Combinatorics and Boson normal ordering: A gentle introduction

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We discuss a general combinatorial framework for operator ordering problems by applying it to the normal ordering of the powers and exponential of the boson number operator. The solution of the problem is given in terms of Bell and Stirling numbers enumerating partitions of a set. This framework reveals several inherent relations between ordering problems and combinatorial objects, and displays the analytical background to Wick's theorem. The methodology can be straightforwardly generalized from the simple example given herein to a wide class of operators.

I. INTRODUCTION

Hilbert space constitutes the arena where quantum phenomena can be described. One common realization is Fock space, which is generated by the set of orthonormal vectors $|n\rangle$ representing states with a specified numbers of particles or objects. A particular role in this description is played by the creation $a^\dagger$ and annihilation a operators representing the process of increasing and decreasing the number of particles in a system, respectively. We consider operators that satisfy the boson commutation relation $[a, a^\dagger] = 1$ describing objects obeying Bose-Einstein statistics, for example, photons or phonons. The fact that the operators a and $a^\dagger$ do not commute is probably the most prominent characteristic of quantum theory, and makes it so strange and successful at the same time.[1,2]

In this paper we are concerned with the *ordering problem* which is one of the consequences of noncommutativity. This problem derives from the fact that the order in which the operators occur is relevant, for example, $a^\dagger a \neq aa^\dagger = a^\dagger a + 1$. The ordering problem plays an important role in the construction of quantum mechanical operators. The physical properties of differently ordered operators may be quite distinct, which we can see by considering their expectation values. An analysis of operator matrix elements reveals their physical properties observed as probabilities. There are two sets of states of primary interest in this context: number states $|n\rangle$ and coherent states $|z\rangle$. The latter, defined as eigenstates of the annihilation operator a, play an important role in quantum optics[3,4,5,6,7] and in the phase space formulation of quantum mechanics.[8]

The calculation of the number or coherent state expectation values reduces to transforming the original expression to the *normally ordered* form in which all annihilation operators are to the right. In this form the evaluation of the matrix elements is immediate. The procedure is called normal ordering.[4,5,6,7,8] Although the process is clear and straightforward, in practice it can be tedious and cumbersome when the expression is complicated, and is even less tractable when we consider operators defined by an infinite series expansion. It is thus desirable to find manageable formulas or guiding principles that lead to solutions of normal ordering problems.

In this paper we present a general framework that is applicable to a broad class of ordering problems. It exploits the fact that the coefficients emerging in the normal ordering procedure appear to be natural numbers which have their origin in combinatorial analysis. In the simplest case of powers or the exponential of the number operator $N = a^\dagger a$ these are Stirling and Bell numbers which enumerate partitions of a set.[9] We use this example to illustrate a systematic approach to the ordering problem. The general methodology is to identify the problem with combinatorial structures and then resolve it using this identification. The solution may be found with the help of the *Dobiński relation*,[10,11] which is a very effective tool and is straightforwardly applicable to a wide range of ordering problems.

As a byproduct of this methodology we obtain a surprising relation between combinatorial structures and operator ordering procedures. This relation is especially interesting because the objects involved in the problem can have clear combinatorial interpretations (for example, as partitions of a set). The expectation is that this remarkable interrelation will shed light on the ordering problem and clarify the meaning of the associated abstract operator expressions.

The framework we present is an example of a fertile interplay between algebra and combinatorics in the context of quantum mechanics. It employs only undergraduate algebra and is not as yet a standard feature of quantum mechanics textbooks.

The paper is organized as follows. Section II briefly recalls the concept of Fock space and introduces the normal

ordering problem. The main part containing the connection to combinatorics is given in Sec. III. It illustrates the methodology by discussing in detail the solution of a generic example. Some applications are provided in Sec. IV. In Sec. V we point out extensions of this approach and suggest further reading.

II. OCCUPATION NUMBER REPRESENTATION

A. States and operators

We consider a pair of one mode boson annihilation a and creation $a^\dagger$ operators satisfying the conventional boson commutation relation

$$[a, a^\dagger] = 1. \tag{1}$$

The operators $a, a^\dagger$, and 1 generate the Heisenberg algebra.

The occupation number representation arises from the interpretation of a and $a^\dagger$ as operators annihilating and creating a particle in a system. From this point of view the Hilbert space $\mathcal{H}$ of states is generated by the number states $|n\rangle$, where $n = 0, 1, 2, \dots$ counts the number of particles, or objects in general. The states are assumed to be orthonormal, $\langle m|n\rangle = \delta_{m,n}$, and constitute a basis in $\mathcal{H}$. This representation is usually called Fock space.

The operators a and $a^\dagger$ satisfying Eq. (1) may be realized in Fock space as

$$a\,|n\rangle = \sqrt{n}|n-1\rangle, \qquad a^\dagger\,|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{2}$$

The number operator N, which counts the number of particles in a system, is defined by

$$N|n\rangle = n|n\rangle, \tag{3}$$

and is represented as $N = a^\dagger a$. It satisfies the commutation relations

$$[a, N] = a, \qquad [a^\dagger, N] = -a^\dagger. \tag{4}$$

The algebra defined by Eqs. (1) and (4) describes objects obeying Bose-Einstein statistics, for example, photons or phonons. It is sometimes called the Heisenberg-Weyl algebra, and occupies a prominent role in quantum optics, condensed matter physics, and quantum field theory.

The second set of states of interest in Fock space are the coherent states $|z\rangle$. They are defined as the eigenstates of the annihilation operator

$$a|z\rangle = z|z\rangle, \tag{5}$$

where z is a complex number (the dual relation is $\langle z|a^\dagger = z^*\langle z|$). These states take the explicit form

$$|z\rangle = e^{-\frac{1}{2}|z|^2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} \, |n\rangle. \tag{6}$$

These states are normalized, $\langle z|z\rangle = 1$, but are not orthogonal and constitute an overcomplete basis in the Hilbert space.[12] Coherent states have many useful properties which are exploited in quantum optics and in other areas of physics.[3,4,5,6,7,8]

B. Normal ordering: Introduction

The noncommutativity of the creation and annihilation operators causes serious ambiguities in defining operator functions in quantum mechanics. To solve this problem the order of the operators has to be fixed. An important practical example of operator ordering is the normally ordered form in which all annihilation operators a stand to the right of the creation operators $a^\dagger$. We now define two procedures on boson expressions yielding a normally ordered form, namely, normal ordering and the double dot operation.[4,5,6,7,8]

By the normal ordering of a general expression $F(a^\dagger, a)$ we mean $F^{(n)}(a^\dagger, a)$ which is obtained by moving all the annihilation operators a to the right using the commutation relation of Eq. (1). This procedure yields an operator whose action is equivalent to the original one, that is, $F^{(n)}(a^\dagger, a) = F(a^\dagger, a)$ as operators, although the form of the expressions in terms of a and $a^\dagger$ may be completely different.

The double dot operation $:F(a^\dagger, a):$ consists of applying the same ordering procedure but without taking into account the commutation relation of Eq. (1), that is, moving all annihilation operators a to the right as if they commuted with the creation operators $a^\dagger$. This notation, although widely used, is not universal.[13] We observe that in general this procedure yields a different operator $F(a^\dagger, a) \neq :F(a^\dagger, a):$.[14]

In addition to the fact that these two procedures yield different results (except for operators that are already in normally ordered form), there is also a practical difference in their use. That is, although the application of the double dot operation is almost immediate, for the normal ordering procedure some algebraic manipulation of the non-commuting operators a and $a^\dagger$ is needed. Here is an example of both procedures in action:

$$aa^\dagger aaa^\dagger a \xrightarrow[{[a,a^\dagger]=1}]{\text{normal ordering}} \underbrace{(a^\dagger)^2 a^4 + 4\,a^\dagger a^3 + 2\,a^2}_{a^\dagger \text{ to the left}, \quad a \text{ to the right}}$$

$$aa^\dagger aaa^\dagger a \xrightarrow[\substack{a,\,a^\dagger \text{ commute} \\ \text{(like numbers)}}]{\text{double dot}} \overbrace{a^\dagger a^\dagger aaaa}\,.$$

In general we say that the normal ordering problem for $F(a^\dagger, a)$ is solved if we can find an operator $G(a^\dagger, a)$ for which the following equality is satisfied

$$F(a^\dagger, a) = :G(a^\dagger, a):\,. \tag{7}$$

The normally ordered form has the merit of enabling immediate calculation of an operator's coherent state ele-

ments which reduce, by virtue of Eq. (5), to substituting $a \to z$ and $a^\dagger \to z^*$ in its functional representation, that is,

$$\langle z|{:}G(a^\dagger,a){:}|z\rangle = G(z^*,z). \tag{8}$$

Thus, by solving the normal ordering problem of Eq. (7), we readily obtain

$$\langle z|F(a^\dagger,a)|z\rangle = G(z^*,z) . \tag{9}$$

This procedure may be illustrated in the example

$$\begin{aligned}\langle z|aa^\dagger aaa^\dagger a \,|z\rangle &= \langle z|(a^\dagger)^2 a^4 + 4a^\dagger a^3 + 2a^2|z\rangle\\ &= (z^*)^2 z^4 + 4\,z^* z^3 + 2\,z^2.\end{aligned}$$

In brief, we have shown that the calculation of coherent state matrix elements reduces to solving the normal ordering problem. The converse statement is also true; that is, if we know the coherent state expectation value of the operator, say Eq. (9), than the normally ordered form of the operator is given by Eq. (7).[4,5]

A standard approach to the normal ordering problem is to use Wick's theorem.[15] In our context, this theorem expresses the normal ordering of an operator by applying the double dot operation to the sum of all possible expressions obtained by removing pairs of annihilation and creation operators where a precedes $a^\dagger$, called contractions in analogy to quantum field theory, for example

$$aa^\dagger aaa^\dagger a = : \underbrace{aa^\dagger aaa^\dagger a}_{\text{no pair removed}} :$$

$$+ : \underbrace{\overbrace{aa}^{}{}^\dagger aaa^\dagger a + \overbrace{aa^\dagger aa}^{}{}^\dagger a + aa^\dagger \overbrace{aa}^{}{}^\dagger a + aa^\dagger a\overbrace{aa}^{}{}^\dagger a}_{\text{1 pair removed}} :$$

$$+ : \underbrace{\overbrace{aa}^{}{}^\dagger \overbrace{aa}^{}{}^\dagger a + \overbrace{aa}^{}{}^\dagger a\overbrace{aa}^{}{}^\dagger a}_{\text{2 pairs removed}} : = (a^\dagger)^2 a^4 + 4\ a^\dagger a^3 + 2\ a^2.$$

This procedure may involve a large number of steps. For polynomial expressions this difficulty may be overcome by using computer algebra, although this use does not provide an analytic structure. For nontrivial functions, such as those having infinite expansions, the problem still remains open.

One approach to the problem relies on the disentangling properties of Lie algebraic operators and application of the Baker-Campbell-Hausdorff formula. Here is a standard example:

$$e^{\lambda(a+a^\dagger)} = e^{\lambda^2/2} :e^{\lambda(a+a^\dagger)}: . \tag{10}$$

However, the use of this kind of disentangling property of the exponential operators is restricted in practice to quadratic expressions in boson operators.[16]

Another method exploits the recurrence relations and solves the normal ordering problem by use of combinatorial identities.[9,17] This promising approach was the inspiration for the systematic combinatorial methodology which is presented in this article.

III. GENERIC EXAMPLE: STIRLING AND BELL NUMBERS

A. Normal ordering: Combinatorial setting

We consider the number operator $N = a^\dagger a$ and seek the normally ordered form of its nth power ($n \geq 1$). We write the latter as

$$\left(a^\dagger a\right)^n = \sum_{k=1}^{n} S(n,k)\,(a^\dagger)^k a^k, \tag{11}$$

which uniquely defines the integer sequences $S(n,k)$ for $k = 1 \ldots n$; these sequences are called the *Stirling numbers*.[11,18] Information about this sequence for each n may be captured in the *Bell polynomials*

$$B(n,x) = \sum_{k=1}^{n} S(n,k)\,x^k. \tag{12}$$

We also define the *Bell numbers* $B(n) = B(n,1)$ as

$$B(n) = \sum_{k=1}^{n} S(n,k). \tag{13}$$

Instead of operators a and $a^\dagger$ we may equally well insert into Eq. (11) the representation of Eq. (1) given by the operator X defined as multiplication by x, and by the derivative $D = \frac{d}{dx}$[19]

$$a^\dagger \longleftrightarrow X, \qquad a \longleftrightarrow D. \tag{14}$$

This substitution does not affect the commutator of Eq. (1), that is, $[D,X] = 1$, which is the only property relevant for the construction. Therefore in this representation Eq. (11) takes the form

$$(XD)^n = \sum_{k=1}^{n} S(n,k)\,X^k D^k. \tag{15}$$

B. Combinatorial analysis

In the following we discuss the properties of the Stirling and Bell numbers.[20] For that purpose we use elementary methods of combinatorial analysis based on a versatile tool known as the Dobiński relation.[10,11] The latter is obtained by acting with Eq. (15) on the exponential function $e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}$ yielding

$$\sum_{k=0}^{\infty} k^n \frac{x^k}{k!} = e^x \sum_{k=1}^{n} S(n,k)\,x^k. \tag{16}$$

[xx all eqs. must be numbered xx] If we recall the definition of the Bell polynomials Eq. (12), we obtain

$$B(n,x) = e^{-x} \sum_{k=0}^{\infty} \frac{k^n}{k!}\,x^k, \tag{17}$$

which is the celebrated *Dobiński relation*.[10,11] It is usually expressed in terms of the Bell numbers, which are given by

$$B(n) = e^{-1} \sum_{k=0}^{\infty} \frac{k^n}{k!}. \tag{18}$$

We observe that both series are convergent and express the integers $B(n)$ or polynomials $B(n,x)$ in a nontrivial way. To mention one of the many applications notice that k^n in Eq. (17) may be replaced by the integral representation $k^n = \int_0^{\infty} d\lambda\, \lambda^n \delta(\lambda - k)$. If we change the order of the sum and integral (allowable because both are convergent), we obtain the solution to the Stieltjes moment problem for the sequence of Bell polynomials

$$B(n,x) = \int_0^{\infty} d\lambda\, W_x(\lambda)\lambda^n, \tag{19}$$

where

$$W_x(\lambda) = e^{-x} \sum_{k=0}^{\infty} \frac{\delta(\lambda - k)}{k!} x^k \tag{20}$$

is a positive weight function located at integer points and is called a *Dirac comb*.[21] Note that Eq. (20) may be identified with the Poisson distribution with mean value equal to x.

A very elegant and efficient way of storing and tackling information about sequences is attained through their generating functions.[11] The exponential generating function of the polynomials $B(n,x)$ is defined as

$$G(\lambda, x) = \sum_{n=0}^{\infty} B(n,x)\frac{\lambda^n}{n!}. \tag{21}$$

It contains all the information about the Bell polynomials. If we use the Dobiński relation, we may calculate $G(\lambda, x)$ explicitly. We substitute Eq. (17) into Eq. (21), change the summation order,[22] and then identify the expansions of the exponential functions to obtain

$$G(\lambda, x) = e^{-x} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} k^n \frac{x^k}{k!} \frac{\lambda^n}{n!} \tag{22a}$$

$$= e^{-x} \sum_{k=0}^{\infty} \frac{x^k}{k!} \sum_{n=0}^{\infty} k^n \frac{\lambda^n}{n!} \tag{22b}$$

$$= e^{-x} \sum_{k=0}^{\infty} \frac{x^k}{k!} e^{\lambda k} = e^{-x} e^{x e^{\lambda}}. \tag{22c}$$

Thus, the exponential generating function $G(\lambda, x)$ takes the compact form

$$G(\lambda, x) = e^{x(e^{\lambda} - 1)}. \tag{23}$$

Note that in the context of the weight function of Eq. (20) $G(\lambda, x)$ is the moment generating function of the Poisson distribution with the parameter x.

An explicit expression for the Stirling numbers $S(n,k)$ may be extracted from the Dobiński relation. Note that in Eq. (17) the relevant series may be multiplied together using the Cauchy multiplication rule to yield

$$B(n,x) = \sum_{l=0}^{\infty} (-1)^l \frac{x^l}{l!} \sum_{k=0}^{\infty} k^n \frac{x^k}{k!} \tag{24a}$$

$$= \sum_{k=0}^{\infty} \sum_{j=1}^{k} \binom{k}{j} (-1)^{k-j} j^n \frac{x^k}{k!} \tag{24b}$$

By comparing the expansion coefficients in Eq. (24b) with Eq. (12), we obtain

$$S(n,k) = \frac{1}{k!} \sum_{j=1}^{k} \binom{k}{j} (-1)^{k-j} j^n, \tag{25}$$

which yields an expression for $S(n,k)$.

If we use any of the above standard formulas Eqs. (25) and (13) for the Stirling or Bell numbers, we can easily calculate them explicitly. We remark that many other interesting results may be derived by straightforward manipulation of the Dobiński relation Eq.(17) or the generating function Eq.(23), see Appendix A.[23] Some of these numbers are given in Table:

	$S(n,k)$,		$1 \leq k \leq n$						$B(n)$
$n=1$	1								1
$n=2$	1	1							2
$n=3$	1	3	1						5
$n=4$	1	7	6	1					15
$n=5$	1	15	25	10	1				52
$n=6$	1	31	90	65	15	1			203
$n=7$	1	63	301	350	140	21	1		877
$n=8$	1	127	966	1701	1050	266	28	1	4140
...	...	...	...	...	...	...	...	...	...

C. Normal ordering: Solution

We return to normal ordering. By using the properties of coherent states in Eqs. (7)–(9), we conclude from Eqs. (11) and (12) that the diagonal coherent state matrix elements generate the Bell polynomials[17]

$$\langle z|(a^{\dagger}a)^n|z \rangle = B(n, |z|^2). \tag{26}$$

If we expand the exponential $e^{\lambda a^{\dagger}a}$ and take the diagonal coherent state matrix element, we find

$$\langle z|e^{\lambda a^{\dagger}a}|z \rangle = \sum_{n=0}^{\infty} \langle z|(a^{\dagger}a)^n|z \rangle \frac{\lambda^n}{n!} = \sum_{n=0}^{\infty} B(n, |z|^2)\frac{\lambda^n}{n!}. \tag{27}$$

We observe that the diagonal coherent state matrix elements of $e^{\lambda a^{\dagger}a}$ yield the exponential generating function of the Bell polynomials (see Eqs. (21) and (23))

$$\langle z|e^{\lambda a^{\dagger}a}|z \rangle = e^{|z|^2(e^{\lambda} - 1)}. \tag{28}$$

Equations (26) and (28) allow us to read off the normally ordered forms

$$(a^\dagger a)^n = \;:B(n, a^\dagger a):\;,\qquad(29)$$

and

$$e^{\lambda a^\dagger a} = \;:e^{a^\dagger a(e^\lambda - 1)}:\;.\qquad(30)$$

Notice that the normal ordering of the exponential of the number operator $a^\dagger a$ amounts to a rescaling of the parameter $\lambda \to e^\lambda - 1$. We stress that this rescaling is characteristic for this specific case only and in general the functional representation may change significantly (see Sec. V). Just for illustration we give results that can be obtained by an analogous calculation[24]

$$e^{\lambda(a^\dagger)^2 a} = \;:\exp\left(\frac{\lambda(a^\dagger)^2 a}{1 - \lambda a^\dagger}\right):\;,\qquad(31)$$

$$e^{\lambda(a^\dagger)^2 a^2} = \;:e^{-a^\dagger a}\sum_{n=0}^{\infty} e^{\lambda n(n-1)}\frac{(a^\dagger a)^n}{n!}:\;.\qquad(32)$$

Equations (29) and (30) provide an explicit solution to the normal ordering problem for powers and the exponential of the number operator. This solution was obtained by identifying the combinatorial objects and resolving the problem on that basis. Furthermore, this surprising connection opens a promising approach to the ordering problem through its combinatorial interpretation.

D. Combinatorial interpretation: Bell and Stirling numbers

We have defined and investigated the Stirling and Bell numbers as solutions to the normal ordering problem. These numbers are well known in combinatorics[11,18] where the $S(n,k)$ are called Stirling numbers of the second kind. Their original definition is given in terms of partitions of a set; that is, the Stirling numbers $S(n,k)$ count the number of ways of putting n different objects into k identical containers (none left empty), see Fig. 1. The Bell numbers $B(n)$ count the number of ways of putting n different objects into n identical containers (some may be left empty). From these definitions the recurrence relation of Eq. (A1) may be readily obtained and further investigated from a purely combinatorial viewpoint. This formal correspondence establishes a direct link to the normal ordering problem of the number operator. As a result we obtain an interesting interpretation of the ordering procedure in terms of combinatorial objects. We remark that other pictorial representations can be also given, for example, in terms of graphs[25] or rook numbers.[26]

In conclusion we point out that this method may be reversed; that is, certain combinatorial families of numbers may be given an algebraic interpretation in the quantum mechanical context.
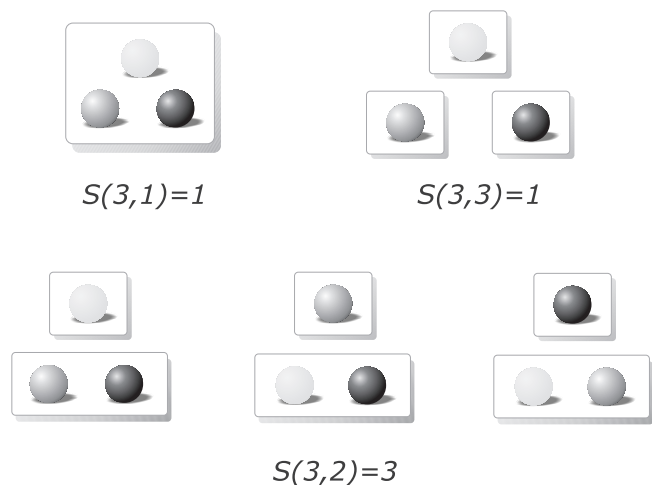

FIG. 1: Illustration of Stirling numbers $S(n,k)$ enumerating partitions of a set of $n = 3$ distinguishable marbles (white, gray and black) into $k = 1, 2, 3$ su bsets.

IV. SOME APPLICATIONS

A. Quantum phase space

A curious application of the coherent state representation is found in the phase space picture of quantum mechanics. For the conjugate pair of observables $\hat{q} = (a^\dagger + a)/\sqrt{2}$ and $\hat{p} = i(a^\dagger - a)/\sqrt{2}$, related to the position and momentum operators of a particle or to quadratures of the electromagnetic field, coherent state expectation values have the simple form $\langle z|\hat{q}|z\rangle + i\langle z|\hat{p}|z\rangle = \sqrt{2}z$ and minimize the uncertainty relation.[27] In this sense the coherent state $|z\rangle$ for $z = (q + ip)/\sqrt{2}$ may be interpreted as the closest quantum approximation to the classical phase state (q, p). These properties are used to construct the quantum analog of phase space through the Husimi distribution, denoted by $Q(q, p)$, which for the quantum state described by the density matrix ρ is defined as[2,8]

$$Q(q, p) = \frac{1}{2\pi}\langle z|\rho|z\rangle.\qquad(33)$$

$Q(q, p)$ is interpreted as the probability density for the system to occupy a region in phase space of width $\Delta\hat{q} = \Delta\hat{p} = \sqrt{1/2}$ centered at (q, p) which on experimental grounds refers to obtaining the result (q, p) from an optimal simultaneous measurement of $\hat{q}$ and $\hat{p}$. Such measurements in quantum optics are obtained using the technique of heterodyne detection.

This construction of the quantum phase space analog raises the problem of efficiently calculating the coherent state expectation values of an operator which, as we have seen in Sec. II B, is in practice equivalent to its normal ordering. Hence ordering techniques are important for practical use.

As an illustration we observe that from Eq. (28) we can readily derive the explicit expression for the Husimi

distribution of the quantum harmonic oscillator in thermal equilibrium. For the Hamiltonian $H = a^\dagger a + 1/2$ the density matrix ρ of a thermal state is $e^{-\beta a^\dagger a}/Z$, where $Z = \text{Tr}\, e^{-\beta a^\dagger a} = 1/(1-e^{-\beta})$ and $\beta = 1/k_B T$. Thus from Eqs. (33) and (28) we obtain

$$Q(q,p) = \frac{1}{2\pi}(1-e^{-\beta})e^{(e^{-\beta}-1)(q^2+p^2)/2}. \qquad (34)$$

It is instructive to compare this quantum phase space distribution with its classical analog. The corresponding Hamiltonian for the classical harmonic oscillator is $H_{\text{cl}} = (q^2 + p^2)/2$, and the probability distribution in the thermal state is $P_{\text{cl}}(q,p) = e^{-\beta(q^2+p^2)/2}/Z_{\text{cl}}$, where $Z_{\text{cl}} = \int e^{-\beta(q^2+p^2)/2}\, dqdp = 2\pi/\beta$. Finally, we obtain

$$P_{\text{cl}}(q,p) = \frac{1}{2\pi}\beta e^{-\beta(q^2+p^2)/2}. \qquad (35)$$

In both cases we obtain gaussians. However, observe that the quantum distribution of Eq. (34) is wider than its classical analog of Eq. (35). It is explained by additional fluctuations due to the uncertainty relation that are inherent in quantum mechanics. For $\beta \to 0$, that is, for large temperatures, the quantum distribution of Eq. (34) correctly goes to the classical distribution in Eq. (35).

An analogous analysis can be done for the whole spectrum of models described by Hamiltonians constructed in the second quantization formalism, provided the normally ordered form of the operators is known. Section III discusses the methodology which is applicable to a wide set of problems, for example, the optical Kerr medium as in Eq. (32) and the open system described by Eq. (31). See Sec. V for a discussion of the range of applicability.

B. Beyond the Wick theorem

As mentioned in Sec. II B the standard approach to normal ordering through Wick's theorem reduces the problem to finding all possible contractions in the operator expression. In practice, the process may be tedious and cumbersome to perform, especially when a large number of operators are involved. Hence systematic methods, like the one described in Sec. III, are of importance in actual applications.

To complete the picture we will show how to connect Wick's approach to the combinatorial setting described in this paper. The bridge is readily provided by the interpretation of Stirling numbers as partitions of a set, as given in Sec. III D. To see the link we consider a string $a^\dagger a\; a^\dagger a\; \dots\; a^\dagger a$ which we label from 1 to n starting from the left, thus obtaining n distinguishable objects

$$\underbrace{a^\dagger a}_{1}\; \underbrace{a^\dagger a}_{2}\; \dots\; \underbrace{a^\dagger a}_{3} \quad \longleftrightarrow \quad ① \; ② \; \dots \; ⓝ \;.$$

Then each choice of contraction in Wick's theorem uniquely divides this set into classes such that objects in the same class are connected by contractions between their operator constituents. See the following examples for illustration

Observe that this construction may be reversed and thus provides a one-to-one correspondence between operator contractions in $(a^\dagger a)^n$ and partitions of the set of n objects.[28] In this way the contractions of Wick's theorem may be seen as partitions of a set, providing the link to the combinatorial framework presented in this paper. The methodology of Sec. III offers an alternative perspective on the normal ordering problem and unlike Wick's approach, exposes its analytical structure, thus yielding practical calculational tools.

C. Operator identities

Manipulations of differently ordered operators often lead to interesting operator identities. For example, taking the limit $\lambda \to -\infty$ in Eq. (30), yields an interesting representation of the vacuum projection operator[4,6]

$$|0\rangle\langle 0| = :e^{-a^\dagger a}:. \qquad (36)$$

Equation (36) leads to a coordinate representation of the squeezing transformation $S(\lambda) = e^{(\lambda^* a^2 - \lambda a^{\dagger 2})/2}$, which is extensively used in quantum optics.[29] It may be obtained using the technique of integration within an ordered product,[30] yielding

$$S(\lambda) = e^{-\lambda/2} \int\limits_{-\infty}^{\infty} dq\, |e^{-\lambda}q\rangle\langle q|, \qquad (37)$$

which offers an interpretation of $S(\lambda)$ as an explicit squeezing of the quadrature.

V. SUMMARY AND OUTLOOK

We have presented a combinatorial framework for operator ordering problems by discussing a simple example of the powers and exponential of the number operator $a^\dagger a$. We have provided a general method for relating normally ordered operator expressions to combinatorial objects and then solved the problem from that viewpoint. The solution involved using the representation of the Heisenberg algebra in terms of operators on the space of polynomials and then applying the Dobiński relation, which provides the exponential generating function and

explicit expressions. This approach provides effective calculational tools and also exposes the analytic structure behind the Wick theorem.

One advantage of this methodology is that it can be straightforwardly generalized to a wide class of operator expressions.[23] The simplest examples are provided by the powers and exponentials of $(a^\dagger)^r a$ and $(a^\dagger)^r a^s$ with r and s integers.[31] It may be further extended to investigate the normal ordering of boson monomials[25] in the form $(a^\dagger)^{r_n} a^{s_n} \ldots (a^\dagger)^{r_2} a^{s_2} (a^\dagger)^{r_1} a^{s_1}$ and more generally homogeneous boson polynomials,[32] that is, linear combinations of boson expressions with the same excess of creation over annihilation operators.[23] Further development of the method applies to the ordering of general operators linear only in the annihilation (or creation) operator, that is, $q(a^\dagger)a + v(a^\dagger)$, where $q(x)$ and $v(x)$ are arbitrary functions. The exponential of an operator of this type constitutes a generalized shift operator and the solution is in the class of Sheffer polynomials.[33] In all of these cases the use of the Dobiński relation additionally provides a solution of the moment problem,[21] as well as a wealth of combinatorial identities for sequences involved in the result (including their deformations[34]).

Ordering problems are naturally inherent in the algebraic structure of quantum mechanics. It is remarkable that they may be described and investigated using objects having a clear combinatorial interpretation. For the generic example considered here these are partitions of a set. For more complicated expressions the interpretation can be provided by introducing correlations between elements or by using a graph representation.

APPENDIX A: COMBINATORIAL IDENTITIES

We enumerate some properties of the Stirling and Bell numbers defined in Sec. III.[35] The reader is invited to check these relations by straightforward manipulation of the Dobiński relation or exponential generating function.[23]

The recurrence relation for the Stirling numbers is

$$S(n+1, k) = kS(n, k) + S(n, k-1), \qquad \text{(A1)}$$

with the initial conditions $S(n, 0) = \delta_{n,0}$ and $S(n, k) = 0$ for $k > n$.

The Bell polynomials may be shown to satisfy the following recurrence relation

$$B(n+1, x) = x \sum_{k=0}^{n} \binom{n}{k} B(k, x), \qquad \text{(A2)}$$

with $B(0, x) = 1$. Consequently for Bell numbers we have $B(n+1) = \sum_{k=0}^{n} \binom{n}{k} B(k)$.

The following exponential generating function of the Stirling numbers $S(n, k)$ is sometimes used in applications

$$\sum_{n=k}^{\infty} S(n, k) \frac{\lambda^n}{n!} = \frac{(e^\lambda - 1)^k}{k!}. \qquad \text{(A3)}$$

In addition, the Stirling numbers $S(n, k)$ may be interpreted as the connection coefficients between two sets x^n and $x^{\underline{n}}$, $n = 1, 2, \ldots$, where $x^{\underline{n}} = x \cdot (x-1) \ldots (x-n+1)$ is the falling factorial; that is, they represent a change of basis in the space of polynomials

$$x^n = \sum_{k=1}^{n} S(n, k) \, x^{\underline{k}}. \qquad \text{(A4)}$$

We also note that the Bell polynomials belong to the class of Sheffer polynomials,[36] which in particular share an interesting property called the Sheffer identity (note the resemblance to the binomial identity)

$$B(n, x+y) = \sum_{k=0}^{n} \binom{n}{k} B(k, y) \, B(n-k, x). \qquad \text{(A5)}$$

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[13] The double dot notation is almost universal in quantum optics and quantum field theory. Nevertheless some authors, for example, Ref. 6, use an alternative notation.

[14] Careless use of the double dot notation may lead to inconsistencies, for example if $A = aa^\dagger$ and $B = a^\dagger a + 1$, we have $A = B$, but $:A: \neq :B:$. Such problems are eliminated if a rigorous definition, beyond this note is given (to be published by A. I. Solomon, P. Blasiak, G. H. E. Duchamp, A. Horzela, and K. A. Penson).

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[19] The simplest representation acts on the space of polynomials and is defined by $Xx^n = x^{n+1}$ and $Dx^n = nx^{n-1}$. It may be naturally extended to the space of formal power series, see Refs. 11,36.

[20] For convenience and to avoid inaccuracy, the definitions of Stirling and Bell numbers are usually extended by the following conventions: $B(0, x) = B(0) = S(0, 0) = 1$ and $S(n, k) = 0$ for $k = 0$ or $k > n > 0$.

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[22] Because the generating functions are formal series, the question of convergence does not arise.

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[24] We suggest derivation of these formulas as a problem to be solved by students during classes on the Fock space methods. Detailed calculations may be found in Refs. 23, 31.

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[27] The conjugate operators $\hat{q}$ and $\hat{p}$, satisfying $[\hat{q}, \hat{p}] = i$, are subject to the Heisenberg uncertainty relation $\Delta_\psi \hat{q} \Delta_\psi \hat{p} \geq 1/2$. For the coherent state $|z\rangle$ the product of uncertainties exactly equals $1/2$. These are the only states with this property that additionally have equal uncertainties $\Delta_\psi \hat{p} = \Delta_\psi \hat{q}$ (in general, we obtain the squeezed states.^{5,7}

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