Boltzmann factor for the kinetic energy of free particles: Maxwell-Boltzmann distribution Masatsugu Sei Suzuki Department of Physics

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We now consider the Boltzmann factor for the kinetic energy of free particles with a mass m. We derive the form of Maxwell-Boltzmann distribution function/

The kinetic energy of the particle is given by

$$E_k = \frac{1}{2}mv^2$$

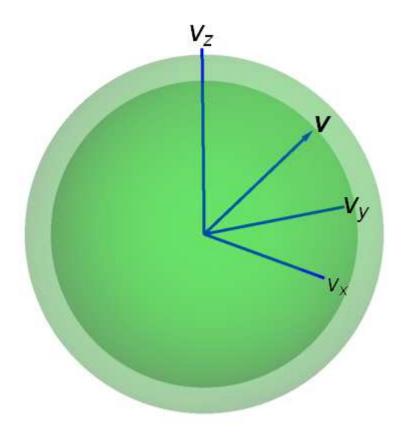
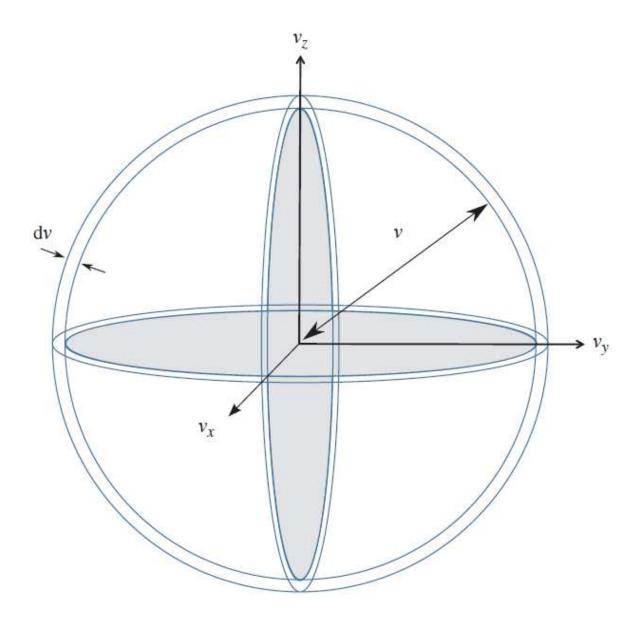


Fig. Velocity space. The kinetic energy is the same for the different state (v - v + dv).



The probability of finding the particles between v and v + dv is

$$f(v)dv = \frac{4\pi v^2 dv \exp(-\frac{\beta mv^2}{2})}{\int\limits_0^\infty 4\pi v^2 dv \exp(-\frac{\beta mv^2}{2})}.$$

Here we have

$$\int_{0}^{\infty} 4\pi v^{2} dv \exp(-\frac{\beta m v^{2}}{2}) = 4\pi \sqrt{\frac{\pi}{2}} (m\beta)^{-3/2} = (\frac{m\beta}{2\pi})^{-3/2}$$

The Maxwell-Boltzmann distribution function is

$$f(v) = \left(\frac{m\beta}{2\pi}\right)^{3/2} 4\pi v^2 \exp\left(-\frac{\beta m v^2}{2}\right)$$
$$= \left(\frac{m}{2\pi k_B T}\right)^{3/2} 4\pi v^2 \exp\left(-\frac{m v^2}{2k_B T}\right)$$

where

$$\int_{0}^{\infty} f(v)dv = 1$$

The average velocity:

$$\langle v \rangle = \int_{0}^{\infty} v f(v) dv = 2\sqrt{\frac{2}{\pi}} (m\beta)^{-1/2} = \sqrt{\frac{8k_B T}{\pi m}}$$

The variance:

$$\left\langle v^2 \right\rangle = \int_0^\infty v^2 f(v) dv = \frac{3}{m\beta} = \frac{3k_B T}{m}$$

This can be rewritten as

$$\frac{1}{2}m\langle v^2 \rangle = \frac{3}{2}k_B T$$
 (equi-partition theorem)

The root-mean square velocity is

$$v_{rns} = \sqrt{\langle v^2 \rangle} = \sqrt{\frac{3k_B T}{m}}$$
.

What is the most probable velocity in which f(v) takes a maximum.

$$\frac{df}{dv} = 0$$

$$2v \exp(-\frac{mv^2}{2k_B T}) + v^2(-\frac{mv}{k_B T}) \exp(-\frac{mv^2}{2k_B T}) = 0$$

or

$$v_{probable} = \sqrt{\frac{2k_BT}{m}}$$

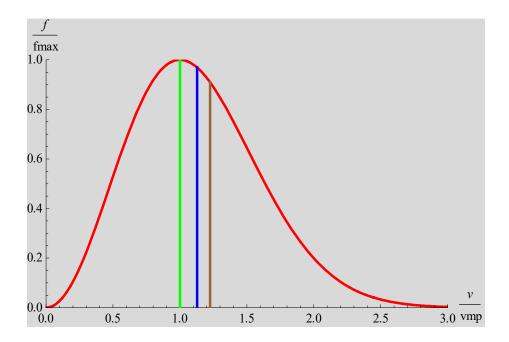


Fig. Plot of the normalized $f(v)/f_{\text{max}}$ as a function of a normalized v/v_{mp} .

Green: most probable speed (v_{mp})

Blue: averaged speed (v_{avg})

Brown: root-mean squared speed (v_{rms})

$$1 < \frac{v_{avg}}{v_{mp}} (= 1.128) < \frac{v_{rms}}{v_{mp}} (= \frac{\sqrt{6}}{2} = 1.225)$$

((**Example**)) Neutron (obeying the Maxwell Boltzmann distribution)

(a) T = 300 K.

$$E = \frac{1}{2}m_n v_p^2 = 25.852 \text{ meV},$$
 $\lambda = \frac{h}{m_n v_p} = 1.77885 \text{ Å}$

(b) T = 20 K (liquid hydrogen or deuterium)

$$E = \frac{1}{2}m_n v_p^2 = 1.72347 \text{ 2 meV},$$
 $\lambda = \frac{h}{m_n v_p} = 6.8895 \text{ Å}$

((Note-1)) The degeneracy of the state

The Boltzmann factor is given by

$$\exp(-\frac{\beta}{2}mv^2)$$

Each states with the velocity having v and v + dv, has the same Boltzmann factor. In other words, there is a degeneracy of states $4\pi v^2 dv$.

((Note-2)) Definition of f(v)

$$N = \int N(\mathbf{v})d\mathbf{v} = \int 4\pi v^2 N(\mathbf{v})$$

or

$$1 = \int 4\pi v^2 dv \frac{N(v)}{N} = \int 4\pi v^2 dv \overline{n}(v) = \int f(v) dv$$

where

$$f(v) = 4\pi v^2 \overline{n}(v)$$
, $\overline{n}(v) = \frac{N(v)}{N}$

N is the total number of particles.

((Mathematica))

A1 =
$$\int_0^\infty 4 \pi v^2 \exp \left[-\frac{\beta}{2} m v^2 \right] dv //$$
Simplify [#, {m > 0, β > 0}] &

$$\frac{2\sqrt{2} \pi^{3/2}}{(m\beta)^{3/2}}$$

$$f1 = \frac{1}{A1} 4 \pi v^2 Exp \left[-\frac{\beta}{2} m v^2 \right]$$

$$e^{-\frac{1}{2} m v^2 \beta} \sqrt{\frac{2}{\pi}} v^2 (m \beta)^{3/2}$$

$$\int_0^\infty f1 \, dv // Simplify[#, \{m > 0, \beta > 0\}] \&$$

$$vav = \int_0^\infty v \, f1 \, dv \, // \, Simplify[\#, \{m > 0, \beta > 0\}] \, \&$$

$$\frac{2\sqrt{\frac{2}{\pi}}}{\sqrt{\mathbf{m}\,\beta}}$$

$$vsq = \int_{0}^{\infty} v^2 f1 dv // Simplify[#, {m > 0, \beta > 0}] &$$

$$\delta v = \sqrt{vsq} // Simplify$$

$$\sqrt{3} \sqrt{\frac{1}{m \beta}}$$

APPENDIX Gauss integrals

$$\int_{0}^{\infty} e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}$$

We take a derivative of this equation with respect to a

$$\int_{0}^{\infty} (-x^{2})e^{-ax^{2}}dx = -\frac{\sqrt{\pi}}{4}a^{-\frac{3}{2}}$$

leading to the formula given by

$$\int_{0}^{\infty} x^{2} e^{-ax^{2}} dx = \frac{\sqrt{\pi}}{4a^{3/2}}.$$