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Partition functions and graphs: A combinatorial approach

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Although symmetry methods and analysis are a necessary ingredient in every physicist's toolkit, rather less use has been made of combinatorial methods. One exception is in the realm of Statistical Physics, where the calculation of the partition function, for example, is essentially a combinatorial problem. In this talk we shall show that one approach is via the normal ordering of the second quantized operators appearing in the partition function. This in turn leads to a combinatorial graphical description, giving essentially Feynman-type graphs associated with the theory. We illustrate this methodology by the explicit calculation of two model examples, the free boson gas and a superfluid boson model. We show how the calculation of partition functions can be facilitated by knowledge of the combinatorics of the boson normal ordering problem; this naturally gives rise to the *Bell* numbers of combinatorics. The associated graphical representation of these numbers gives a perturbation expansion in terms of a sequence of graphs analogous to zero-dimensional Feynman diagrams.

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1 Introduction

According to the axiomatic approach, it is possible to reconstruct a quantum field theory from the vacuum expectation values. When we *normally order* a set of operators so that all the annihilation operators are to the right, then in such a vacuum expectation value only the constant term remains.¹⁾ Similarly, when we normally order a string of boson operators a, a^\dagger satisfying $[a, a^\dagger] = 1$, then the vacuum expectation reduces to the constant term; and likewise we may recover the expectation in the coherent state $|z\rangle$ by replacing a by the c -number z . Therefore the ability to normally order a string of operators is a powerful calculational tool in physics. It was recognized early on that the procedure of normally ordering a string of bosons leads to classical combinatorial numbers, the Stirling and Bell numbers [1]. Apart from the generation of interesting combinatorial sequences, and their extensions [2], the associated graph theory representations of these numbers have analogies to the Feynman diagrams of a zero-dimensional quantum field theory.

In this note we shall present a standard graphical representation of the Bell numbers which we show is in some sense *generic*. That is, we use these graphs to provide a representation of a perturbation expansion for the partition function of a free boson gas, and show that the same sequence of graphs can be used to give a perturbation expansion for a general partition function.

We illustrate this approach by applying it to a superfluid boson system.

2 Combinatorial sequences, generating functions and graphs

2.1 Some combinatorial sequences

Sequences of numbers of combinatorial interest are common in mathematics; for example, some sequences depending on one parameter are

1. $\{n\}$ The integers.
2. $\{n!\}$ The number of ways of putting n different objects into n different containers (leaving none empty).
3. $\{2^n\}$ The number of maps from an n -element set to $\{0, 1\}$.
4. $\{B(n)\}$ The Bell numbers; the number of ways of putting n different objects into n identical containers (some may be left empty).

These are all familiar except perhaps the last, the Bell numbers. These have the values

$$B(n) = 1, 2, 5, 15, 52, 203, \dots, \quad n = 1, 2, \dots$$

and $B(n) \leq n!$.

¹⁾ Note that this process of normally ordering, denoted by \mathcal{N} , does *not* change the value of the operator. Thus $\mathcal{N}(f(a, a^\dagger)) = f(a, a^\dagger)$.

We may also define sequences which depend on, say, two parameters, for example the 'choose' symbols ${}^n C_k \equiv \frac{n!}{(n-k)! k!}$. Related to the Bell numbers are the *Stirling numbers of the second kind* $S(n, k)$, which are defined as the number of ways of putting n different objects into k identical containers, leaving none empty. From the definition we have

$$B(n) = \sum_{k=1}^n S(n, k). \quad (1)$$

2.2 Normal order

Although somewhat unfamiliar to physicists, the Bell and Stirling numbers are fundamental in quantum theory. This is because they arise naturally in the *normal ordering problem*. For canonical bosons $[a, a^\dagger] = 1$ the Stirling numbers of the second kind $S(n, k)$ intervene through [3]

$$(a^\dagger a)^n = \sum_{k=1}^n S(n, k) (a^\dagger)^k a^k. \quad (2)$$

The corresponding Bell numbers $B(n) = \sum_{k=1}^n S(n, k)$ are simply the expectation values

$$B(n) = \langle z | (a^\dagger a)^n | z \rangle_{z=1} \quad (3)$$

taken in the coherent state defined by

$$a|z\rangle = z|z\rangle \quad (4)$$

for $z = 1$. In fact, for physicists, these equations may be taken as the *definitions* of the Stirling and Bell numbers.

2.3 Generating functions

Corresponding to a sequence of combinatorial numbers $\{a_n\}$ we may define the *exponential generating function (egf)*

$$A(x) = \sum_{n=0}^{\infty} a_n \frac{x^n}{n!}. \quad (5)$$

This provides a compact formula for the combinatorial sequence. For example for the sequences above

1. $a_n = n, \quad A(x) = xe^x,$
2. $a_n = n!, \quad A(x) = 1/(1-x),$
3. $a_n = 2^n, \quad A(x) = e^{2x},$

4. $a_n = B(n)$, $A(x) = \exp(e^x - 1)$.

Except for the last, which we shall prove in what follows, these exponential generating functions are immediate. Note that we consider the expansion in a *formal* sense; we are not concerned here about the convergence of the series defined by the egf's. We may similarly define egf's corresponding to 2-parameter sequences, thus:

$$A(x, y) = \sum_{n=0}^{\infty} \left(\sum_{k=0}^{\infty} a_{n,k} y^k \right) \frac{x^n}{n!}. \tag{6}$$

For the 2-parameter sequences above we obtain:

1. $a_{n,k} \equiv {}^n C_k$, $A(x, y) = \exp((1 + y)x)$,
2. $a_{n,k} \equiv S(n, k)$, $A(x, y) = \exp(y(e^x - 1))$.

In the latter function, the coefficient of the n -th power of x is an n -degree polynomial in y , a Bell polynomial, $B_n(y)$.

Therefore we have the generating function for the Bell numbers and Bell polynomials

$$\begin{aligned} A_B(x) &= \sum_{n=0}^{\infty} B(n) \frac{x^n}{n!} = \\ &= \exp\left(x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots\right) \end{aligned} \tag{7}$$

and

$$\begin{aligned} A_B(x, y) &= \sum_{n=0}^{\infty} \left(\sum_{k=0}^{\infty} S(n, k) y^k \right) \frac{x^n}{n!} = \\ &= \sum_{n=0}^{\infty} B_n(y) \frac{x^n}{n!} = \\ &= \exp(y(e^x - 1)). \end{aligned} \tag{8}$$

2.4 Graphs

We now give a graphical representation of the Bell numbers. Consider labelled lines which emanate from a white dot, the origin, and finish on a black dot, the vertex. We shall allow only one line from each white dot but impose no limit on the number of lines ending on a black dot. Clearly this simulates the definition of $S(n, k)$ and $B(n)$, with the white dots playing the role of the distinguishable objects, whence the lines are labelled, and the black dots that of the indistinguishable containers. The identification of the graphs for 1,2 and 3 lines is given in the Figure 1.

We have concentrated on the Bell number sequence and its associated graphs since, as we shall show, there is a sense in which this sequence of graphs is *generic*.

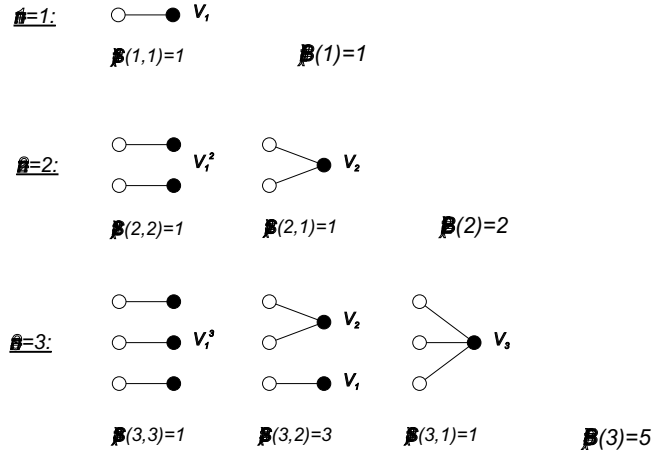


Fig. 1. Graphs for $B(n)$, $n = 1, 2, 3$.

That is, we can represent *any* combinatorial sequence by the same sequence of graphs as in the Figure 1, with suitable vertex multipliers (denoted by the V terms in the same figure). One reason the graphical representation is useful is that there exist some rather powerful results which apply to graphs and their associated generating functions. We give one such result now.

2.5 Connected graph theorem

This states that if $C(x) = \sum_{n=1}^{\infty} c(n)x^n/n!$ is the exponential generating function of *labelled connected* graphs, *viz.* $c(n)$ counts the number of connected graphs of order n , that is with n lines, then

$$A(x) = \exp(C(x)) \quad (9)$$

is the exponential generating function for *all* graphs [4].

We may apply this very simply to the case of the $B(n)$ graphs in Figure 1. For each order n , the *connected* graphs clearly consist of a single graph. Therefore for each n we have $c(n) = 1$; whence, $C(x) = \exp(x) - 1$. It follows that the generating function for *all* the graphs $A(x)$ is given by

$$A(x) = \exp(\exp(x) - 1), \quad (10)$$

which is therefore the generating function for the Bell numbers.

Given a general generating function $C(x) = \sum_{n=1}^{\infty} V_n x^n/n!$ we may represent this by the same sequence of graphs as in Figure 1, but now with vertex factors $V_n = c(n)$, as shown in Figure 1.

This is of course a trivial observation, since any sequence of graphs each term of which consists of a single connected graph will, with the appropriate multipliers V_n ,

give by definition the exponential generating function of many combinatorial sequences. This however shows the generic nature of the $B(n)$ sequence, as previously noted in [5]; and will prove of value in our discussion of partition functions.

3 Partition functions

We first illustrate the use of normal ordering in the context of *partition functions* by the most simple example. We define as usual the partition function Z associated with a Hamiltonian H by $Z \equiv \text{Tr} \exp(-\beta H)$.

3.1 Free boson gas and Bell polynomials

We take as our example the Hamiltonian for the single-mode free boson gas $H = \epsilon a^\dagger a$ (ignoring an additive constant), $\epsilon > 0$. The usual computation of the partition function, exploiting the completeness property $\sum_{n=0}^{\infty} |n\rangle\langle n| = I$, is immediate:

$$Z = \text{Tr} \exp(-\beta \epsilon a^\dagger a) = \quad (11)$$

$$= \sum_{n=0}^{\infty} \langle n | e^{-\beta \epsilon \hat{n}} | n \rangle = \quad (12)$$

$$= \sum_{n=0}^{\infty} e^{-\beta \epsilon n} = \quad (13)$$

$$= (1 - e^{-\beta \epsilon})^{-1}. \quad (14)$$

However, we may, somewhat perversely in this simple case, use *any* complete set to perform the trace. Choosing coherent states, for which the completeness or *resolution of unity* property is

$$\frac{1}{\pi} \int d^2 z |z\rangle\langle z| = I \equiv \int d\mu(z) |z\rangle\langle z| \quad (15)$$

the appropriate trace calculation is

$$Z = \frac{1}{\pi} \int d^2 z \langle z | \exp(-\beta \epsilon a^\dagger a) | z \rangle = \quad (16)$$

$$= \frac{1}{\pi} \int d^2 z \langle z | : \exp(a^\dagger a (e^{-\beta \epsilon} - 1)) : | z \rangle, \quad (17)$$

where we have used the following well-known relation [6, 7] for the *forgetful* normal ordering operator $: f(a, a^\dagger) :$ which means “normally order the creation and annihilation operators in f forgetting the commutation relation $[a, a^\dagger] = 1$ ”²):

$$\mathcal{N}(\exp(x a^\dagger a)) =: \exp(a^\dagger a (e^x - 1)) :. \quad (18)$$

²) Of course, this procedure may alter the value of the operator to which it is applied.

We therefore obtain, integrating over the angle variable θ and the radial variable $r = |z|$,

$$Z = \frac{1}{\pi} \int_0^{2\pi} d\theta \int_0^\infty r dr \exp(r^2(e^{-\beta\epsilon} - 1)), \quad (19)$$

which gives us $Z = (1 - e^{-\beta\epsilon})^{-1}$ as before.

We rewrite the above equation to show the connection with our previously-defined combinatorial numbers. Writing $y = r^2$ and $x = -\beta\epsilon$, Eq.(19) becomes

$$Z = \int_0^\infty dy \exp(y(e^x - 1)). \quad (20)$$

This is an integral over the classical generating function for the Bell polynomials

$$\exp(y(e^x - 1)) = \sum_{n=0}^\infty B_n(y) \frac{x^n}{n!}, \quad (21)$$

where $B_n(1) = B(n)$, as defined in Eq.(3). This leads to the combinatorial form for the partition function

$$Z = \int_0^\infty dy \sum_{n=0}^\infty B_n(y) \frac{x^n}{n!}. \quad (22)$$

Although Eq.(22) is remarkably simple in form, it is often by no means a straightforward matter to evaluate the analogous integral for other than the free boson system considered here. Further, it is also clear that we may not interchange the integral and the summation, as each individual y integral diverges. We shall therefore concentrate in what follows on the *partition function integrand* (PFI) $F(z) = \langle z | \exp(-\beta H) | z \rangle$, whence $Z = \int F(z) d\mu(z)$, to give a graphical description of a perturbation approach. The function F maps coherent states $|z\rangle$ to (real) numbers, and is related to, but not identical with, the previously-introduced *free energy functional* [8] associated with the Hamiltonian system.

3.2 General partition functions

We now apply this graphical approach to the general partition function in second quantized form. With the usual definition for the partition function

$$Z = \text{Tr} \exp(-\beta H). \quad (23)$$

In general the Hamiltonian is given by $H = \epsilon w(a, a^\dagger)$, where ϵ is the energy scale, and w is a string (= sum of products of positive powers) of boson creation and annihilation operators. The partition function integrand F for which we seek to give a graphical expansion, is

$$Z(x) = \int F(x, z) d\mu(z), \quad (24)$$

where

$$\begin{aligned}
 F(x, z) &= \langle z | \exp(xw) | z \rangle = && (x = -\beta\epsilon) \\
 &= \sum_{n=0}^{\infty} \langle z | w^n | z \rangle \frac{x^n}{n!} = \\
 &= \sum_{n=0}^{\infty} W_n(z) \frac{x^n}{n!} = \\
 &= \exp\left(\sum_{n=1}^{\infty} V_n(z) \frac{x^n}{n!}\right), \tag{25}
 \end{aligned}$$

with obvious definitions of W_n and V_n . The sequences $\{W_n\}$ and $\{V_n\}$ may each be recursively obtained from the other [9]. This relates the sequence of multipliers $\{V_n\}$ of Figure 1 to the Hamiltonian of Eq.(23). The lower limit 1 in the V_n summation is a consequence of the normalization of the coherent state $|z\rangle$.

We conclude this discussion with an example.

3.3 Superfluid boson system

We may write the Hamiltonian for a superfluid boson system as [10]

$$H = \epsilon \left\{ \frac{1}{2} c_1 a^2 + \frac{1}{2} \bar{c}_1 (a^\dagger)^2 + c_2 (a^\dagger a + \frac{1}{2}) \right\}. \tag{26}$$

As in the non-interacting boson gas example, this represents a single mode of the system; the complete Hamiltonian is a direct sum of non-interacting terms. The constants c_1 and c_2 are complex and real respectively, but otherwise arbitrary. Noting that the Hamiltonian Eq.(26) is an element of the non-compact Lie algebra $su(1,1)$ enables an expression for the partition function integrand to be readily obtained (see the Appendix). To illustrate the graphical series for this PFI, we shall choose real arguments; that is we put z and the constant c_1 real in Eq.(33) below to get

$$F(x, y) = \sqrt{\frac{1}{\mu}} \exp \left[y \left(y_1 + \frac{1}{\mu} - 1 \right) \right], \tag{27}$$

where $y = z^2$ and y_1, μ are functions of x . The PFI $F(x, y)$ of Eq.(27) generates an integer sequence for even c_1, c_2 as may be easily verified using algebraic software. For example, choosing $c_1 = 2, c_2 = 4$ we have

$$F(x, y) = \exp \left(\frac{V_1(y)x}{1!} + \frac{V_2(y)x^2}{2!} + \frac{V_3(y)x^3}{3!} + \dots \right), \tag{28}$$

with

$$\begin{aligned}
 V_1(y) &= 2 + 6y, \\
 V_2(y) &= 2 + 36y, \\
 V_3(y) &= 16 + 288y, \\
 V_4(y) &= 144 + 3024y, \\
 &\dots
 \end{aligned} \tag{29}$$

leading to a corresponding Bell-type graphical expansion.

4 Discussion

The normal ordering of creation and annihilation operators leads naturally to Stirling and Bell numbers. Therefore these combinatorial numbers, and their graphical representations, are ubiquitous in second-quantized quantum physics. In this talk we emphasized this fact by application to a perturbative expansion for the partition function of statistical physics. We did this through the introduction of the *partition function integrand* or PFI, a function which when integrated over the complete set of coherent states gives the partition function proper. The evaluation of the PFI depends on the normal ordering of the the exponentiated hamiltonian given in terms of second-quantized operators. In general this is a difficult if not intractable problem, although approaches based on the *Product Theorem* of combinatorial graph theory lead to some simplification³). However, even with the straightforward methods illustrated here, solutions are obtainable in many cases of physical interest. In particular, we illustrated this approach in the case of the free boson gas, and a superfluid boson model. We also gave a graphical representation for the perturbation expansion of the PFI, an expansion in terms of $x = -\beta\epsilon$, essentially energy scale times inverse temperature. The graphical series is that of the Bell numbers, together with appropriate multipliers $V_n(z)$, where z is the coherent state parameter which must be integrated over to obtain the partition function. We showed how to determine these multipliers in terms of the Hamiltonian. We conclude that there is a sense in which the Bell graph series is generic for the evaluation of PFI's.

The operators of this theory are quantized, but have no explicit dependence on space or time, which justifies considering the theory as a zero-dimensional field theory, with the graphs as being analogous to zero-dimensional Feynman diagrams.

Appendix: Partition function integrand for a superfluid boson system

The partition function integrand $F(x, z)$ corresponding to the hamiltonian Eq.(26) is the expectation of the following operator

$$\begin{aligned} \exp(-\beta H) &= \exp\left\{\frac{1}{2}xc_1a^2 + \frac{1}{2}x\bar{c}_1(a^\dagger)^2 + xc_2(a^\dagger a + \frac{1}{2})\right\} = \\ &= \exp\left\{\frac{1}{2}x_1a^2 + \frac{1}{2}\bar{x}_1(a^\dagger)^2 + x_2(a^\dagger a + \frac{1}{2})\right\} = \left(\text{for } \begin{array}{l} x_1 = xc_1, \\ x_2 = xc_2, \end{array}\right) \\ &= \exp\{x_1K^- + \bar{x}_1K^+ + 2x_2K^0\}, \end{aligned} \tag{30}$$

where we have identified the generators $\{K^+, K^-, K^0\}$ of $su(1, 1)$ with the appropriate operators $\{\frac{1}{2}(a^\dagger)^2, \frac{1}{2}a^2, \frac{1}{2}(a^\dagger a + \frac{1}{2})\}$. The normally ordered form of Eq.(30) is

$$\exp(-\beta H) = e^{\bar{y}_1K^+} e^{2y_2K^0} e^{y_1K^-}. \tag{31}$$

³) See the talk by A. Horzela *et al* in this conference.

Since the equality of Eq.(30) and Eq.(31) is a group-theoretical result, we may use the 2×2 representation

$$\{K^+, K^-, K^0\} = \left\{ \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \right\}, \quad (32)$$

in which to implement the equality, thus evaluating y_1 and y_2 . The result is

$$y_1 = xc_1 \sinh \left(\frac{\delta}{\mu\delta} \right), \quad y_2 = -\ln \mu,$$

where

$$\delta = x\sqrt{c_2^2 - |c_1|^2}, \quad \mu = \cosh \delta - xc_2 \frac{\sinh \delta}{\delta}.$$

We therefore have for the Partition Function Integrand

$$\begin{aligned} F(x, z) &= \langle z | \exp \left\{ \frac{1}{2} x_1 a^2 + \frac{1}{2} \bar{x}_1 (a^\dagger)^2 + x_2 (a^\dagger a + \frac{1}{2}) \right\} | z \rangle = \\ &= \langle z | e^{\bar{y}_1 (a^\dagger)^2 / 2} e^{y_2 (a^\dagger a + 1/2)} e^{y_1 a^2 / 2} | z \rangle = \\ &= e^{\frac{1}{2} \bar{y}_1 z^2} e^{|z|^2 (e^{y_2} - 1)} e^{y_1 z^2 / 2} e^{\frac{1}{2} y_2}. \end{aligned} \quad (33)$$

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