

Dirichlet's integral formula and the evaluation of the phase volume

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The phase volume in the microcanonical ensemble is not easily obtained even in the cases where the Hamiltonian function is separable. Dirichlet's integral formula constitutes a consistent method to evaluate the phase volume for simple situations. Several examples where Dirichlet's integral formula is used to obtain the phase volume are presented in this paper.

I. INTRODUCTION

Classical statistical mechanics usually starts with a system at constant energy (E), number of particles (N) and external parameter (a_k). A very significant property of the microcanonical ensemble is the phase volume $\Phi(E, a_k, N)$ which is defined as^{1,2}

$$\Phi(E, a_k, N) = \int \cdots \int dq dp, \quad (1)$$

$$H(p, q, a_k) \leq E.$$

The phase volume is the volume in Γ space enclosed by the surface $H(p, q, a_k) = E$. $H(p, q, a_k)$ is the Hamiltonian function of the system, p and q are the set of generalized momenta and coordinates. The phase volume is a rather geometric quantity, which only receives its physical significance in connection with the microcanonical ensemble because the entropy may be defined³ as

$$S = k \ln \Phi. \quad (2)$$

Equation (2) presents the entropy as a function of the independent variables E, a_k, N . It constitutes the basic equation of the entropic representation. In practice, Φ is not easily evaluated even in the case of simple systems. Besides the theoretical importance of the microcanonical ensemble, the evaluation of Φ is rather inconvenient for explicit applications.

Even in simple cases where the Hamiltonian function is separable (independent particles) textbooks do not offer a consistent method of solving Eq. (1), but different and unrelated methods which vary from case to case.

The use of Dirichlet's integral formula has been successful in the evaluation of certain kinds of multiple integrals (areas, volumes, moments of inertia, etc.) over certain domains.

In this paper Dirichlet's integral formula is used consistently to evaluate the phase volume for different simple situations. In the examples presented in this paper no integrations need to be worked, just a table of Γ functions is necessary.

II. DIRICHLET'S INTEGRAL FORMULA

It is well known⁴ that the integral

$$I = \int \cdots \int f(t_1 + t_2 + \cdots + t_n) t_1^{\alpha_1 - 1} \times t_2^{\alpha_2 - 1} \cdots t_n^{\alpha_n - 1} dt_1 dt_2 \cdots dt_n, \quad (3)$$

where f is continuous, $\alpha_r > 0$ ($r = 1, 2, \dots, n$), and the integration is performed over all positive values of the variables such that $\sum_{i=1}^n t_i \leq 1$, is given by

$$I = \frac{\Gamma(\alpha_1)\Gamma(\alpha_2)\cdots\Gamma(\alpha_n)}{\Gamma(\alpha_1 + \alpha_2 + \cdots + \alpha_n)} \int_0^1 f(\tau) \tau^{\sum \alpha - 1} d\tau. \quad (4)$$

We are interested in the case where $f(\tau) = 1$. Then formula (4) adopts the form

$$I = \frac{\Gamma(\alpha_1)\Gamma(\alpha_2)\cdots\Gamma(\alpha_n)}{\Gamma(\alpha_1 + \alpha_2 + \cdots + \alpha_n)} \frac{1}{\sum \alpha}. \quad (5)$$

Taking into account the recurrence relation for Γ functions

$$\Gamma(\alpha + 1) = \alpha \Gamma(\alpha), \quad \alpha > 0, \quad (6)$$

Eq. (5) may be written

$$I = \Gamma(\alpha_1)\Gamma(\alpha_2)\cdots\Gamma(\alpha_n) / \Gamma(\alpha_1 + \alpha_2 + \cdots + \alpha_n + 1). \quad (7)$$

For future examples we shall need to evaluate the integral

$$I_R = \int \cdots \int t_1^{\alpha_1 - 1} t_2^{\alpha_2 - 1} \cdots t_n^{\alpha_n - 1} \times dt_1 dt_2 \cdots dt_n \quad (8)$$

over the set of all the positive values of the variables such that

$$(t_1/b_1)^{\beta_1} + (t_2/b_2)^{\beta_2} + \cdots + (t_n/b_n)^{\beta_n} \leq 1, \quad (9)$$

where it is assumed that t_i, b_i, β_i are positive. By means of a change of variable of the form

$$(t_i/b_i)^{\beta_i} = r_i, \quad (i = 1, 2, \dots, n), \quad (10)$$

Eq. (8) may be written

$$I_R = \frac{b_1^{\alpha_1} b_2^{\alpha_2} \cdots b_n^{\alpha_n}}{\beta_1 \beta_2 \cdots \beta_n} \times \int \cdots \int r_1^{\alpha_1/\beta_1 - 1} r_2^{\alpha_2/\beta_2 - 1} \cdots r_n^{\alpha_n/\beta_n - 1} dr_1 dr_2 \cdots dr_n, \quad (11)$$

where the integration is performed over the set of all positive values of the variables such that $r_1 + r_2 + \cdots + r_n \leq 1$.

The integration in Eq. (11) has been previously evaluated [see Eq. (7)] so it may be written

$$I_R = \frac{b_1^{\alpha_1} b_2^{\alpha_2} \dots b_n^{\alpha_n}}{\beta_1 \beta_2 \dots \beta_n} \times \frac{\Gamma(\alpha_1/\beta_1) \Gamma(\alpha_2/\beta_2) \dots \Gamma(\alpha_n/\beta_n)}{\Gamma(\alpha_1/\beta_1 + \alpha_2/\beta_2 + \dots + \alpha_n/\beta_n + 1)}. \quad (12)$$

If the integration is performed over the set of positive and negative values of the variables such that $r_1 + r_2 + \dots + r_n \leq 1$, by symmetry considerations, the integration may be evaluated as 2^n times the result of integrating over the first hyperoctant, i.e., 2^n times Eq. (12).

III. EXAMPLES

A set of examples is presented where the phase volume is obtained by means of Dirichlet's integral formula. In these examples the Hamiltonian function is separable and Dirichlet's integral formula constitutes a consistent method to obtain the phase volume.

A. Classical ideal gas

A N -particle ideal gas is enclosed in a three-dimensional box of volume V , m is the mass of each particle. The total energy of the gas is E . The Hamiltonian function is

$$H = \sum_{i=1}^{3N} \frac{p_i^2}{2m} + E_p, \quad (13)$$

where

$$E_p = \begin{cases} 0 & \text{inside the box} \\ \infty & \text{in the box walls} \end{cases}$$

The phase volume is

$$\Phi = \int \dots \int dq_{3N} \int \dots \int dp_1 \dots dp_{3N}, \quad 0 \leq H \leq E. \quad (14)$$

When the position coordinates are integrated out, Eq. (14) yields

$$\Phi = V^N \int \dots \int dp_1 \dots dp_{3N}, \quad 0 \leq \sum_{i=1}^{3N} \frac{p_i^2}{2m} \leq E. \quad (15)$$

Equation (15) is of the same form as Eq. (8) over the

domain defined by Eq. (9). When parameters are identified, it results in $\alpha_i = 1$, $t_i = p_i$, $\beta_i = 2$, $b_i = (2mE)^{1/2}$, ($i = 1, 2, \dots, 3N$) and so, the phase volume is

$$\Phi = \frac{2^{3N} V^N (2mE)^{3N/2} [\Gamma(1/2)]^{3N}}{2^{3N} \Gamma(3N/2 + 1)}, \quad (16)$$

the 2^{3N} factor in Eq. (16) accounts for the fact that the integration in Eq. (15) is performed over the set of positive and negative values of the generalized momenta.

Usually is assumed that $3N/2 + 1$ is an integer because N is very large, and so Eq. (16) may be written.

$$\Phi = \frac{V^N (2\pi mE)^{3N/2}}{(3N/2)!}. \quad (17)$$

B. Mixture of two ideal gases

The gas mixture is enclosed in a three-dimensional box of volume V . N_1 and N_2 are the number of particles of each molecular species.

In this system the Hamiltonian function is

$$H = \sum_{i=1}^{3N_1} \frac{p_i^2}{2m_1} + \sum_{j=1}^{3N_2} \frac{p_j^2}{2m_2} + E_p, \quad (18)$$

where

$$E_p = \begin{cases} 0 & \text{inside the box} \\ \infty & \text{in the box walls} \end{cases}$$

and m_1 and m_2 are the molecular masses of the species 1 and 2.

The phase volume is

$$\Phi = V^{N_1+N_2} \int \dots \int \prod_i^{3N_1} dp_i \prod_j^{3N_2} dp_j. \quad (19)$$

Integration in Eq. (19) is over the domain defined by

$$\sum_{i=1}^{3N_1} \left(\frac{p_i}{(2m_1E)^{1/2}} \right)^2 + \sum_{j=1}^{3N_2} \left(\frac{p_j}{(2m_2E)^{1/2}} \right)^2 \leq 1. \quad (20)$$

When the parameters in Eqs. (8) and (9) are identified, they are $\alpha_k = 1$, $t_k = p_i$, $\beta_k = 2$, $b_k = (2m_1E)^{1/2}$, $k = 1, 2, \dots, 3N_1$, $\alpha_k = 1$, $t_k = p_j$, $\beta_k = 2$, $b_k = (2m_2E)^{1/2}$, $k = 3N_1 + 1, \dots, 3N_1 + 3N_2$ and the phase volume is given as

$$\Phi = (2^{3N_1+3N_2})(2m_1E)^{3N_1/2}(2m_2E)^{3N_2/2} V^{N_1+N_2} [\Gamma(1/2)]^{3N_1+3N_2} \{2^{3N_1+3N_2} [(3N_1 + 3N_2)/2 + 1]\}^{-1}. \quad (21)$$

As the integration in Eq. (19) is over the set of positive and negative values of generalized momenta a factor $2^{3N_1+3N_2}$ is present in Eq. (21).

Usually is supposed that $(3N_1 + 3N_2)/2$ is an integer because $3(N_1 + N_2)/2$ is a very large number, and so Eq. (21) gives

$$\Phi = \frac{V^{N_1+N_2} m_1^{3N_1/2} m_2^{3N_2/2} (2\pi E)^{3(N_1+N_2)/2}}{[3(N_1 + N_2)/2]!}. \quad (22)$$

C. Monodimensional ultrarelativistic gas

In a N -particle monodimensional ultrarelativistic gas, the particle energy is proportional to the linear momentum modulus, i.e., $e_i = c|p_i|$. The particles are restricted to move between $x = 0$ and $x = L$. The total energy of the system is E and the Hamiltonian function is

$$H = \sum_{i=1}^N c|p_i| + E_p, \quad (23)$$

where

$$E_p = \begin{cases} 0, & 0 \leq q \leq L \\ \infty, & q = 0, q = L \end{cases}$$

The phase volume is

$$\Phi = \int \dots \int dq_1 \dots dq_N dp_1 \dots dp_N, \quad 0 \leq \sum_i c|p_i| \leq E, \quad (24)$$

when the position coordinates are integrated out, Eq. (24) yields

$$\Phi = L^N \int \cdots \int dp_1 \cdots dp_N, \quad (25)$$

$$0 \leq \sum_i c|p_i| \leq E.$$

After identifying the parameters in Eqs. (8) and (9), $\alpha_i = 1$, $t_i = p_i$, $\beta_i = 1$, $b_i = E/c$, $i = 1, 2, \dots, N$ is obtained, and Eq. (20) may be written

$$\Phi = \frac{2^N L^N (E/c)^N [\Gamma(1)]^N}{\Gamma(N+1)}. \quad (26)$$

The 2^N factor in Eq. (26) accounts for the fact that the integration is performed over the set of positive and negative values of the generalized momenta.

Equation (26) finally takes the following expression:

$$\Phi = \frac{(2LE/c)^N}{N!}. \quad (27)$$

D. Three-dimensional ultrarelativistic gas

A N -particle ultrarelativistic gas is enclosed in a three-dimensional box of volume V . The particle energy is proportional to the linear momentum modulus, i.e., $e_i = c|p_i| = cp_i$. The total energy of the system is E and the Hamiltonian function is

$$H = \sum_{i=1}^N cp_i + E_p, \quad (28)$$

where

$$E_p = \begin{cases} 0 & \text{inside the box} \\ \infty & \text{in the box walls.} \end{cases}$$

The phase volume is given as

$$\Phi = V^N \int \cdots \int (dp_{1x} dp_{1y} dp_{1z}) \cdots (dp_{Nx} dp_{Ny} dp_{Nz}), \quad (29)$$

$$0 \leq \sum_{i=1}^N cp_i \leq E; p_i = (p_{ix}^2 + p_{iy}^2 + p_{iz}^2)^{1/2}$$

Taking into account the fact that in the momentum space of each particle the number of phase points with momentum between p_i and $p_i + dp_i$ is given by $4\pi p_i^2 dp_i$, Eq. (29) may be written

$$\Phi = (4\pi V)^N \int \cdots \int p_1^2 \cdots p_N^2 dp_1 dp_2 \cdots dp_N, \quad (30)$$

$$0 \leq \sum_{i=1}^N cp_i \leq E.$$

When the parameters in Eqs. (8) and (9) are identified, it results in $\alpha_i = 3$, $t_i = p_i \geq 0$, $\beta_i = 1$, $b_i = E/c$, ($i = 1, 2, \dots, N$) and finally

$$\Phi = \frac{(8\pi V)^N (E/c)^N}{3N!}. \quad (31)$$

E. Monodimensional harmonic oscillators

The Hamiltonian function of a system composed of N monodimensional harmonic oscillators is

$$H = \sum_{i=1}^N \frac{p_i^2}{2m} + \frac{m\omega^2 q_i^2}{2}, \quad (32)$$

where m is the mass and ω the frequency.

The phase volume is given as

$$\Phi = \int \cdots \int dq_1 \cdots dq_N dp_1 \cdots dp_N, \quad (33)$$

$$0 \leq H \leq E,$$

where integration is over the domain defined by

$$\sum_{i=1}^N \left\{ \left[\left(\frac{p_i^2}{2mE} \right)^{1/2} \right]^2 + \left(\frac{q_i}{(1/\omega)(2E/m)^{1/2}} \right)^2 \right\} \leq 1. \quad (34)$$

when the parameters in Eqs. (8) and (9) are identified, they are $\alpha_j = 1$, $t_j = p_i$, $\beta_j = 2$, $b_j = (2mE)^{1/2}$, $j = 1, 2, \dots, N$, $\alpha_j = 1$, $t_j = q_i$, $\beta_j = 2$, $b_j = (1/\omega)(2E/m)^{1/2}$, $j = N+1, \dots, 2N$.

The phase volume is finally obtained as

$$\Phi = \frac{(2\pi E/\omega)^N}{N!}. \quad (35)$$

F. Bidimensional harmonic oscillator

The Hamiltonian function of a bidimensional harmonic oscillator is

$$H = (p_1^2 + p_2^2)/2m + m\omega_1^2 q_1^2/2 + m\omega_2^2 q_2^2/2, \quad (36)$$

where m is the mass and ω_1 and ω_2 are the frequencies.

The phase volume is given by

$$\Phi = \int \cdots \int dq_1 dq_2 dp_1 dp_2, \quad (37)$$

$$0 \leq H \leq E,$$

the last integration being over the domain defined by

$$\left[p_1/(2mE)^{1/2} \right]^2 + \left[p_2/(2mE)^{1/2} \right]^2 + \left(\frac{q_1}{(1/\omega_1)(2E/m)^{1/2}} \right)^2 + \left(\frac{q_2}{(1/\omega_2)(2E/m)^{1/2}} \right)^2 \leq 1. \quad (38)$$

Identifying the parameters in Eqs. (8) and (9), in a straightforward manner, we have

$$\Phi = 2\pi^2 E^2 / \omega_1 \omega_2. \quad (39)$$

G. Monodimensional anharmonic oscillator

The Hamiltonian function of this system is

$$H = p^2/2m + Aq^n, \quad n > 2, \quad (40)$$

where m is the mass and A is a constant.

The phase volume is

$$\Phi = \int \cdots \int dq dp, \quad (41)$$

$$0 \leq H \leq E,$$

where the domain of integration is given by

$$\left(\frac{p}{(2mE)^{1/2}} \right)^2 + \left(\frac{q}{(E/A)^{1/n}} \right)^n \leq 1. \quad (42)$$

When the parameters in Eqs. (8) and (9) are identified, the phase volume is

$$\Phi = \frac{2(2mE)^{1/2} (E/A)^{1/n} \Gamma(1/2) \Gamma(1/n)}{n \Gamma[(3n+2)/2n]}. \quad (43)$$

H. Simple pendulum

The Hamiltonian function of a simple pendulum is

$$H = p_\alpha^2/2ml^2 + mgl(1 - \cos\alpha), \quad (44)$$

where the meaning of p_α , m , g , l , and α is standard. The potential energy origin has been taken in the equilibrium position ($\alpha = 0$).

For small vibrations the Hamiltonian function will take the following form

$$H = p_\alpha^2/2ml^2 + mgl\alpha^2/2. \quad (45)$$

The phase volume is given as

$$\Phi = \int \dots \int dp_\alpha d\alpha, \quad (46)$$

$$0 \leq H \leq E,$$

where the integration is performed over the domain defined by

$$\left(\frac{p_\alpha}{(2ml^2E)^{1/2}}\right)^2 + \left(\frac{\alpha}{(2E/mgl)^{1/2}}\right)^2 \leq 1. \quad (47)$$

When the parameters in Eqs. (8) and (9) are identified, the phase volume is

$$\Phi = 2\pi E(l/g)^{1/2}. \quad (48)$$

If the potential energy origin were taken as $\alpha = \pi/2$ instead of $\alpha = 0$, the Hamiltonian function of this system would be given by

$$H = p_\alpha^2/2ml^2 - mgl(1 - \alpha^2/2), \quad (49)$$

where the validity of the small amplitude approximation has been assumed.

In this case the phase volume will be

$$\Phi = 2\pi(E' + mgl)(l/g)^{1/2}. \quad (50)$$

The different expressions for the phase volume [see Eqs. (48) and (50)] are due to the different potential energy origins used to evaluate the phase volume. When it is taken into account that the difference in energy between both potential energy levels is given by mgl , Eqs. (48) and (50) are identical because of $E = E' + mgl$.

¹R. Becker, *Theory of heat* (Springer Verlag, New York, 1967), p. 113.

²A. Munster, *Statistical thermodynamics* (Springer Verlag, New York, 1969), Vol. 1, p. 44.

³See Ref. 2, pp. 53ff for this definition and others related to it.

⁴E. T. Whittaker, G. N. Watson, *A course of modern analysis* (Cambridge University, Cambridge, England, 1969), p. 258.