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Statistics of non-interacting bosons and fermions in micro-canonical, canonical and grand-canonical ensembles: A survey

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Abstract. The statistical properties of non-interacting bosons and fermions confined in trapping potentials are most easily obtained when the system may exchange energy and particles with a large reservoir (grand-canonical ensemble). There are circumstances, however, where the system under consideration may be considered as being isolated (micro-canonical ensemble). This paper first reviews results relating to micro-canonical ensembles. Some of them were obtained a long time ago, particularly by Khinchin in 1950. Others were obtained only recently, often motivated by experimental results relating to atomic confinement. A number of formulas are reported for the first time in the present paper. Formulas applicable to the case where the system may exchange energy but not particles with a reservoir (canonical ensemble) are derived from the micro-canonical ensemble expressions. The differences between the three ensembles tend to vanish in the so-called Thermodynamics limit, that is, when the number of particles and the volume go to infinity while the particle number density remains constant. But we are mostly interested in systems of moderate size, often referred to as being *mesoscopic*, where the grand-canonical formalism is not applicable. The mathematical results rest primarily on the enumeration of partitions of numbers.

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1. Introduction

Let us first recall that in Quantum Statistical Mechanics isolated systems should be treated in the *microcanonical* formalism, systems that may exchange energy with a heat bath in the *canonical* formalism and systems that may exchange both energy and particles with a bath in the *grand-canonical* formalism. In the latter case simple formulas

are easily obtained. For large systems the three ensembles are generally equivalent so that the grand-canonical formalism suffices for most applications. However, there is presently much interest in systems consisting of only a few particles, bosons or fermions. Recent experimental observations of atomic Bose-Einstein condensation motivated much theoretical work relating to *mesoscopic* devices. The fluctuation of the number of bosons occupying the ground level of harmonic traps was particularly considered. In such cases the grand-canonical ensemble is inappropriate and one must consider instead the less-easily handled micro-canonical and canonical formalisms.

Many results about canonical and microcanonical ensembles are known but they are scattered in the literature and often require intricate mathematical methods. The present paper provides an essentially exhaustive and mathematically simple derivation of the statistics of non-interacting particles in the three ensembles. Fermions and bosons are treated on the same footing but particles such as photons and phonons that do not carry generalized charges are considered in a separate section. In our approach *system* energy levels and their degeneracies are considered. A short study of compound systems helps clarify how degeneracy occurs. The mathematical method rests on exact results relating to the microcanonical statistics, canonical and grand-canonical expressions being subsequently derived through averaging. This line of attack is often evoked as being the most natural one but it has apparently not been pursued in detail before. Microcanonical statistics was treated by Khinchin in 1950 [1] but other statistics and degeneracies were not considered at that time. The microcanonical theory rests on the assumptions that the particles are undistinguishable and interact only weakly so that one-particle energies add up. The number of microcanonical configurations is assumed to be finite.

The purpose of this paper is not purely educational. Although the mathematical formalism requires only elementary combinatorics and the handling of generating series, the method naturally gives rise to several new results. This is the case in particular for formulas that facilitate estimations of certain quantities relevant to the canonical and grand-canonical ensembles. Complete results are given in the important case of evenly-spaced non-degenerate levels, one-dimensional harmonic potentials being a basic example. Recursive relations for occupancies are obtained that generalize results recently reported by Schönhammer [2]. It has been noticed long ago that microstates are in that case described by the partition of integers [3, 4]. It is also known that hard-core interacting bosons in harmonic potentials may be treated as non-interacting fermions [5]. Furthermore, the micro-canonical statistics of a band of states is particularly relevant to spin systems [6] and semiconductor devices.

The paper is essentially self-contained. Various formulas about occupancies, statistical weights, and partition functions for bosons and fermions are obtained in Sections 2 to 4, beginning with the microcanonical and ending up with the grand-canonical ensemble. Chargeless particles are treated in Section 5, and Section 6 addresses issues relating to compound systems and degeneracy. Section 7 deals with the case of evenly-spaced levels. Relations between fermionic and bosonic statistics are

given in Appendix A, links between von Neumann-Shannon entropy and the classical formulations of entropy in Thermodynamics in Appendix B.

2. Microcanonical statistics

Consider an isolated system comprising N undistinguishable particles. The energy ε_s of a particle in (quantum) state s is assumed to be non-negative without loss of generality. In what follows $\mathbb{S}$ denotes the set of states and $\mathbb{E}$ the set of energy levels. The *degeneracy* g_ε of an energy level ε is the number of states corresponding to that level. For example the energy of a state $s \equiv (k_1, \ldots, k_d)$, where $k_1, \ldots, k_d$ are non-negative integers, of a d-dimensional isotropic harmonic oscillator is given by the formula $\varepsilon = \hbar\omega(k + d/2)$ where $\hbar\omega$ is a constant and $k = k_1 + \cdots + k_d$. The degeneracy of the energy level ε is equal to the number of ways of obtaining k by summing up d nonnegative integers, namely $g_\varepsilon = (k + d - 1)!/(k!(d - 1)!)$.

A system is characterized by N and the total energy U it contains. Because of our assumption that the one-particle energies add up, U is the sum of N ε-values ($\varepsilon \in \mathbb{E}$), some of them possibly occuring more than once. In the sequel $\mathbb{U}$ denotes the set of *all* finite sums of elements of $\mathbb{E}$, with the convention that $\mathbb{U}$ contains 0. Given $N \in \mathbb{N}$ and $U \in \mathbb{U}$ several configurations may occur when U is a sum of N values in $\mathbb{E}$. Letting ν_s denote the number of particles in state s, a (N, U)-microstate is a family $\nu = (\nu_s)_{s\in\mathbb{S}}$ of non-negative integers (in other words, ν is a mapping from $\mathbb{S}$ to $\mathbb{N}$) fullfilling the conditions

$$\sum_{s\in\mathbb{S}} \nu_s = N, \quad \text{and} \quad \sum_{s\in\mathbb{S}} \nu_s\varepsilon_s = U. \tag{1}$$

As an example consider a system of particles whose energy levels are $\varepsilon = 2k-1+l^2$, with k, l positive integers (this is the case for charged single-spin particles in uniform magnetic fields under some conditions). Figure 1 shows the 22 partitions of $U = 22$ among $N = 3$ particles. Because of the degeneracies some of the partitions shown are associated with *several* microstates. The number ν_s of bosons in some state s is unconstrained while the numbers of fermions in a state may only be 0 or 1. Accordingly, the first marked ($\downarrow$) partition corresponds to two bosonic microstates since the ε=18 level is twice degenerate and to zero fermionic microstate since the ε=2 level is not degenerate. The second marked partition in Fig. 1 may correspond to a fermionic microstate because two *distinct* states have energy ε=10, namely $s_{1,3}$ (i.e., k=1, l=3) and $s_{5,1}$ (i.e., k=5, l=1), or to three bosonic microstates where the two-particles states for ε=10 are respectively: $(s_{1,3}, s_{5,1})$, $(s_{1,3}, s_{1,3})$ and $(s_{5,1}, s_{5,1})$.

The system *statistical weight* $W(N, U)$, i.e., the number of distinct (N, U)-microstates, is assumed to be finite. This implies finite degeneracies. Indeed, $W(1, U)$ is zero if U is not a one-particle energy level, otherwise it is the degeneracy at this level. Notice that since $0 \in \mathbb{U}$ by convention $W(0, 0) = 1$. Summing up the numbers on top of Fig. 1 we see that $W(3, 22)$ is equal to 34 for bosons and 21 for fermions. The purpose of formulas given below is to provide such numbers directly.

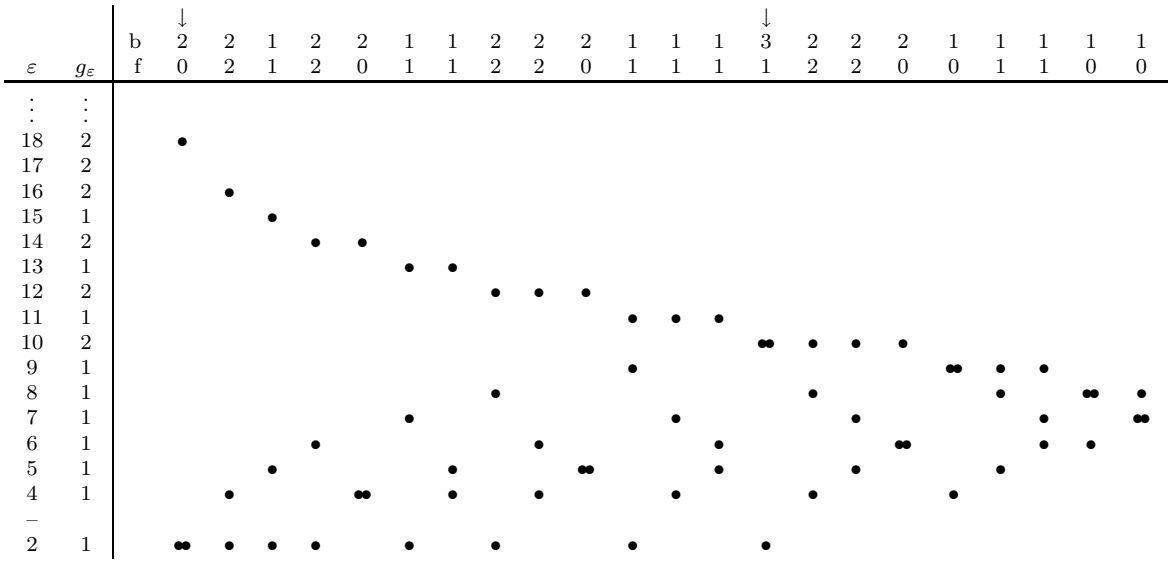

Figure 1. This figure represents the ($N = 3,\ U = 22$)-microstates: The energy levels ε and their degeneracy g_ε are shown on the left. At the top of the figure the number of microstates corresponding to each partition is given for bosons (b) and fermions (f).

The *microcanonical occupancy* $N_\varepsilon(N,U)$ of energy level ε is defined as the average number of particles at this energy level, the $W(N,U)$ microstates being equally likely. (If $W(N,U) = 0$ we have $N_\varepsilon(N,U) = 0$). In Fig. 1 the occupancy of level $\varepsilon = 10$ is 12/34 for bosons and 6/21 for fermions. Letting $\Omega(N,U)$ denote the set of all (N,U)-microstates the occupancy may be written

$$N_\varepsilon(N,U) = \frac{1}{W(N,U)} \sum_{s,\,\varepsilon_s=\varepsilon} \sum_{\nu\in\Omega(N,U)} \nu_s, \tag{2}$$

the first summation index s running through the states of energy ε. Conditions (1) and definition (2) result in

$$\sum_{\varepsilon\in\mathbb{E}} N_\varepsilon(N,U) = N, \quad \text{and} \quad \sum_{\varepsilon\in\mathbb{E}} N_\varepsilon(N,U)\varepsilon = U. \tag{3}$$

For example, the first relation in (3) derives from

$$W(N,U)\sum_{\varepsilon\in\mathbb{E}} N_\varepsilon(N,U) = \sum_{\varepsilon\in\mathbb{E}} \sum_{s,\,\varepsilon_s=\varepsilon} \sum_{\nu\in\Omega(N,U)} \nu_s = \sum_{s\in\mathbb{S}} \sum_{\nu\in\Omega(N,U)} \nu_s = \sum_{\nu\in\Omega(N,U)} \sum_{s\in\mathbb{S}} \nu_s.$$

Notice that at most $NW(N,U)$ summands contribute to each of the above sums. In the sequel the symbol + refers to bosons and the symbol − to fermions. The symbol ± should be replaced by + for bosons and by − for fermions.

The present article rests mainly on the following recursion relation, to be proven later in this section

$$N_\varepsilon^\pm(N,U) = \frac{W^\pm(N-1,U-\varepsilon)}{W^\pm(N,U)} \left(g_\varepsilon \pm N_\varepsilon^\pm(N-1,U-\varepsilon)\right). \tag{4}$$

Since $W(N-n,U-n\varepsilon)$ vanishes for $n>N$, iterating N times the above formula yields

$$N_\varepsilon^\pm(N,U)=\frac{g_\varepsilon}{W^\pm(N,U)}\sum_{n=1}^{N}(\pm1)^{n-1}W^\pm(N-n,U-n\varepsilon). \tag{5}$$

Combining (3) and (5) provides recursive formulas for the statistical weight

$$W^\pm(N,U)=\frac{1}{N}\sum_{n=1}^{N}\sum_{\varepsilon\in\mathbb{E}}(\pm1)^{n-1}g_\varepsilon W^\pm(N-n,U-n\varepsilon) \tag{6}$$

$$=\frac{1}{U}\sum_{n=1}^{N}\sum_{\varepsilon\in\mathbb{E}}(\pm1)^{n-1}\varepsilon g_\varepsilon W^\pm(N-n,U-n\varepsilon). \tag{7}$$

For example, the first one obtains as follows:

$$NW^\pm(N,U)=\sum_{\varepsilon\in\mathbb{E}}N_\varepsilon^\pm(N,U)W^\pm(N,U)=\sum_{\varepsilon\in\mathbb{E}}g_\varepsilon\sum_{n=1}^{N}(\pm1)^{n-1}W^\pm(N-n,U-n\varepsilon).$$

Notice that the sums above involve only the values of ε for which $N_\varepsilon(N,U)\neq0$, that is, at most $NW(N,U)$ ε-values. Formula (6) appears in [7, 8] in a different form (summation is done on one-particle states instead of system energy levels) for bosons, and in [9] for fermions without degeneracy. Although less interesting than (6) for a direct computation of $W(N,U)$, formula (7) will prove useful later.

To establish (4) consider a state s. For bosons (1) shows that the relation $\nu_s=\nu'_s-1$ defines a one-to-one correspondence between the set of $(N-1,U-\varepsilon)$-microstates ν and the set of (N,U)-microstates ν' with $\nu'_s>0$. Thus

$$\sum_{\nu'\in\Omega^+(N,U)}\nu'_s=\sum_{\nu\in\Omega^+(N-1,U-\varepsilon)}(1+\nu_s)=W^+(N-1,U-\varepsilon)+\sum_{\nu\in\Omega^+(N-1,U-\varepsilon)}\nu_s. \tag{8}$$

The above result amounts to removing one particle in state s from each (N,U)-microstate that exhibits such a particle and counting the remaining particles in state s. For fermions the number of (N,U)-microstates with one particle in state s equals the number of $(N-1,U-\varepsilon)$-microstates with no particle in state s, that is, all of them except those having one particle in that state. Thus

$$\sum_{\nu'\in\Omega^-(N,U)}\nu'_s=W^-(N-1,U-\varepsilon)-\sum_{\nu\in\Omega^-(N-1,U-\varepsilon)}\nu_s. \tag{9}$$

By (2), summing extremal members in (8) and (9) for all states s of energy ε the result in (4) is obtained.

Formulas (4) and (5) have apparently not been published before in their general form. Related expressions are given by Khinchin [1] under the assumption of evenly-spaced non-degenerate energy levels. Khinchin accounts for degeneracy by repeating energy levels. This amounts to consider quantum states instead of energy levels [7]. For bosons Eq. (5) has appeared in a different form in [7]. For the case of non-degenerate fermionic systems the formulas (4,5) were given in [9].

It is thus clear that microcanonical statistics rely on the sole knowledge of statistical weights, the computation of which requiring only the energy-levels values and their degeneracy.

3. Canonical statistics

When the system may exchange energy with a medium of arbitrarily large size at temperature T (heat bath), the probability that a particular (N,u)-microstate occurs at equilibrium is proportional to q^u, where

$$q \equiv \exp(-\frac{1}{k_{\mathrm{B}}T}),$$

according to Boltzmann and Gibbs. The *partition function*

$$Z(N,q) \equiv \sum_{u\in\mathbb{U}} W(N,u)q^u \tag{10}$$

normalizes the probability. Notice that, even though all sums are finite in the previous section, the summation index u takes on infinitely many contributing values. Summability requires that the energy levels ε form a finite or unbounded countable set. If the levels are discrete this means that they must form a finite or unbounded increasing sequence. Convergence of the partition function occurs if, and only if, $Z(1,q)$ converges. Indeed, $0 \le Z^-(N,q) \le Z^+(N,q) \le Z(1,q)^N$. We assume in the sequel that $Z(1,q)$ converges.

The system is characterized by the number N of particles and the temperature T, or N and q equivalently. The average energy $U(N,q)$ follows from

$$U(N,q) = \frac{1}{Z(N,q)} \sum_{u\in\mathbb{U}} uW(N,u)q^u = q\frac{d}{dq}\ln Z(N,q). \tag{11}$$

The system may be characterized by N and U since $U(N,q)$ is an increasing function of q. Indeed, the energy variance, a positive quantity, is given by

$$\begin{aligned}\mathrm{Var}(U) &= \frac{1}{Z(N,q)} \sum_{u\in\mathbb{U}} u(u-1)W(N,u)q^u + U(N,q) - U(N,q)^2 \\ &= \frac{1}{Z(N,q)}\frac{d^2}{dq^2}Z(N,q) + U(N,q) - U(N,q)^2 \quad = q\frac{d}{dq}U(N,q).\end{aligned}$$

Energy variance is therefore linked to heat capacity $c(N,T) \equiv dU(N,q)/dT$ by $\mathrm{Var}(U) = k_{\mathrm{B}}T^2c(N,T)$. It is worthwhile to point out that two systems in the canonical ensemble have the same heat capacity if, and only if, their partition functions coincide except for a multiplicative factor of the form aq^b, where a and b are real numbers that do not depend on T. This result follows easily from (11).

The *canonical occupancy* $N_\varepsilon(N,q)$ at level ε is the average number of particles at this level. It may therefore be calculated by averaging the microcanonical occupancies at level ε with $W(N,u)q^u$ as a weight. Accordingly, relations (3) result in

$$\sum_{\varepsilon\in\mathbb{E}} N_\varepsilon(N,q) = N, \quad \text{and} \quad \sum_{\varepsilon\in\mathbb{E}} N_\varepsilon(N,q)\varepsilon = U(N,q). \tag{12}$$

Since $W(N,u)$ vanishes for $u<0$, it is not difficult to see ‡ with the help of formula (4) that

$$N_\varepsilon^\pm(N,q) = q^\varepsilon \frac{Z^\pm(N-1,q)}{Z^\pm(N,q)} \left(g_\varepsilon \pm N_\varepsilon^\pm(N-1,q)\right), \tag{13}$$

$$= \frac{g_\varepsilon}{Z^\pm(N,q)} \sum_{n=1}^{N} (\pm 1)^{n-1} q^{n\varepsilon} Z^\pm(N-n,q). \tag{14}$$

Equation (14) is derived by iterating (13) or averaging (5). A relation similar to (13) is given in [10] for the case of non-degenerate energy levels. But the assumption made in that paper that $N_\varepsilon^\pm(N,q)$ and $N_\varepsilon^\pm(N-1,q)$ are identical is valid for large N-values only. The relations (14) and (5) were given in [11].

In general, a closed form expression of $Z(N,q)$ has not been established, but this quantity can be evaluated recursively. Using $W(0,0)=1$ and $W(0,u)=0$ if $u>0$, we obtain from (6)

$$Z(0,q)=1, \quad \text{and} \quad Z(1,q)=\sum_{\varepsilon\in\mathbb{E}} g_\varepsilon q^\varepsilon. \tag{15}$$

Summing up (14) for ε running through $\mathbb{E}$ and making use of the first formula in (12), we obtain for $N\geq 1$

$$Z^\pm(N,q) = \frac{1}{N} \sum_{n=1}^{N} (\pm 1)^{n-1} Z^\pm(N-n,q) Z(1,q^n). \tag{16}$$

This formula may also be derived directly from (6). Alternative proofs are given in [12, 13, 14, 15]. Making use of (7) instead provides a similar formula for the computation of $Z'(N,q) \equiv \frac{d}{dq} Z(N,q)$. Comparing this formula with the derivative of (16) results in an other expression. These new formulas are respectively

$$Z'^\pm(N,q) = \sum_{n=1}^{N} (\pm q)^{n-1} Z^\pm(N-n,q) Z'(1,q^n) \tag{17}$$

$$= \frac{1}{N-1} \sum_{n=1}^{N-1} (\pm 1)^{n-1} Z'^\pm(N-n,q) Z(1,q^n). \tag{18}$$

The above relations (16) and (18) allow, in turn, the numerical computation of $U(N,q)$ with the help of (11).

Note incidentally that $Z(1,q)$ depends only on the energy levels and their degeneracy, not on the nature of the particles. Moreover, formulas (16) and (14) show that the main difficulty in the computation of $Z(N,q)$ and $N_\varepsilon(N,q)$ rests on the numerical evaluation of $Z(1,q^n)$, that is, of the one-particle partition function at temperature T/n, for n going from 1 to N. There is a formula giving $Z(N,q)$ in terms of $Z(1,q)$ only:

$$Z^\pm(N,q) = \sum_{(\nu_k)_{k\geq 1}\in \mathbf{P}(N)} \prod_{k\geq 1} \frac{(\pm 1)^{k-1} Z(1,q^k)^{\nu_k}}{\nu_k!\, k^{\nu_k}}, \tag{19}$$

‡ Index shifts in the calculation, such as $\sum_{u\in\mathbb{U}} W(N-1,u-\varepsilon)q^u = q^\varepsilon \sum_{u\in\mathbb{U}} W(N-1,u)q^u$, are justified by the following remark. Let $u'\in\mathbb{U}$. If there exists $N\in\mathbb{N}^*$ such that $W(N,u-u')\neq 0$, then $u\in\mathbb{U}$ if, and only if, $u-u'\in\mathbb{U}$.

where $\mathbf{P}(N)$ stands for the set of unrestricted partitions of N, corresponding to the non-degenerate bosonic (N,U)-microstates with $\mathbb{E}=\mathbb{N}$ and $U=N$; see, e.g., [16]. This formula, which may be established by induction on N (the proof is tedious but obvious), is a special case of more general relations that are not relevant to this paper. Related formulas are given in [14, 17] and linked to symmetric polynomials in [18].

4. Grand-canonical statistics

If the system may exchange energy and particles with a bath at temperature T and fugacity z, the probability that a (n,u)-microstate occurs is proportional to $z^n q^u$. The grand-partition function

$$\mathcal{Z}(z,q)=\sum_{n\geq 0}\sum_{u\in\mathbb{U}} W(n,u) z^n q^u$$

that normalizes the probability reads

$$\mathcal{Z}^+(z,q)=\prod_{\varepsilon\in\mathbb{E}}\frac{1}{(1-zq^\varepsilon)^{g_\varepsilon}},\qquad \mathcal{Z}^-(z,q)=\prod_{\varepsilon\in\mathbb{E}}(1+zq^\varepsilon)^{g_\varepsilon}. \tag{20}$$

These formulas can be recovered by averaging both sides of (16) with z^N as a weight and using (15) so that

$$\begin{aligned}\sum_{n\geq 0} nZ^\pm(n,q)z^n &= \sum_{n\geq 0}\sum_{i=1}^{n}(\pm 1)^{i+1}Z^\pm(n-i,q)\sum_{\varepsilon\in\mathbb{E}} g_\varepsilon q^{i\varepsilon}\\ &= -\sum_{\varepsilon\in\mathbb{E}} g_\varepsilon \sum_{n\geq 0} z^n \sum_{i=1}^{n}(\pm q^\varepsilon)^i Z^\pm(n-i,q)\\ &= -\sum_{\varepsilon\in\mathbb{E}} g_\varepsilon \Big(\sum_{n\geq 1}(\pm zq^\varepsilon)^n\Big)\Big(\sum_{n\geq 0} Z^\pm(n,q)z^n\Big)\\ &= z\sum_{n\geq 0} Z^\pm(n,q)z^n \sum_{\varepsilon\in\mathbb{E}} g_\varepsilon \frac{\mp q^\varepsilon}{1\mp zq^\varepsilon}.\end{aligned}$$

Dividing both sides by $z\sum_{n\geq 0} Z^\pm(n,q)z^n$ we recognize that the two sides of each equality shown in (20) have the same logarithmic derivative with respect to z, so that they are proportional to one another. It follows that they are identical since they have the same constant term 1.

The *grand-canonical* occupancy at level ε is calculated by averaging the microcanonical occupancy $N_\varepsilon(n,u)$ with $z^n q^u W(n,u)$ as a weight, that is, by averaging the canonical occupancy $N_\varepsilon(n,q)$ with $Z(n,q)z^n$ as a weight. Using (13) and introducing the chemical potential $\mu\equiv k_{\mathrm{B}}T\ln z$, we obtain the celebrated Bose-Einstein and Fermi-Dirac distributions

$$N_\varepsilon^+(z,q)=\frac{g_\varepsilon}{q^{\mu-\varepsilon}-1},\qquad N_\varepsilon^-(z,q)=\frac{g_\varepsilon}{q^{\mu-\varepsilon}+1}. \tag{21}$$

It follows from $\ln\mathcal{Z}^\pm(z,q)=\mp\sum_{\varepsilon\in\mathbb{E}} g_\varepsilon\ln(1\mp zq^\varepsilon)$ that the average number of particles and average energy are respectively

$$\sum_{\varepsilon\in\mathbb{E}} N_\varepsilon(z,q)=z\frac{d}{dz}\ln\mathcal{Z}(z,q),\qquad \sum_{\varepsilon\in\mathbb{E}}\varepsilon N_\varepsilon(z,q)=q\frac{d}{dq}\ln\mathcal{Z}(z,q). \tag{22}$$

The expansion of $\ln(1 \mp zq^\varepsilon)$ in power series of zq^ε provides with an expression of $\ln \mathcal{Z}(z,q)$ in terms of the one-particle canonical partition function, namely

$$\ln \mathcal{Z}^{\pm}(z,q) = \sum_{n\geq 1} (\pm 1)^{n-1} Z(1,q^n) \frac{z^n}{n}. \tag{23}$$

Accordingly, the average number of particles and energy may be computed as

$$N(z,q) = \sum_{n\geq 1} (\pm 1)^{n-1} Z(1,q^n) z^n, \tag{24}$$

$$U(z,q) = \sum_{n\geq 1} (\pm 1)^{n-1} Z'(1,q^n) (zq)^n. \tag{25}$$

5. Photons and phonons.

Particles that do not bear generalized charge such as photons or phonons can be created or annihilated without violating conservation rules. Accordingly, the number N of such particles is not conserved in the micro-canonical and canonical ensembles. A U-microstate is now a family $\nu = (\nu_s)_{s\in\mathbb{S}}$ of non-negative integers satisfying the sole condition

$$\sum_{s\in\mathbb{S}} \nu_s \varepsilon_s = U. \tag{26}$$

The microcanonical statistical weight $W(U)$ is obtained by summing up $W(n,U)$ over all n values. Let $\varepsilon_0 = \min \mathbb{E}$ be the lowest one-particle energy level. If $\varepsilon_0 > 0$ then $n\varepsilon_0$ exceeds U at sufficiently large values of n so that $W(U)$ is finite. This arguments also applies to fermionic systems with $\varepsilon_0 = 0$ because the number of fermions that occupy this level cannot exceed its degeneracy. But if ε_0 were equal to zero in bosonic systems the addition of a particle at level ε_0 would entail that $W(n,U) \leq W(n+1,U)$ and $W(U)$ would be equal to zero or infinity. We therefore assume that the ground-state energy of chargeless bosons is non-zero. No generality is lost since such particles cannot be detected at zero energy.

The microcanonical occupancy of the energy level ε is the average number of particles at level ε. Arguments similar to the ones given in Section 2 show that (3)-(5) may be written as

$$\sum_{\varepsilon\in\mathbb{E}} N_\varepsilon(U)\varepsilon = U,$$

$$N_\varepsilon^{\pm}(U) = \frac{W^{\pm}(U-\varepsilon)}{W^{\pm}(U)} (g_\varepsilon \pm N_\varepsilon^{\pm}(U-\varepsilon)) \tag{27}$$

$$= \frac{g_\varepsilon}{W^{\pm}(U)} \sum_{n=1}^{\lfloor U/\varepsilon \rfloor} (\pm 1)^{n-1} W^{\pm}(U-n\varepsilon). \tag{28}$$

Equation (7) becomes

$$W^{\pm}(U) = \frac{1}{U} \sum_{\varepsilon\leq U} \varepsilon g_\varepsilon \sum_{n=1}^{\lfloor U/\varepsilon \rfloor} (\pm 1)^{n-1} W^{\pm}(U-n\varepsilon). \tag{29}$$

Canonical ensemble and grand-canonical ensemble with fugacity $z = 1$ are presently equivalent. Indeed, averaging as in §3 the above relations with q^u as a weight gives

$$Z(q) = \sum_{u\in\mathbb{U}} W(u)q^u, \quad U(q) = q\frac{d}{dq}\ln Z(q), \quad \sum_{\varepsilon\in\mathbb{E}} N_\varepsilon(q)\varepsilon = U(q), \tag{30}$$

and

$$N_\varepsilon^+(q) = \frac{g_\varepsilon}{q^{-\varepsilon}-1}, \qquad N_\varepsilon^-(q) = \frac{g_\varepsilon}{q^{-\varepsilon}+1}. \tag{31}$$

Inserting the latter expressions in the third equation of (30) and integrating, the expression of $\ln Z^\pm(q)$ is obtained from the second equation of (30) yielding

$$Z^+(q) = \prod_{\varepsilon\in\mathbb{E}} \frac{1}{(1-q^\varepsilon)^{g_\varepsilon}}, \qquad Z^-(q) = \prod_{\varepsilon\in\mathbb{E}} (1+q^\varepsilon)^{g_\varepsilon}. \tag{32}$$

If we expand $\ln(1 \pm q^\varepsilon)$ in power series of q^ε as was done earlier in §4 we obtain

$$\ln Z^\pm(q) = \sum_{n\geq 1} \frac{(\pm 1)^{n-1}}{n} Z(1, q^n). \tag{33}$$

The average energy may be derived from this expression according to (30) and the average number of particles is obtained from a summation of (31) and expansion of $q^\varepsilon/(1 \pm q^\varepsilon)$. These two quantities are given by

$$N(q) = \sum_{n\geq 1} (\pm 1)^{n-1} Z(1, q^n), \qquad U(q) = \sum_{n\geq 1} (\pm 1)^{n-1} Z'(1, q^n) q^n. \tag{34}$$

6. Compound systems

A compound system is a mixture of several sub-systems comprising undistinguishable particles, the particles of any two sub-systems being distinguishable. We assume that mixing does not affect the one-particle energy-level values and consider two sub-systems only, generalization to a greatest number of sub-systems being straightforward.

Consider a system composed of two sub-systems with a total of $N_1 + N_2 \equiv N$ particles and energy $U_1 + U_2 \equiv U$. If neither energy nor particles are allowed to be exchanged the number $W(N, U)$ of configurations of the compound system is the product of the statistical weights of the sub-systems and the occupancies add up, that is

$$W(N, U) = W_1(N_1, U_1) W_2(N_2, U_2), \tag{35}$$

$$N_\varepsilon(N, U) = N_{1,\varepsilon}(N_1, U_1) + N_{2,\varepsilon}(N_2, U_2). \tag{36}$$

Suppose now that the number of particles in each sub-system is constant but that some energy may be transferred from one sub-system to the other. For example the two sub-systems may comprise electrons of spin 1/2 and -1/2 respectively, spin flip being not allowed. Each possible energy splitting between the two sub-systems has to be taken in

account. Since all the possible configurations are equally likely to occur any (N_1, u_1)-microstate of the first sub-system has a statistical weight $W_2(N_2, U - u_1)$. Therefore, the number of possible configurations of the system and the occupancy of level ε are

$$W(N,U) = \sum_{u_1+u_2=U} W_1(N_1,u_1)W_2(N_2,u_2), \tag{37}$$

$$N_\varepsilon(N,U) = \sum_{u_1+u_2=U} \frac{W_1(N_1,u_1)W_2(N_2,u_2)}{W(N,U)}(N_{1,\varepsilon}(N_1,u_1) + N_{2,\varepsilon}(N_2,u_2)). \tag{38}$$

As one may expect for sub-systems that only exchange energy the canonical-ensemble formulas are simple. Remembering that at equilibrium the temperatures and chemical potentials of the two sub-systems equalize, the above expressions give

$$Z(N,q) = Z_1(N_1,q)Z_2(N_2,q), \tag{39}$$

$$N_\varepsilon(N,q) = N_{1,\varepsilon}(N_1,q) + N_{2,\varepsilon}(N_2,q). \tag{40}$$

If the sub-systems may exchange particles, for instance if spin flip is allowed in a system of electrons, similar arguments show that the statistical weight and the occupancy of level ε are

$$W(N,U) = \sum_{n_1+n_2=N} \sum_{u_1+u_2=U} W_1(n_1,u_1)W_2(n_2,u_2), \tag{41}$$

$$N_\varepsilon(N,U) = \sum_{n_1+n_2=N} \sum_{u_1+u_2=U} \frac{W_1(n_1,u_1)W_2(n_2,u_2)}{W(N,U)}(N_{1,\varepsilon}(n_1,u_1) + N_{2,\varepsilon}(n_2,u_2)). \tag{42}$$

Partition and grand-partition functions are easily derived:

$$Z(N,q) = \sum_{n_1+n_2=N} Z_1(n_1,q)Z_2(n_2,q), \tag{43}$$

$$\mathcal{Z}(z,q) = \mathcal{Z}_1(z,q)\mathcal{Z}_2(z,q). \tag{44}$$

Such a compound systems is equivalent to a single system with the following characteristics: $\mathbb{E}$ is the union of the sets of energy levels of the subsystems and the degeneracies are added. Because of the possible exchange of energy and particles the two sub-systems become undistinguishable from one another. This fact is ascertained by the expression obtained for the grand-partition function of the compound system. But this conclusion does not apply when the sub-systems only exchange energy as illustrated in [9].

7. Non-degenerate system with evenly-spaced levels

7.1. Microcanonical relations

When the energy levels are evenly spaced we may assume without loss of generality that the energy levels are non-negative integers. We may indeed take the energy-level spacing as the energy unit. On the other hand shifting the energy levels by one is tantamount to shifting the total energy of the system by the number of particles. The number of configurations and the occupancies are unaffected.

We first restrict our attention to a band of evenly-spaced one-particle energy levels, namely $\mathbb{E} = \{0, 1, \ldots, B\}$. Let us recall that a partition of $U \in \mathbb{N}$ is a non-increasing sequence of nonnegative integers summing up to U. If bosons are considered, a (N, U)-microstate is a partition of U with at most N parts none of them exceeding B. Thus the statistical weight is the number of such partitions. An example is given in Figure 1.

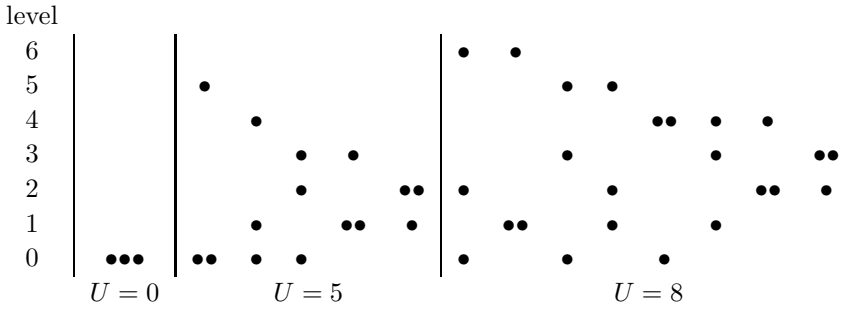

Figure 2. Bosons, $(N = 3, U)$-microstates for $B = 6$.

With a usual notation, the statistical weight

$$W^+(N, U) = p(B, N, U) \tag{45}$$

vanishes when $U < 0$ and $U > NB$. Several classical properties of the $p(B, N, U)$'s are given in [16]. For fermions, only the partitions of U with distinct parts are to be considered. Considering upward shifts from the smallest energy $U_{\min} \equiv N(N-1)/2$ and letting $P \equiv B - N + 1$ denote the maximum number of adjacent empty levels, it is easy to see that these partitions are the partitions of the *added* energy $R \equiv U - U_{\min}$ into at most N parts none of them exceeding P, that is

$$W^-(N, U) = p(B - N + 1, N, U - N(N-1)/2) = p(P, N, R). \tag{46}$$

Figure 3 illustrates the above argument with reference to Figure 2. The numbers in parentheses count the number of energy jumps from the initial positions and relate the fermionic (3,8)-microstates to the corresponding bosonic (3,5)-microstates.

In the present situation of evenly-spaced levels further micro-canonical relations may be established. The following reasoning may be formalized by using the definition in (1) of microstates. Consider first a bosonic system consisting of N particles and energy U. Recall that $W^+(N-1, U-\varepsilon)$ is the number of (N, U)-microstates with at least one particle at level ε. There are therefore $W^+(N, U) - W^+(N-1, U)$ microstates with no particle at level 0. Shifting downward the energy levels by 1 these microstates provide all the $(N, U-N)$-microstates except those that have one particle at least at level B. In other words

$$W^+(N, U) - W^+(N-1, U) = W^+(N, U-N) - W^+(N-1, U-N-B). \tag{47}$$

Let us denote for short $M_k(N, U) \equiv W(N, U) N_k(N, U)$. Substituting $N - n$ and $U - n(k+1)$ in place of N and U in (47) and summing both sides with n running

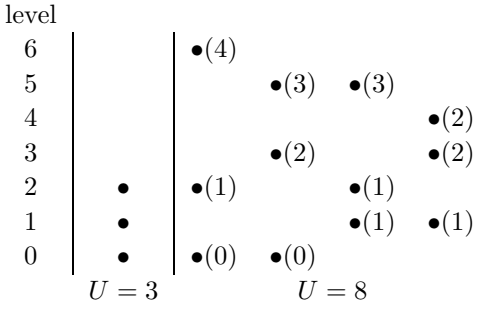

Figure 3. Fermions, $(N = 3, U)$-microstates for $B = 6$.

from 0 to N, we obtain from (5) a relation involving the same number N of particles but successive levels $k, k+1$. This relation reads for $0 \leq k < B$

$$\begin{array}{l} W^+(N,U) + M^+_{k+1}(N,U) - M^+_{k+1}(N,U+k+1) \quad = \\ W^+(N,U-N) + M^+_k(N,U-N) - M^+_k(N,U-N-B+k). \end{array} \tag{48}$$

Indeed, using (5) we have successively

$$\begin{aligned} \sum_{n\geq 0} W^+(N-n,U-n(k+1)) \qquad &= W^+(N,U) + W^+(N,U)N^+_{k+1}(N,U), \\ \sum_{n\geq 0} W^+(N-1-n,U-n(k+1)) &= \sum_{n\geq 1} W^+(N-n,U+k+1-n(k+1)) \\ &= W^+(N,U+k+1)N^+_{k+1}(N,U+k+1), \end{aligned}$$

the right-hand terms in (47) being handled analogously.

Consider now a fermionic system consisting of N particles and with total energy U. We have

$$W^-(N,U) + W^-(N-1,U-B-1) = W^-(N,U-N) + W^-(N-1,U-N+1). \tag{49}$$

Indeed, the left-hand side of this expression counts the union of the (N,U)-microstates and the fictitious (N,U)-configurations with 1 particle at the fictitious additional level $B+1$. Depending on whether the above (N,U)-configurations have 0 particle at level 0 or not, shifting downward the levels by 1 results either in a $(N,U-N)$-microstate or in a $(N,U-N)$-configuration with 1 particle at the fictitious level -1. This gives the right-hand side. Notice further that analogously the occupancy of the lowest level satisfies the relation

$$M_0(N,U) + M_0(N-1,U-B-1) = W^-(N-1,U-N+1), \tag{50}$$

because shifting the levels yields all the (N,U)-configurations with 1 particle at level -1. In the same way as in (48) one derives from (47), we obtain from (49) for $0 \leq k < B$

$$\begin{array}{l} W^-(N,U) - M^-_{k+1}(N,U) + M^-_{k+1}(N,U-B+k) \quad = \\ W^-(N,U-N) - M^-_k(N,U-N) + M^-_k(N,U-N+1+k). \end{array} \tag{51}$$

Replacing $M_0(N,U)$ in (50) by its value given by (4) and substituting N to $N-1$ we obtain

$$M_0(N,U) = M_0(N,U-B-1) + W^-(N,U) - W^-(N,U-N).$$

This relation shows that formula (51) still holds for $k+1=0$.

7.2. Canonical relations

It is well known that the generating series for U of the numbers $p(B,N,U)$ in (45) is the gaussian polynomial

$$\sum_{U=0}^{NB} p(B,N,U)q^U = \frac{(q)_{B+N}}{(q)_B(q)_N},$$

where $(q)_n$ is the commonly employed notation for the product $(1-q)(1-q^2)\dots(1-q^n)$ and $(q)_0=1$. Accordingly,

$$Z^+(N,q) = \frac{(q)_{B+N}}{(q)_B(q)_N}, \qquad Z^-(N,q) = q^{N(N-1)/2}\frac{(q)_{B+1}}{(q)_{B+1-N}(q)_N}. \tag{52}$$

In order to keep the paper self-contained let us point out that the latter expressions may be easily derived from the previous microcanonical relations. According to (45) and (46) it suffices to consider $Z^+(N,q)$. Firstly

$$Z(1,q) = 1+q+\dots+q^B = \frac{1-q^{B+1}}{1-q}.$$

Secondly, averaging (47) with q^U as a weight and collecting the results we obtain the recurrence relation

$$Z^+(N,q) = \frac{1-q^{B+N}}{1-q^N}Z^+(N-1,q),$$

from which the derivation of $Z^+(N,q)$ in (52) is straightforward.

Averaging (48) and (51) with q^U as a weight, dividing by $Z(N,q)$ and multiplying by q^{k+1}, provides simple recursive formulas for the computation of canonical occupancies. These formulas are new for bosons, and generalize [2] for fermions. For $0 \le k < B$ they are

$$(1-q^{k+1})N^+_{k+1}(N,q) \qquad = q^{k+1}(1-q^N) - q^N(q^{k+1}-q^{B+1})N^+_k(N,q), \tag{53}$$

$$(q^{k+1}-q^{B+1})N^-_{k+1}(N,q) = q^{k+1}(1-q^N) - q^N(1-q^{k+1})N^-_k(N,q). \tag{54}$$

As noticed after (51) the latter formula holds for $k+1=0$ so that

$$N^-_0(N,q) = \frac{1-q^N}{1-q^{B+1}}.$$

There is apparently no such simple expression for $N^+_0(N,q)$. This quantity may be calculated from (13) with the initial value $N^+_0(1,q) = 1/Z(1,q)$. The expression obtained directly from (14) is

$$N^+_0(1,q) = \frac{(q)_N}{(q)_{N+B}}\sum_{n=0}^{N-1}\frac{(q)_{B+n}}{(q)_n}.$$

7.3. Unbounded energy levels.

If we let $B \to \infty$ in the previous formulas we obtain expressions applicable to infinitely many energy levels

$$W^+(N,U) = p_N(U), \quad W^-(N,U) = p_N(U - N(N-1)/2) = p_N(R),$$
$$Z^+(N,q) = \frac{1}{(q)_N}, \qquad Z^-(N,q) = \frac{q^{N(N-1)/2}}{(q)_N}.$$

The recursive formulas obtained in the last subsection were given before in [2] for fermionic systems in the limit of infinite B-values.

If we introduce the additional energy R in place of the total energy U in fermionic systems the statistical weights and partition functions exhibit the same form for bosons and fermions. This explains the similarities previously noted, for instance the fact that Bose and Fermi gases (with the same number N of particles) in square-law potentials have the same heat capacity. Considering R instead of U enables one to let $N \to \infty$ in the case of fermionic systems [19, 20, 21, 22]. This limit provides with the simplest form of all previous formulas.

8. Conclusion

Non-interacting fermions and bosons statistics have been obtained in the three classical ensembles. The originality of the method rests on the derivation of complete and explicit microcanonical formulas by direct enumeration of the microstates. Canonical and grand-canonical relations are further derived by simple averaging. Several results are new, older works are referred to.

Using the microcanonical relations requires the sole knowledge of system energy levels and degeneracies. Only average occupation numbers have been reported, but formulas for joint and higher moments may be obtained by similar arguments [1]. Microcanonical formulas have been given that arise naturally. One of them leads to a recursive relation for the derivative of the canonical partition function. We have also shown that most canonical and grand-canonical quantities may be calculated from the one-particle canonical partition functions at temperatures T/n, $n \geq 1$. This result is still valid for particles that do not bear generalized charges.

One-dimensional harmonic oscillators Schönhammer's results [2] have been generalized in several aspects. Bosons are also treated. Related microcanonical relations are given. The case of finitely many levels is treated. Extension to arbitrary degeneracy shall be the object of future research.

Other, less classical, statistical ensembles might be handled analogously. For example, in the grand microcanonical ensemble [23] the system may exchange particles with a bath. The fugacity z and the energy U of the system are fixed but the number n of its particles is allowed to fluctuate. The probability that a particular (n,U)-microstate occurs is proportional to z^n. Accordingly, the grand microcanonical statistics can be derived from averaging the microcanonical relations in §2 with z^n as a weight.

Appendix A. Relations between fermionic and bosonic statistical weights.

Given the set $\mathbb{E}$ of the one-particle energy levels, there is a simple relation between the numbers $W^-(N,U)$ and $W^+(N,U)$. It reads

$$W^-(N,U) = \sum_{n=0}^{\lfloor N/2\rfloor} (-1)^n \sum_{u=0}^{U/2} W^-(n,u) W^+(N-2n, U-2u), \tag{A.1}$$

where $\lfloor N/2\rfloor$ denotes the greatest integer non-exceeding $N/2$, and the second $\sum$ symbol stands for a summation for all values of $u \in \mathbb{U}$ between 0 and $U/2$. Let us sketch a proof of relation (A.1). Suppose the Pauli exclusion principle applies to all energy levels except ε. Then the possible (N,U)-configurations split up into those that obey strictly the Pauli principle and those that exhibit at least two particles at level ε. Removing two particles at level ε in the latter, denoting by $W^\varepsilon(N,U)$ the number of (N,U)-configurations of our supposed system and enumerating, result in

$$W^-(N,U) = W^\varepsilon(N,U) - W^\varepsilon(N-2, U-2\varepsilon). \tag{A.2}$$

Further relaxing the Pauli principle at other levels one by one and iterating formula (A.2), we get

$$W^-(N,U) = \sum_{E\subseteq\mathbb{E}} (-1)^{|E|} W^+(N-2|E|, U-2\textstyle\sum_{\varepsilon\in E}\varepsilon), \tag{A.3}$$

where $|E|$ stands for the number of levels in E. Finally formula (A.3) may alternatively be written as formula (A.1) by letting $n = |E|$, $u = \sum_{\varepsilon\in E}\varepsilon$, and remarking that there are $W^-(n,u)$ ways to get u from the n elements in E. All sums terminate because $W(N,U) = 0$ for negative N or U.

Averaging formula (A.1) we readily derive the identity

$$Z^-(N,q) = \sum_{n=0}^{\lfloor N/2\rfloor} (-1)^n Z^+(N-2n,q) Z^-(n,q^2). \tag{A.4}$$

Denoting by $\mathcal{Z}^\pm(z,q)$ the grand-canonical partition function further averaging yields

$$\mathcal{Z}^-(z,q) = \mathcal{Z}^+(z,q)\mathcal{Z}^-(-z^2,q^2),$$

a fairly straightforward identity in view of (20). In the present case we recognize that it is easier to proceed the other way around, namely from grand-canonical to microcanonical relations. As an illustration, from the similar identities

$$1 = \mathcal{Z}^+(z,q)\mathcal{Z}^-(-z,q), \qquad \mathcal{Z}^+(z,q) = \mathcal{Z}^-(z,q)\mathcal{Z}^+(z^2,q^2),$$

we derive by expanding the series products and identifying the coefficients of z^N, for positive N,

$$\begin{aligned} 0 &= \sum_{n=0}^{N} (-1)^n Z^+(n,q) Z^-(N-n,q), \\ Z^+(N,q) &= \sum_{n=0}^{\lfloor N/2\rfloor} Z^-(N-2n,q) Z^+(n,q^2). \end{aligned}$$

The microcanonical counterparts of these relations are obtained by identifying the coefficients of q^U.

Appendix B. Entropy

For the reader's convenience we link in what follows statistical quantities with thermodynamical ones. This can be done by examinating the expression of entropy in both formalisms. The von Neumann-Shannon entropy is defined as

$$S = -\sum_{\omega} p_\omega \ln p_\omega,$$

where p_ω is the probability of a state of the system and ω runs through the set of all such states.

In the micro-canonical ensemble with N particles and total energy U, the microstates are equally likely so that $p_{\omega(N,U)} = 1/W(N,U)$ and $S = \ln W(N,U)$, namely the Boltzmann entropy.

In the canonical ensemble with N particles and temperature T, $p_{\omega(N,u)} = q^u/Z(N,q)$. Thus

$$\begin{aligned} S &= -\sum_{u\in\mathbb{U}} W(N,u)\frac{q^u}{Z(N,q)} \ln \frac{q^u}{Z(N,q)} = \ln Z(N,q) - \frac{q \ln q}{Z(N,q)} \frac{d}{dq} Z(N,q) \\ &= \ln Z(N,q) + \frac{1}{k_{\mathrm{B}}T} U(N,q). \end{aligned}$$

This is the classical expression of the entropy of a closed thermodynamic system with Helmholz free energy $A(N,q) = -k_{\mathrm{B}}T \ln Z(N,q)$.

In the grand-canonical ensemble with fugacity z and temperature T, the probability $p_{\omega(n,u)} = z^n q^u/\mathcal{Z}(z,q)$. Accordingly, we obtain as above

$$S = -\sum_{u\in\mathbb{U}} \sum_{n\geq 0} W(n,u)\frac{z^n q^u}{\mathcal{Z}(z,q)} \ln \frac{z^n q^u}{\mathcal{Z}(z,q)} = \ln \mathcal{Z}(z,q) + \frac{1}{k_{\mathrm{B}}T} U(z,q) - \frac{\mu}{k_{\mathrm{B}}T} N(z,q).$$

The relevant thermodynamical potential (grand potential) is given by the logarithm of the partition function. Accordingly, entropies of subsystems add up if their partition functions multiply. The appropriate conditions are given in Section 6.

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