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.

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

where β 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.

$$P(E)\mathrm{d}E \propto e^{-\beta E}\,\mathrm{d}E$$

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

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

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

$$\mathrm{d}\vec{v} = \mathrm{d}v_x\,\mathrm{d}v_y = v\,\mathrm{d}v\,\mathrm{d}\theta$$

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

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

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

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

After normalisation we find the **Rayleigh distribution**

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