

# Simulation of a many-particle system using space partitioning

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## 1 Scientific model

### 1.1 Maxwell-Boltzmann distribution

The well-known **Maxwell-Boltzmann distribution** describes the molecular speed for a monoatomic classical ideal gas in thermodynamic equilibrium.

$$f(v) dv = \left(\frac{\beta m}{2\pi}\right)^{3/2} 4\pi v^2 e^{-\beta \frac{mv^2}{2}} dv$$

where  $\beta$  is given by  $\beta \equiv \frac{1}{k_B T}$ ,  $T$  is the temperature,  $k_B$  is the Boltzmann constant and  $m$  is the molecular mass of the gas.

In this section, we derive a similar expression for a two-dimensional gas. Consider a gas consisting of a single molecule of mass  $m$  in a container in contact with a heat bath of temperature  $T$ . The probability of the particle being in a state with energy  $E$  is given by the Boltzmann distribution.

$$P(E) dE \propto e^{-\beta E} dE$$

Since the energy of particle is only a function of the velocity  $\vec{v}$ ,  $E = \frac{mv^2}{2}$ , we can deduce

$$P(\vec{v}) d\vec{v} \propto e^{-\beta \frac{m|\vec{v}|^2}{2}} d\vec{v}$$

But we're interested in the speed distribution, not the velocity distribution. For this, we use a substitution to polar coordinates

$$d\vec{v} = dv_x dv_y = v dv d\theta$$

where  $v = |\vec{v}|$  is the speed. So

$$f(v) dv d\theta \propto v e^{-\beta \frac{mv^2}{2}} dv d\theta$$

Since the distribution is independent of the parameter  $\theta$ , we can integrate over it and remove it from the equation.

$$f(v) dv \propto v e^{-\beta \frac{mv^2}{2}} dv$$

After normalisation we find the **Rayleigh distribution**

$$f(v) dv = \beta m v e^{-\beta \frac{mv^2}{2}} dv$$

## 1.2 Elastic collision

The most basic interaction that needs to be modeled in a many particle system is the elastic collision between hard spheres or disks. Consider two particles denoted by subscripts 1 and 2. Let  $m_i$  be the masses,  $v_c$  be the the velocity of the center of mass (COM) frame,  $v_i$  the velocities before the collision,  $v'_i$  the velocities before collision in the COM frame,  $w_i$  the velocities after the collision and  $w'_i$  the velocities after collision in the COM frame. We assume the speed of both bodies is non-relativistic.

The one-dimensional results are well known

$$v_c = \frac{m_1 v_1 + m_2 v_2}{m_1 + m_2}$$

$$v_1 = \exp c$$