Combinatorics and Boson Normal Ordering: A Gentle Introduction

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We discuss a general combinatorial framework for operator ordering problems by illustrating it on a simple example of 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 elementary exposition reveals inherent relations between ordering problems and combinatorial objects, displaying the analytical background to Wick's theorem. The methodology herein presented is comprehensible at the undergraduate level and can be straightforwardly generalized to a wide class of operators.

I. INTRODUCTION

Hilbert space constitutes the arena where quantum phenomena occur. One common realization is Fock space generated by the set of orthonormal vectors $|n\rangle$ representing states with specified numbers of particles, or objects in general. 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 satisfying the conventional boson commutation relation $[a, a^\dagger] = 1$ describing objects obeying Bose-Einstein statistics, *e.g.* photons or phonons.

Operators a and $a^\dagger$ exhibit a typically quantum mechanical feature in that they *do not* commute. This is probably the most prominent characteristic of quantum theory, and one that 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 derives from the fact that the order in which operators occur is relevant, *e.g.* $a^\dagger a \neq aa^\dagger = a^\dagger a + 1$. The ordering problem plays a vital role in the construction of quantum mechanical operators. The physical properties of differently ordered operators may be quite distinct, which may easily be seen by consideration of their expectation values. Analysis of operator matrix elements reveals their physical properties observed as probabilities yielded by experiment. There are two sets of states of primary interest in this context; namely, number states $|n\rangle$ and coherent states $|z\rangle$. The latter, defined as eigenstates of the annihilation operator a, play an important role *e.g.* in quantum optical investigations[3–7] or in the phase space formulation of quantum mechanics.[8]

Calculation of the number or coherent state expectation values in practice comes down to transforming the original expression to the *normally ordered* form in which all annihilation operators stand to the right. In this form evaluation of the matrix elements is immediate. The procedure itself is called *normal ordering*.[4–8] Although the process is clear and straightforward, in practice it may be very tedious and cumbersome. This is evident when the expression is complicated and is even less tractable when one considers operators defined through an infinite series expansion. It is thus highly desirable to find manageable formulas or, at least, some guiding principles leading to solutions of the normal ordering problems.

In this paper we present a general framework which 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 guiding example to illustrate a systematic approach to the ordering problem. The general methodology consists in identifying the problem with combinatorial structures and then resolving it on this basis. The solution may be found with the help of the *Dobiński formula*, which proves to be a very effective tool and, moreover, has the merit of being 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 is especially interesting as the objects involved in the problem may have clear combinatorial interpretations (*e.g.* 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 herein presented is an example of a fertile interplay between algebra and combinatorics implemented in the quantum mechanical context. It employs undergraduate algebra only and may thus fulfill an educational function. To our knowledge this approach 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 Section III. It illustrates the methodology by discussing in detail the solution of a generic example. Some applications are provided in Section IV. In the concluding Section 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

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

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 $n = 0, 1, 2, ...$ counts the number of particles, or objects in general. The states are assumed to be orthonormal $\langle n|k\rangle = \delta_{n,k}$ and constitute a basis in $\mathcal{H}$. This representation is usually called Fock space.

Operators a and $a^\dagger$ satisfying Eq.(1) may be realized in Fock space as follows:

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

Consequently the *number operator* N counting the number of particles in a system and defined by

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

is represented as $N = a^\dagger a$. It satisfies the following 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, *e.g.* 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 $\langle z|a^\dagger = z^*\langle z|$). Explicitly they take the 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 not orthogonal and constitute an overcomplete basis in the Hilbert space.[10] Coherent states have many useful properties which are exploited in quantum optics as well as in other areas of physics.[3–8]

B. Normal ordering: Introduction

The noncommutativity of creation and annihilation operators causes serious ambiguities in defining operator functions in Quantum Mechanics. To solve this problem one has additionally to fix the order of the operators involved. 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.[4–8]

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). We stress the fact that this procedure yields an operator whose action is equivalent to the original one, *i.e.* $F^{(n)}(a^\dagger, a) = F(a^\dagger, a)$ as operators, although the form of the expressions in terms of a and $a^\dagger$ may be completely different.

On the other hand 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), *i.e.* moving all annihilation operators a to the right as if they commuted with the creation operators $a^\dagger$. This notation, while widely used, is not universal.[11] We observe that in general this procedure yields a different operator $F(a^\dagger, a) \neq\, :F(a^\dagger, a):$.[12]

As just remarked, these two procedures provide completely different results (except for operators which are already in normally ordered form). There is also a practical difference in their use. That is, while 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:

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

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

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 of the operator has the merit of enabling immediate calculation of its coherent state elements. This boils down, by virtue of Eq.(5), to substituting $a \to z$ and $a^\dagger \to z^*$ in its functional representation, *i.e.*

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

Thus, having solved the normal ordering problem of Eq.(7) we readily obtain

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

This may be illustrated on the above example

$$\begin{aligned}\langle z|\ aa^\dagger aaa^\dagger a\ |z\rangle &= \langle z|\ (a^\dagger)^2a^4 + 4\ a^\dagger a^3 + 2\ a^2\ |z\rangle \\ &= (z^*)^2z^4 + 4\, z^*z^3 + 2\, z^2\ . \end{aligned} \tag{10}$$

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; *i.e.* 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 problem is by use of *Wick's theorem.*[13] In our context, this 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, *e.g.*

$$\begin{aligned} aa^\dagger aaa^\dagger a = &:\underbrace{aa^\dagger aaa^\dagger a}_{\text{no pair removed}}: \\ + &:\underbrace{\not{a}\not{a}^\dagger aaa^\dagger a + \not{a}a^\dagger aa\not{a}^\dagger a + aa^\dagger\not{a}a\not{a}^\dagger a + aa^\dagger a\not{a}\not{a}^\dagger a}_{\text{1 pair removed}}: \\ + &:\underbrace{\not{a}\not{a}^\dagger\not{a}a\not{a}^\dagger a + \not{a}\not{a}^\dagger a\not{a}\not{a}^\dagger a}_{\text{2 pairs removed}}: = (a^\dagger)^2a^4 + 4\ a^\dagger a^3 + 2\ a^2. \end{aligned}$$

This procedure may involve a large number of steps. For polynomial expressions this difficulty may be overcome by using computer algebra, although this does not provide an analytic structure. Moreover, for nontrivial functions, *e.g.* 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:

$$e^{\lambda(a+a^\dagger)} = e^{\lambda^2/2}\ :e^{\lambda(a+a^\dagger)}:\ . \tag{11}$$

The use of this kind of disentangling property of the exponential operators is, however, restricted in practice to quadratic expressions in boson operators.[14]

Another method exploits recurrence relations and solves the normal ordering problem by use of combinatorial identities.[9,15] 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 n-th power ($n \geq 1$). We may write this as

$$\left(a^\dagger a\right)^n = \sum_{k=1}^{n} S(n,k)\,(a^\dagger)^k a^k \tag{12}$$

which expression uniquely defines the integer sequences $S(n,k)$ for $k = 1...n$ which are called *Stirling numbers.*[16,17] For each n information about this sequence may be captured in the so called *Bell polynomials*

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

and one also defines the *Bell numbers* $B(n) = B(n,1)$, *i.e.*

$$B(n) = \sum_{k=1}^{n} S(n,k). \tag{14}$$

Instead of operators a and $a^\dagger$ we may equally well insert into Eq.(12) the representation of Eq.(1) given by operator X defined as multiplication by x, and by the derivative $D = \frac{d}{dx}$[18]

$$a^\dagger \longleftrightarrow X, \qquad a \longleftrightarrow D. \tag{15}$$

This substitution does not affect the commutator of Eq.(1), *i.e.* $[D, X] = 1$, which is the only property relevant for the construction. Therefore in this representation the relation of Eq.(12) takes the form

$$(XD)^n = \sum_{k=1}^{n} S(n,k)\,X^kD^k. \tag{16}$$

Having placed the problem on an analytical footing we proceed to its solution.

B. Combinatorial analysis

In the following we are concerned with properties of the above-defined Stirling and Bell numbers.[19] For that purpose we use elementary methods of combinatorial analysis based on a versatile tool which is the Dobiński relation. It is readily obtained by acting with Eq.(16) on the exponential function $e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}$ yielding

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

Recalling the definition of the Bell polynomials Eq.(13) we obtain

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

which is the celebrated *Dobiński formula*.[17,20] It is usually stated for Bell numbers in the form

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

We observe that both series are convergent and express integer numbers $B(n)$ or polynomials $B(n,x)$ in a very nontrivial way which has many applications. Just to mention one: notice that k^n in Eq.(17) may be replaced by the integral representation $k^n = \int_0^{\infty} d\lambda\ \lambda^n \delta(\lambda - k)$. Then changing the order of the sum and integral (allowable since 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.

Having established the Dobiński formula we proceed to further investigation of Stirling and Bell numbers. All the properties of these sequences may be readily obtained from a straightforward application of Eq.(17).

A very elegant and efficient way of storing and tackling information about sequences is attained through their *generating functions*.[17] The *exponential generating function* of 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. Using the Dobiński relation we may calculate it explicitly. Substituting Eq.(17) into Eq.(21), changing the summation order[22] and then identifying the expansions of the exponential functions we obtain

$$\begin{aligned} G(\lambda,x) &= e^{-x} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} k^n \frac{x^k}{k!} \frac{\lambda^n}{n!} \\ &= e^{-x} \sum_{k=0}^{\infty} \frac{x^k}{k!} \sum_{n=0}^{\infty} k^n \frac{\lambda^n}{n!} \\ &= e^{-x} \sum_{k=0}^{\infty} \frac{x^k}{k!} e^{\lambda k} = e^{-x} e^{x e^{\lambda}}. \end{aligned} \tag{22}$$

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

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

Note that put in the context of the weight function of Eq.(20) it 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. Notice that in Eq.(17) the relevant series may be multiplied together using the Cauchy multiplication rule, which yields

$$\begin{aligned} B(n,x) &= \sum_{l=0}^{\infty} (-1)^l \frac{x^l}{l!} \cdot \sum_{k=0}^{\infty} k^n \frac{x^k}{k!} \\ &= \sum_{k=0}^{\infty} \sum_{j=1}^{k} \binom{k}{j} (-1)^{k-j} j^n \frac{x^k}{k!} \end{aligned} \tag{24}$$

Comparing the expansion coefficients with Eq.(13) we get

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

Thus the *explicit expression* for $S(n,k)$ is obtained.

Using any of the standard formulas for Stirling or Bell numbers one can easily calculate them explicitly. Here are some:

	$S(n,k)$,	$1 \le k \le n$								$B(n)$
$n=1$	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
...	...	...	...	...	...	...	...	...	...	...

We conclude our investigation of the combinatorial structure of Stirling and Bell numbers at this point and pass on to the normal ordering problem. However, we remark that many other interesting results may be derived by straightforward manipulation of the Dobiński formula or the generating function, see Appendix A.[23]

C. Normal ordering: Solution

We return to normal ordering. Using the properties of coherent states, see Eqs.(7)-(9), we conclude from Eqs.(12) and (13) that diagonal coherent state matrix elements generate Bell polynomials[15]

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

Moreover, expanding the exponential $e^{\lambda a^\dagger a}$ and taking the diagonal coherent state matrix element we have

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

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))

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

Eqs.(26) and (28) allow one to read off the normally ordered forms

$$(a^\dagger a)^n = \,:B(n,a^\dagger a):\tag{29}$$

and

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

Notice that the normal ordering of the exponential of the number operator $a^\dagger a$ amounts to a rescaling of the parameter $\lambda \longrightarrow e^\lambda - 1$. It should be stressed that this is characteristic for this specific case only and in general the functional representation may change significantly (see Section V for further reading). Just for illustration we quote results which can be obtained by analogous calculation[24]

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

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

Eqs.(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 identification of combinatorial objects in the problem and resolving it 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

In previous sections we defined and investigated Stirling and Bell numbers as solutions to the normal ordering problem. On the other hand these numbers are well known in combinatorics[16,17] 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, see Fig.1, *i.e.*

- Stirling numbers $S(n,k)$ count the number of ways of putting n different objects into k identical containers (none left empty).

- 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 *e.g.* in terms of graphs[25] or rook numbers.[26]

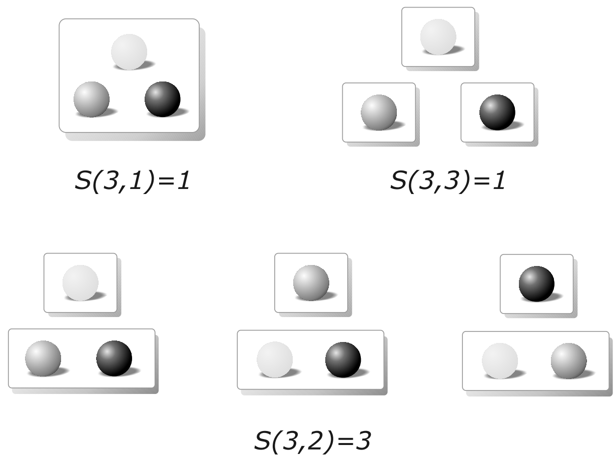

FIG. 1: Illustration of Stirling numbers $S(n,k)$ enumerating partitions of a set of $n=3$ distinguishable marbles (white, gray and black) into $k=1,2,3$ subsets.

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

IV. SOME APPLICATIONS

A. Quantum phase space

A curious application of coherent state representation is found in the phase space picture of quantum mechanics. It is due to the fact that it is intimately connected with the conjugate pair of observables $\hat{q} = (a^\dagger + a)/\sqrt{2}$ and $\hat{p} = i(a^\dagger - a)/\sqrt{2}$ related to position and momentum operators of a particle or to quadratures of the electromagnetic field. Coherent state expectation values of these operators have the simple form $\langle z|\hat{q}|z\rangle + i\langle z|\hat{p}|z\rangle = \sqrt{2}\,z$ and moreover 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]

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

It is interpreted as the probability density for the system to occupy a fuzzy region in phase space, of width $\Delta\hat{q} = \Delta\hat{p} = \sqrt{1/2}$, centered at (q, p). Physically it means obtaining the result (q, p) from an optimal simultaneous measurement of q and 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 effective calculation of the coherent state expectation values of an operator which, as we have seen in Section II B, is in practice equivalent to its normal ordering. Hence ordering techniques are important for its practical use.

As an illustration we observe that from Eq.(28) one readily derives the explicit expression for the Husimi distribution of the quantum harmonic oscillator in thermal equilibrium. Indeed, 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 $Z = \mathrm{Tr}\, e^{-\beta a^\dagger a} = 1/(1-e^{-\beta})$ and $\beta = 1/k_B T$. Thus from Eqs.(33) and (28) we obtain

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

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

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

In both cases we obtain gaussians, however it should be observed that the quantum distribution of Eq.(34) is wider than its classical analog of Eq.(35). It is explained by additional fluctuations due to uncertainty relation inherent in quantum mechanics. Moreover, for $\beta \to 0$, *i.e.* for large temperatures, the quantum distribution of Eq.(34) correctly reconstructs the classical of Eq.(35).

Analogous analysis can be made for the whole spectrum of models described by hamiltonians constructed in the second quantization formalism, provided the normally ordered form of the operators are known. Section III offers the methodology applicable to a wide set of problems *e.g.* for the optical Kerr medium as in Eq.(32) or for the open system described by Eq.(31). See Section V for the discussion of the range of applicability.

B. Beyond the Wick theorem

As mentioned in Section 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, however, 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 Section III, are of importance in actual applications.

Completing the whole picture we will show how to connect Wick's approach with 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 Section III D. To see this we consider a string $a^\dagger a\ a^\dagger a\ ...\ a^\dagger a$ consisting of n blocks $a^\dagger a$ which we label from 1 to n starting from the left, thus obtaining n distinguishable objects

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

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

$a^\dagger a\ a^\dagger a\ a^\dagger a\ a^\dagger a\ a^\dagger a \leftrightarrow ①②③④⑤ \leftrightarrow$ [①②] [③] [④⑤]

$a^\dagger a\ a^\dagger a\ a^\dagger a\ a^\dagger a\ a^\dagger a \leftrightarrow ①②③④⑤ \leftrightarrow$ [①②③] [④⑤]

$a^\dagger a\ a^\dagger a\ a^\dagger a\ a^\dagger a\ a^\dagger a \leftrightarrow ①②③④⑤ \leftrightarrow$ [①③] [②④⑤]

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 Section III offers an alternative perspective on the normal ordering problem and, contrary to Wick's approach, exposes its analytical structure yielding practical calculational tools.

C. Operator identities

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

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

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

$$S(\lambda) = e^{-\lambda/2} \int_{-\infty}^{\infty} dq \; |\, e^{-\lambda} q\,\rangle\langle\, q\,| \tag{37}$$

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

V. SUMMARY AND OUTLOOK

In this note we have presented a combinatorial framework for operator ordering problems by illustrating it on a simple example of the powers and exponential of the number operator $a^\dagger a$. We have provided a general scheme for relating normally ordered operator expressions to combinatorial objects and then solved the problem from that viewpoint. We achieved this using the representation of the Heisenberg algebra in terms of operators on the space of polynomials and then applying the Dobiński relation which provided the exponential generating function and explicit expressions. This approach provides not only effective calculational tools but also exposes the analytic structure behind the Wick theorem.

This methodology has the merit of straightforward generalization 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 $(a^\dagger)^{r_N} a^{s_N} ... (a^\dagger)^{r_2} a^{s_2} (a^\dagger)^{r_1} a^{s_1}$ and more generally *homogeneous boson polynomials*,[32] *i.e.* 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, *i.e.* $q(a^\dagger)a + v(a^\dagger)$ 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 given within the class of Sheffer polynomials.[33] In all these cases 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 using graph representation.

Appendix A: Combinatorial identities

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

First, we state the *recurrence relation* for Stirling numbers

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

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

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

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

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

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

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

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

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

We note also that 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)

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

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[10] Coherent states $|z\rangle$ are not orthogonal for different z and the overlapping factor is $\langle z|z'\rangle = e^{z^* z' - \frac{1}{2}|z|^2 - \frac{1}{2}|z'|^2}$. They constitute an overcomplete basis in the sense of resolution of the identity $\frac{1}{\pi}\int_{\mathbb{C}} d^2z\ |z\rangle\langle z| = 1$.

[11] The double dot notation is almost universal in quantum optics and quantum field theory. Nevertheless some authors, *e.g.* Louisell in Ref.[6], use alternative notation.

[12] 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 $: A :\neq: B :$. However such problems are eliminated if a rigorous definition, beyond the remit of this note, is given (to be published).

[13] Wick's theorem is usually formulated for the time ordered, also called chronologically ordered, products of field operators, see *e.g.* J. D. Bjorken and S. D. Drell, *Relativistic Quantum Fields* (McGraw-Hill, 1968). In our context, however, operators do not depend on the space-time coordinate and chronological ordering reduces to the normal ordering procedure discussed in this paper. See e.g. Ref.[2].

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[18] 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 further naturally extended to the space of formal power series, see Refs.[17,36].

[19] 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] Since the generating functions are *formal* series, the question of convergence does not arise.

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[27] Conjugate operators $\hat{q}$ and $\hat{p}$, satisfying $[\hat{q},\hat{p}] = i$, are subject to the Heisenberg uncertainty relation $\Delta_\psi \hat{q} \cdot \Delta_\psi \hat{p} \geq 1/2$. For coherent state $|z\rangle$ product of uncertainties is equal exactly to 1/2. Moreover these are the only states with this property which additionally have equal uncertainties $\Delta_\psi \hat{p} = \Delta_\psi \hat{q}$ (in general one obtains the squeezed states[5,7]).

[28] Detailed proof of this bijection should take into consideration the specific structure of contractions between blocks $a^\dagger a$ which make the order in such constructed class irrelevant.

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