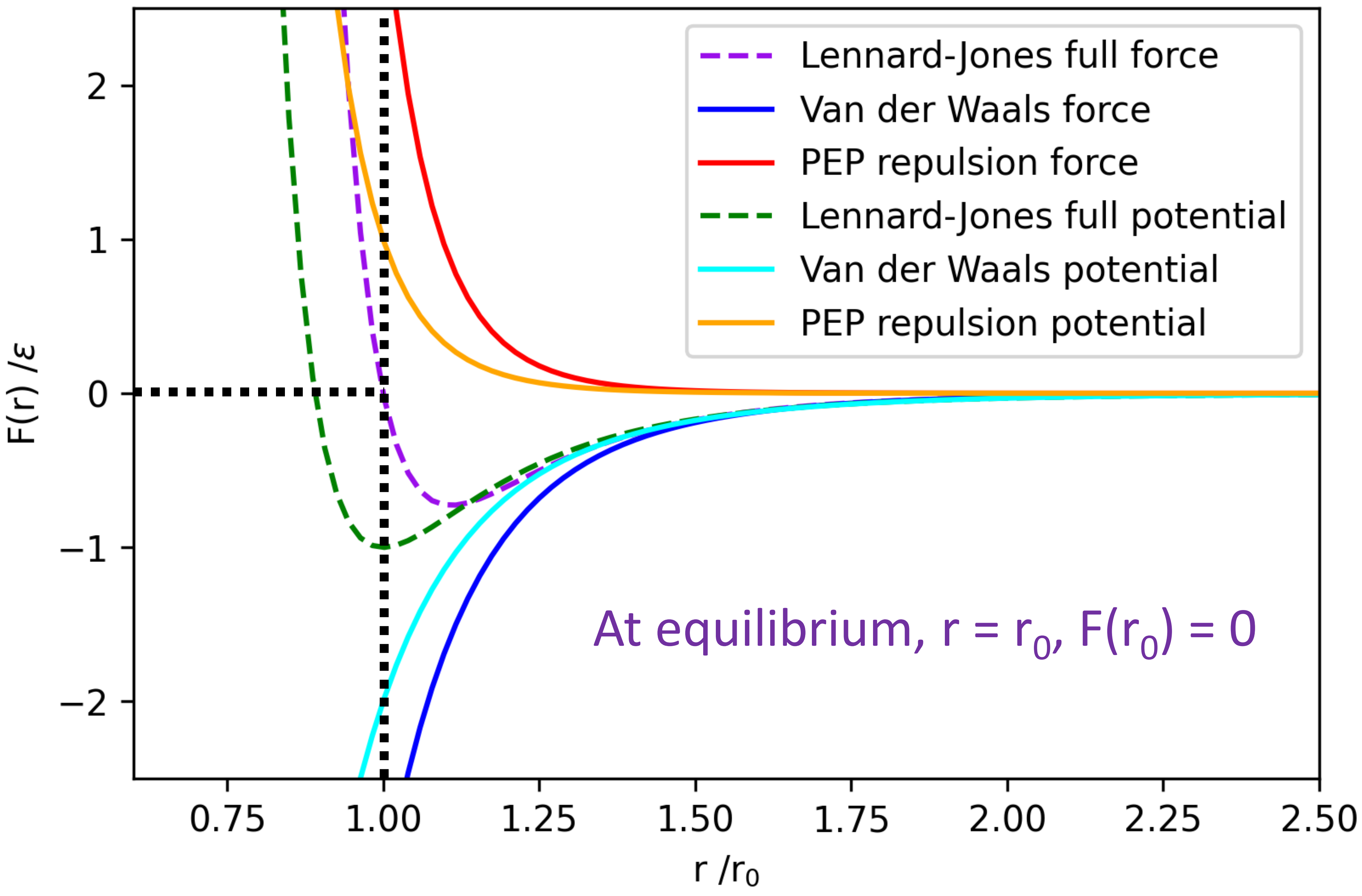
$$F(r) = 12\varepsilon\left(\frac{r_0^{12}}{r^{13}} - \frac{r_0^{6}}{r^{7}}\right)$$

$$V(r) = \varepsilon\left[\left(\frac{r_0}{r}\right)^{12} - 2\left(\frac{r_0}{r}\right)^{6}\right]$$

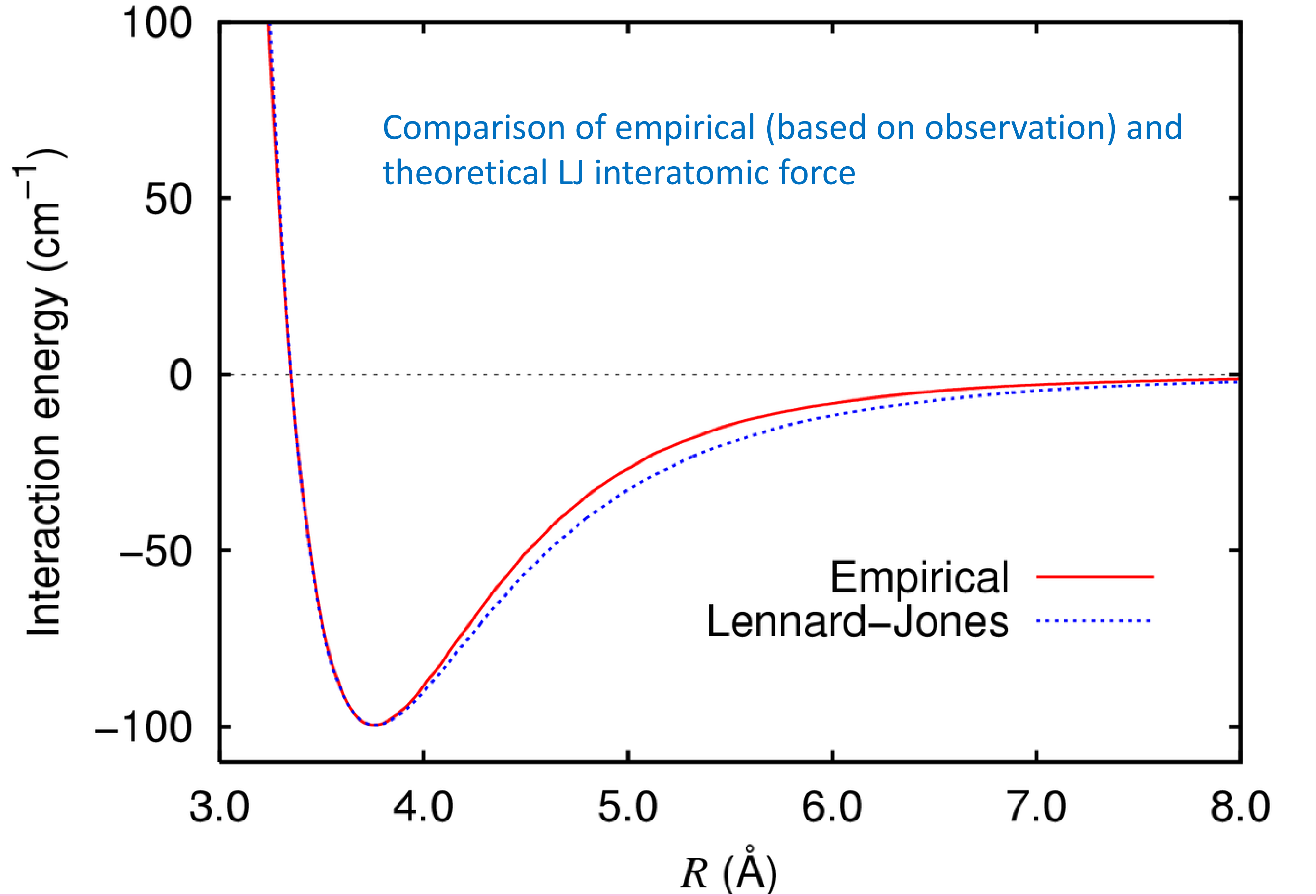
$$F(r) = 12\varepsilon\left(\frac{r_0^{12}}{r^{13}} - \frac{r_0^{6}}{r^{7}}\right)$$







Lennard-Jones full force
Van der Waals force
PEP repulsion force
Lennard-Jones full potential
Van der Waals potential
PEP repulsion potential
At equilibrium, r = r0, F(r0) = 0
F(r) /ε
r /r0
2
1
0
−1
−2
0.75
1.00
1.25
1.50
1.75
2.00
2.25
2.50



https://upload.wikimedia.org/wikipedia/commons/thumb/9/93/Argon_dimer_potential_and_Lennard-Jones.png/320px-Argon_dimer_potential_and_Lennard-Jones.png

Limitations of the Lennard-Jones potential

Infinite range potential means it is computationally expensive to calculate
-> usually get around this by truncating (killing off) the potential

For large molecules (e.g. proteins), the range of attraction is too large compared with the diameter of the proteins (the protein-protein distance)

Summary

Saw the relationship between force and potential, and how to visual this graphically (through derivatives)

Briefly discussed some limitations of the Lennard-Jones potential

Discussed derivation of the constants, A and B, for the general form of the Lennard-Jones potential