Thermodynamics and Statistical Mechanics

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Contents

0.1 Ideal Gas

- Point particles that don't fill up space
- Non interacting particles
- Newtonian physics, $m\frac{\mathrm{d}v}{\mathrm{d}t} = F$
- The particles have a Kinetic Energy $T = \frac{1}{2}mv^2$

We have a Box with length ℓ and a particle interacting with the surface A with its v_x velocity.

The time between colissions with the surface is $\Delta t = \frac{2\ell}{v_x}$. We calculate the Pressure with

$$P = \frac{F}{A} = \frac{m\Delta v}{A\Delta t} = \frac{m2v_x^2}{A2\ell} = \frac{mv_x^2}{V} \tag{1}$$

And then

$$PV = mv_x^2 = kT \tag{2}$$

from this we gather

- Equipartition principle: every squared degree of freedom has $\frac{1}{2}kT$ Energy.

And the total Energy for the particle is

$$E = \sum_i \frac{1}{2}m < v_i^2 >= \frac{3}{2}m < v^2 >= \frac{3}{2}kT \tag{3}$$

1 Molecular Dynamics

Lennard Jones Potential

$$U(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) \tag{4}$$

For example

- Argon
  - $\sigma = 0.34$ nm
  - $/k_B = 120$K
  - $m = 40u$
- Methane
  - $\sigma = 0.38$
  - $\epsilon/k_B = 148$K
  - $m = 16u$