Recursion formulas for quantum statistical partition functions

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Peter Borrmann and Gert Franke

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Peter Borrmann
University of Bremen, Dept. of Physics, D-W2800 Bremen 33, Germany

Gert Franke
University of Oldenburg, Dept. of Physics, D-W2900 Oldenburg, Germany

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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.

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

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

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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.

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