New probability distributions in astrophysics: III. The truncated Maxwell-Boltzmann distribution

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Abstract The Maxwell-Boltzmann (MB) distribution for velocities in ideal gases is usually defined between zero and infinity. A double truncated MB distribution is here introduced and the probability density function, the distribution function, the average value, the rth moment about the origin, the root-mean-square speed and the variance are evaluated. Two applications are presented: (i) a numerical relationship between root-mean-square speed and temperature, and (ii) a modification of the formula for the Jeans escape flux of molecules from an atmosphere.

Keywords: 05.20.-y Classical statistical mechanics; 05.20.Dd Kinetic theory;

1 Introduction

The Maxwell-Boltzmann (MB) distribution, see [1,2], is a powerful tool to explain the kinetic theory of gases. The range in velocity of this distribution spans the interval $[0, \infty]$, which produces several problems:

1. The maximum velocity of a gas cannot be greater than the velocity of light, $c$
2. The kinetic theory is developed in a classical environment, which means that the involved velocities should be smaller than $\approx 1/10 c$

These items point toward the hypothesis of an upper bound in velocity for the MB. We will now report some approaches, including an upper bound in velocity: the ion velocities parallel to the magnetic field in a low density surface of a ionized plasma [3]; propagation of longitudinal electron waves in a collisionless, homogeneous, isotropic plasma, whose velocity distribution function is a truncated MB [4]; fast ion production in laser plasma [5]; the release of a dust particle from a plasma-facing wall [6]; an explanation of an anomaly in the Dark Matter (DAMA) experiment [7]; a distorted MB distribution of epithermal ions observed associated with the collapse of energetic ions [8]; and deviations to MB distribution that could have observable effects which can be measured trough the vapor spectroscopy at an interface [9].

However, these approaches do not clearly cover the effect of introducing a lower and an upper boundary in the MB distribution, which is the subject that will be analyzed in this paper.

This paper is structured as follows. Section 2 reviews the basic statistics of the MB distribution and it derives a new approximate expression for the median. Section 3 introduces the double truncated MB and it derives the connected statistics. Section 4 derives the relationship for root-mean-square speed versus temperature in the double truncated MB. Finally, Section 5.2 derives a new formula for Jeans flux in the exosphere.

2 The Maxwell-Boltzmann distribution

Let $V$ be a random variable defined in $[0, \infty]$; the MB probability density function (PDF), $f(v; a)$, is

$$f(v; a) = \frac{\sqrt{2v^2e^{-\frac{v^2}{2a^2}}}}{\sqrt{\pi a^3}}$$

(1)

where $a$ is a parameter and $v$ denotes the velocity, see [1,2]. Conversion to the physics is done by introducing the variable $a$, which is defined as

$$a = \sqrt{\frac{kT}{m}}$$

(2)
where $m$ is the mass of the gas molecules, $k$ is the Boltzmann constant and $T$ is the thermodynamic temperature. With this change of variable, the MB PDF is

$$f_p(v; m, k, T) = \frac{\sqrt{2}a^2 e^{-\frac{1}{2} \frac{v^2}{m k T}}}{\sqrt{\pi} \left( \frac{kT}{m} \right)^{\frac{3}{2}}} ,$$

where the index $p$ stands for physics. The distribution function (DF), $F(x; a)$, is

$$F(v; a) = \frac{\sqrt{2} \left( \frac{kT}{m} \right)^{\frac{3}{2}} \sqrt{\pi} \sqrt{2} \erf \left( \frac{1}{2} \sqrt{2} \frac{v}{\sqrt{kT}} \right) m - 2 v e^{-\frac{1}{2} \frac{v^2}{kT}}}{2 \sqrt{\pi} \left( \frac{kT}{m} \right)^{\frac{3}{2}} a} .$$

The average value or mean, $\mu$, is

$$\mu(a) = 2 \frac{\sqrt{2}a}{\sqrt{\pi}} ,$$

$$\mu(m, k, T)_p = 2 \frac{\sqrt{2}}{\sqrt{\pi}} \frac{kT}{m} ,$$

the variance, $\sigma^2$, is

$$\sigma^2(a) = \frac{a^2 (-8 + 3 \pi)}{\pi} ,$$

$$\sigma^2(m, k, T)_p = \frac{kT (-8 + 3 \pi)}{m \pi} .$$

The $r$th moment about the origin for the MB distribution is, $\mu'_r$, is

$$\mu'_r(a) = \frac{2^{r/2+1} a^r \Gamma \left( r/2 + \frac{3}{2} \right)}{\sqrt{\pi}} ,$$

$$\mu'_r(m, k, T)_p = \frac{2^{r/2+1} \left( \frac{kT}{m} \right)^r \Gamma \left( r/2 + \frac{3}{2} \right)}{\sqrt{\pi}} ,$$

where

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt ,$$

is the gamma function, see [10]. The root-mean-square speed, $v_{rms}$, can be obtained from this formula by inserting $r = 2$

$$v_{rms}(a) = \sqrt{3} a ,$$

$$v_{rms}(m, k, T)_p = \sqrt{3} \sqrt{\frac{kT}{m}} ,$$

see eqn.(7-10-16) in [11]. This equation allows us to derive the temperature once the root-mean-square speed is measured

$$T = \frac{1}{3} \frac{v_{rms}^2 m}{k} .$$

The coefficient of variation (CV) is

$$CV = \frac{\sigma(a)}{\mu(a)} = \sqrt{\frac{3}{8} \pi - 1} ,$$
which is constant. The first three rth moments about the mean for the MB distribution, \( \mu_r(a) \), are

\[
\begin{align*}
\mu_2(a) &= \frac{a^2 (-8 + 3 \pi)}{\pi} \\
\mu_3(a) &= -2 \frac{a^3 \sqrt{2} (5 \pi - 16)}{\pi^{3/2}} \\
\mu_4(a) &= \frac{a^4 (15 \pi^2 + 16 \pi - 192)}{\pi^2}.
\end{align*}
\]

(12a) \hspace{1cm} (12b) \hspace{1cm} (12c)

The mode is at

\[
\begin{align*}
v(a) &= \sqrt{2} a \\
v(m, k, T)_p &= \sqrt{2} \sqrt{\frac{kT}{m}}.
\end{align*}
\]

(13a) \hspace{1cm} (13b)

An approximate expression for the median can be obtained by a Taylor series of the DF around the mode. The approximation formula is

\[
\begin{align*}
v(a) &= -\frac{1}{4} a \left( -6 + e \left( \text{erf}(1) - \frac{1}{2} \right) \sqrt{\pi} \right) \sqrt{2} , \\
v(m, k, T)_p &= -\frac{1}{4} \sqrt{\frac{kT}{m}} \left( -6 + e \left( \text{erf}(1) - \frac{1}{2} \right) \sqrt{\pi} \right) \sqrt{2} ,
\end{align*}
\]

(14a) \hspace{1cm} (14b)

which has a percent error, \( \delta \), of \( \delta \approx 0.04\% \) in respect to the numerical value. The entropy is

\[
\begin{align*}
\ln \left( \sqrt{2} \sqrt{\pi a} \right) - \frac{1}{2} + \gamma \\
\ln \left( \sqrt{2} \sqrt{\frac{kT}{m}} \right) - \frac{1}{2} + \gamma ,
\end{align*}
\]

(15a) \hspace{1cm} (15b)

where \( \gamma \) is the Euler-Mascheroni constant, which is defined as

\[
\gamma = \lim_{n \to \infty} \left( 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n} - \ln n \right) = 0.57721 \ldots ,
\]

(16)

see \[10\] for more details. The coefficient of skewness is

\[
\frac{(-10 \pi + 32) \sqrt{2}}{(-8 + 3 \pi)^{3/2}} \approx 0.48569 ,
\]

(17)

and the coefficient of kurtosis is

\[
\frac{15 \pi^2 + 16 \pi - 192}{(-8 + 3 \pi)^2} \approx 3.10816 .
\]

(18)

According to \[12\], a random number generation can be obtained via inverse transform sampling when the distribution function or cumulative distribution function, \( F(x) \), is known: (i) a pseudo number generator gives a random number \( R \) between zero and one; (ii) the inverse function \( x = F^{-1}(R) \) is evaluated; and (iii) the procedure is repeated for different values of \( R \). In our case, the inverse function should be evaluated in a numerical way by solving for \( v \) the following nonlinear equation

\[
\begin{align*}
F(v; a) - R &= 0 \\
F(v; m, k, T)_p - R &= 0 ,
\end{align*}
\]

(19a) \hspace{1cm} (19b)

where \( F(v) \) and \( F_p(v) \) are the two DF represented by equations (4a) and (4b). As a practical example, by inserting in equation (19a) \( a = 1 \) and \( R = 0.5 \), we obtain in a numerical way \( v = 1.538 \).
3 The double truncated Maxwell-Boltzmann distribution

Let \( V \) be a random variable that is defined in \([v_l, v_u]\); the double truncated version of the Maxwell-Boltzmann PDF, \( f_t(v; a, v_l, v_u) \), is

\[
f_t(v; a, v_l, v_u) = v^2 e^{-\frac{1}{2} \frac{v^2}{a^2}},
\]

where

\[
C = \frac{-2}{CD},
\]

where

\[
CD = a^2 \left( -a \sqrt{\pi} \sqrt{2} \text{erf} \left( \frac{1}{2} \sqrt{\frac{v_l}{a}} \right) + a \sqrt{\pi} \sqrt{2} \text{erf} \left( \frac{1}{2} \sqrt{\frac{v_u}{a}} \right) + 2 \sqrt{v_l} e^{-\frac{1}{2} \frac{v_l^2}{a^2}} - 2 \sqrt{v_u} e^{-\frac{1}{2} \frac{v_u^2}{a^2}} \right),
\]

and \( \text{erf}(x) \) is the error function, which is defined as

\[
\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt,
\]

see [10]. The physical meaning of \( a \) is still represented by equation (2); however, due to the tendency to obtain complicated expressions, we will omit the double notation. The DF, \( F_t(v; a, v_l, v_u) \), is

\[
F_t(v; a, v_l, v_u) = C a^2 \left( \sqrt{\pi} \sqrt{2} \text{erf} \left( \frac{1}{2} \sqrt{\frac{v_l}{a}} \right) - 2 \sqrt{v_u} e^{-\frac{1}{2} \frac{v_u^2}{a^2}} \right).
\]

The average value \( \mu_t(a, v_l, v_u) \), is

\[
\mu_t(a, v_l, v_u) = C a^2 \left( 2 e^{-\frac{1}{2} \frac{v_l^2}{a^2}} a^2 - 2 e^{-\frac{1}{2} \frac{v_u^2}{a^2}} a^2 + a^{-1} \frac{v_l^2}{a^2} v_l^2 - e^{-\frac{1}{2} \frac{v_u^2}{a^2}} v_u^2 \right).
\]

The \( r \)th moment about the origin for the double truncated MB distribution is, \( \mu'_r(a, v_l, v_u) \),

\[
\mu'_r(a, v_l, v_u) = \frac{MN}{r+3},
\]

where

\[
MN = C 2^{\frac{r}{2}} + \frac{3}{2} a^2 \times 
\left( \left( \frac{v_l^2}{a^2} \right)^{-\frac{1}{2}} - v_l e^{-\frac{1}{2} \frac{v_l^2}{a^2}} M_{\frac{1}{2}, \frac{1}{2} + \frac{1}{2}} \left( \frac{1}{2} \frac{v_l^2}{a^2} \right) \right) 
- v_l e^{-\frac{1}{2} \frac{v_l^2}{a^2}} M_{\frac{1}{2}, \frac{1}{2} + \frac{1}{2}} \left( \frac{1}{2} \frac{v_l^2}{a^2} \right) \left( \frac{v_l^2}{a^2} \right)^{-\frac{1}{2}} \left( \frac{v_l^2}{a^2} \right)^{-\frac{1}{2}} \right),
\]

where \( M_{\mu, \nu}(z) \) is the Whittaker M function, see [10]. The root-mean-square speed, \( v_{rms,t}(a, v_l, v_u) \), can be obtained from this formula by inserting \( r = 2 \), and is

\[
(v_{rms,t}(a, v_l, v_u)) = \sqrt{\frac{NV}{5 \left( \frac{v_l^2}{a^2} \right)^{3/4}}}.
\]
where

\[ NV = 2C^2 \frac{3}{4} a^2 \left( v_{u}^{3} e^{-1/4 \frac{v_{u}^2}{v^2}} M_{3/4, 5/4} \left( \frac{1/2 v_{u}^2}{a^2} \right) \left( \frac{v_{u}^2}{a^2} \right)^{3/4} \right) \]

\[ -v_{u}^{3} e^{-1/4 \frac{v_{u}^2}{v^2}} M_{3/4, 5/4} \left( \frac{1/2 v_{u}^2}{a^2} \right) \left( \frac{v_{u}^2}{a^2} \right)^{3/4} \right) . \]  

(29)

The variance \( \sigma_{v}^2(a, v_{l}, v_{u}) \) is defined as

\[ \sigma_{v}^2(a, v_{l}, v_{u}) = \mu'_{2, t}(a, v_{l}, v_{u}) - (\mu'_{1, t}(a, v_{l}, v_{u}))^2 \]  

(30)

and has the following explicit form

\[ \sigma_{v}^2(a, v_{l}, v_{u}) = \]

\[ 4 \left( (v_{l} + 2 v_{u}) a^2 + v_{l} v_{u} (v_{l} + \frac{1}{2} v_{u}) \right) (a^2 + 1/2 v_{u}^2) C^2 a^4 e^{-\frac{1}{4} \frac{v_{l}^2 + v_{u}^2}{a^2}} \]

\[ -2 \left( (v_{l} + \frac{1}{2} v_{u}) a^2 + \frac{1}{4} v_{l} (v_{l} + 2 v_{u}) \right) C^2 a^4 (a^2 + \frac{1}{2} v_{u}^2) e^{-\frac{1}{4} \frac{v_{l}^2 + v_{u}^2}{a^2}} \]

\[ + (a^2 + \frac{1}{2} v_{u}^2) \left( C \text{erf} \left( \frac{1}{2} \frac{\sqrt{2} v_{l}}{a} \right) a^3 \sqrt{2} \sqrt{\pi} \right) \]

\[ - C \text{erf} \left( \frac{1}{2} \frac{\sqrt{2} v_{u}}{a} \right) a^3 \sqrt{2} \sqrt{\pi} + 4 \right) C (a^2 + \frac{1}{2} v_{u}^2) e^{-\frac{v_{u}^2}{a^2}} \]

\[ + (a^2 + \frac{1}{2} v_{u}^2) \left( C \text{erf} \left( \frac{1}{2} \frac{\sqrt{2} v_{l}}{a} \right) a^3 \sqrt{2} \sqrt{\pi} \right) \]

\[ - C \text{erf} \left( \frac{1}{2} \frac{\sqrt{2} v_{u}}{a} \right) a^3 \sqrt{2} \sqrt{\pi} + 4 \right) C e^{-\frac{v_{u}^2}{a^2}} + \frac{3}{4} \sqrt{\pi} \sqrt{2} \left( - \text{erf} \left( \frac{1}{2} \frac{\sqrt{2} v_{u}}{a} \right) \right) \]

\[ + \text{erf} \left( \frac{1}{2} \frac{\sqrt{2} v_{l}}{a} \right) a^3 \sqrt{2} \sqrt{\pi} \right) C a^2 . \]  

(31)

Although the coefficients of skewness and kurtosis for the truncated MB exist, they have a complicated expression.

4 A laboratory application

The temperature as a function of root-mean-square speed for the MB is given by equation (10). In the truncated MB distribution, the temperature can be found by solving the following nonlinear equation

\[ v_{\text{rms}, t}(k, m, T, v_{l}, v_{u}) = v_{\text{rms}, m} \]  

(32)

where \( v_{\text{rms}, m} \) is not a theoretical variable but is the root-mean-square speed measured in the laboratory and \( v_{\text{rms}, t} \) is given by equation (25). The laboratory measures of \( v_{\text{rms}, m} \) started with \( \frac{388}{5} m/s \) at \( 400 \, ^\circ C \) was found for a metallic vapor. In the truncated MB distribution, there are three parameters that can be measured in the laboratory from a kinematical point of view, as follows:
Figure 1. The theoretical root-mean-square speed as a function of the upper limit in velocity (continuous line) and standard value of the temperature (dotted line) when $a=340$ and $v_l = 0$.

the lowest velocity, $v_l$; the highest velocity, $v_u$; and the root-mean-square speed, $v_{rms,m}$. Setting for simplicity $v_l=0$, we will now explore the effect of the variation of $v_u$ on the root-mean-square speed; see Figure 1. The first example of the influence of the upper limit in velocity on the temperature is given by potassium gas \[14,15\], in which molecular mass is $6.492429890 \times 10^{-26}$ kg. In Figure 2 we evaluate in a numerical way the temperature when $v_l=0$ and $v_u$ is variable in the case of a measured value of $v_{rms,m}$.

Figure 2. Temperature as a function of the upper limit in velocity for Potassium (continuous line) and standard value of the temperature (dotted line) when $v_l = 0$ and $v_{rms,m} = 589.115111\text{m/s}$.

The second example is given by diatomic nitrogen, $N_2$, in which molecular mass is $4.651737684 \times 10^{-26}$ kg. In Figure 3 we evaluate the temperature when $v_l=0$ and $v_u$ is a variable in the case of a measured value of $v_{rms,m}$.

5 The Jeans escape

The standard formula for the escape of molecules from the exosphere is reviewed in the framework of the MB distribution. A new formula for the Jeans escape is derived in the framework of the truncated MB.
Figure 3. Temperature as a function of the upper limit in velocity for diatomic nitrogen, $N_2$, (continuous line) and standard value of the temperature (dotted line) when $v_l = \text{and } v_{rms,m} = 695.9756308\text{m/s}$

5.1 The standard case

In the exosphere, a molecule of mass $m$ and velocity $v_e$ is free to escape when

$$\frac{1}{2}mv_e^2 - GMm/R_ex = 0,$$

(33)

where $G$ is the Newtonian gravitational constant, $M$ is the mass of the Earth, $R_{ex} = R + H$ is the radius of the exosphere, $R$ is the radius of the Earth and $H$ is the altitude of the exosphere. The flux of the molecules that are living in the exosphere $\Phi_j$ is

$$\Phi_j = \frac{1}{4}N_{ex}\mu_e,$$

(34)

where $N_{ex}$ is the number of molecules per unit volume and $\mu_e$ is the average velocity of escape. In the presence of a given number of molecules per unit volume, the standard MB distribution in velocities in a unit volume, $f_m$, is

$$f_m(v; m, k, T, N_{ex}) = N_{ex}\sqrt{2m/kT}\exp\left(-\frac{v^2}{2kT}\right).$$

(35)

The average value of escape is defined as

$$\mu_e = \frac{\int_{v_0}^{\infty} vf_m(v; m, k, T, N_{ex})dv}{\int_{0}^{\infty} f_m(v; m, k, T, N_{ex})dv}.$$  

(36)

In this integral, the following changes are made to the variables

$$\lambda = \frac{1}{2}\frac{mv_e^2}{kT}.$$  

(37)

Therefore,

$$\mu_e = 2(\lambda_e + 1)e^{-\lambda_e}\sqrt{2\frac{kT}{\pi m}},$$

(38)

with

$$\lambda_e = 2\frac{GM}{R_{ex}v_0^2},$$

(39)

where $v_0$ is the mode as represented by equation (13b). The flux is now

$$\Phi_j = \frac{N_{ex}(\lambda_e + 1)e^{-\lambda_e}v_0}{2\sqrt{\pi}}.$$  

(40)
For more details see [16][17][18][19]. On adopting the parameters of Table 1 the Jeans escape flux for hydrogen is

$$\Phi_j = 3.98 \times 10^{11} \text{molecules m}^{-2}\text{s}^{-1},$$

(41)

and

$$\lambda_e = 7.78.$$  

(42)

The Jeans escape flux for Earth at $T = 900$ K varies between $\Phi_j \approx 2.7 \times 10^{11} \text{molecules m}^{-2}\text{s}^{-1}$; see [20] or Fig.1 in [21], and $\Phi_j \approx 4.1 \times 10^{11} \text{molecules m}^{-2}\text{s}^{-1}$, see [22]. Therefore, our choice of parameters is compatible with the suggested interval in flux.

| Parameter | value |
|-----------|-------|
| $R_{\text{ex}}$ | 6900 km |
| $T$ | 900 K |
| $N_{\text{ex}}$ | $10^{11}$ m$^{-3}$ |

5.2 The truncated case

The average value of escape for a truncated MB distribution, $\mu_{e,t}$, is

$$\mu_{e,t} = \frac{\int_{v_\lambda}^{\infty} v f(t,v,m,k,T,N_{\text{ex}},v_l,v_u)dv}{\int_{0}^{\infty} f(t,v,m,k,T,N_{\text{ex}},v_l,v_u)dv}.$$  

(43)

This integral can be solved by introducing the change of variable as given by equation (37)

$$\mu_{e,t} = -\frac{2}{4\sqrt{\lambda_\lambda} e^{-\lambda_\lambda} - 2\sqrt{\lambda_\lambda} e^{-\lambda_\lambda} - \sqrt{\pi} \text{erf} (\sqrt{\lambda_l}) + \sqrt{\pi} \text{erf} (\sqrt{\lambda_u})} \sqrt{\frac{kT}{m}}.$$  

(44)

where $\lambda_l$ is the lower value of $\lambda$ and $\lambda_u$ is the upper value of $\lambda$. The flux of the molecules that are living the exosphere in the truncated MB, $\Phi_{j,t}$, is

$$\Phi_{j,t} = \frac{N_{\text{ex}} ((\lambda_u + 1) e^{-\lambda_u} - e^{-\lambda_u} (\lambda_e + 1)) \sqrt{2}}{4\sqrt{\lambda_\lambda} e^{-\lambda_\lambda} + 2\sqrt{\pi} \text{erf} (\sqrt{\lambda_l}) - 2\sqrt{\pi} \text{erf} (\sqrt{\lambda_u}) - 4\sqrt{\lambda_\lambda} e^{-\lambda_\lambda} \sqrt{\frac{kT}{m}}}. $$  

(45)

The increasing flux of molecules is outlined when one parameter, $\lambda_t$, is variable; see Figure 4. In other words, an increase in $\lambda_t$ produces an increase in the flux of the molecules. The dependence of the flux when two parameters are variable, $\lambda_l$ and $\lambda_u$, is reported in Figure 5.

These Jeans escape fluxes for Earth are compatible with the observed values that were reported in Section 5.1.

6 Conclusions

This paper derived analytical formulae for the following quantities for a double truncated MB distribution: the PDF, the DF, the average value, the $r$th moment about the origin, the root-mean-square speed and the variance. The traditional correspondence between root-mean-square speed and temperature is replaced by the nonlinear Equation (32). The new formula (45) for the Jeans escape flux of molecules from an atmosphere is now a function of the lower and upper boundary in velocity.
Figure 4. The flux of molecules as a function of $\lambda_l$ with parameters as in Table 1, $\lambda_e = 7.78$ and $\lambda_u = 1000\lambda_e$.

Figure 5. The flux of molecules as a function of $\lambda_l$ and $\lambda_u$ with parameters as in Table 1.
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