On the equivalence of the microcanonical and the canonical ensembles: a geometrical approach

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Abstract

In this paper, we consider the volume enclosed by the microcanonical ensemble in phase space as a statistical ensemble. This can be interpreted as an intermediate image between the microcanonical and the canonical pictures. By maintaining the ergodic hypothesis over this ensemble, that is, the equiprobability of all its accessible states, the equivalence of this ensemble in the thermodynamic limit with the microcanonical and the canonical ensembles is suggested by means of geometrical arguments. The Maxwellian and the Boltzmann-Gibbs distributions are obtained from this formalism. In the appendix, the derivation of the Boltzmann factor from a new microcanonical image of the canonical ensemble is also given.

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The microcanonical and the canonical ensembles represent two clearly different physical situations in a statistical system\(^1\). The microcanonical ensemble is presented in the literature as modeling an isolated system that conserves its energy in time. The canonical ensemble models a system in contact with a heat reservoir containing an infinite energy, which allows to fluctuate the energy of the system but maintains its mean value constant in time. In the thermodynamic limit, and under certain assumptions on the entropy function\(^2\), both formalisms converge and they give the same macroscopic statistical results\(^1,2\).

Here, we interpret the volume enclosed by the microcanonical ensemble in phase space as a statistical ensemble. It implies the existence of some kind of heat reservoir with an upper limit energy in order that the system can visit all the accessible states enclosed in that volume. The geometrical reason why this picture is equivalent to the microcanonical ensemble in the thermodynamic limit is discussed. Thus, if the microcanonical ensemble is supposed to be represented by the equiprobability over the hypersurface on which the system evolves as consequence of conserving an energy \(E\) (as recently explained in Refs. \(^3,5\)), then the volume-based ensemble can be interpreted as the equiprobability over the whole volume which is enclosed by that hypersurface. This means that, in the latter ensemble, the system can visit states with different energies, with an upper limit \(E\) given by the energy defined in its equivalent microcanonical picture. As we have said, we can think that in this image the system is exchanging energy with a heat (or energy) reservoir containing a maximum energy \(E\). This constraint is removed in the thermodynamic limit when the number of degrees of freedom and the energy \(E\) are supposed to become infinite. Let us observe that this infinite limit establishes also the equivalence between this ensemble and the canonical ensemble (when certain conditions of smoothness in the entropy function are implicit\(^2\)), just because in this case the reservoir contains an infinite energy and then both pictures become identical. Hence, when the number of dimensions of the system increases infinitely, almost all the volume enclosed by that hypersurface is located in the vanishingly thin layer close to the hypersurface, and, in consequence, surface and volume, tend to coincide. This is the reason why the microcanonical ensemble and the volume-based ensemble, and by extension the canonical ensemble, give the same results for systems well-behaved\(^2\) in the thermodynamic limit.

We proceed to obtain different classical results from this volume-based statistical ensemble. We start by deriving (recalling) the Maxwellian (Gaussian) distribution from geometri-
cal arguments over the volume of an $N$-sphere. Following the same insight, we also explain the origin of the Boltzmann-Gibbs (exponential) distribution by means of the geometrical properties of the volume of an $N$-dimensional pyramid. We finish claiming a possible general statistical result that follows from the properties of the volume enclosed by a one-parameter dependent family of hypersurfaces, in which $N$-spheres and $N$-dimensional pyramids are included. In the appendix, an alternative microcanonical image of the canonical ensemble is also given.

**Derivation of the Maxwellian distribution**

Let us suppose a one-dimensional ideal gas of $N$ non-identical classical particles with masses $m_i$, with $i = 1, \ldots, N$, and total maximum energy $E$. If particle $i$ has a momentum $m_i v_i$, we define a kinetic energy:

$$K \equiv p_i^2 \equiv \frac{1}{2} m_i v_i^2,$$

where $p_i$ is the square root of the kinetic energy. If the total maximum energy is defined as $E \equiv R^2$, we have

$$p_1^2 + p_2^2 + \cdots + p_{N-1}^2 + p_N^2 \leq R^2.$$  

(2)

We see that the system has accessible states with different energy, which is supplied by the heat reservoir. These states are all those enclosed into the volume of the $N$-sphere given by Eq. (2). The formula for the volume $V_N(R)$ of an $N$-sphere of radius $R$ is

$$V_N(R) = \frac{\pi^{\frac{N}{2}}}{\Gamma\left(\frac{N}{2} + 1\right)} R^N,$$

where $\Gamma(\cdot)$ is the gamma function. If we suppose that each point into the $N$-sphere is equiprobable, then the probability $f(p_i)dp_i$ of finding the particle $i$ with coordinate $p_i$ (energy $p_i^2$) is proportional to the volume formed by all the points on the $N$-sphere having the $i$th-coordinate equal to $p_i$. Our objective is to show that $f(p_i)$ is the Maxwellian distribution, with the normalization condition

$$\int_{-R}^{R} f(p_i)dp_i = 1.$$  

(4)

If the $i$th particle has coordinate $p_i$, the $(N-1)$ remaining particles share an energy less than the maximum energy $R^2 - p_i^2$ on the $(N-1)$-sphere

$$p_1^2 + p_2^2 \cdots + p_{i-1}^2 + p_{i+1}^2 \cdots + p_N^2 \leq R^2 - p_i^2.$$  

(5)
whose volume is $V_{N-1}(\sqrt{R^2 - p_i^2})$. It can be easily proved that
\[ V_N(R) = \int_{-R}^{R} V_{N-1}(\sqrt{R^2 - p_i^2}) dp_i. \] (6)

Hence, the volume of the $N$-sphere for which the $i$th coordinate is between $p_i$ and $p_i + dp_i$ is $V_{N-1}(\sqrt{R^2 - p_i^2}) dp_i$. We normalize it to satisfy Eq. (4), and obtain
\[ f(p_i) = \frac{V_{N-1}(\sqrt{R^2 - p_i^2})}{V_N(R)}, \] (7)
whose final form, after some calculation is
\[ f(p_i) = C_N R^{-1} \left(1 - \frac{p_i^2}{R^2}\right)^{\frac{N-1}{2}}, \] (8)
with
\[ C_N = \frac{1}{\sqrt{\pi}} \frac{\Gamma\left(\frac{N+2}{2}\right)}{\Gamma\left(\frac{N+1}{2}\right)}. \] (9)

For $N \gg 1$, Stirling’s approximation can be applied to Eq. (9), leading to
\[ \lim_{N \gg 1} C_N \simeq \frac{1}{\sqrt{\pi}} \sqrt{\frac{N}{2}}. \] (10)

If we call $\epsilon$ the mean energy per particle, $E = R^2 = N\epsilon$, then in the limit of large $N$ we have
\[ \lim_{N \gg 1} \left(1 - \frac{p_i^2}{R^2}\right)^{\frac{N-1}{2}} \simeq e^{-p_i^2/2\epsilon}. \] (11)

The factor $e^{-p_i^2/2\epsilon}$ is found when $N \gg 1$ but, even for small $N$, it can be a good approximation for particles with low energies. After substituting Eqs. (10)–(11) into Eq. (8), we obtain the Maxwellian distribution in the asymptotic regime $N \to \infty$ (which also implies $E \to \infty$):
\[ f(p)dp = \sqrt{\frac{1}{2\pi\epsilon}} e^{-p^2/2\epsilon} dp, \] (12)
where the index $i$ has been removed because the distribution is the same for each particle, and thus the velocity distribution can be obtained by averaging over all the particles.

Depending on the physical situation the mean energy per particle $\epsilon$ takes different expressions. For a one-dimensional gas in thermal equilibrium we can calculate the dependence of $\epsilon$ on the temperature, which, as in the microcanonical ensemble, can be calculated by differentiating the entropy with respect to the energy. The entropy can be written as
\[ S = -kN \int_{-\infty}^{\infty} f(p) \ln f(p) \, dp, \] where \( f(p) \) is given by Eq. (12) and \( k \) is the Boltzmann constant. If we recall that \( \epsilon = E/N \), we obtain

\[ S(E) = \frac{1}{2} kN \ln \left( \frac{E}{N} \right) + \frac{1}{2} kN(\ln(2\pi) + 1). \] (13)

The calculation of the temperature \( T \) gives

\[ T^{-1} = \left( \frac{\partial S}{\partial E} \right)_N = \frac{kN}{2E} = \frac{k}{2\epsilon}. \] (14)

Thus \( \epsilon = kT/2 \), consistent with the equipartition theorem. If \( p^2 \) is replaced by \( \frac{1}{2}mv^2 \), the Maxwellian distribution is a function of particle velocity, as it is usually given in the literature:

\[ g(v)dv = \sqrt{\frac{m}{2\pi kT}} e^{-mv^2/2kT} dv. \] (15)

This shows that the geometrical image of the volume-based statistical ensemble allows us to recover the same result than that obtained from the microcanonical and canonical ensembles. Also, it confirms for this case the equivalence among all these ensembles in the thermodynamic limit.

**Derivation of the Boltzmann-Gibbs distribution**

Here we start by assuming \( N \) agents, each one with coordinate \( x_i, i = 1, \ldots, N \), with \( x_i \geq 0 \) representing the wealth or money of the agent \( i \), and a total available amount of money \( E \):

\[ x_1 + x_2 + \cdots + x_{N-1} + x_N \leq E. \] (16)

Under random evolution rules for the exchanging of money among agents, let us suppose that this system evolves in the interior of the \( N \)-dimensional pyramid given by Eq. (16). The role of the heat reservoir, that in this model supplies money instead of energy, could be played by the state or by the bank system in western societies. The formula for the volume \( V_N(E) \) of an equilateral \( N \)-dimensional pyramid formed by \( N + 1 \) vertices linked by \( N \) perpendicular sides of length \( E \) is

\[ V_N(E) = \frac{E^N}{N!}. \] (17)

We suppose that each point on the \( N \)-dimensional pyramid is equiprobable, then the probability \( f(x_i)dx_i \) of finding the agent \( i \) with money \( x_i \) is proportional to the volume formed
by all the points into the \((N - 1)\)-dimensional pyramid having the \(i\)th-coordinate equal to \(x_i\). Our objective is to show that \(f(x_i)\) is the Boltzmann factor (or the Maxwell-Boltzmann distribution), with the normalization condition

\[
\int_0^E f(x_i)dx_i = 1. \tag{18}
\]

If the \(i\)th agent has coordinate \(x_i\), the \(N - 1\) remaining agents share, at most, the money \(E - x_i\) on the \((N - 1)\)-dimensional pyramid

\[
x_1 + x_2 \cdots + x_{i-1} + x_{i+1} \cdots + x_N \leq E - x_i, \tag{19}
\]

whose volume is \(V_{N-1}(E - x_i)\). It can be easily proved that

\[
V_N(E) = \int_0^E V_{N-1}(E - x_i)dx_i. \tag{20}
\]

Hence, the volume of the \(N\)-dimensional pyramid for which the \(i\)th coordinate is between \(x_i\) and \(x_i + dx_i\) is \(V_{N-1}(E - x_i)dx_i\). We normalize it to satisfy Eq. \((18)\), and obtain

\[
f(x_i) = \frac{V_{N-1}(E - x_i)}{V_N(E)}, \tag{21}
\]

whose final form, after some calculation is

\[
f(x_i) = N E^{-1} \left(1 - \frac{x_i}{E}\right)^{N-1}, \tag{22}
\]

If we call \(\epsilon\) the mean wealth per agent, \(E = N\epsilon\), then in the limit of large \(N\) we have

\[
\lim_{N \gg 1} \left(1 - \frac{x_i}{E}\right)^{N-1} \simeq e^{-x_i/\epsilon}. \tag{23}
\]

The Boltzmann factor \(e^{-x_i/\epsilon}\) is found when \(N \gg 1\) but, even for small \(N\), it can be a good approximation for agents with low wealth. After substituting Eq. \((23)\) into Eq. \((22)\), we obtain the Maxwell-Boltzmann distribution in the asymptotic regime \(N \to \infty\) (which also implies \(E \to \infty\)):

\[
f(x)dx = \frac{1}{\epsilon} e^{-x/\epsilon}dx, \tag{24}
\]

where the index \(i\) has been removed because the distribution is the same for each agent, and thus the wealth distribution can be obtained by averaging over all the agents. This distribution has been found to fit the real distribution of incomes in western societies\(^6\).

Depending on the physical situation the mean wealth per agent \(\epsilon\) takes different expressions and interpretations. For instance, doing a thermodynamic simile, we can calculate
the dependence of $\epsilon$ on the temperature, which, as in the microcanonical ensemble, can be obtained in this case by differentiating the entropy with respect to the total wealth. The entropy can be written as $S = -kN \int_0^\infty f(x) \ln f(x) \, dx$, where $f(x)$ is given by Eq. (24) and $k$ is the Boltzmann constant. If we recall that $\epsilon = E/N$, we obtain

$$S(E) = kN \ln \left( \frac{E}{N} \right) + kN. \quad (25)$$

The calculation of the temperature $T$ gives

$$T^{-1} = \left( \frac{\partial S}{\partial E} \right)_N = \frac{kN}{E} = \frac{k}{\epsilon}. \quad (26)$$

Thus $\epsilon = kT$, and the Boltzmann-Gibbs distribution is obtained as it is usually given in the literature:

$$f(x) \, dx = \frac{1}{kT} e^{-x/kT} \, dx. \quad (27)$$

This shows that the geometrical image of the volume-based statistical ensemble allows us to recover the same result than that obtained from the microcanonical and canonical ensembles. Also, it confirms for this case the equivalence among all these ensembles in the thermodynamic limit.

**General derivation of the asymptotic distribution: an open problem**

Now the problem is stated in a general way. Let $b$ be a real constant. If we have a set of positive variables $(x_1, x_2, \ldots, x_N)$ verifying

$$x_1^b + x_2^b + \cdots + x_{N-1}^b + x_N^b \leq E \quad (28)$$

with an adequate mechanism assuring the equiprobability of all the possible states $(x_1, x_2, \ldots, x_N)$ into the volume given by expression (28), will we have for the generic variable $x$ the distribution

$$f(x) \, dx \sim \epsilon^{-1/b} e^{-x^b/\epsilon} \, dx, \quad (29)$$

when we average over the ensemble in the limit $N \to \infty$?

Let us suppose that the answer to this last question is affirmative (as it will be probably shown in a next paper). If we define

$$c_b = \left[ \int_0^\infty e^{-y^b/b} \, dy \right]^{-1}, \quad (30)$$
then expression (29), redefined as

$$f(x)dx = c_b \epsilon^{-1/b} e^{-x^b/b\epsilon} dx,$$  \hspace{1cm} (31)

is normalized, i.e., $\int_0^\infty f(x)dx = 1$. Following the thermodynamic simile done in the cases $b = 1, 2$, we can calculate the dependence of $\epsilon$ on the temperature by differentiating the entropy with respect to the energy. The entropy can be written as $S = -kN \int_0^\infty f(x) \ln f(x) \, dx$, where $f(x)$ is given by Eq. (31) and $k$ is the Boltzmann constant. If we recall that $\epsilon = E/N$, we obtain

$$S(E) = \frac{kN}{b} \ln \left( \frac{E}{N} \right) + \frac{kN}{b} (1 - b \ln c_b),$$ \hspace{1cm} (32)

where it has been used that $\epsilon = \langle x^b \rangle = \int_0^\infty x^b f(x) dx$. Let us recall at this point that, for the case $b = 2$, the limits used in the normalization integral of $f(x)$ in expression (4), and, therefore, in the calculation of $S(E)$, are from $-\infty$ to $\infty$ instead from 0 to $\infty$ that are used here. This does not introduce any change in the final result, only redefines the constant $c_b=2$, which now is $\sqrt{\frac{2}{\pi}}$ instead of the factor $\frac{1}{\sqrt{2\pi}}$ from expression (12).

The calculation of the temperature $T$ gives

$$T^{-1} = \left( \frac{\partial S}{\partial E} \right)_N = \frac{kN}{bE} = \frac{k}{b\epsilon}.$$ \hspace{1cm} (33)

Thus $\epsilon = kT/b$, a result that recovers the theorem of equipartition of energy for the quadratic case $b = 2$. The distribution for all $b$ is finally obtained:

$$f(x)dx = c_b \left( \frac{b}{kT} \right)^{1/b} e^{-x^b/kT} dx.$$  \hspace{1cm} (34)

This shows that the geometrical image of the volume-based statistical ensemble allows us to recover the same result than that obtained from the microcanonical and canonical ensembles\cite{3,5}. Also, it confirms for this case the equivalence among all these ensembles in the thermodynamic limit.

**APPENDIX: A microcanonical image of the canonical ensemble**

We are interested in this paper with alternative views of the different statistical ensembles. Here we give a different image of the canonical ensemble from that that is its usual presentation in the literature.
Let us suppose that a system with mean energy $\bar{E}$, and in thermal equilibrium with a heat reservoir, is observed during a very long period $\tau$ of time. Let $E_i$ be the energy of the system at time $i$. Then we have:

$$E_1 + E_2 + \cdots + E_{\tau-1} + E_\tau = \tau \cdot \bar{E}.$$  

(35)

If we repeat this process of observation a huge number (toward infinity) of times, the different vectors of measurements, $(E_1, E_2, \ldots, E_{\tau-1}, E_\tau)$, with $0 \leq E_i \leq \tau \cdot \bar{E}$, will finish by covering equiprobably the whole surface of the $\tau$-dimensional hyperplane given by Eq. (35). If it is now taken the limit $\tau \to \infty$, the asymptotic probability $p(E)$ of finding the system with an energy $E$ (where the index $i$ has been removed),

$$p(E) \sim e^{-E/\bar{E}},$$

(36)

is found by means of the geometrical arguments exposed in Ref. 5. Doing a thermodynamic simile, the temperature $T$ can also be calculated. It is obtained that

$$\bar{E} = kT.$$  

(37)

The stamp of the canonical ensemble, namely, the Boltzmann factor,

$$p(E) \sim e^{-E/kT},$$

(38)

is finally recovered from this new image of the canonical ensemble.

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