Partition functions and symmetric polynomials

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Abstract. We find a close correspondence between certain partition functions of ideal quantum gases and certain symmetric polynomials. Due to this correspondence it can be shown that a number of thermodynamic identities which have recently been considered are essentially of combinatorical origin and known for a long time as theorems on symmetric polynomials. For example, a recurrence relation for partition functions appearing in the textbook of P. Landsberg is nothing else but Newton's identity in disguised form. Conversely, a certain theorem on symmetric polynomials translates into a new and unexpected relation between fermionic and bosonic partition functions, which can be used to express the former by means of the latter and vice versa.

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1. Introduction

The theory of ideal quantum gases, although a standard section in every modern textbook on statistical mechanics, is far from being a closed field of research. On one hand, there are continuous attempts towards a deeper understanding of the foundations of the field and to disclose unexpected regularities and relations between known facts. As examples we quote the work of M. H. Lee [1, 2, 3] on a unified treatment of Fermi and Bose gases and our earlier paper on a fermion-boson symmetry for harmonic oscillators of odd space dimensions [4]. Also this article is intended to contribute to such foundational questions

On the other hand, there are various applications of the theory of ideal gases in almost all areas of modern physics, despite the apparent over-simplification of non-interacting particles. In nuclear physics the shell model is a prominent representative, which at low excitation energies describes the motion of noninteracting fermions in a common (mean) field [5]. In solid state physics of one space dimension interacting fermions may be described as noninteracting bose gases (Luttinger liquids) [6, 7, 8]. The crucial point is that the specific heat of N fermions and bosons is the same for equidistant energy spectra, for recents works see [9, 10].

In atomic physics the concept of ideal quantum gases helped to understand experiments on magnetically trapped atomic vapours [11, 12, 13, 14]. Here the system can be well described as an ideal quantum gas contained in an external harmonic oscillator potential, for an overview see [15]. Also the case of constant and small particle number N turns out to be of interest, thereby excluding the use of a grand canonical ensemble (N fluctuating) and/or the thermodynamic limit ($N \to \infty$). Examples of applications, except the above-mentioned trapped systems, are quantum dots [16] and fluorescence from a few electrons [17]. For a comparison of canonical and grand canonical results in a two-state system see also [18].

In the context of these small quantum systems it is sometimes of interest to explicitely calculate the $N-$particle partition function $Z_N^{\pm}$, where $+$ stands for bosons and $-$ for fermions. For this purpose a certain recurrence relation for $Z_N^{\pm}$ has recently been used by several authors [19, 20, 9, 4, 17]. It seems that none of the authors, including us, was aware that this recurrence relation could be traced back to the time-honoured textbook of P. Landsberg [21]. Even more remarkable we find that, in some sense, Landsberg's formula was already discovered by Isaac Newton. Of course, Newton did not know anything about partition functions and Fermi/Bose statistics. However, there is an intimate connection between partition functions and symmetric polynomials, which allows to translate certain theorems on symmetric functions into statements about physical partition functions and vice versa. This will be the main subject of the present article.

The basic idea will be spelled out in section 2. Since we write this article for people who may be experts in either field, combinatorics and statistical mechanics, but not in both, we will give some rather elementary introductions into the field of symmetric

polynomials (section 3) and partition functions (section 4). Section 4 also contains the "dictionary" needed for the translation between statements of the respective fields. Thus we obtain the following results, which now appear obvious, but have not yet been explicitely mentioned in the physics literature, namely that Z_N^+ may be expressed by the $Z_n^-, n \leq N$ and vice versa. The most compact expression of this is the statement that the grand canonical partition functions satisfy $\mathcal{Z}^+(z)\mathcal{Z}^-(-z) = 1$. In section 5 we add some closing remarks.

2. The basic idea

Before going into details we will describe the basic idea of the correspondence between partition functions and symmetric polynomials and illustrate this idea for the simple example of a system with $L = 3$ energy levels and $N = 2$ particles.

It is well-known that the eigenstates of the $N-$particle Hamiltonian $H_N^{\pm}$ ($+$ for bosons, $-$ for fermions) of N non-interacting particles can be labelled by occupation number sequences $(n_1, n_2, \ldots, n_L)$, where $\sum_{\ell=1}^{L} n_\ell = N$ and $n_\ell = 0, 1$ for fermions. The latter condition expresses the Pauli principle. Equivalently, the eigenstates are in 1 : 1-correspondence to the monomials $x_1^{n_1} x_2^{n_2} \ldots x_L^{n_L}$ of degree N, where the $x_1, x_2, \ldots, x_L$ are (symbolic) commuting variables. In our example, we obtain the monomials x_1x_2, x_1x_3, x_2x_3 for the fermionic case, and, additionally, x_1^2, x_2^2, x_3^2, for the bosonic case.

The eigenvalue of $H_N^{\pm}$ corresponding to the eigenstate labelled by $x_1^{n_1} x_2^{n_2} \ldots x_L^{n_L}$ is given by $\sum_{\ell=1}^{L} E_\ell n_\ell$, if E_ℓ denotes the ℓ-th energy eigenvalue of the one-particle-Hamiltonian. Hence the corresponding eigenvalue of $\exp(-\beta H_N^{\pm})$, where, as usual, $\beta = \frac{1}{k_B T}$ denotes the inverse temperature, will be

$$\exp(-\beta \sum_{\ell=1}^{L} E_\ell n_\ell) = (e^{-\beta E_1})^{n_1} \ldots (e^{-\beta E_L})^{n_L}. \tag{1}$$

This eigenvalue is nothing else but the value of the monomial $x_1^{n_1} x_2^{n_2} \ldots x_L^{n_L}$ evaluated at $x_1 = e^{-\beta E_1}, \ldots, x_L = e^{-\beta E_L}$. To obtain the trace $\operatorname{Tr} \exp(-\beta H_N^{\pm})$ we have to sum over all eigenstates, or, equivalently, over all monomials of degree N (subject to the constraint $n_\ell = 0, 1$ in the fermionic case). Interchanging summation and evaluation, we may first consider the bosonic polynomial b_N (resp. the fermionic f_N) obtained by summing up all monomials of degree N (satisfying the above constraint in the case of f_N) and then, in a second step, evaluate this polynomial at $x_\ell = e^{-\beta E_\ell}, \ell = 1, \ldots, L$ in order to obtain $\operatorname{Tr} \exp(-\beta H_N^{\pm})$. The latter is usually called the partition function of the system. In our example, $b_2 = x_1^2 + x_2^2 + x_3^2 + x_1x_2 + x_1x_3 + x_2x_3$ and $f_2 = x_1x_2 + x_1x_3 + x_2x_3$. Both polynomials are symmetric w. r. t. any permutation of their arguments x_1, x_2, x_3. This also holds in the general case.

Thus we have established a connection between systems of N non-interacting bosons (resp. fermions) and certain symmetric polynomials b_N (resp. f_N). Specification of the one-particle Hamiltonian then corresponds to an evaluation of these polynomials at $x_\ell = e^{-\beta E_\ell}, \ell = 1, \ldots, L$ and yields the particular partition function.

3. Symmetrical polynomials

We collect some well-known definitions and results on symmetric polynomials which are relevant for our purposes. Throughout we consider polynomials in a finite number of (symbolic) variables $x_1, \ldots, x_n$. Most results also hold for the case of infinitely many variables ($n = \infty$) which is of physical interest, where the polynomials become formal power series. We will only indicate those cases where $n = \infty$ becomes problematic.
A polynomial p is called symmetric iff $p(x_1, \ldots, x_n) = p(x_{\sigma(1)}, \ldots, x_{\sigma(n)})$ for all permutations $\sigma \in \mathcal{S}_n$. The elementary symmetric polynomials f_m can be defined through their generating function

$$\prod_{\ell=1}^{n}(x + x_\ell) = \sum_{m=0}^{n} f_m x^{n-m}, \quad m = 0, \ldots, n. \tag{2}$$

For example,

$$f_0 = 1, \tag{3}$$
$$f_1 = x_1 + x_2 + \ldots + x_n, \tag{4}$$
$$f_2 = \sum_{i<j} x_i x_j, \tag{5}$$
$$\vdots$$
$$f_n = x_1 x_2 \cdots x_n. \tag{6}$$

The letter "f" for elementary symmetric polynomials is unusual, but chosen here to stress the association to "fermions". One important property of the f's is that $(f_1, \ldots, f_n)$ forms a basis in the sense that any symmetric polynomial can be uniquely written as a polynomial of the f_m. For example, if $n = 2$,

$$x_1^2 + x_2^2 = (x_1 + x_2)^2 - 2x_1 x_2 = f_1^2 - 2f_2. \tag{7}$$

Of course, there exist other bases of symmetric polynomials. For our purposes, the following ones are the most important:

Let b_ℓ denote the sum of all monomials of degree ℓ, for example

$$b_0 = 1, \tag{8}$$
$$b_1 = x_1 + x_2 + \ldots + x_n, \tag{9}$$
$$b_2 = \sum_{i\leq j} x_i x_j, \tag{10}$$
$$\vdots$$

Obviously the b_ℓ are symmetric polynomials, sometimes called complete symmetric polynomials (our "b" refers to "bosons"). Also the sequence $(b_0, \ldots, b_n)$ forms a basis in the ring of all symmetric polynomials in n variables, as we will see below. For example, if $n = 2$,

$$x_1^2 + x_2^2 = 2(x_1^2 + x_2^2 + x_2 x_2) - (x_1 + x_2)^2 = 2b_2 - b_1^2. \tag{11}$$

Another basis is given by the power sums

$$s_\ell = \sum_{i=1}^{n} x_i^\ell, \quad \ell = 0, \ldots, n. \tag{12}$$

($s_0 = n$ has to be redefined in the case $n = \infty$.) In order to prove that $(s_0, \ldots, s_n)$ forms a basis, it would suffice to show that every elementary symmetric polynomial f_m could be expressed as a polynomial of the s_ℓ. This, in turn, follows immediately from the Newton identities, as they are called in Ref. [22],

$$m f_m = \sum_{k=0}^{m-1} (-1)^{k+1} f_k s_{m-k}, \quad 1 \le m \le n. \tag{13}$$

These identities could be viewed as recursion relations for the f_m. Iterative substitution then yields the f_m solely in terms of the s_ℓ, for example

$$f_3 = \frac{1}{6}(s_1^3 - 3 s_1 s_2 + 2 s_3). \tag{14}$$

Explicit formulae for these representations will be given below.

Now consider the case of the b_m. Here we have analogous identities which immediately imply that $(b_0, \ldots, b_n)$ will form a basis:

$$\sum_{k=0}^{m} (-1)^k f_k b_{m-k} = 0, \quad 1 \le m \le n. \tag{15}$$

These identities can most compactly be written in terms of the generating functions

$$F(z) = \sum_{r=0}^{\infty} f_r z^r = \prod_{\ell=1}^{\infty} (1 + x_\ell z), \tag{16}$$

$$B(z) = \sum_{r=0}^{\infty} b_r z^r = \prod_{\ell=1}^{\infty} (1 - x_\ell z)^{-1} \tag{17}$$

as

$$B(z) F(-z) = 1. \tag{18}$$

Finally we give the explicit representations of the f_m and b_m in terms of the power sums s_ℓ, as well as the representations of the f_m in terms of the b_k and vice versa. To write these representations in compact form, it is convenient to use partitions. A partition λ of a positive integer N, written as $\lambda \vdash N$, is a way to write N as a sum, irrespective of order, in other words, a non-increasing sequence of positive integers $(\lambda_1, \lambda_2, \ldots, \lambda_p)$ such that $\sum_{i=1}^{p} \lambda_i = N$. $\ell(\lambda) \equiv p$ is called the length of a partition. Another notation for λ is $(1^{m_1} 2^{m_2} \ldots)$ where m_i counts the occurence of the integer i in

the partition $(\lambda_1, \lambda_2, \ldots, \lambda_p)$. Further let $\zeta(\lambda) \equiv (\prod_{i=1}^{p} i^{m_i} m_i!)^{-1}$ and $\mu(m)$ denote the multinomial coefficient

$$\mu(m) \equiv \frac{(\sum_i m_i)!}{\prod_i m_i!}. \tag{19}$$

Products of special symmetric polynomials introduced above according to a partition λ will be written with a subscript λ, for example,

$$f_\lambda \equiv \prod_{\ell=1}^{p} f_{\lambda_\ell}. \tag{20}$$

Then

$$\left.\begin{array}{c} b_N \\ f_N \end{array}\right\} = \sum_{\lambda \vdash N} (\pm 1)^{N+\ell(\lambda)} \zeta(\lambda) s_\lambda, \tag{21}$$

where the +sign refers to the b's and the $-$sign to the f's, and

$$\left.\begin{array}{c} b_N \\ f_N \end{array}\right\} = \sum_{\lambda \vdash N} (-1)^{N+\ell(\lambda)} \mu(m) \left\{\begin{array}{c} f_\lambda \\ b_\lambda \end{array}\right. . \tag{22}$$

Note the symmetry of the transformations $f \to b$ and $b \to f$. This is a consequence of the invariance of the identities (15) with respect to the interchange $b \leftrightarrow f$ and of $b_0 = f_0 = 1$. Note that (22), according to (17), is essentially equivalent to a well-known explicit expansion formula for the reciprocal value of a power series. These and other explicit relations between special symmetric polynomials are often also written in terms of determinants, see [23].

4. Partition functions

The canonical partition function plays a fundamental role in statistical mechanics since most thermodynamic functions can be derived from it. It is defined by

$$Z(\beta) \equiv \mathrm{Tr} \exp(-\beta H), \tag{23}$$

where H denotes the Hamiltonian of the system. Sometimes one writes $Z_N(\beta)$ in order to stress the dependance on the number N of particles in the system. The grand canonical partition function is defined by

$$\mathcal{Z}(z, \beta) \equiv \sum_{N=0}^{\infty} Z_N(\beta) z^N, \tag{24}$$

where the variable z is physically interpreted as the fugacity of the system.

Here we will only consider ideal gases, i. e. the case where H is the sum of N (identical) single-particle Hamiltonians

$$H = \sum_{n=1}^{N} h_n, \tag{25}$$

for example, N fermions in a common potential or mean field.

Let E_ℓ denote the energy eigenvalues of h_n, counted in such a way that several E_ℓ have the same value in case of degeneracy. Then the bosonic(+) or fermionic(−) partition functions depend only on the E_ℓ and can be written as

$$Z_N^-(\beta) = \sum_{i_1<i_2<\ldots<i_N} \exp(-\beta \sum_{\ell=1}^{N} E_{i_\ell}) \tag{26}$$

or

$$Z_N^+(\beta) = \sum_{i_1\le i_2\le\ldots\le i_N} \exp(-\beta \sum_{\ell=1}^{N} E_{i_\ell}). \tag{27}$$

Let us consider for the moment only systems with a finite number of energy eigenvalues $E_1, \ldots, E_n$. Expanding the exponentials in (26),(27) into products and introducing the abbreviations

$$x_\ell = \exp(-\beta E_\ell), \quad \ell = 1, \ldots, n, \tag{28}$$

it is easy to see, c. f. section 2, that

$$Z_N^- = f_N(x_1, \ldots, x_n), \tag{29}$$

and

$$Z_N^+ = b_N(x_1, \ldots, x_n). \tag{30}$$

Hence the fermionic/bosonic partitions functions for particular systems are obtained if the corresponding symmetric polynomials f_N/b_N are evaluated at the values (28), where only β is left variable. The grand canonical partition functions obviously correspond to the generating functions of special symmetric polynomials introduced in (16). It is then obvious that suitable relations between symmetric polynomials can be translated into relations between partition functions which are independent of the particular physical system, e. g. of the common potential or the dimension of the physical space, as long as the systems are ideal gases.

For systems with infinite-dimensional Hilbert spaces, i. e. $n = \infty$, the polynomials degenerate into formal power series. Evaluation at the values (28) leads to partition functions only if these series converge. But then the translation of combinatorical results into physical ones is still possible.

Having identified the physical interpretation of the f's and the b's it remains to investigate the power sums s_j. Since $x_\ell^j = \exp(-j\beta E_\ell)$ we conclude

$$s_j(e^{-\beta E_1}, \ldots, e^{-\beta E_\ell}, \ldots) = Z_1^\pm(j\beta). \tag{31}$$

Note that $Z_1^+ = Z_1^-$.

Now we can interprete all results mentioned in the last section as relations between the physical partition functions. We will not reproduce these relations anew but say a few words on each. The Newton identities (13) are viewed as recursion relations for partition functions which allow the explicit calculation of $Z_N^\pm(\beta)$ if $Z_1(\beta)$ is known for all β. In this context they appear for the first time in the textbook of P. Landsberg [21]. Later they have been re-discovered and applied recently to systems of few quantum

particles, see e.g. [19, 20, 24, 25, 9]. An explicit representation equivalent to (21) appears within a physical context in [9] and [4]. Equations (15) and (22) express relations between bosonic and fermionic partition functions which have, to our knowledge, not yet been considered in the physical literature. Note, however, that the identity (18) can be rewritten as

$$\mathcal{Z}^+(z,\beta)\mathcal{Z}^-(-z,\beta) = 1, \tag{32}$$

which obviously follows from the product representations and is implicitely contained in the above-mentioned articles based on a "unified treatment" of Fermi and Bose statistical mechanics of ideal gases [1, 2, 3]. We remark that (32) implies $Z_1^+ = Z_1^-$ which is closely related to the fact that in the classical limit (i. e. $z \to 0$) the distinction between Fermi and Bose gases disappears. Further we note that from the product representation (16,17) and (18) one immediately derives the well-known fact that $\mathcal{Z}^-$ has zeros at $z_\ell = -\exp(\beta E_\ell)$ and no poles, and hence $\mathcal{Z}^+$ has poles at $z_\ell = \exp(\beta E_\ell)$ and no zeros. Poles and zeros lie outside the physical domain of $z \in (0,\infty)$ for fermions and $z \in (0,1)$ for bosons.

5. Concluding remarks

In this article we have suggested a new way of looking at the partition functions of ideal quantum gases. The construction of these functions is split into two steps. In the first step we consider a finite or infinite set of abstract energy levels as symbolic variables and define certain symmetric polynomials (or formal power series) in these variables: the b_N for bosons and the f_N for fermions. The symmetry involved is a symmetry between energy levels, not between particles. It is due to the fact that for non-interacting particles all possible occupations of the energy levels are counted on an equal footing. This first step is the same for each physical system.

The second step consists in an evaluation of the symmetric polynomials b_N and f_N at the values $e^{-\beta E_\ell}$ for the variable x_ℓ. Only within this step the numerical energy values of the concrete physical systems, their degeneracies et cetera enter into the expression for the partition functions. Now the different possible occupations of the energy levels contribute to the partition function with different weights. The mentioned physically relevant combinatorical results are independent from the second step and hold for all considered systems.

Finally we would like to mention that the wording "partition function" is due to Darwin and Fowler [26] and is obviously connected to the "partition" of energy into the energy levels of a system. Thus the combinatorical element was present from the outset, although the connection to the combinatorical partitions occuring in the explicit formulae of section 3 seems to be novel.

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References

[1] M. H. Lee, *Polylogarithmic analysis of chemical-potential and fluctuations in a d-dimensional free Fermi gas at low temperatures*, J. Math. Phys. (N.Y.) **36**, 1217 (1995)
[2] M. H. Lee, *Equivalence of ideal gases in two dimensions and Landen's relations*, Phys. Rev. E **55**, 1518 (1997)
[3] M. H. Lee, *Polylogarithms and Riemann's ζ function*, Phys. Rev. E **56**, 3909 (1997)
[4] H.-J. Schmidt, J. Schnack, *Thermodynamic fermion-boson symmetry in harmonic oscillator potentials*, Physica A **265**, 584 (1999)
[5] P. Ring, P. Schuck, *The Nuclear Many-Body Problem*, Texts and monographs in physics, Springer (1980)
[6] S. Tomonaga, *Remark on Bloch's method of sound waves applied to many fermion problems*, Prog. Theor. Phys. **5**, 544 (1950)
[7] J. Luttinger, *An exactly soluble model of a many-fermion system*, J. Math. Phys. **4**, 1154 (1963)
[8] K. Schönhammer, V. Meden, *Fermion-boson transmutation and comparison of statistical ensembles in one dimension*, Am. J. Phys. **64**, 1168 (1996)
[9] H.-J. Schmidt, J. Schnack, *Investigations on finite ideal quantum gases*, Physica A **260**, 479 (1998)
[10] M. Crescimanno, A. S. Landsberg, *Spectral equivalence of bosons and fermions in one-dimensional harmonic potentials*, Phys. Rev. A. **63**, 035601 (2001)
[11] M. Anderson, J. Ensher, M. Matthews, C. Wieman, E. Cornell, *Observation of Bose-Einstein condensation in a dilute atomic vapour*, Science **269**, 198 (1995)
[12] K. Davis, M.-O. Mewes, M. Andrews, N. van Druten, D. Durfee, D. Kurn, W. Ketterle, *Bose-Einstein condensation of a gas of sodium atoms*, Phys. Rev. Lett. **75**, 3969 (1995)
[13] W. Ketterle, N. van Druten, *Bose-Einstein condensation of a finite number of particles trapped in one or three dimensions*, Phys. Rev. A **54**, 656 (1996)
[14] C. Bradley, C. Sackett, R. Hulet, *Bose-Einstein condensation of Lithium: Observation of limited condensate number*, Phys. Rev. Lett. **78**, 985 (1997)
[15] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, S. Stringari, *Theory of Bose-Einstein condensation in trapped gases*, Rev. Mod. Phys. **71**, 463 (1999)
[16] Y. Alhassid, *The statistical theory of quantum dots*, Rev. Mod. Phys. **72**, 895 (2000)
[17] J. Arnaud, L. Chusseau, F. Philippe, *Fluorescence from a few electrons*, Phys. Rev. B **62**, 13482 (2000)
[18] P. T. Landsberg, P. Harshman, *Canonical versus Grand Canonical Occupation Numbers for Simple Systems*, J. Stat. Phys. **53**, 475 (1988)
[19] P. Borrmann, G. Franke, *Recursion formulas for quantum statistical partition functions*, J. Chem. Phys. **98**, 2484 (1993)
[20] F. Brosens, L. Lemmens, J. T. Devreese, *Thermodynamics of coupled identical oscillators within the path integral formalism*, Phys. Rev. E **55**, 227 (1997)
[21] P. T. Landsberg, *Thermodynamics with quantum statistical illustrations*, Interscience Publishers, New York, London (1961)
[22] D. Cox, J. Little, D. O'Shea, *Ideals, Varieties, and Algorithms*, Springer (1992)
[23] I. G. Macdonald, *Symmetric Functions and Hall Polynomials*, Clarendon Press (1979)
[24] S. Grossmann, M. Holthaus, *Fluctuations of the particle number in a trapped Bose-Einstein condensate*, Phys. Rev. Lett. **79**, 3557 (1997)

[25] M. Wilkens, C. Weiss, *Particle number fluctuations in an ideal Bose gas*, J. Mod. Opt. **44**, 1801 (1997)

[26] C. G. Darwin, R. H. Fowler, *On the partition of enery*, Phil. Mag. **44**, 450 (1922)