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Per Olof Fröman

A simple derivation of a general equilibrium equation, with two astrophysical applications

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Read 10 February 1954 by Oskar KLEIN

A simple derivation of a general equilibrium equation, with two astrophysical applications

By Per Olof Fröman

Summary. — If the statistical mechanical formula (1), which has been derived by O. KLEIN, is combined with the well-known thermodynamical equilibrium condition (2) containing the chemical potentials μ_r , one immediately obtains the general equilibrium equation (3), which contains as special cases SAHA's formula (4) and another well-known formula (5) of great astrophysical importance.

Using the powerful concept of a Gibbs' grand canonical ensemble, O. KLEIN has derived the following formula¹:

$$N_{r,s} = \left(\frac{2\pi m_r \, k \, T}{h^2}\right)^{\frac{3}{2}} g_{r,s} \, e^{\frac{\mu_r - E_{r,s}}{k \, T}},\tag{1}$$

from which it follows that

$$N_{r} = \sum_{s} N_{r,s} = \left(\frac{2\pi m_{r} k T}{h^{2}}\right)^{\frac{3}{2}} e^{\frac{\mu_{r}}{k}T} \sum_{s} g_{r,s} e^{-\frac{E_{r,s}}{k}T},$$
(1a)

where

- $N_{r,s}$ is the mean number of particles (per unit volume) of kind r which are in the internal quantum state s, regardless of the translatory motion of the particle
- $g_{r,s}$ is the statistical weight of the internal quantum state s of the particles of kind r

 $E_{r,s}$ is the energy of the internal quantum state s of the particles of kind r μ_r is the chemical potential of the particles of kind r

- m_r is the mass of a particle of kind r
- T is the absolute temperature
- k is Boltzmann's constant

h is Planck's constant.

We now consider a possible reaction

$$\sum \varkappa_r A_r = 0,$$

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¹ O. KLEIN, G. BESKOW and L. TREFFENBERG, Arkiv för mat., astr. o. fys., Band 33 B, No. 1 (1946–47); O. KLEIN, Supplemento al volume VI, Serie IX del Nuovo Cimento, N. 2 (1949). For one kind of particle the formula was also given in Professor KLEIN's lectures on statistical mechanics in 1951–52.

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between the different kinds of particles. Here, A_r is the symbol for a particle of kind r, and \varkappa_r are coefficients (of which some are positive and some negative). For the above reaction we have the well-known thermodynamic equilibrium condition¹

$$\sum_{\mathbf{r}} \varkappa_{\mathbf{r}} \mu_{\mathbf{r}} = 0. \tag{2}$$

Combining (1) and (2), we immediately obtain the following general equilibrium equation²

$$\prod_{r} (N_{r,s})^{\varkappa_{r}} = \prod_{r} \left\{ \left(\frac{2 \pi m_{r} k T}{h^{2}} \right)^{\frac{3}{2}} g_{r,s} e^{-\frac{E_{r,s}}{k T}} \right\}^{\frac{\kappa_{r}}{k}}$$
(3)

We obtain

$$\prod_{r} (N_{r})^{\varkappa_{r}} = \prod_{r} \left\{ \left(\frac{2 \pi m_{r} k T}{h^{2}} \right)^{\frac{3}{2}} \sum_{s} g_{r,s} e^{-\frac{E_{r,s}}{k T}} \right\}^{\varkappa_{r}}$$
(3a)

from (1a) and (2), and

$$\frac{N_{r,s}}{N_r} = \frac{g_{r,s}e^{-\frac{2r_rs}{kT}}}{\sum g_{r,s}e^{-\frac{E_{r,s}}{kT}}}$$
(3 b)

from (1) and (1a). The formulae (3a) and (3b) together constitute an equilibrium equation which is as general as (3).

We shall now use (3) to obtain two well-known equilibrium equations of considerable astrophysical importance.

I. Let r denote those atoms of a certain kind which have lost r electrons. If (3) is applied to the special reaction in which such an ion loses a further electron, one immediately obtains SAHA's formula in the form

$$N_{e} \frac{N_{r+1,s'}}{N_{r,s}} = \left(\frac{2\pi m_{e} \, k \, T}{h^{2}}\right)^{\frac{3}{2}} \cdot \frac{2 \, g_{r+1,s'}}{g_{r,s}} e^{-\frac{E_{r+1,s'}-E_{r,s}}{k \, T}} \tag{4}$$

if the electron mass is neglected in comparison with the atomic mass. N_e denotes the mean number of free electrons per unit volume, and m_e denotes the electron mass.

II. Let $N(n_K, n_L, \ldots)$ denote the mean number of atoms or ions of a certain kind (per unit volume) with n_K electrons bound in the K-shell, n_L electrons bound in the L-shell, etc. If (3) is applied to the special reaction in which such an atom or ion loses all its electrons, one immediately obtains

$$\frac{N(n_{K}, n_{L}, n_{M}, \ldots)}{N(0, 0, 0, \ldots)} = \left(\frac{N_{e}}{2\left(\frac{2\pi m_{e} k T}{h^{2}}\right)^{\frac{3}{2}}}\right)^{n_{K}+n_{L}+n_{M}+\ldots} .$$

$$\cdot \left(\frac{2 \cdot 1^{2}}{n_{K}}\right) \cdot \left(\frac{2 \cdot 2^{2}}{n_{L}}\right) \cdot \left(\frac{2 \cdot 3^{2}}{n_{M}}\right) \cdots e^{\frac{n_{K} \chi_{K}+n_{L} \chi_{L}+n_{M} \chi_{M}+\ldots}{k T}}$$
(5)

¹ This equilibrium condition can be derived by the use of Gibbs' grand canonical ensemble. See O. KLEIN, Supplemento al volume VI, serie IX del Nuovo Cimento, N. 2 (1949). ² For the sake of simplicity we have suppressed the subscript r on the index s.

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if the mass of the electrons is neglected in comparison with the atomic mass. Here $\chi_K, \chi_L, \chi_M, \ldots$ denote the (mean) ionization potentials for the K-, L-, M-, ... shells. The formula (5) is very important for calculations of the ionization (and the opacity) of stellar matter.

This note was initiated by Professor O. KLEIN's lectures on statistical mechanics given in 1951–52 at Stockholms Högskola. I am indebted to Professor KLEIN for valuable discussions and for his kind criticism of my manuscript.

CERN (European Council for Nuclear Research), Theoretical Study Group at the Institute for Theoretical Physics, University of Copenhagen.

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