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Boltzmann, Gibbs, and Darwin-Fowler Approaches in Parastatistics

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Derivations of the equilibrium values of occupation numbers are made using three approaches, namely, the BOltzmann "elementary" one, the ensemble method of Gibbs, and that of Darwin and Fowler as well.

Derivam-se os valores de equilíbrio dos números de ocupação em três diferentes abordagens, a saber, a "elementar" de Boltzmann, o método dos ensembles de Gibbs, e também o de Darwin e Fowler. Fica assim estabelecida, a equivalência desses métodos em paraestatística.

1. INTRODUCTION

There are essentially three methods used in equilibrium statistical mechanics, namely, the Boltzmann method of identifying the equilibrium state with the most probable one; the Gibbs ensemble method of postulating a canonical distribution; and the Darwin-Fowler method' of identifying the equilibrium state with the average state. Most textbooks on statistical mechanics include discussions of the first two methods. The inclusion into the text of the last method, which Schrödinger[2] seems to advocate, is less usual. The equivalence of those methods is usually demonstrated for the ideal Boltzmann, Bose-Einstein, and Fermi-Dirac statistics. However, the equivalence is not guaranteed when the methods are applied to different statistics such as parastatistics[3], where eachenergy level can afford up to some number k of particles, and can be regarded as a generalization of the above mentioned statistics. It seems desirable to confirm the equivalence of those methods for parastatistics. In most textbooks however discussions on parastatistics are rather rare.

In his book Isihara[4] presents a brief discussion on parastatistics and derives the equilibrium occupation numbers based on Boltzmann's method; however, some clarification seems to be needed in his derivation. In the following, we shall consider parastatistics for a system of non-distinguishable particles and derive the equilibrium occupation numbers, by using the three methods mentioned above. In the derivations, the equivalence of those methods shall become clearer, specially between Boltzmann, and Darwin-Fowler, approaches.

2. DERIVATION OF THE DISTRIBUTION FUNCTION

2.1 The Boltzmann method

In this approach, energy levels are grouped into cells such that the j^{th} cell contains m_j levels. Identical particles belonging to the same j^{th} cell are assumed to have the same average energy, ε_j. The n_j particles of the j^{th} cell are distributed over all levels, in the cell, in all possible allowed ways ω_j, contributing with an energy $\varepsilon_j n_j$ to the system.

Thus, for a system of N identical particles, with a total energy E, one has:

$$E = \sum_j \varepsilon_j n_j \quad , \tag{2.1}$$

$$N = \sum_j n_j \quad , \tag{2.2}$$

$$W\{n_j\} = \prod_j \omega_j \quad , \tag{2.3}$$

where $W\{n_j\}$ is the total number of ways of distributing the particles specified by the set $\{n_j\}$.

The equilibrium occupation numbers are then to be evaluated from the following maximization condition:

$$\delta \ln W + \sum_j (\alpha + \beta\varepsilon_j)\delta n_j = 0 \quad , \tag{2.4}$$

where a and β are Lagrange multipliers associated with constraints (2.1) and (2.2). The major task is to find an expression for ω_i as a function of n_i. For Bose-Einstein and Fermi-Dirac statistics, ω_i is usually derived separately by elementary methods. For parastatistics which allows up to k particles in each level, we shall use the method of generating functions. It is not difficult to see that the pertinent generatingfunction is given by

$$f(z) = (1 + z + z^2 + \ldots z^k)^{m_j} = \left[\frac{1 - z^{k+1}}{1 - z}\right]^{m_j},$$

and ω_j is the coefficient of the term z^{n_j}. Hence,

$$\omega_j = \frac{1}{n_j!}\left[\frac{d^{n_j}}{dz^{n_j}} f(z)\right]_{z=0}$$

$$= m_j n_j! \sum_{v=0}^{\left[\frac{n_j}{k+1}\right]} (-)^v \frac{[m_j + n_j - v(k+1) - 1]!}{v!(m_j - v)![n_j - v(k+1)]!} \qquad (2.6)$$

Although expression (2.6) is exact, it is too complicated to be useful. We thus rewrite (2.6) according to Cauchy's theorem[6]:

$$\omega_j = \frac{1}{2\pi i}\oint_C \frac{f(z)\,dz}{z^{n_j+1}} = \frac{1}{2\pi i}\oint_C \exp\left[m_j g_j(z)\right] dz\,, \qquad (2.7)$$

where C is a closed path around the origin, and

$$g_j(z) = \ln\left[\frac{1 - z^{k+1}}{1-z}\right] - \left[\frac{n_j + 1}{m_j}\right] \ln z\,. \qquad (2.8)$$

Since m_i is supposed to be large, and $g_j(z)$ is analytic in the cut plane,

an integral of the typeof (2.7) can be approximately evaluated by the method of the steepest descents[7], which yields the result:

$$\omega_j \approx (2\pi m_j\, g_j''(z_{0j})^{-1/2} \exp\left[m_j\, g_j(z_{0j}) + i\alpha_j\right] , \tag{2.9}$$

where a is the angle that the steepest descent line makes with the real axis, and z_{0j} is the saddle point of $g_3(z)$, determined by:

$$\frac{d}{dz_{0j}} g_j = 0 = \frac{1}{1-z_{0j}} - \frac{(k+1)z_{0j}^{k}}{1-z_{0j}^{k+1}} - \frac{n_j + 1}{m_j}\,\frac{1}{z_{0j}} \tag{2.10}$$

Hence

$$\frac{n_j + 1}{m_j} = \frac{1}{z_{0j}^{-1} - 1} - \frac{k + 1}{z_0^{-(k+1)} - 1} . \tag{2.11}$$

Substituing (2.7) into (2.4), we obtain

$$\sum_j \left[\frac{\omega_j'}{\omega_j} + (\alpha + \beta\varepsilon_j)\right]\delta n_j = 0 , \tag{2.12}$$

where

$$\omega_j' = -\frac{1}{2\pi i}\oint_C \frac{f(z)\ln z}{z^{n_j+1}}\, dz \approx$$

$$\approx -\left[2\pi m_j\, g_j''(z_{0j})\right]\exp\left[m_j\, g_j(z_{0j}) + i\alpha_j\right]\ln z_{0j} . \tag{2.13}$$

Since $g_3(z)$ is the same for each j, cf. Eq. (2.8), the same holds for α_j and z_{0j}.

From (2.9), (2.12) and (2.13), we obtain

$$z_{0j} = \exp(\alpha + \beta\varepsilon_j) \ . \tag{2.14}$$

By combining (2.11) end (2.14), it follows that

$$\frac{n_j + 1}{m_j} \simeq \frac{n_j}{m_j} \simeq \frac{1}{\exp\left[-(\alpha + \beta\varepsilon_j)\right] - 1} - \frac{k + 1}{\exp\left[-(k+1)(\alpha + \beta\varepsilon_j)\right] - 1} \ , \tag{2.15}$$

which is the result we set forth to derive.

2.2 The Gibbs Method

In this approach, the total energy of the system is not a constant, and a canonical distribution is postulated. There is no need to group levels into cells nor to find the associated multiplicities, One starts from the partition function, defined as

$$Q_N = \sum_{\{n_\rho\}} \exp\left[-\beta' \sum_\rho \varepsilon_\rho n_\rho\right] \ , \tag{2.16}$$

where ρ is the index of the energy levels, and the summation is to be carried out over the set $\{n_\rho\}$ of all possible values of n_ρ which are consistent with the conditions

$$N = \sum_\rho n_\rho \ , \tag{2.17}$$

and

$$n_\rho = 0, 1, 2 \ldots k \ . \tag{2.18}$$

The summations (2.16) are, however, cumbersome because of condition (2.17). To remove this difficulty, we transform (2.16) into the grand canonical partition function:

$$Z = \sum_{N=0}^{\infty} z^N Q_N = \sum_{N=0}^{\infty} \sum_{\{n_\rho\}} z^N \exp\left[-\beta' \sum_\rho n_\rho \varepsilon_\rho\right]$$

$$= \sum_{N=0}^{\infty} \sum_{\{n_\rho\}} \prod_{\rho} \left[Z e^{-\beta' \varepsilon_\rho} \right]^{n_\rho} \quad . \tag{2.19}$$

The double summation (2.19) can be converted into a single one, free from the restriction (2.17):

$$Z = \prod_{\rho} \left[\sum_{n_\rho=0}^{k} \left[Z e^{-\beta' \varepsilon_\rho} \right]^{n_\rho} \right] = \prod_{\rho} \frac{\left[Z e^{-\beta' \varepsilon_\rho} \right]^{k+1} - 1}{Z e^{-\beta' \varepsilon_\rho} - 1} \tag{2.20}$$

The average total number of particles can be obtained from

$$\langle N \rangle = Z \frac{\partial}{\partial z} (\ell n Z) = \sum_{\rho} \left[\frac{1}{Z^{-1} e^{\beta' \varepsilon_\rho} - 1} - \frac{k+1}{(Z e^{-\beta' \varepsilon_\rho})^{-k+1} - 1} \right] . \tag{2.21}$$

Hence, the equilibrium occupation number is given by

$$n_\rho = \frac{1}{(Z e^{-\beta' \varepsilon_\rho})^{-1} - 1} - \frac{k+1}{(Z e^{-\beta' \varepsilon_\rho})^{-k+1} - 1} \tag{2.22}$$

This is the same as (2.15), if we identify $Z = e^{\alpha}$ and $\beta' = -\beta$

2.3 The Darwin-Fowler Method

In this approach, the physical conditions are the same as those of the Boltzmann method, namely, the total number of particles and the total energy are fixed constants. However, the ortifice of grouping energy levels into cells is eliminated. Without this artifice, the relative probability of any allowedstate of the system becomes the same. There is no most probable state to be identified as the equilibrium state. One takes averages with respect to all permissible states and identifies the equilibrium state with this average state. In parastatistics, each level admits up to k particles, i.e., $n_\rho = 0, 1 \ldots k$. When the permitted va-

lues of n_ρ are given in the set $\{n_\rho\}$, a state is uniquely defined. Thus, denoting the number of ways to realize a state $\{n_\rho\}$, by $W\{n_\rho\}$, we have :

$$W\{n_\rho\} = \prod_\rho \gamma(n_\rho) \ , \tag{2.23}$$

where

$$\begin{aligned} \gamma(n_\rho) &= 1 \ , \qquad if \ n_\rho = 0,1,\ldots,k \ , \\ &= 0 \qquad\quad otherwise \ . \end{aligned} \tag{2.24}$$

The states defined by assigning values to n_ρ must be compatible with the restrictions

$$\begin{aligned} N &= \sum n_\rho \ , \\ E &= \sum n_\rho \varepsilon_\rho \ . \end{aligned} \tag{2.25}$$

Hence, the average occupation number can be defined as

$$\langle n_\rho \rangle = \frac{1}{G} \sum_{\{n_\rho\}}{}' n_\rho W\{n_\rho\} \tag{2.26}$$

where

$$G = \sum_{\{n_\rho\}}{}' W\{n_\rho\} \ , \tag{2.27}$$

and the summations are to be carried out over all possible states $\{n_\rho\}$ which are compatible with (2.25). The task is, then, to evaluate (2.26) and (2.27). For this purpose, we now introduce a generating function defined by

$$F(x,y,\varepsilon_\rho) = \sum_{\{n_\rho\}} W\{n_\rho\} \, x^{n_1+n_2\ldots} \, y^{n_1\varepsilon_1+n_2\varepsilon_2\ldots}$$

$$= \sum \prod_{\rho} \gamma(n_\rho) (xy^{\varepsilon_\rho})^{n_\rho}$$

$$= \prod_{\rho} \sum_{n_\rho=0}^{\infty} \gamma(n_\rho) (xy^{\varepsilon_\rho})^{n_\rho} \quad , \tag{2.28}$$

where the summations are now to be carried out over all states without restrictions, (2.25). Similar to the Boltzmann method, G can be identified with the coefficient of $x^N y^E$, in (2.28). Hence, applying Cauchy's theorem, we have

$$G = \left(\frac{1}{2\pi i}\right)^2 \oint dx \oint dy \; x^{-N-1} \; y^{-E-1} \; F(x, y, \varepsilon_\rho) \quad . \tag{2.29}$$

Applying the method of steepest descent, we obtain

$$G \approx x_0^{-N-1} \; y_0^{-E-1} \; F(x_0, y_0, \varepsilon_\rho) \quad , \tag{2.30}$$

where (x_0, y_0) is the saddle point to be determined from the equations

$$x_0 \frac{\partial F}{\partial x_0} - (N + 1) F = 0 \quad , \tag{2.31}$$

$$y_0 \frac{\partial F}{\partial y_0} - (E + 1) F = 0 \quad . \tag{2.32}$$

From (2.31), we have

$$N + 1 \simeq N = \frac{x_0}{F} \frac{\partial F}{\partial x_0} = x_0 \frac{\partial \ell n F}{\partial x_0} \quad . \tag{2.33}$$

Substituing (2.28) into (2.33), we obtain

$$N = \sum_{\rho} x_0 \frac{\partial}{\partial x_0} \ell n \left[\sum_{n_\rho=0}^{\infty} \gamma(n_\rho) (xy^{\varepsilon_\rho})^{n_\rho} \right]$$

$$= \sum_{\rho} x_0 \frac{\partial}{\partial x_0} \ln \left[\frac{1 - (x_0 y_0^{\varepsilon_\rho})^k + 1}{1 - x_0 y_0^{\varepsilon_\rho}} \right]$$

$$= \sum_{\rho} \left[\frac{xy^{\varepsilon_\rho}}{1 - x_0 y_0^{\varepsilon_\rho}} - \frac{(k+1)(x_0 y_0^{\varepsilon_\rho})^{k+1}}{1 - (x_0 y_0^{\varepsilon_\rho})^k + 1} \right] . \qquad (2.34)$$

Hence,

$$\langle n_\rho \rangle = \frac{1}{(x_0 y_0^{\varepsilon_\rho})^{-1} - 1} - \frac{k+1}{(x_0 y_0^{\varepsilon_\rho})^{-(k+1)} - 1} , \qquad (2.35)$$

which is the same result as given in (2.15) and (2.22), if we identify $x = e^{\alpha}$ and $y_0 = e^{\beta}$.

3. CONCLUSION

The equivalence of the three methods, mentioned in the Introduction, is shown for an ideal gas of identical particles which satisfy parastatistics. The three methods, therefore, can be regarded as equivalent, independent of the statistics.

The Boltzmann "elementary" method, when applied to parastatistics, becomes rather complex as compared to its application to Bose-Einstein or Fermi-Dirac statistics. The mathematical apparatus needed becomes similar to that needed for the Darwin-Fowler method.

Though our derivations may seem a bit complicated, it is hoped that they may clarify some points left out in the derivation by Isihara.

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