భారతీయ సాంకేతిక విజ్ఞాన సంస్థ హైదరాబాద్
भारतीय प्रौद्योगिकी संस्थान हैदराबाद
Indian Institute of Technology Hyderabad

Biomolecular Simulation BT2123

Lecture 4 : Lennard-Jones potential and combination rules, microcanonical ensemble, density of states

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Quiz

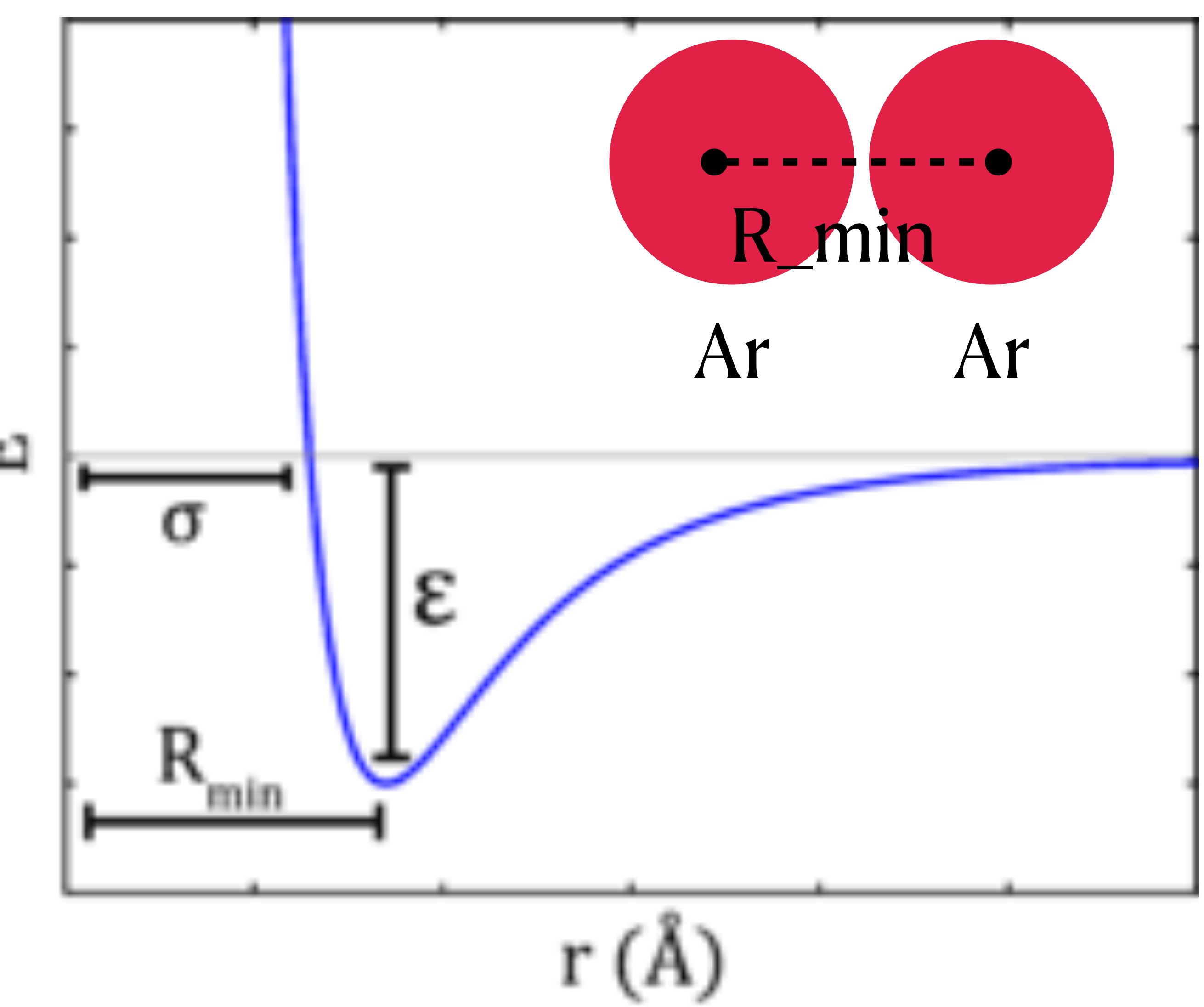
1. What will be the volume of the 864 Ar gas atoms, given that the density is 1.40 mg/m^3
2. How many water molecules will be there in 1 nm^3 area.

Lennard-Jones Pontential

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

$$V = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

$$\sigma = 2^{\frac{1}{6}} r_{min}$$



$$V = \epsilon \left[\left(\frac{r_{min}}{r}\right)^{12} - 2\left(\frac{r_{min}}{r}\right)^{6} \right]$$

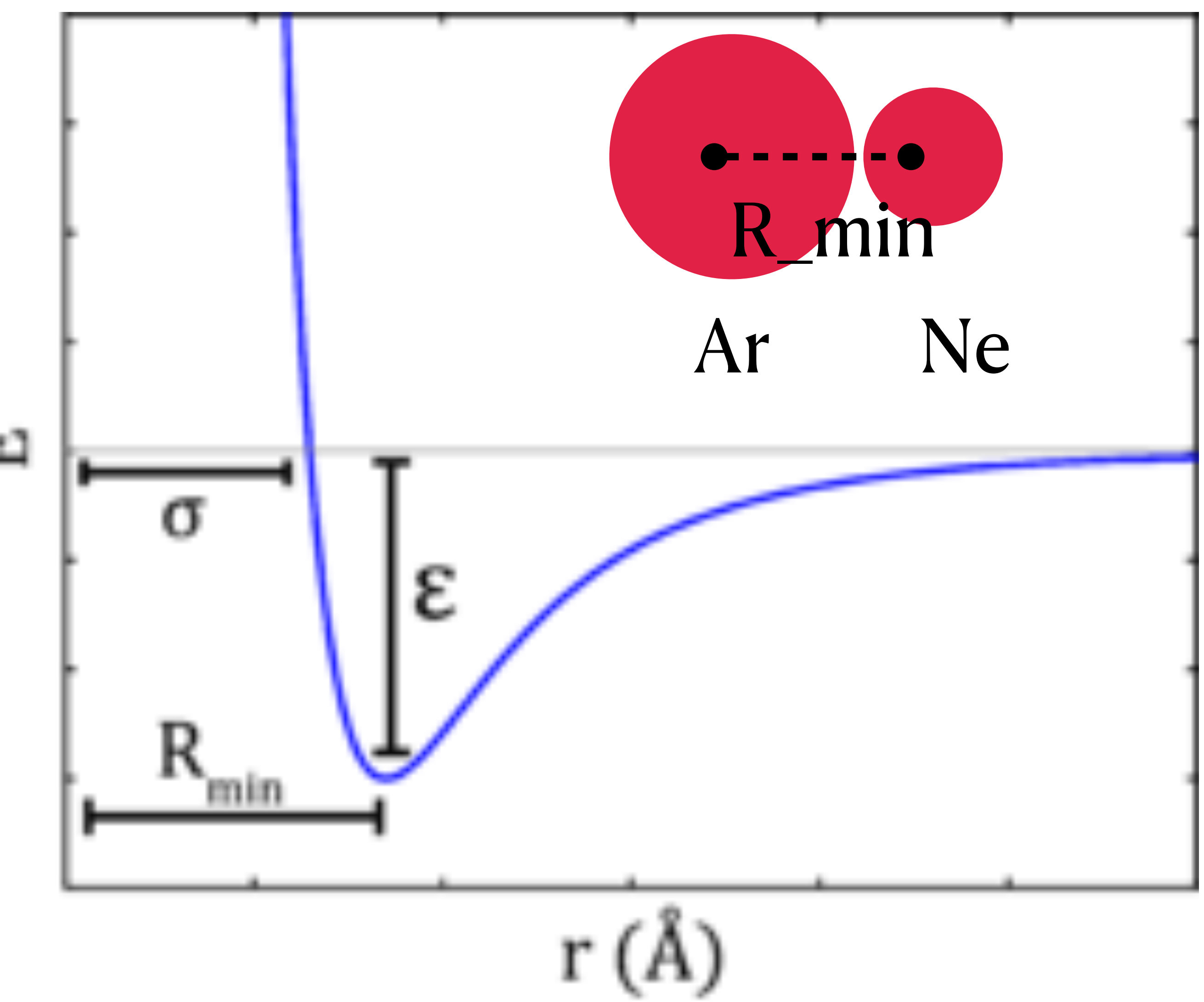
$$F = -\nabla(V)$$

$$= 12\frac{\epsilon}{r} \left[\left(\frac{r_{min}}{r}\right)^{12} - \left(\frac{r_{min}}{r}\right)^{6} \right]$$

Combination rule

$$R_{i,j} = \frac{R_i}{2} + \frac{R_j}{2}$$

$$\epsilon_{i,j} = \sqrt{\epsilon_i \epsilon_j}$$



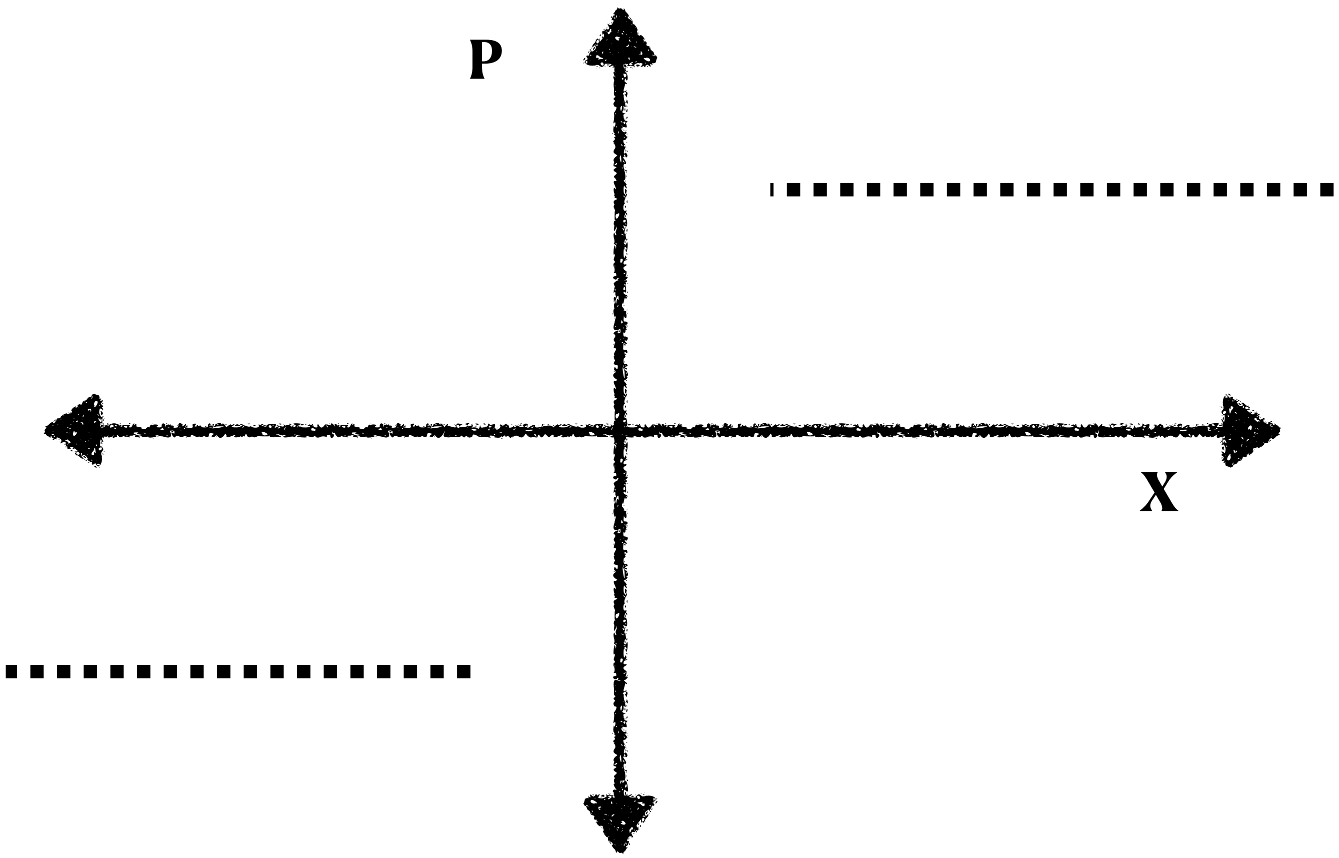
Soft spheres

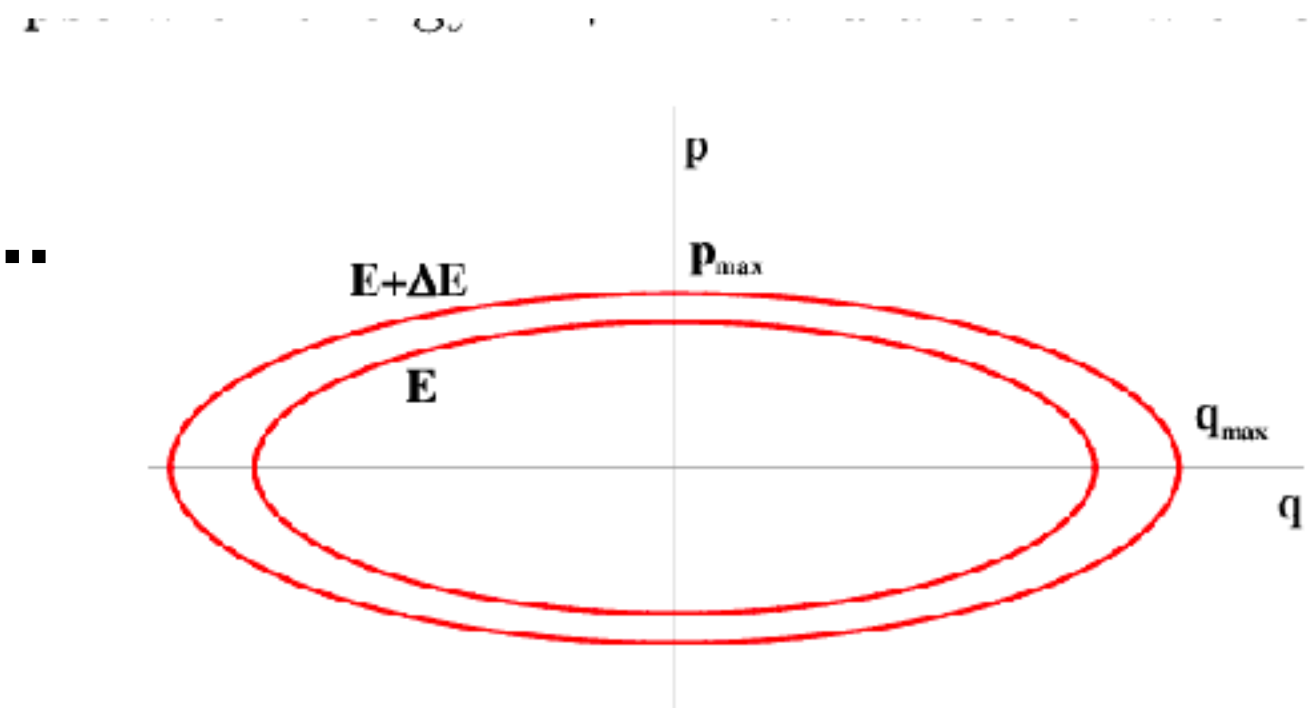
Vs

Hard Sphere

Phase Space

$$F(x) = -kx$$





$$X = (r_1, r_2, ...r_N, p_1, p_2..., p_N)$$

$$F(x) = 0$$

Statistical mechanics

Statistical mechanics provides a microscopic basis for thermodynamics which otherwise is a phenomenological theory.

Statistical mechanics is concerned with the large numbers of objects that can be constituents of the macroscopic system.

Microcanonical ensemble

Calculate the intermolecular potential between two Argon (Ar) atoms separated by a distance of 4.0 Å (use ϵ=0.997 kJ/mol and σ=3.40 Å).