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Microcanonical single-particle distributions for an ideal gas in a gravitational field

F L Román, J A White and S Velasco

Departamento di Física Aplicada, Facultad de Ciencias, Universidad de Salamanca, 37008 Salamanca, Spain

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Abstract. The single-particle energy, velocity and height probability distributions for an ideal gas in a gravitational field are obtained within the microcanonical ensemble framework. The asymptotic expressions for these distributions in the thermodynamic limit are also reported.

Resumen. Haciendo uso de la colectivdad microcanónica, en este trabajo se obtienen la distribución de probabilidad para la energía, la velocidad y la altura de un partícula para un gas ideal en un campo gravitatorio. También se obtienen las correspondientes distribuciones en el límite termodinámico.

1. Introduction

In most textbooks on statistical mechanics, the microcanonical ensemble serves as a necessary and academic first step to introduce the ensemble theory, but it is rarely used in the study of specific systems. Two main reasons can be argued for this lack of applications. First, many real systems are not kept at constant total energy. Second, from a mathematical (operative) point of view the expressions appearing in this ensemble are less familiar to the students than those appearing in other ensembles. On the other hand, the use of computer simulations in this field have become usual in statistical mechanics classrooms, with the aim of both illustrating *experimentally* the behaviour of the system and supporting the theoretical expressions. In this context, it must be noted that the majority of these computer simulations are designed for a finite system having a constant total energy. Then, it is clear that a correct interpretation of the results can only be achieved by comparing the computer simulation data with the microcanonical formulae. This correct comparison could be essential in studies of small systems.

Perhaps the most typical example to which the above paragraph applies is the calculation of the probability distribution, $\omega(\vec{p})$, of the momentum $\vec{p}$ of one of the particles of an ideal gas. Students know that such a distribution has the *Maxwell* form (or the *Maxwell–Boltzmann* form if one is concerned with the distribution of the absolute magnitude of the velocity: $v = |\vec{p}|/m$). Strictly speaking the *Maxwell* expression is the distribution of particle momenta in the canonical ensemble. However, in the microcanonical ensemble this distribution has a form that differs from the *Maxwell* one, approaching *Maxwell's* form in the thermodynamic limit. Therefore, the momentum distribution generated in microcanonical simulations must be compared with the appropriate microcanonical form and not with the *Maxwell* form. In a recent issue of this journal (Velasco *et al* 1993), the importance of this question in studies of systems with a reduced number of particles has been discussed. This is the case, for instance, when the simulations are performed with a reduced number of particles in order to make the simulation in a reasonable time, or when one is interested in the behaviour of small systems, such as clusters.

The aim of the present work is to analyse, following the above discussions, the single-particle distributions for a particularly interesting system: an ideal gas in a gravitational field. There are several pedagogical reasons for this study. First, this system is more *realistic* than the usual ideal gas. Second, not only *momentum (or velocity) and energy distributions* but also a position (height) distribution appears in this problem (remember that, in the absence of a gravitational field, for the ideal gas all positions inside a vessel are equally probable). Third, this system is very useful in illustrating some properties of probability distribution functions (factorization, statistical correlations, etc). Furthermore, we note

that the single-particle distributions for this system in the canonical ensemble appear in many textbooks on statistical mechanics (see, for instance, Becker 1967, pp 94–8 and 142); in particular, the height distribution in the canonical ensemble has the well known *barometric* form.

We start, in section 2, by calculating the microcanonical density function for an ideal gas (in any dimension) in a vertical gravitational field. The single-particle height and momentum (or velocity) distributions are then derived by integrating this density function over appropriate phase coordinates. The integrations appearing in the calculations are carried out by means of a procedure based in the *Dirichlet* integral (Fernández-Pineda *et al* 1979). The single-particle energy distribution is obtained from the well known energy distribution law of a component in the microcanonical ensemble. The moments associated to each distribution are derived and some interesting observations on the statistical correlation between height and velocity are also reported. In section 3 we calculate the asymptotic expressions of the microcanonical distributions in the thermodynamic limit, obtaining the canonical forms characterizing this system. In particular, we show that the momentum and velocity distributions are identical to the *Maxwell* and *Maxwell–Boltzmann* distributions of an ideal gas (without gravitational field) whereas the height distribution takes the *barometric* form. The moments corresponding to the canonical distributions are also calculated, showing that height and velocity are now statistically independent variables. Finally, in section 4, a comparison between microcanonical and canonical distributions for a two-dimensional ideal gas in a gravitational field is made.

2. Single-particle distributions in the microcanonical ensemble

We consider a f-dimensional ($f = 1, 2, 3$) ideal gas consisting of N identical structureless particles contained into a vertical vessel of linear dimensions L_α ($\alpha = 1, \ldots, f$). The system is placed in a gravitational field of intensity g directed downward. The classical Hamiltonian of the system is

$$H = K + E_p + E_w + \sum_{\alpha=1}^{fN} \frac{p_\alpha^2}{2m} + \sum_{i=1}^{N} mgz_i + E_w \tag{1}$$

where m is the mass of a particle, p_α a Cartesian component of the momentum of a particle, z_i the height of the ith particle with respect to the bottom of the vessel, and

$$E_w = \begin{cases} 0 & \text{inside the vessel,} \\ \infty & \text{in the vessel walls.} \end{cases}$$

Furthermore, we assume that the vertical dimension L_z of the vessel is such that: $L_z = \infty$.

2.1. The density function

In the microcanonical ensemble the macrostate of the system is defined by a constant energy (E), a fixed number of particles (N) and a fixed *volume* (V). The equilibrium density function is given by

$$\rho(q,p) = \frac{1}{\Omega(E,V,N)} \delta[H(q,p) - E] \tag{2}$$

where $(q,p) \equiv (q_1, \ldots, q_{fN};\ p_1, \ldots, p_{fN})$ denotes the phase coordinates of the system, $\delta(x)$ is the Dirac delta function, and $\Omega(E,V,N)$ is the *density of states*, which is equal, by definition, to the number of microstates compatible with the macrostate (E,V,N). It is well known that the density of states can be obtained from,

$$\Omega(E,V,N) = \left(\frac{\partial \Phi(E,V,N)}{\partial E}\right)_{V,N} \tag{3}$$

where $\Phi(E,V,N)$ is the *phase volume*, which is defined as the number of microstates with energy equal to or less than E,

$$\Phi(E,V,N) = \int \cdots \int_{0 \le H(q,p) \le E} \mathrm{d}q_1 \ldots \mathrm{d}q_{fN} \mathrm{d}p_1 \ldots \mathrm{d}p_{fN}. \tag{4}$$

Fernández-Pineda *et al* developed a very elegant approach to evaluate the phase volume (4) based on the Dirichlet integral formula. This method makes use of the integral

$$\int \cdots \int_{0 \le \sum_{j=1}^{n} (t_j/b_j)^{\beta_j} \le 1} t_1^{\alpha_1 - 1} \ldots t_n^{\alpha_n - 1} \mathrm{d}t_1 \ldots \mathrm{d}t_n = \frac{\prod_{j=1}^{n} b_j^{\alpha_j} \prod_{j=1}^{n} \Gamma(\alpha_j/\beta_j)}{\prod_{j=1}^{n} \beta_j\, \Gamma\left(1 + \sum_{j=1}^{n} \alpha_j/\beta_j\right)} \tag{5}$$

where $\Gamma(x)$ is the Euler gamma function. In the present case, taking into account the Hamiltonian (1), when the horizontal position coordinates are integrated out, equation (4) gives:

$$\Phi(E,N) = A^N \int \cdots \int_{0 \le \sum_{\alpha=1}^{fN} (p_\alpha/\sqrt{2mE})^2 + \sum_{i=1}^{N} (z_i/E/mg) \le 1} \times \mathrm{d}z_1 \ldots \mathrm{d}z_N \mathrm{d}p_1 \ldots \mathrm{d}p_{fN}$$

where $A = \prod_{\alpha=1}^{f-1} L_\alpha$. The above equation has the same form as equation (5). When parameters are

identified, one easily gets:

$$\Phi(E,N)=\frac{A^N(2\pi)^{fN/2}m^{(f-2)N/2}}{g^N\Gamma(\frac{1}{2}fN+N+1)}E^{(f+2)N/2} \quad (7)$$

where a factor 2^{fN} has been taken into account because the integration over the momenta in equation (5) is performed over positive and negative values of these variables. From equations (3) and (7), one obtains

$$\Omega(E,N)=\frac{A^N(2\pi)^{fN/2}m^{(f-2)N/2}}{g^N\Gamma(\frac{1}{2}fN+N)}E^{[(f+2)N/2]-1} \quad (8)$$

for the density of states.

2.2. Velocity and height probability distributions

The height and momentum density distribution $\omega_m(z_1,\vec{p}_1)(\vec{p}_1\equiv(p_1,\ldots,p_f))$ for one particle can be obtained from the microcanonical density function (2) by integrating over all phase coordinates except $(z_1,\vec{p}_1)$ and over spatial coordinates $q\neq(z_2,\ldots,z_N)$

$$\begin{aligned}\omega_m(z_1,\vec{p}_1)&=\frac{1}{\Omega(E,N)}\int\cdots\int\delta[H(q,p)-E]\\&\quad\times dq_2\ldots dq_{fN}dp_{f+1}\ldots dp_{fN}\\&=\frac{A^N}{\Omega(E,N)}\int\cdots\int\frac{\partial}{\partial E}\theta[E-H(q,p)]\\&\quad\times dz_2\ldots dz_N dp_{f+1}\ldots dp_{fN}\\&=\frac{A^N}{\Omega(E,N)}\frac{\partial}{\partial E}\\&\quad\times\int\cdots\int_{0\leq\sum_{\alpha=f+1}^{fN}(p_\alpha/\sqrt{2mE_1'})^2+\sum_{i=2}^{N}(z_i/E_1'/mg)\leq 1}\\&\quad\times dz_2\ldots dz_N dp_{f+1}\ldots dp_{fN}\end{aligned} \quad (9)$$

where $\theta(x)$ is the Heaviside step function, $E_1'=E-(\vec{p}_1^2/2m)-mgz_1$, and where the subscript m means *microcanonical*. The integral in equation (9) has the same form as equation (5). Identifying parameters and taking into account equation (8), one obtains

$$\begin{aligned}\omega_m(z_1,\vec{p}_1)&=\frac{\Gamma(\frac{1}{2}fN+N)}{\Gamma(\frac{1}{2}fN+N-\frac{1}{2}(f+2))}\\&\quad\times\frac{mg}{(2\pi m)^{f/2}E^{(f+2)/2}}\\&\quad\times\left(1-\frac{\vec{p}_1^2}{2mE}-\frac{mgz_1}{E}\right)^{[(f/2)+1]N-[(f/2)+2]}\end{aligned} \quad (10)$$

Furthermore, taking into account that

$$\int_{(\text{angles})}d\vec{p}=\frac{2\pi^{f/2}}{\Gamma(f/2)}p^{f-1}dp \quad (11)$$

and that $p=mv$, from equation (10) one gets:

$$\begin{aligned}\omega_m(z_1,v_1)&=\frac{\Gamma(\frac{1}{2}fN+N)}{\Gamma(f/2)\Gamma(\frac{1}{2}fN+N-(f+2)/2)}\\&\quad\times\frac{m^{(f+2)/2}gv_1^{f-1}}{2^{(f-2)/2}E^{(f+2)/2}}\\&\quad\times\left(1-\frac{mv_1^2}{2E}-\frac{mgz_1}{E}\right)^{[(f/2)+1]N-[(f/2)+2]}\end{aligned} \quad (12)$$

for the height and velocity (modulus) density distribution for one particle.

The single-particle height distribution $\omega_m(z_1)$ can be obtained by integrating distribution (12) over the velocity v_1. Taking into account the integral

$$\int_0^a x^m(a^n-x^n)^p dx=\frac{\Gamma[(m+1)/n]\Gamma(p+1)}{n\Gamma[(m+1)/n+p+1]}a^{m+1+np} \quad (13)$$

one obtains,

$$\begin{aligned}\omega_m(z_1)&=\int_0^{\sqrt{2(E-mgz_1)}}\omega_m(z_1,v_1)dv_1\\&=\left(\frac{fN}{2}+N-1\right)\frac{mg}{E}\left(1-\frac{mgz_1}{E}\right)^{[(f/2)+1]N-2}\end{aligned} \quad (14)$$

In a similar way, and using equation (13), the single-particle velocity distribution $\omega_m(v_1)$ can be obtained by integrating distribution (12) over the spatial coordinate z_1,

$$\begin{aligned}\omega_m(v_1)&=\int^{(E/mg)-(v_1^2/2g)}\omega_m(z_1,v_1)dz_1\\&=\frac{\Gamma[(fN/2)+N]}{\Gamma(f/2)\Gamma[(fN/2)+N-(f/2)]}\frac{m^{f/2}v_1^{f-1}}{2^{(f-2)/2}E^{f/2}}\\&\quad\times\left(1-\frac{mv_1^2}{2E}\right)^{[(f/2)+1](N-1)}\end{aligned} \quad (15)$$

This velocity distribution differs from the Schlüter distribution, characteristic of an ideal gas (without gravitational field) in the microcanonical ensemble (Schlüter 1948, Velasco *et al* 1993), which is given by:

$$\begin{aligned}\omega_m^{(0)}(v_1)&=\frac{\Gamma(fN/2)}{\Gamma(f/2)\Gamma[(fN/2)-(f/2)]}\frac{m^{f/2}v_1^{f-1}}{2^{(f-2)/2}E^{f/2}}\\&\quad\times\left(1-\frac{mv_1^2}{2E}\right)^{(fN/2)-[(f/2)+1]}\end{aligned} \quad (16)$$

Next we shall derive the moments $\langle z_1^n\rangle_m$ and $\langle v_1^n\rangle_m$ of distributions (14) and (15) respectively. Using

equation (13), simple calculations lead to:

$$\langle z_1^n\rangle_m = \int_0^{E/mg} z_1^n \omega_m(z_1)\mathrm{d}z_1 = \frac{\Gamma(n+1)\Gamma[(fN/2)+N]}{\Gamma[(fN/2)+N+n]}\left(\frac{E}{mg}\right)^n \qquad (17)$$

$$\langle v_1^n\rangle_m = \int_0^{\sqrt{2E/m}} v_1^n \omega_m(v_1)\mathrm{d}v_1 = \frac{\Gamma[(f+n)/2]\Gamma[(fN/2)+N]}{\Gamma(f/2)\Gamma[(fN/2)+N+(n/2)]}\left(\frac{2E}{m}\right)^{n/2}. \qquad (18)$$

Particularly interesting are the first moment of the height distribution and the second moment of the velocity distribution, which take the form:

$$\langle z_1\rangle_m = \frac{2}{(f+2)}\left(\frac{E}{Nmg}\right) \qquad (19)$$

$$\langle v_1^2\rangle_m = \frac{2f}{(f+2)}\left(\frac{E}{Nm}\right). \qquad (20)$$

From equation (19) one gets

$$\langle E_p\rangle_m = \sum_{i=1}^{N} mg\langle z_i\rangle_m = \frac{2E}{(f+2)} \qquad (21)$$

for the mean potential energy, and

$$\langle K\rangle_m = \sum_{i=1}^{N} \tfrac{1}{2}m\langle v_i^2\rangle_m = \frac{fE}{(f+2)} \qquad (22)$$

for the mean kinetic energy. Note that: $\langle K\rangle_m + \langle E_p\rangle_m = E$ and $\langle K\rangle_m = (f/2)\langle E_p\rangle_m$.

Comparison of distributions (12), (14) and (15) shows the fact that:

$$\omega_m(z_1, v_1) \neq \omega_m(z_1)\omega_m(v_1) \qquad (23)$$

which indicates that, in a microcanonical scheme, the height and the velocity of one particle are not *statistically independent* variables for an ideal gas in a gravitational field; one says that they are *correlated* variables. As a measure of this correlation we can consider the cross moment,

$$\langle z_1 v_1\rangle_m = \int_0^{E/mg} z_1\mathrm{d}z_1 \int_0^{\sqrt{2(E-mgz_1)/m}} v_1\omega_m(z_1,v_1)\mathrm{d}v_1 = \frac{\Gamma[(f+1/2)]\Gamma[(fN/2)+N]}{\Gamma(f/2)\Gamma[(fN/2)+N+\frac{3}{2}]}\left(\frac{2^{1/2}E^{3/2}}{m^{3/2}g}\right). \qquad (24)$$

One can easily check that: $\langle z_1 v_1\rangle_m \neq \langle z_1\rangle_m\langle v_1\rangle_m$.

2.3. Energy probability distribution

Since the energy of one particle depends both on its velocity and its height, it is not possible to derive the single-particle energy distribution from the height and velocity distribution (12) in a straightforward way. Students of introductory courses in statistical mechanics know that if an isolated system Σ can be descomposed, in the sense discussed by Khinchin (1949, pp 38–43), into two components Σ_I and Σ_{II}, the probability density of the energy E_I of the component Σ_I has the form (Khinchin 1949, p 75, Becker 1967, p 138):

$$p(E_I) = \frac{\Omega_I(E_I)\Omega_{II}(E-E_I)}{\Omega(E)}. \qquad (25)$$

In particular, considering one particle as component Σ_I and the remaining $(N-1)$ particles as component Σ_{II}, equation (25) leads to the following single-particle energy distribution:

$$p(E_1) = \frac{\Omega_1(E_1)\Omega_{(N-1)}(E-E_1)}{\Omega_N(E)} \qquad (26)$$

where Ω_1, $\Omega_{(N-1)}$ and Ω_N denote the density of states for a system consisting of *one*, $(N-1)$ and N particles, respectively. We remark that the above equation is verified when the interparticle energy interaction can be neglected, so that the energy of the system is given by the sum of the energies of constituent particles.

Substitution of equation (8) into equation (26) leads to:

$$p_m(E_1) = \frac{\Gamma[(fN/2)+N]}{\Gamma[(f/2)+1]\Gamma\{(fN/2)+N-[(f+2)/2]\}} \times \frac{1}{E}\left(\frac{E_1}{E}\right)^{f/2}\left(1-\frac{E_1}{E}\right)^{[(f/2)+1](N-1)-1} \qquad (27)$$

which is the single-particle energy distribution for the considered finite system in the microcanonical ensemble. Note that this distribution differs from the Schlüter energy distribution characteristic of an ideal gas without gravitational field (Velasco *et al* 1993) which is given by:

$$p_m^{(0)}(E_1) = \frac{\Gamma(fN/2)}{\Gamma(f/2)\Gamma[(fN/2)-(f/2)]}\frac{1}{E}\left(\frac{E_1}{E}\right)^{(f/2)-1} \times \left(1-\frac{E_1}{E}\right)^{(fN/2)-[(f/2)+1]} \qquad (28)$$

Using integral (13), the moments of distribution (27) can be obtained by a simple calculation,

$$\langle E_1^n\rangle_m = \int_0^E E_1^n p_m(E_1)\mathrm{d}E_1 = \frac{\Gamma[(f/2)+n+1]\Gamma[(fN/2)+N]}{\Gamma[(f/2)+1)\Gamma[(fN/2)+N+n]}E^n. \qquad (29)$$

In particular, the first two moments are given by:

$$\langle E_1\rangle_m = E/N \qquad (30)$$

$$\langle E_1^2\rangle_m = \frac{(f+4)N}{(fN+2N+2)}\left(\frac{E}{N}\right)^2. \qquad (31)$$

Based on equations (19) and (20), one can check that: $\langle E_1\rangle_m = \frac{1}{2}m\langle v_1^2\rangle_m + mg\langle z_1\rangle_m$.

3. The thermodynamic limit

In the thermodynamic limit (TL)

$$N \to \infty, \qquad E \to \infty \qquad \frac{E}{N} = \text{finite} \neq 0 \tag{32}$$

the *microcanonical* distributions must approach the *canonical* forms, since the infinite system acts as a thermal bath for the single particle. Introducing the limits

$$\lim_{n,a\to\infty;n/a=\text{finite}} \left(1 - \frac{x}{a}\right)^n = e^{-nx/a} \tag{33}$$

$$\lim_{n,a\to\infty;n/a=\text{finite}} \frac{\Gamma(n)}{\Gamma(n-\nu)} a^{-\nu} = \left(\frac{n}{a}\right)^\nu \tag{34}$$

the TL of single-particle distributions (10), (12), (14), (15) and (27) are, respectively,

$$\omega_c(z_1, \vec{p}_1) = \frac{mg}{(2\pi m)^{f/2}} \left[\left(\frac{f}{2}+1\right)\frac{N}{E}\right]^{(f+2)/2} \times \exp\left[-\left(\frac{f}{2}+1\right)\frac{N}{E}\left(\frac{\vec{p}_1^{\,2}}{2m} + mgz_1\right)\right] \tag{35}$$

$$\omega_c(z_1, v_1) = \frac{m^{(f+2)/2} g}{\Gamma(f/2) 2^{(f-2)/2}} \left[\left(\frac{f}{2}+1\right)\frac{N}{E}\right]^{(f+2)/2} \times v_1^{f-1} \exp\left[-\left(\frac{f}{2}+1\right)\frac{N}{E}\left(\frac{mv_1^2}{2} + mgz_1\right)\right] \tag{36}$$

$$\omega_c(z_1) = \left(\frac{f}{2}+1\right)\frac{Nmg}{E} \exp\left[-\left(\frac{f}{2}+1\right)\frac{Ngmz_1}{E}\right] \tag{37}$$

$$\omega_c(v_1) = \frac{m^{f/2}}{\Gamma(f/2) 2^{(f-2)/2}} \left[\left(\frac{f}{2}+1\right)\frac{N}{E}\right]^{f/2} \times v_1^{f-1} \exp\left[-\left(\frac{f}{2}+1\right)\frac{Nmv_1^2}{2E}\right] \tag{38}$$

$$p_c(E_1) = \frac{1}{\Gamma[(f/2)+1]} \left[\left(\frac{f}{2}+1\right)\frac{N}{E}\right]^{(f+2)/2} \times E_1^{f/2} \exp\left[-\left(\frac{f}{2}+1\right]\frac{NE_1}{E}\right]$$

where the label 'c' means *canonical.*

Using the definition of temperature in the microcanonical ensemble,

$$\frac{1}{k_B T} = \left(\frac{\partial \ln \Phi}{\partial E}\right)_{V,N} = \frac{1}{\Phi}\left(\frac{\partial \Phi}{\partial E}\right)_{V,N} = \frac{\Omega}{\Phi} \tag{40}$$

and taking into account expressions (7) and (8), one obtains

$$\frac{1}{k_B T} = \left(\frac{f}{2}+1\right)\frac{N}{E} \tag{41}$$

which remains finite in the thermodynamic limit. Substitution of equation (41) into equations (35)–(39) leads to the following expressions for the single-particle distributions of an ideal gas in a gravitational field within the canonical ensemble framework:

$$\omega_c(z_1, \vec{p}_1) = \frac{mg}{(2\pi m)^{f/2}} \left(\frac{1}{k_B T}\right)^{(f+2)/2} \times \exp\left[-\left(\frac{\vec{p}_1^{\,2}}{2m} + mgz_1\right)\Big/ k_B T\right] \tag{42}$$

$$\omega_c(z_1, v_1) = \frac{m^{(f+2)/2} g}{\Gamma(f/2) 2^{(f-2)/2}} \left(\frac{1}{k_B T}\right)^{(f+2)/2} \times v_1^{f-1} \exp\left[-\left(\frac{mv_1^2}{2} + mgz_1\right)\Big/ k_B T\right] \tag{43}$$

$$\omega_c(z_1) = \frac{mg}{k_B T} \exp\left(-\frac{mgz_1}{k_B T}\right) \tag{44}$$

$$\omega_c(v_1) = \frac{m^{f/2}}{\Gamma(f/2) 2^{(f-2)/2}} \left(\frac{1}{k_B T}\right)^{f/2} \times v_1^{f-1} \exp\left(-\frac{-mv_1^2}{2k_B T}\right) \tag{45}$$

$$p_c(E_1) = \frac{1}{\Gamma[(f/2)+1]} \left(\frac{1}{k_B T}\right)^{(f+2)/2} \times E_1^{f/2} \exp\left(-\frac{E_1}{k_B T}\right). \tag{46}$$

We notice that distributions (42) and (43) have the usual *Maxwell* form, while the height distribution (44) has the well known *barometric* form (Becker 1967, p 142). It is also interesting to compare the velocity distribution (45) and the energy distribution (46) with those characterizing an ideal gas in absence of gravitational field, that is

$$\omega_c^{(0)}(v_1) = \frac{m^{f/2}}{\Gamma(f/2) 2^{(f-2)/2}} \left(\frac{1}{k_B T}\right)^{f/2} \times v_1^{f-1} \exp\left(-\frac{mv_1^2}{2k_B T}\right) \tag{47}$$

$$p_c^{(0)}(E_1) = \frac{1}{\Gamma(f/2)} \left(\frac{1}{k_B T}\right)^{f/2} E_1^{(f-2)/2} \exp\left(-\frac{E_1}{k_B T}\right). \tag{48}$$

(These distributions can be easily obtained as the TL

of distributions (16) and (28), respectively.) One can see that the velocity distributions (45) and (47) have the same form, i.e. within the canonical scheme the single-particle velocity distribution of an ideal gas is not sufficient to discern whether the system is or is not in a gravitational field (remember that both distributions are different in the microcanonical scheme). However, the single-particle energy distributions (46) and (48) are not equal as it happens in the microcanonical scheme.

Next we shall derive the moments of the single-particle canonical distributions. From equations (44), (45) and (46), one gets:

$$\langle z_1^n\rangle_c = \int_0^\infty z_1^n \omega_c(z_1)\,dz_1 = \frac{\Gamma(n+1)}{[(f/2)+1]^n}\left(\frac{E}{Nmg}\right)^n \tag{49}$$

$$\langle v_1^n\rangle_c = \int_0^\infty v_1^n \omega_c(v_1)\,dv_1 = \frac{\Gamma[(f+n)/2]}{\Gamma(f/2)}\frac{1}{[(f/2)+1]^{n/2}} \times \left(\frac{2E}{Nm}\right)^{n/2} \tag{50}$$

$$\langle E_1^n\rangle_c = \int_0^\infty E_1^n p_c(E_1)\,dE_1 = \frac{\Gamma[(f/2)+n+1]}{\Gamma[(f/2)+1]} \times \frac{1}{[(f/2)+1]^n}\left(\frac{E}{N}\right)^n. \tag{51}$$

Comparison of these moments with those of the corresponding microcanonical distributions leads to:

$$\frac{\langle z_1^n\rangle_m}{\langle z_1^n\rangle_c} = \frac{\Gamma[(fN/2)+N]}{\Gamma[(fN/2)+N+n]}[(f/2)+1]^n N^n \overset{N\to\infty}{\longrightarrow} 1 \tag{52}$$

$$\frac{\langle v_1^n\rangle_m}{\langle v_1^n\rangle_c} = \frac{\Gamma[(fN/2)+N]}{\Gamma[(fN/2)+N+(n/2)]}[(f/2)+1]^{n/2} \times N^{n/2} \overset{N\to\infty}{\longrightarrow} 1 \tag{53}$$

$$\frac{\langle E_1^n\rangle_m}{\langle E_1^n\rangle_c} = \frac{\Gamma[(fN/2)+N]}{\Gamma[(fN/2)+N+n]}[(f/2)+1]^n N^n \overset{N\to\infty}{\longrightarrow} 1. \tag{54}$$

From the above expressions, it is interesting to note that: $\langle z_1\rangle_m = \langle z_1\rangle_c$, $\langle v_1^2\rangle_m = \langle v_1^2\rangle_c$ and $\langle E_1\rangle_m = \langle E_1\rangle_c$, while the other moments only coincide in the thermodynamic limit.

Finally, from distributions (7), (37) and (38), it is also interesting to note that:

$$\omega_c(z_1, v_1) = \omega_c(z_1)\omega_c(v_1) \tag{55}$$

which shows that, at difference with the microcanonical case (see equation (23)), the height and the velocity of a particle become *uncorrelated* variables in the canonical ensemble.

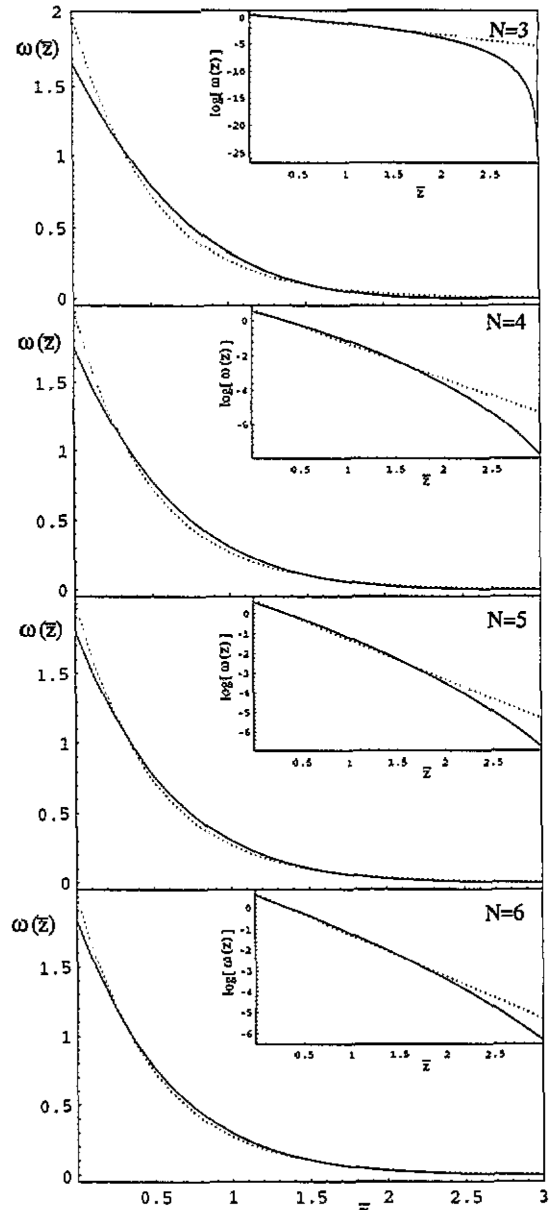

Figure 1. Single-particle height distributions for a two-dimensional ideal gas consisting of 3, 4, 5 and 6 particles in a gravitational field: microcanonical distribution (solid lines) and canonical (*barometric*) distribution (dotted lines). The inset shows the corresponding log plots.

4. Case of a two-dimensional ideal gas

We now proceed to compare the microcanonical and canonical distributions reported in the above sections for the case of a two-dimensional ($f = 2$) ideal gas in a gravitation field. In order to do this comparison we use *reduced* heights, velocities and energies, defined

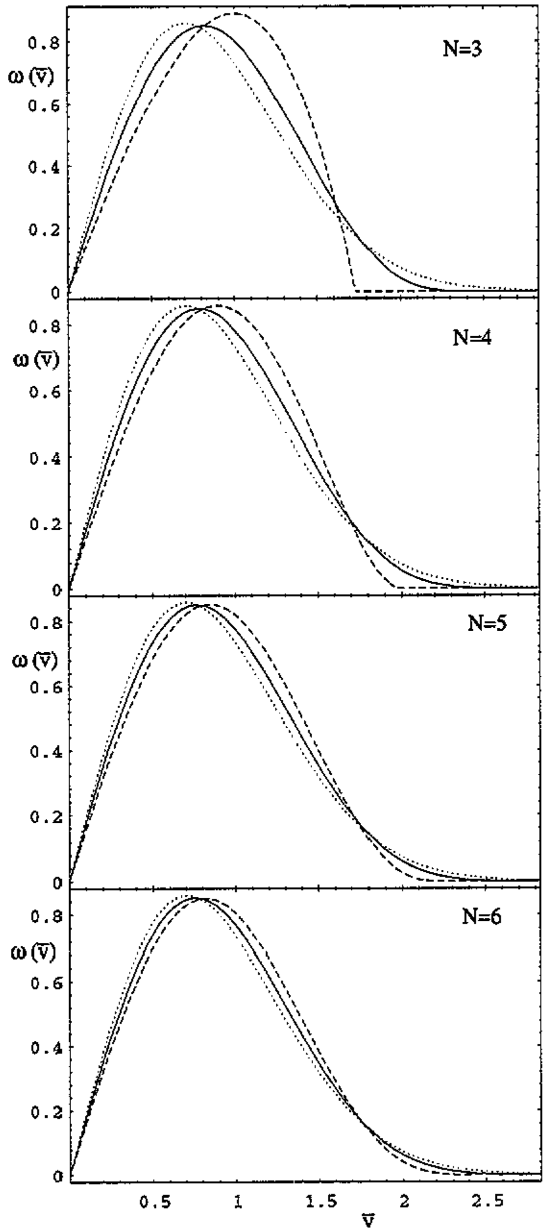

Figure 2. Same as figure 1 but for the single-particle velocity distribution. The dashed lines correspond to the microcanonical velocity distribution for an ideal gas in the absence of a gravitational field.

by:

$$\bar{z}_1 = \frac{Nmgz_1}{E}, \qquad \bar{v}_1 = \sqrt{\frac{Nm}{E}}v_1, \qquad \bar{E}_1 = \frac{NE_1}{E}. \tag{56}$$

Then, the single-particle height (14), velocity (15) and energy (27) distributions, with $f = 2$, in the micro-

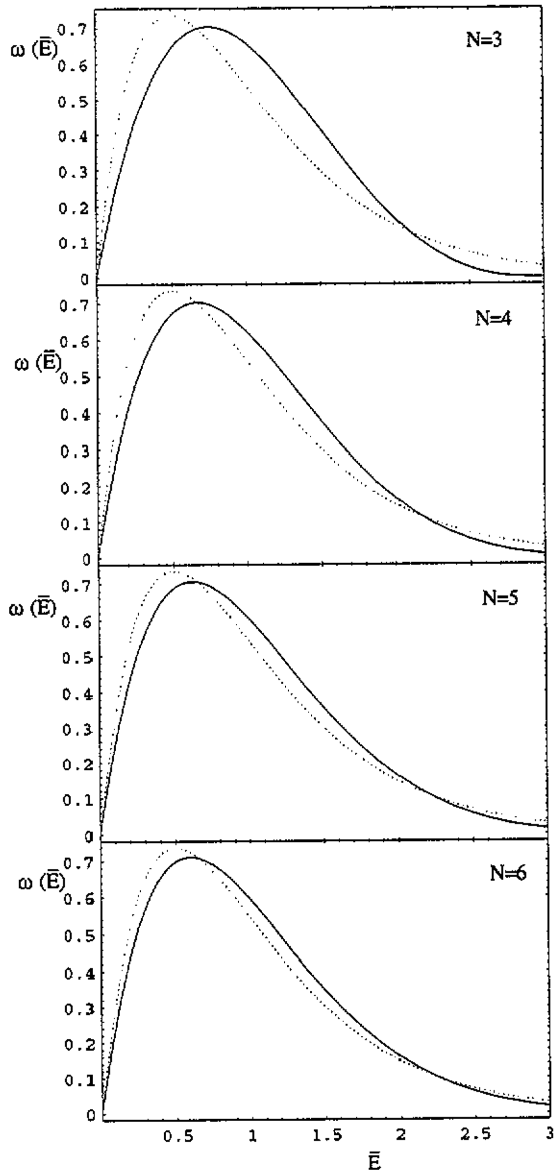

Figure 3. Same as figure 1 but for the single-particle energy distribution.

canonical ensemble become, respectively,

$$\omega_{\mathrm{m}}(\bar{z}_1) = \frac{(2N-1)}{N}\left(1 - \frac{\bar{z}_1}{N}\right)^{2(N-1)} \tag{57}$$

$$\omega_{\mathrm{m}}(\bar{v}_1) = \frac{(2N-1)}{N}\bar{v}_1\left(1 - \frac{\bar{v}_1^2}{2N}\right)^{2(N-1)} \tag{58}$$

$$p_{\mathrm{m}}(\bar{E}_1) = \frac{(2N-1)(2N-2)}{N^2}\bar{E}_1\left(1 - \frac{\bar{E}_1}{N}\right)^{2N-3} \tag{59}$$

while the corresponding distributions in the canonical ensemble (equations (37), (38) and (39), respectively) take the forms:

$$\omega_c(\bar{z}_1) = 2\exp(-2\bar{z}_1) \tag{60}$$

$$\omega_c(\bar{v}_1) = 2\bar{v}_1 \exp(-\bar{v}_1^2) \tag{61}$$

$$p_c(\bar{E}_1) = 4\bar{E}_1 \exp(-2\bar{E}_1). \tag{62}$$

Figure 1 shows a comparison between the microcanonical (57) and canonical (60) height distributions for $N = 3$, 4, 5 and 6. We can see that the microcanonical distribution approaches the *barometric* distribution (60) very quickly as N increases. Probably, a more illustrative way of comparing the above distributions is showing the corresponding $\log \omega(\bar{z}_1)$. This is also shown in figure 1, where one can appreciate the deviation of the microcanonical height distribution from the linear behaviour of the logarithmic *barometric* distribution.

Figure 2 shows the comparison between the microcanonical (58) and canonical (61) velocity distributions for $N = 3$, 4, 5 and 6. We can see that the microcanonical distribution approaches the *Maxwell* distribution (61) very quickly as N increases.

In order to illustrate the influence of the gravitational field, we have also plotted in figure 2 the single-particle microcanonical velocity distribution of an ideal gas in the absence of gravitational field (equation (16) with $f = 2$),

$$\omega_m^{(0)}(\bar{v}_1) = \frac{(N-1)}{N}\bar{v}_1\left(1 - \frac{\bar{v}_1^2}{2N}\right)^{N-2}. \tag{63}$$

Two main effects can be observed. First, the presence of a gravitational field shifts the maximum of the microcanonical velocity distribution toward the low velocity region; i.e. the presence of a gravitational field *cools* the gas. Second, the microcanonical velocity distribution with gravitational field is closer to the *Maxwell* distribution than the microcanonical velocity distribution without gravitational field.

Finally, figure 3 shows the comparison between the microcanonical (59) and canonical (62) energy distributions for $N = 3$, 4, 5 and 6, respectively.

5. Conclusions

We have derived, in the microcanonical ensemble framework, the single-particle height, velocity and energy distributions of an ideal gas in a gravitational field. Calculations are based on well known concepts in standard statistical mechanics courses and the necessary mathematical background is accessible to students of these courses. Among the obtained results we remark that for this system the height and the velocity are not statistically independent variables. We have also shown that the microcanonical distributions approach the canonical forms (with the characteristic exponential factor) in the thermodynamic limit. Although there are differences between these distributions and the canonical forms, it is remarkable that they are very close even for a reduced number of particles.

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