The General Boson Normal Ordering Problem

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We solve the boson normal ordering problem for $F \left[ (a^\dagger)^r a^s \right]$, with $r, s$ positive integers, $[a, a^\dagger] = 1$, i.e. we provide exact and explicit expressions for its normal form $N \{ F \left[(a^\dagger)^r a^s \right] \}$, where in $N(F)$ all $a$’s are to the right. The solution involves integer sequences of numbers which are generalizations of the conventional Bell and Stirling numbers whose values they assume for $r = s = 1$. A comprehensive theory of such generalized combinatorial numbers is given including closed-form expressions (extended Dobinski - type formulas) and generating functions. These last are special expectation values in boson coherent states.

Consider a function $F(x)$ having a Taylor expansion around $x = 0$, i.e. $F(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} x^k$. In this note we will collect the formulas concerning our solution of the normal ordering problem for $F \left[ (a^\dagger)^r a^s \right]$, where $a, a^\dagger$ are the boson annihilation and creation operators, $[a, a^\dagger] = 1$, and $r$ and $s$ are positive integers. The normally ordered form of the operator $F \left[ (a^\dagger)^r a^s \right]$ is denoted by $N \{ F \left[(a^\dagger)^r a^s \right] \}$, where in $N(F)$ all the $a$’s are to the right. It satisfies the operator identity:

$$N \{ F \left[(a^\dagger)^r a^s \right] \} = F \left[(a^\dagger)^r a^s \right]. \quad (1)$$

Furthermore, an auxiliary symbol $O(a, a^\dagger)$ will be used, which means expand $O$ in powers of $a$ and $a^\dagger$ and order normally assuming they commute [1],[2].

The combinatorial numbers $S(n, k)$, known as Stirling numbers of the second kind, and their sums $B(n)$, the Bell numbers, arise naturally in the normal ordering procedure for $r = s = 1$, as follows [3]:

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

$$B(n) = \sum_{k=1}^{n} S(n, k), \quad (3)$$

which may be taken as definitions of $S(n, k)$ and $B(n)$. In the present work we shall treat the case of general $(r, s)$, consequently generalizing these combinatorial numbers.

For the moment we restrict ourselves to the case $r \geq s$, the other alternative being treated later. We do not give the proofs of the formulas here; they will be given elsewhere [4]. The case $r = s = 1$ is known [1],[2] and some features of the $r > 1, s = 1$ case have been published [5]. When needed we shall refer to [1],[2] and [5] where particular cases of our more general formulas are discussed.

We define the set of positive integers $S_{r,s}(n, k)$ entering the expansion:

$$\left[ (a^\dagger)^r a^s \right]^n = N \left\{ \left[ (a^\dagger)^r a^s \right]^n \right\} = (a^\dagger)^{n(r-s)} \sum_{k=s}^{ns} S_{r,s}(n, k)(a^\dagger)^k a^k, \quad (4)$$

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for \( n = 1, 2, \ldots \). Once the \( S_{r,s}(n,k) \) are known, the normal ordering of \( [(a^\dagger)^r a^s]^n \) is achieved. The same applies to any operator \( F \left[(a^\dagger)^r a^s\right] \) if \( F(x) \) has a Taylor expansion around \( x = 0 \). The row sums of the triangle \( S_{r,s}(n,k) \) are given by:

\[
B_{r,s}(n) = \sum_{k=s}^{n} S_{r,s}(n,k),
\]

which for any \( t \) extend to the polynomials of order \( ns \) defined by:

\[
B_{r,s}(n,t) = \sum_{k=s}^{n} S_{r,s}(n,k)t^k.
\]

All the subsequent formulas are consequences of the following relation, linking the polynomial of Eq.(6) to a certain infinite series:

\[
e^{-t} \sum_{k=s}^{\infty} \frac{1}{k!} \prod_{j=1}^{n} [(k + (j - 1)(r - s)) \cdot (k + (j - 1)(r - s) - 1) \cdot \ldots \cdot (k + (j - 1)(r - s) - s + 1)] t^k =
\]

\[
= \sum_{k=s}^{n} S_{r,s}(n,k)t^k, \quad n = 1, 2, \ldots
\]

which for \( r, s \geq 1 \) and \( t = 1 \) is an analogue of the celebrated Dobinski relation, which expresses the combinatorial Bell numbers \( B_{1,1}(n) \) as a sum of an infinite series [6],[7],[8]:

\[
B_{1,1}(n) = \frac{1}{e} \sum_{k=0}^{\infty} \frac{k^n}{k!}.
\]

For a review of various characteristics of Bell numbers \( B_{1,1}(n) \) see [9]. It seems that Bell and Stirling numbers are now beginning to appear in textbooks of mathematical physics [10].

By setting \( t = 1 \) in Eq.(7) we obtain expressions for the generalized Bell numbers \( B_{r,s}(n) \), \( n = 1, 2, \ldots \) :

\[
r > s : \quad B_{r,s}(n) = B_{r,s}(n,1) = \frac{1}{e} \sum_{k=s}^{\infty} \frac{1}{k!} \prod_{j=1}^{n} (k + (j - 1)(r - s)) \cdot \ldots \cdot (k + (j - 1)(r - s) - s + 1) \cdot \frac{(r - s)^{s(n-1)}}{e} \sum_{k=0}^{\infty} \frac{1}{k!} \prod_{j=1}^{n} \Gamma(n + \frac{k+j}{r-s}) \Gamma(1 + \frac{k+j}{r-s})
\]

\[
= \frac{(r-s)^{s(n-1)}}{e} \sum_{k=0}^{\infty} \frac{1}{k!} \prod_{j=1}^{n} \Gamma(n + \frac{k+j}{r-s}) \Gamma(1 + \frac{k+j}{r-s})
\]

\[
r = s : \quad B_{r,r}(n) = B_{r,r}(n,1) = \frac{1}{e} \sum_{k=0}^{\infty} \frac{1}{k!} \prod_{j=1}^{n} (k + r) \cdot \frac{(k+r)!}{k!}^{-1}
\]

For all \( r, s \) we set \( B_{r,s}(0) = 1 \) by convention. In Eq.(9) we use the notation \( m^\bullet := m(m-1)(m-2)\ldots(m-s+1) \) for the falling factorial [11], and in Eq.(10) \( \Gamma(y) \) is the Euler gamma function.

The numbers \( S_{r,s}(n,k) \) are non-zero for \( s \leq k \leq ns \), and satisfy by convention \( S_{r,s}(n,0) = \delta_{n,0} \). We shall refer to them as generalized Stirling numbers of the second kind. Their exact expressions in the form of a finite sum are:

\[
S_{r,s}(n,k) = \frac{(-1)^k}{k!} \sum_{p=s}^{k} (-1)^p \binom{k}{p} \prod_{j=1}^{n} (p + (j - 1)(r - s)) \cdot \frac{(-1)^{k}}{k!} \left\{ \left( x^r \frac{d^s}{dx^s} \right)^n \left( x^{-1} - x \right)^k \sum_{p=0}^{s-1} \binom{k}{p} (-x)^p \right\}_{x=1}
\]

from which for \( r = s = 1 \) one obtains the standard form of the classical Stirling numbers of the second kind [8]:

\[
S_{1,1}(n,k) = \frac{(-1)^k}{k!} \sum_{p=1}^{k} (-1)^p \binom{k}{p} p^n,
\]
and for \( r = 2, s = 1 \),

\[
S_{2,1}(n, k) = \frac{n!}{k!} \left( \frac{n-1}{k-1} \right), \tag{15}
\]

which are the so-called unsigned Lah numbers \([5],[8]\).

That the numbers \( S_{r,s}(n, k) \) are natural extensions of \( S_{1,1}(n, k) \) can be neatly seen by observing their action on the space of polynomials generated by falling factorials. Let \( x \) be any real number. Then,

\[
\prod_{j=1}^{n} (x + (j - 1)(r - s)) = \sum_{k=s}^{n} S_{r,s}(n, k)x^k. \tag{16}
\]

This last equation when specified to \( r = s \) gives a particularly transparent interpretation of \( S_{r,r}(n, k) \) as connection coefficients:

\[
(x^r)^n = \sum_{k=r}^{n} S_{r,r}(n, k)x^{\underline{k}}. \tag{17}
\]

For \( r = s = 1 \) it boils down to the defining equations for \( S_{1,1}(n, k) \) in terms of \( x^\underline{k} \), used by J. Stirling himself \([11]\):

\[
x^n = \sum_{k=1}^{n} S_{1,1}(n, k)x^{\underline{k}}. \tag{18}
\]

The relations for \( S_{r,s}(n, k) \) become particularly appealing for \( r = s \): Eq.(12) can be reformulated as:

\[
S_{r,r}(n, k) = \frac{(-1)^k}{k!} \sum_{p=r}^{k} (-1)^p \left( \binom{k}{p} \right) (p^\underline{k})^n, \tag{19}
\]

which differs from Eq.(14) in that the sum in Eq.(19) starts from \( p = r \) and \( p^n \) becomes \((p^\underline{k})^n\). The recurrence relations for \( S_{r,r}(n, k) \) are the following:

\[
\begin{align*}
S_{r,r}(1, r) &= 1, & S_{r,r}(n, k) &= 0, & k < r, & nr < k \leq (n+1)r, \tag{20} \\
S_{r,r}(n + 1, k) &= \sum_{p=0}^{r} \binom{k + p - r}{p} r^\underline{p} S_{r,r}(n, k + p - r), & r \leq k \leq nr, & n > 1. \tag{21}
\end{align*}
\]

where the definition \( r^\underline{p} := 1 \) is made. Note that for \( r = s = 1 \) we get the known relation for conventional Stirling numbers i.e.: \( S_{1,1}(n + 1, k) = kS_{1,1}(n, k) + S_{1,1}(n, k - 1) \) with appropriate initial conditions \([11]\).

The ”non-diagonal” generalized Bell numbers \( B_{r,s}(n) \) can always be expressed as special values of generalized hypergeometric functions \( \, _pF_q \). Algebraic manipulation of Eqs.(9)-(11) yields the following examples. For \( r > 1, s = 1 \), \( B_{r,1}(n) \) is a combination of \( r - 1 \) different hypergeometric functions of type \( \, _1F_{r-1}(\ldots, x) \), each of them evaluated at the same value of argument \( x = (r-1)^{1-r} \); here are some lowest order cases:

\[
\begin{align*}
B_{2,1}(n) &= \frac{n!}{e} \, _1F_1(n + 1; 2; 1) = (n - 1)!L^{(1)}_{n-1}(-1), \tag{22} \\
B_{3,1}(n) &= \frac{2^{n-1}}{e} \left( \frac{2\Gamma(n + \frac{1}{2})}{\sqrt{\pi}} \right) _1F_2 \left( \begin{array}{c} n + 1, 1 \\ \frac{3}{2}, \frac{1}{2}, \frac{1}{4} \end{array} \right) + n! \, _1F_2 \left( \begin{array}{c} n + 1, \frac{3}{2} \\ 2, 1 \end{array} \right), \tag{23}
\end{align*}
\]

etc. In Eq.(22) \( L^{(\alpha)}(y) \) is the associated Laguerre polynomial.

Similarly the series \( B_{2r,r}(n) \) can be written down in a compact form using the confluent hypergeometric function of Kummer:

\[
B_{2r,r}(n) = \frac{(rn)!}{e \cdot r!} \, _1F_1(rn + 1, r + 1; 1). \tag{24}
\]

In contrast, the ”diagonal” numbers \( B_{r,r}(n) \) of Eq.(11), which also can be rewritten as:

\[
B_{r,r}(n) = \frac{1}{e} \sum_{k=0}^{\infty} \frac{1}{(k + r - 1)!} [k(k + 1) \ldots (k + r - 1)]^n, \quad n = 1, 2, \ldots \tag{25}
\]
cannot be expressed through hypergeometric functions. However, the sequences $B_{r,s}(n)$ possess a particularity that they can always be expressed in terms of conventional Bell numbers and $r$-nomial (binomial, trinomial . . . ) coefficients. For example:

$$B_{2,2}(n) = \sum_{k=0}^{n-1} \binom{n-1}{k} B_{1,1}(n+k).$$

(26)

Some low-order triangles of $S_{r,s}(n,k)$ and their associated $B_{r,s}(n)$ are presented in Table 1.

It turns out that various generating functions for $B_{r,s}(n)$ and $S_{r,s}(n,k)$ can be related to special quantum states, which are called coherent states [1], defined as linear combinations of the eigenstates of the number operator, $N = a^\dagger a$, $N|n\rangle = n|n\rangle$, $\langle n|n'\rangle = \delta_{n,n'}$ and defined as:

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

(27)

(with $\langle z|z\rangle = 1$), for $z$ complex. The states $|z\rangle$ satisfy:

$$a|z\rangle = z|z\rangle.$$

(28)

It has been noticed in [13] that,

$$\langle z|(a^\dagger a)^n|z\rangle \equiv B_{1,1}(n)$$

(29)

and the exponential generating function (egf) of the numbers $B_{1,1}(n)$, i.e. $\sum_{n=0}^{\infty} B_{1,1}(n) \frac{\lambda^n}{n!}$ satisfies

$$\langle z|e^{\lambda a^\dagger a}|z\rangle = \langle z| : e^{a^\dagger a(e^\lambda - 1)} : |z\rangle \equiv e^{\lambda - 1} = \sum_{n=0}^{\infty} B_{1,1}(n) \frac{\lambda^n}{n!},$$

(30)

which is a restatement of the known fact that [1],[2],[5]:

$$e^{\lambda a^\dagger a} = N \left( e^{\lambda a^\dagger a} \right) = : e^{a^\dagger a(e^\lambda - 1)} :.$$

(31)

How does it generalize to $r, s \geq 1$ ?

Eqs.(4) and (5) give directly:

$$\langle z| [(a^\dagger)^r a^s]^n |z\rangle \equiv B_{r,s}(n),$$

(32)

valid for all $r, s$.

We first treat the case $r = s = 1, 2, \ldots$. Note in this context that a Hermitian Hamiltonian $(a^\dagger)^r a^r$ is of great importance in quantum optics, as for $r = 2, 3, \ldots$ it provides a description of non-linear Kerr-type media[12]. Using Eq.(19) we can find the following egf of $S_{r,r}(n,k)$:

$$\sum_{n=[k/r]} S_{r,r}(n,k) = \sum_{n=k/r}^{\infty} \frac{(-1)^k}{k!} \binom{k}{p} e^{xp(p-1)\ldots(p-r+1) - 1},$$

(33)

where $[y]$ is the ceiling function [11], defined as the nearest integer greater or equal to $y$. This yields via exchange of order of summation:

$$e^{\lambda (a^\dagger)^r a^r} = N \left( e^{\lambda (a^\dagger)^r a^r} \right) = 1 + \sum_{k=r}^{\infty} \frac{(-1)^k}{k!} \left[ \sum_{p=r}^{k} (-1)^p \binom{k}{p} \left( e^{xp(p-1)\ldots(p-r+1) - 1} \right) \right] (a^\dagger a)^k :$$

(34)

and

$$\langle z|e^{\lambda (a^\dagger)^r a^r}|z\rangle \equiv 1 + \sum_{k=r}^{\infty} \frac{(-1)^k}{k!} \left[ \sum_{p=r}^{k} (-1)^p \binom{k}{p} \left( e^{\lambda p - 1} \right) \right].$$

(35)
Another case which can be written in a closed form is \( r > 1, s = 1 \), for which the egf for \( S_{r,1}(n,k) \) reads:
\[
\sum_{n=\lfloor k/r \rfloor}^{\infty} \frac{x^n}{n!} S_{r,1}(n,k) = \frac{1}{k!} \left\{ (1 - (r-1)x)^{-\frac{1}{r-1}} - 1 \right\}.
\] (36)

One then obtains [5],[14]:
\[
e^{\lambda(a^\dagger a)^r} = N \left( e^{\lambda(a^\dagger a)^r} \right) = \exp \left\{ (1 - \lambda(a^\dagger a)^{r-1}(r-1))^{-\frac{1}{r-1}} - 1 \right\} a^\dagger a \right\}. \]
(37)

For arbitrary \( r > s \) the following formula is still valid:
\[
e^{\lambda(a^\dagger a)^r} = N \left( e^{\lambda(a^\dagger a)^r} \right) = 1 + \sum_{n=1}^{\infty} \frac{\lambda^n}{n!} (a^\dagger a)^{n(r-s)} \left( \sum_{k=s}^{n} S_{r,s}(n,k) (a^\dagger a)^k \right) : \]
(38)

where the explicit form of \( S_{r,s}(n,k) \) may be used, see Eqs.(12)-(13).

A close look at Eqs.(35) and (32) reveals that \( n > s \geq r \) examination of Eqs.(9)-(10) confirms that the numbers \( B_{r,s}(n) \) increase so rapidly with \( n \) that one cannot define their egf’s meaningfully. In particular, this is reflected by Eq.(38) which is true in its operator form, but one needs to exercise care when calculating its matrix elements as the convergence of the result may require limitations on \( \lambda \).

A well-defined and convergent procedure for such sequences is to consider what we call hypergeometric generating functions (hgf), i.e. the egf for the ratios \( B_{r,s}(n)/n^t \), where \( t \) is an appropriately chosen integer. A case in point is the series \( B_{3,2}(n) \) which may be written explicitly from Eq.(10) as:
\[
B_{3,2}(n) = \frac{1}{e} \sum_{k=0}^{\infty} \frac{(n+k)! (n+k+1)!}{k! (k+1)! (k+2)!}.
\] (40)

Its hgf \( G_{3,2}(\lambda) \) is then:
\[
G_{3,2}(\lambda) = \sum_{n=0}^{\infty} \left[ \frac{B_{3,2}(n)}{n!} \right] \frac{\lambda^n}{n!} = \frac{1}{e} \sum_{k=0}^{\infty} \frac{1}{(k+2)!} F_1(k+2,k+2;1+\lambda).
\] (41)

Similarly one can work out other examples of hgf. See [15] for other instances where this type of hgf appear.

All the previous considerations also apply to the case \( r < s \). In this case we define the generalized Stirling numbers by (note the difference with Eq.(4)):
\[
r \leq s : \quad [(a^\dagger a)^r a^s]^n = N \left\{ [(a^\dagger a)^r a^s]^n \right\} = \sum_{k=r}^{nr} S_{r,s}(n,k)(a^\dagger a)^k a^k \right\} a^{n(s-r)},
\] (42)

By taking the Hermitian conjugate of Eq.(4), with the change \( r \leftrightarrow s \), we obtain
\[
r \leq s : \quad [(a^\dagger a)^r a^s]^n = \sum_{k=r}^{nr} S_{s,r}(n,k)(a^\dagger a)^k a^k \right\} a^{n(s-r)},
\] (43)

whence the symmetry relation:
\[
S_{r,s}(n,k) = S_{s,r}(n,k), \quad s \leq k \leq ns, \quad (r \leq s).
\] (44)

The normal ordering of \( F[a^s(a^\dagger a)^r] \) involves the antinormal to normal order, in the terminology of [16]. With this in mind we define the anti-Stirling numbers of the second kind \( \tilde{S}_{r,s}(n,k) \) as:
\[
r \geq s : \quad [a^s(a^\dagger a)^r]^n = (a^\dagger a)^{n(r-s)} \sum_{k=0}^{ns} \tilde{S}_{s,r}(n,k)(a^\dagger a)^k a^k \right\},
\] (45)
and similarly anti-Bell numbers: \( \tilde{B}_{r,s}(n) = \sum_{k=0}^{ns} \tilde{S}_{r,s}(n,k) \) for \( r \geq s \).

It can be demonstrated [4] that they satisfy the following symmetry properties:

\[
\tilde{S}_{s,r}(n,k) = \tilde{S}_{r,s}(n,k), \quad 0 \leq k \leq ns, \quad (r \geq s),
\]

(46)

\[
\tilde{S}_{r,s}(n,k) = S_{r,s}(n+1,k+s), \quad 0 \leq k \leq ns, \quad (r \geq s),
\]

(47)

and \( \tilde{B}_{r,s}(n) = B_{r,s}(n+1) \).

If in Eq.(1) \( F(x) \) has a Taylor expansion of \( F(x) \) around \( x_0 \neq 0 \), then

\[
F \left[ (a^r a^s) \right] = \mathcal{N} \left\{ F \left[ (a^r a^s) \right] \right\} = \sum_{k=0}^{\infty} \frac{F^{(k)}(x_0)}{k!} \mathcal{N} \left\{ [(a^r a^s - x_0)^k \right\},
\]

(48)

and our above results should be supplemented by the appropriate binomial expansion coefficients.

All the \( B_{r,s}(n) \) described here are the \( n \)-th moments of positive functions on the positive half axis; some solutions of the associated Stieltjes moment problem have been recently discussed at some length [17]. In addition we have found that even larger classes of combinatorial sequences are solutions of the moment problem and they can be used for the construction of new families of coherent states [18].

We are considering the possible combinatorial interpretation of the above results.

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Table 1.

| Triangles of generalized Stirling and Bell numbers, as defined by Eqs.(4) and(5). |
### $r=1, s=1$

| $n$  | $S_{1.1}(n,k)$ | $B_{1.1}(n)$ |
|------|----------------|--------------|
| 1    | 1              | 1            |
| 2    | 1 1            | 2            |
| 3    | 1 3 1          | 5            |
| 4    | 1 7 6 1        | 15           |
| 5    | 1 15 25 10 1   | 52           |
| 6    | 1 31 90 65 15 1| 203          |

| $n$  | $S_{1.1}(n,k)$ | $B_{1.1}(n)$ |
|------|----------------|--------------|
| 1    | 1              | 1            |
| 2    | 2 1            | 3            |
| 3    | 6 6 1          | 13           |
| 4    | 24 36 12 1     | 73           |
| 5    | 120 240 120 20 1| 501          |
| 6    | 720 1800 1200 300 30 1| 4051        |

### $r=2, s=2$

| $n$  | $S_{2.2}(n,k)$ | $B_{2.2}(n)$ |
|------|----------------|--------------|
| 1    | 1              | 1            |
| 2    | 2 4 1          | 7            |
| 3    | 4 32 38 12 1   | 87           |
| 4    | 8 208 652 576 188 24 1| 1657     |
| 5    | 16 1280 9080 16944 12052 3840 580 40 1| 43833  |
| 6    | 32 7744 11656 542800 420080 322848 98296 16000 1390 60 1| 1515903|

### $r=3, s=2$

| $n$  | $S_{3.2}(n,k)$ | $B_{3.2}(n)$ |
|------|----------------|--------------|
| 1    | 1              | 1            |
| 2    | 6 6 1          | 13           |
| 3    | 72 168 96 18 1 | 355          |
| 4    | 1440 5760 6120 2520 456 36 1| 16333       |
| 5    | 43200 259200 424800 285120 92520 15600 1380 60 1| 1121881    |
| 6    | 1814400 15120000 34776000 33566400 16304400 4379760 682200 62400 3270 90 1| 106708921  |