FÍSICA ESTADÍSTICA I-PCF

TAREA 10

Fecha de entrega: miércoles 13 de noviembre de 2013

- **Problemas**

1. Calcule la función de partición de tres partículas indistinguibles,

$$Z_3(\beta) = \mathrm{Tr}\{e^{-\beta \hat{\boldsymbol{H}}_3}\},$$

donde $\hat{\boldsymbol{H}}_3$ es el hamiltoniano de tres partículas independientes (sin interacción entre ellas). Considere el caso cuando las partículas se encuentran en una caja tridimensional e impenetrable de volumen $V = L^3$.

   a) Describa explícitamente los estados sobre los cuales se realiza la traza para cada caso (bosones y fermiones).

   Ver problema 7.3 (pág. 357) del libro: A Modern Course in Statistical Physics (2da edición) de L. Reichl.

2. Demuestre que la función de partición canónica de N partículas indistinguibles puede escribirse como:

$$Z_N(\beta) = \sum_{k=1}^{N} (\pm 1)^{k+1} Z_1(k\beta) Z_{N-k}(\beta)$$

con $Z_0 = 1$. (Ver Borrmann y Franke J. Chem. Phys. 98 (3), 1993. Anexo)

3. Partiendo de la función de partición canónica $Z_N(\beta)$, deduzca la distribución de Fermi-Dirac

$$\langle n_k \rangle = \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1}$$

y la de Bose-Einstein

$$\langle n_k \rangle = \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1},$$

siguiendo el método presentado en el apéndice B de la referencia Eur. J. Phys. 33, Number 3, 709 (2012). Anexo

NOTES

Recursion formulas for quantum statistical partition functions

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I. INTRODUCTION

We consider a system of N particles for which the energy can be written as a sum of one particle energies such as ideal gases or simple shell models. We aim at a recursion of Z in terms of Z for subsystems. The idea may be seen as a vague analogy to cluster expansion methods.

A. Theorem

The one particle energy of the kth particle being in state r_k will be denoted by $\epsilon(r_k)$, the partition function by $Z(N)$. Then for the partition function holds

$$Z(N)=\frac{1}{N}\sum_{k=1}^{N}(\pm 1)^{k+1}S(k)Z(N-k)\,, \tag{1}$$

with $Z(0)=1$ and $S(k)$, which can be identified as the Boltzmannian partition function of a cluster of size k, given by

$$S(k):=\sum_{j}\exp[-\beta\, k\epsilon(\,j)]\,. \tag{2}$$

The minus and the plus sign stand for Fermi–Dirac and Bose–Einstein statistics, respectively. The sum in Eq. (2) runs over all possible states.

B. Proof

1. Fermi–Dirac statistics

In the case of Fermi–Dirac statistics the partition function may be written as [1]

$$Z_{\mathrm{FD}}(N)=\frac{1}{N!}\sum_{r_1}\sum_{r_2\neq r_1}\cdots\sum_{r_N\neq r_1,r_2,\ldots,r_{N-1}}\times\exp\left(-\beta\sum_{k=1}^{N}\epsilon(r_k)\right). \tag{3}$$

Splitting the inner sum into two terms gives

$$Z_{\mathrm{FD}}(N)=\frac{1}{N}\left[\frac{1}{(N-1)!}\sum_{r_1}\sum_{r_2\neq r_1}\cdots\sum_{r_{N-1}\neq r_1,r_2,\ldots,r_{N-2}}\exp\left(-\beta\sum_{k=1}^{N-1}\epsilon(r_k)\right)\right]$$
$$\times\left\{\sum_{r_N}\exp[-\beta\epsilon(r_N)]-\sum_{j=1}^{N-1}\exp[-\beta\epsilon(r_j)]\right\}. \tag{4}$$

The term in square brackets is just $Z_{\mathrm{FD}}(N-1)$, the first term in the curly brackets is $S(1)$. Thus Eq. (4) takes the form

$$Z_{\mathrm{FD}}(N)=\frac{1}{N}S(1)Z_{\mathrm{FD}}(N-1)-\frac{1}{N!}\sum_{j=1}^{N-1}\left\{\sum_{r_1}\sum_{r_2\neq r_1}\cdots\sum_{r_{N-1}\neq r_1,r_2,\ldots,r_{N-2}}\exp\left(-\beta\sum_{k=1}^{N-1}\epsilon(r_k)\right)\exp[-\beta\epsilon(r_j)]\right\}.$$

Because of permutational symmetry the term in the brackets is independent of *j*. Hence, the outer sum gives simply a factor *(N−1)* and *j* can be chosen arbitrary.

$$Z_{\mathrm{FD}}(N)=\frac{1}{N}S(1)Z_{\mathrm{FD}}(N-1)-\frac{N-1}{N!}\sum_{r_1}\sum_{r_2\neq r_1}\cdots\sum_{r_{N-1}\neq r_1,r_2,\ldots,r_{N-2}}\exp\left(-\beta\sum_{k=1}^{N-2}\epsilon(r_k)\right)\exp[-2\beta\epsilon(r_{N-1})]$$
$$=\frac{1}{N}S(1)Z_{\mathrm{FD}}(N-1)-\frac{1}{N}S(2)Z_{\mathrm{FD}}(N-2)+\frac{(N-1)(N-2)}{N!}$$
$$\times\sum_{r_1}\sum_{r_2\neq r_1}\cdots\sum_{r_{N-2}\neq r_1,r_2,\ldots,r_{N-3}}\exp\left(-\beta\sum_{k=1}^{N-3}\epsilon(r_k)\right)\exp[-3\beta\epsilon(r_{N-3})]\,.$$

Repeated use of these transformations yields Eq. (1).

2. Bose–Einstein statistics

For bosons the partition function takes the form,[1]

$$Z_{\mathrm{BE}}(N)=\sum_{r_1,r_2,\ldots,r_N} g(r_1,r_2,\ldots,r_N)\exp\left(-\beta\sum_{k=1}^{N}\epsilon(r_k)\right) \quad (5)$$

where g is

$$g(r_1,r_2,\ldots,r_N)=\frac{1}{N!}\prod_{k=0} N_k!$$

and N_k being the number of particles in state k. Using the definition of g in a recursive way

$$g(r_1,r_2,\ldots,r_N)=\frac{1}{N}g(r_1,\ldots,r_{N-1})\left(1+\sum_{j=1}^{N-1}\delta_{r_j r_N}\right)$$

and dividing the sums in Eq. (5) in two parts gives

$$Z_{\mathrm{BE}}(N)=\sum_{r_1,r_2,\ldots,r_{N-1}} g(r_1,r_2,\ldots,r_{N-1})\exp\left(-\beta\sum_{k=1}^{N-1}\epsilon(r_k)\right)\sum_{r_N}\frac{1}{N}\left(1+\sum_{j=1}^{N-1}\delta_{r_j r_N}\right)\exp[-\beta\epsilon(r_N)]$$

$$=\frac{1}{N}S(1)Z_{\mathrm{BE}}(N-1)+\frac{1}{N}\sum_{j=1}^{N-1}\sum_{r_1,r_2,\ldots,r_{N-1}} g(r_1,r_2,\ldots,r_{N-1})\exp\left(-\beta\sum_{k=1}^{N-1}\epsilon(r_k)\right)\exp[-\beta\epsilon(r_j)]\,.$$

In the second step again advantage has been taken of the permutational symmetries. Proceeding in the same manner as done above for Fermi–Dirac statistics yields the theorem.

II. CONCLUSIONS

The recursion formula given in the theorem is exact. For practical purposes the sums may be done only over finite number of states which yields a good approximation up to temperatures where the occupation numbers of higher states are sufficiently small. Using the derived recursion formulas for the partition functions the computational effort increases approximately with the number $n_{\max}$ of states taken into account for the functions $S(k)$, $(k=1,\ldots,N)$, and with the square of the particle number for Eq. (1). In contrast, the numerical effort to evaluate the usual Eqs. (3) and (5) directly, increases roughly with $(n_{\max})^N$.

The given recursion formulas may be applied in cluster physics as well as in the framework of simple models in nuclear physics. Recently, Mendel[2] applied our results in a special model of quantum chromo dynamics.

ACKNOWLEDGMENT

We thank E. R. Hilf for fruitful discussions.

[1] F. Reif, *Fundamentals of statistical and thermal physics* (McGraw-Hill, Singapore, 1965).
[2] E. Mendel, preprint, Universität, Oldenburg, 1992.

Chemical potential for the interacting classical gas and the ideal quantum gas obeying a generalized exclusion principle

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Appendix B. Derivation of mean occupancy for an ideal quantum gas with intermediate quantum statistics of order *j*

Our starting point to derive $\langle n_k \rangle_j$ is the observation that Z_N can be written as a sum over all possible values of n_k for each k, i.e.

$$Z_N = \sum_{n_1=0}^{j} \sum_{n_2=0}^{j} \ldots \, \mathrm{e}^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots)} \delta_{n_1+n_2+\cdots,N}, \tag{B.1}$$

where $\delta_{i,j}$ is the Kronecker delta and the factor $\delta_{n_1+\cdots+n_k+\cdots,N}$ has been introduced to guarantee the conservation of N. To proceed further [4], we write the last expression as

$$Z_N = \sum_{n_k=0}^{j} \mathrm{e}^{-\beta n_k \epsilon_k} \left[\sum_{n_1=0}^{j} \sum_{n_2=0}^{j} \ldots \, \mathrm{e}^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots)} \delta_{n_1+n_2+\cdots,N-n_k} \right] \tag{B.2}$$

$$= \sum_{n_k=0}^{j} \mathrm{e}^{-\beta n_k \epsilon_k} \left[\sum_{\{n_l\}}{}' \mathrm{e}^{-\beta E'_{\{n_l\}}} \delta_{n_1+n_2+\cdots,N-n_k} \right]. \tag{B.3}$$

The term within square brackets corresponds to the partition function of $N - n_k$ particles with the energy level k excluded, $Z^{(k)}_{N-n_k}$; we use the superindex $^{(k)}$ to denote all quantities which have been computed in this way. In terms of this, we have

$$Z_N = \sum_{n_k=0}^{j} \mathrm{e}^{-\beta n_k \epsilon_k} Z^{(k)}_{N-n_k}. \tag{B.4}$$

A general formula to compute average number of particles that occupy the energy level k, given by $\langle n_k \rangle_j = Z_N^{-1} \sum_{n_1=0}^{j} \sum_{n_2=0}^{j} \ldots n_k \mathrm{e}^{-\beta(n_1\epsilon_1+n_2\epsilon_2+\cdots)}$, is derived by noting that

$$\langle n_k \rangle_j = -\frac{1}{\beta} \frac{\partial \ln Z_N}{\partial \epsilon_k}; \tag{B.5}$$

thus,

$$\langle n_k \rangle_j = \frac{1}{Z_N} \sum_{n_k=0}^{j} n_k \mathrm{e}^{-\beta n_k \epsilon_k} Z^{(k)}_{N-n_k}. \tag{B.6}$$

The evaluation of equation (B.6) requires us to compute $Z^{(k)}_{N-n_k}$ from $n_k = 0$ to j which makes the calculation rather cumbersome (see [19] and [4] for details). We avoid this difficulty by noting that the ratio $Z^{(k)}_{N-n_k}/Z^{(k)}_N$ can be written as the product of the ratios of partition functions that differ only in one particle, i.e.

$$\frac{Z^{(k)}_{N-n_k}}{Z^{(k)}_N} = \frac{Z^{(k)}_{N-1}}{Z^{(k)}_N} \cdot \frac{Z^{(k)}_{N-2}}{Z^{(k)}_{N-1}} \cdots \frac{Z^{(k)}_{N-n_k}}{Z^{(k)}_{N-n_k+1}}. \tag{B.7}$$

Consider the energy of $N - n_k$ particles distributed over the energy levels distinct to ϵ_k

$$E^{(k)}_{N-n_k} = \frac{\sum_{\{n_l\}}{}' E'_{\{n_l\}} \mathrm{e}^{-\beta E'_{\{n_l\}}} \delta_{n_1+n_2+\cdots,N-n_k}}{\sum_{\{n_l\}}{}' \mathrm{e}^{-\beta E'_{\{n_l\}}} \delta_{n_1+n_2+\cdots,N-n_k}} = -\frac{\partial}{\partial \beta} \ln Z^{(k)}_{N-n_k}. \tag{B.8}$$

The difference $\Delta E^{(k)} = E^{(k)}_{N-n_k} - E^{(k)}_{N-n_k+1}$, i.e. the change in energy when withdrawing only one particle, is given by

$$\Delta E^{(k)} = -\frac{\partial}{\partial \beta} \ln \frac{Z^{(k)}_{N-n_k}}{Z^{(k)}_{N-n_k+1}}. \tag{B.9}$$

Since the energy change has been done at constant T and V, we must have that $\beta\Delta E^{(k)} + \ln\left[Z^{(k)}_{N-n_k}/Z^{(k)}_{N-n_k+1}\right] = \Delta S^{(k)}/k_{\mathrm{B}}$, where $\Delta S^{(k)}$ denotes the entropy change of the system when withdrawing only one particle.

Using the first law of thermodynamics, we can identify the chemical potential with

$$\mu^{(k)}_{N-n_k+1} = k_{\mathrm{B}}T \ln \frac{Z^{(k)}_{N-n_k}}{Z^{(k)}_{N-n_k+1}}, \tag{B.10}$$

which corresponds exactly with the expression $\mu^{(k)}_{N-n_k+1} = F^{(k)}_{N-n_k+1} - F^{(k)}_{N-n_k}$ with $F^{(k)}_N = -k_{\mathrm{B}}T \ln Z^{(k)}_N$ the Helmholtz free energy of N particles. Thus, equation (B.7) can be written as

$$\frac{Z^{(k)}_{N-n_k}}{Z^{(k)}_N} = \mathrm{e}^{\beta\mu_N}\,\mathrm{e}^{\beta\mu_{N-1}}\cdots\mathrm{e}^{\beta\mu_{N-n_k+1}}. \tag{B.11}$$

In the thermodynamic limit $N \to \infty$, we can write $\mathrm{e}^{\beta\mu_N} = \cdots = \mathrm{e}^{\beta\mu_{N-n_k+1}} \approx \mathrm{e}^{\beta\mu}$, and therefore

$$Z_N = Z^{(k)}_N \sum_{n_k=0}^{j} \mathrm{e}^{-\beta n_k(\epsilon_k-\mu)} = Z^{(k)}_N \frac{\mathrm{e}^{-\beta(\epsilon_k-\mu)(j+1)} - 1}{\mathrm{e}^{-\beta(\epsilon_k-\mu)} - 1}. \tag{B.12}$$

Consequently, by the use of (B.6) and after some algebra, we finally get

$$\langle n_k\rangle_j = \frac{1}{\mathrm{e}^{\beta(\epsilon_k-\mu)} - 1} - \frac{j+1}{\mathrm{e}^{\beta(\epsilon_k-\mu)(j+1)} - 1}. \tag{B.13}$$

The generalization presented here shows how the chemical potential μ emerges from the particle conservation requirement for any order of the IQS.

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