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Addition of a large number of identical angular momenta. Statistical distributions

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Abstract. The quantum mechanical addition of an arbitrary (very large) number of identical angular momenta is considered. The resulting states jm usually occur many times. In this paper the corresponding multiplicities P_j and Q_m are investigated. Several explicit formulae for Q_m are given. The asymptotic approximations for multiplicities P_j and Q_m , which are the Wigner and Gauss distributions respectively, are derived. All parameters of the distributions are explicitly obtained. A comparison of theoretical multiplicities with the exact ones is made when the number of angular momenta is relatively small.

1. Introduction

Let us consider *n* identical spins, each having the angular momentum *s*. Under the quantum mechanical vector addition of these angular momenta the resulting angular momenta j = ns, ns - 1, ... 0 (or $\frac{1}{2}$) occur with multiplicities P_{jn}^s . Further, we label the number of states of the system with whole magnetic quantum number *m* as Q_{mn}^s .

The basic relations between the numbers P and Q are

$$\sum_{m=-ns}^{ns} Q_{mn}^{s} = \sum_{j=0(\frac{1}{2})}^{ns} (2j+1) P_{jn}^{s} = \chi^{n},$$
(1)

$$P_{jn} = Q_{mn} - Q_{m+1,n} |_{m=j}$$
⁽²⁾

where $\chi = 2s + 1$. For very large *n* and $s = \frac{1}{2}$ we have the statistical approximation

$$Q_{mn}^{1/2} = 2^n (\pi n/2)^{-1/2} \exp(-2m^2/n), \qquad (3)$$

see for example Kittel (1977).

Bloch (1954) has considered the distribution of total angular momentum in the nucleus which consists of many particles each having an angular momentum. He has derived the asymptotic formula for the number N_i (analogous to our P_i) of levels with angular momentum j and energy up to a given value, which has the form of the Wigner distribution

$$N_j \sim (2j+1) \exp[-(j+\frac{1}{2})^2/2\sigma^2].$$
(4)

Cleary and Wybourne (1971), using group theoretical methods and the theory of numbers, have investigated, for large n, the distribution of the angular momentum multiplicities which arise in the irreducible representation [n, 0, 0, ..., 0] of SU(2s + 1). They have found that the numbers Q_m have a normal distribution and, as a

consequence, the numbers P_j are distributed with respect to j according to the Wigner-type form.

Büttner (1967) and Mikhailov (1974) have derived generating functions, recurrence relations and tables for multiplicities which have been considered from the asymptotic point of view by Cleary and Wybourne (1971).

Mikhailov (1977) and Rashid (1977), using different methods, have found an explicit formula for the numbers P_i :

$$P_{jn}^{s} = \sum_{k} (-1)^{k} \binom{n}{k} \binom{(s+1)n - j - \chi k - 2}{n-2}.$$
(5)

In § 2 of this paper we write several explicit formulae for the numbers Q_m , one of which is very similar to formula (5). In § 3 the generating functions and, as a consequence, the recurrence relations for the numbers Q_m and P_j are determined. The asymptotic formulae for the numbers Q and P are derived in §§ 4 and 5. The formulae have the forms of Gauss and Wigner distributions accordingly, as well as the asymptotic formulae for angular momentum multiplicities in the irreducible representation $[n, 0, 0, \ldots 0]$ of the group SU(2s + 1) (Cleary and Wybourne 1971). All the distribution parameters obtained in this paper are explicitly determined in terms of the numbers of particles n and their angular momenta s. In the particular case when $s = \frac{1}{2}$, the expression for the numbers Q inevitably proves to be formula (3).

2. Exact expression for the numbers Q

In addition to formula (5) for P_{jn}^{s} the generalising numbers $P_{jn}^{s\nu}$ (Mikhailov 1977) were introduced:

$$\boldsymbol{P}_{jn}^{s,0} \equiv \boldsymbol{P}_{jn}^{s}, \qquad \boldsymbol{P}_{jn}^{s,\nu-1} = \boldsymbol{P}_{jn}^{s,\nu-1} - \boldsymbol{P}_{j+1,n}^{s,\nu-1}$$
(6)

$$P_{jn}^{s\nu} = \sum_{k} (-1)^{k} \binom{n}{k} \binom{(s+1)n - \chi k - j - \nu - 2}{n - \nu - 2}.$$
(7)

As may be seen from the last expression, the numbers $P_{jn}^{s\nu}$ have a simple transformation when j and ν are changed. In particular, the relations (6) and (7) are true when ν is negative. This may be proved by the same method as in Mikhailov (1977) for positive ν . Setting $\nu = 0$ in (6), we find recurrence relations which are identical to (2). Further, observing that initial values of P and Q (when j = ns, m = ns) are equal,

$$P_{ns,n}^{s,-1} = P_{ns,n}^{s} = Q_{ns,n}^{s} = 1,$$

we obtain

$$Q_{mn}^{s} = P_{mn}^{s,-1} = \sum_{k} (-1)^{k} \binom{n}{k} \binom{(s+1)n - \chi k - m - 1}{n-1}.$$
(8)

With the help of (12) from Mikhailov (1977) we find that

$$Q_{mn}^{1/2} = \binom{n}{n/2 - m}.$$

For s = 1, m = 0 the numbers Q_{mn}^s have an interesting structure. From the beginning we give the sequence of the first 13 numbers $Q_{0,n}^1 = Q_n = 1, 1, 3, 7, 19, 51, 141$,

393, 1107, 3139, 8953, 25653, 73789 (n = 0, 1, ..., 12). This concise table allows us to check the hypothetical expression

$$Q_n = \sum_{k=0}^{\lfloor n/2 \rfloor} A_k \binom{n}{2k},\tag{9}$$

where

$$A_k = \sum_{i=0}^k Q_i \binom{k}{i}.$$
 (10)

Finally we have

$$Q_n = \sum_k \sum_i Q_i \binom{k}{i} \binom{n}{2k}.$$
(11)

This is the self-reproducing series of numbers. It may be constructed from $Q_0 = 1$. Further, the numbers A_k proved to have another and more simple form

$$A_k = \binom{2k}{k}.$$
(12)

The last expression together with (10) gives the formula for the summation of the numbers Q_n with binomial coefficients as the summation weights. Using (9) and (12) we have

$$Q_n = \sum_{k} \frac{n!}{k!(n-2k)!k!},$$
(13)

which allows the generalisation for the case when m and s are arbitrary integer or half-integer numbers

$$Q_{mn}^{s} = \sum_{n_{\mu}} \frac{n!}{n_{s}! n_{s-1}! \dots n_{-s}!},$$
(14)

$$\sum_{\mu} \mu n_{\mu} = m, \qquad \sum_{\mu} n_{\mu} = n.$$
(15)

3. Generating functions

From (14) we may see that the numbers Q are equal to the coefficients in the decomposition of the polynomial of degree n

$$\left(\sum_{\mu=-s}^{s}\phi_{\mu}^{s}\right)^{n}=\sum_{m=-ns}^{ns}Q_{mn}^{s}\phi_{mn}^{s},$$
(16)

where

$$\phi_{\mu}^{s} = x^{s+\mu} y^{s-\mu}, \qquad \phi_{mn}^{s} = x^{ns+m} y^{ns-m}$$

Then the generating function for all numbers Q may be written in the form

$$\exp\left(\sum_{\mu}\phi_{\mu}^{s}\right) = \sum_{n=0}^{\infty}\sum_{m}\frac{1}{n!}Q_{mn}^{s}\phi_{mn}^{s}.$$
(17)

The condition (2) in combination with (16) leads to the relation

$$(x-y)\left(\sum_{\mu} \phi_{\mu}^{s}\right) = \sum_{j=0(1/2)}^{ns} P_{jn}^{s}(x\phi_{jn}^{s} - y\phi_{-j,n}^{s})$$
(18)

from which we can easily deduce the generating function for the numbers P_{in}^{s} ;

$$(x - y) \exp\left(\sum \phi_{\mu}^{s}\right) = \sum_{n=0}^{\infty} \sum_{j} \frac{1}{n!} P_{jn}^{s} (x \phi_{jn}^{s} - y \phi_{-j,n}^{s}).$$
(19)

The recurrence relations can be derived from the last four formulae. Let for example $n_1 + n_2 = n$ then (16) leads to the equality

$$\sum_{m_1} Q^s_{m_1,n_1} \phi^s_{m_1,n_1} \cdot \sum_{m_2} Q^s_{m_2,n_2} \phi^s_{m_2,n_2} = \sum_m Q^s_{mn} \phi^s_{mn},$$

$$m_1 + m_2 = m,$$

from which we have

$$\sum_{n_1, m_2} Q^s_{m_1, n_1} Q^s_{m_2, n_2} = Q^s_{mn}.$$
(20)

For $n_2 = 1$ the equality $Q_{m_2,n_2}^s = 1$ $(m_2 = -s, -s + 1, ..., s)$ is true; then from (20) we obtain

$$Q_{m-s,n-1}^{s} + Q_{m-s+1,n-1}^{s} + \ldots + Q_{m+s,n-1}^{s} = Q_{mn}^{s}.$$
 (21)

This recurrence relation bears a great resemblance to the analogous relation (7) of Mikhailov (1977) for the numbers P_{jn}^{s} .

4. Asymptotic formula for Q

We mentioned in the Introduction that the numbers Q_{mn}^s are distributed in accordance with the Gauss form for $s = \frac{1}{2}$ and $n \to \infty$ (3). The comparison with the exact values of Qshows that for $s > \frac{1}{2}$ the approach to the normal distribution, provided n is increasing, is faster than for $s = \frac{1}{2}$. Further, without special proof, we use as a basis the theorem that the normal distribution is the true asymptotic formula for the numbers Q. Our aim will be to find the parameters of this distribution.

Thus we start from the formula

$$Q_{mn}^{s} = Q_{0n}^{s} \exp(-m^{2}/c_{n}^{s}).$$
(22)

Having rewritten the normalisation condition (1) for $n \rightarrow \infty$ in the integral form

$$\int_{-\infty}^{+\infty} Q_{mn}^{s} \, \mathrm{d}m = \chi^{n} \tag{23}$$

we obtain

$$Q_{0n}^{s} = \chi^{n} (\pi c_{n}^{s})^{-1/2}.$$
(24)

For $s = \frac{1}{2}, 1, \ldots, 4$ and $n = 1, 2, \ldots, 10-20$ (depending on s) the tables of exact numbers Q_{mn}^s have been calculated by the author. These tables may be used as the experimental material to check the proposed theoretical formulae. In particular the exact numbers must obey condition (22) for m = 1. It is not difficult to obtain the sequence of parameters c_n^s which is given in table 1 for s = 1, but the basic contents of the tables are the differences $\delta(c_n^s) = c_n^s - c_{n-1}^s$.

With the help of the table we may see that for increasing *n* the differences δ approximate to the numbers $\Delta_s : \Delta_1 = \frac{4}{3}, \Delta_{3/2} = \frac{5}{2}, \Delta_2 = 4$. By means of a similar straightforward method we found that $\Delta_3 = 8, \Delta_4 = \frac{40}{3}$. Also from (3) we have $\Delta_{1/2} = \frac{1}{2}$.

Assuming that $\delta(c_n^s)$ approximates to the constant value in all cases under consideration, we adopt the second supposition which is concluded in the equality

$$c_n^s = \Delta_s \,.\, n \tag{25}$$

where *n* is very large. Then it is not difficult to see that all the numbers Δ_s may be written in the simple form

$$\Delta_s = 2s(s+1)/3. \tag{26}$$

Table 1. The parameters c_n^s and their differences $\delta(c_n^s)$ which were obtained for m = 1 assuming (22) to be true. The numbers Q_{0n}^s and Q_{1n}^s were extracted from the tables of exact numbers Q.

<i>s</i> = 1	n c δc	10 14·34	11 15·67 1·338	12 17·00 1·330	13 18·34 1·3335	14 19·67 1·3321	15 21.00 1.3330	16 22·34 1·3333
$s = \frac{3}{2}$	n 2δc		8 5·173	10 5∙014	12 4·995			
$s=\frac{3}{2}$	n 2δc		7 4·77	9 4·97	11 4·994	13 4∙997		
<i>s</i> = 2	n δc		6 3·13	7 4·35	8 3·88	9 4·02	10 3·98	11 3·99

Summarising the formulae (22), (24–26) we write the asymptotical formula, which was sought for, in the explicit form

$$Q_{mn}^{s} = \chi^{n} [2ns(s+1)/3]^{-1/2} \exp[-3m^{2}/2ns(s+1)].$$
⁽²⁷⁾

The last formula can be proved quite strictly by means of the recurrence relations (21). As before, the starting points of our proof are the two assumptions (22) and (25). Substituting (22) in (21) and using the expression for the normalisation constant (24) we obtain

$$\sum_{\mu=-s}^{s} \exp[-(m+\mu)^2/\Delta_s(n-1)] = (2s+1)[(n-1)/n]^{1/2} \exp(-m^2/\Delta_s n).$$

If we divide both sides of the equality by the exponential from the right-hand side and make small simplifications, we get

$$\exp\left(-\frac{m^2}{\Delta_s n(n-1)}\right) \sum_{\mu} \exp\left(\frac{2m\mu - \mu^2}{\Delta_s (n-1)}\right) = (2s+1)[(n-1)/n]^{1/2}.$$
 (28)

Supposing *m* sufficiently small in comparison with *ns* (maximum of *m*), taking into account that $\Delta_s > 1$ for $s \ge 1$, we substitute unity for the first exponential in (28), expand the other exponentials in powers of $(2m\mu - \mu^2)/\Delta_s(n-1)$ and break the series off after

linear terms. Moreover, taking into account that $\Sigma_{\mu} \mu = 0$ we obtain

$$(2s+1) - [\Delta_s(n-1)]^{-1} \sum_{\mu} \mu^2 = (2s+1)[(n-1)/n]^{1/2},$$
(29)

and finally

$$\Delta_{s} = \lim_{n \to \infty} \left[(n-1)\{1 - [(n-1)/n]^{1/2}\}(2s+1) \right]^{-1} \sum_{\mu} \mu^{2}$$
$$= \left[\frac{2}{(2s+1)} \right] \left[\frac{s(s+1)(2s+1)}{3} \right] = \frac{2s(s+1)}{3}.$$
(30)

The comparison of the Gauss distribution (27) with the exact numbers Q shows satisfactory agreement. First of all, the numbers Q_{0n}^s , calculated with the help of (24), approximate more exactly to the true multiplicities while n is increasing (checked for $s = \frac{3}{2}$, 2) or s is increasing (checked for n = 8). Further for s = 4, n = 8 the inner half of the succession of the theoretical numbers $Q_{mn}^s(|m| \le ns/2)$ does not deviate from the exact number succession more than 4% and for s = 4, n = 9 by more than 3.5%. But it must be mentioned that the wings of the Gauss curve (|m| > ns/2) give appreciably increased values when n and s are comparatively small.

5. Asymptotic formula for P

We have obtained an approximate (for small n) expression for multiplicities Q(27), which for $n \to \infty$ is an asymptotic formula. With the help of (2) we try to find an analogous approximation for the numbers P. Substituting (22), (25) into (2) one finds that

$$P_{jn}^{s} = Q_{0n}^{s} \exp(-j^{2}/c_{n}^{s}) \{1 - \exp[-(2j+1)/c_{n}^{s}]\}$$

= $Q_{0n}^{s} (2j+1/c_{n}^{s}) \exp(-j^{2}/c_{n}^{s}) \{1 - (2j+1)/2c_{n}^{s} + \ldots\}.$ (31)

Let us neglect $(2j+1)/2c_n^s$ because of

$$(2j+1)/2c_n^s \le \frac{3ns}{2ns(s+1)} = \frac{3}{2(s+1)} \le 1.$$

Here j has been replaced by its maximum ns. The approximation adopted is quite accurate when j < ns/3 or ns/4 and the more exact, the greater s.

If the series in curly brackets of (31) is broken off, the formulae do not satisfy the normalisation condition (1), which we rewrite for $n \to \infty$ in the integral form

$$\int_{0}^{\infty} (2j+1) P_{jn}^{s} \, \mathrm{d}j = \chi^{n}.$$
(32)

Defining the new normalisation constant P_{0n}^{s} from (32), we obtain finally

$$P_{jn}^{s} = P_{0n}^{s}(2j+1) \exp(-j^{2}/c_{n}^{s}),$$

$$P_{0n}^{s} = \chi^{n} [(\pi c_{n}^{s})^{1/2} (c_{n}^{s} + \frac{1}{2}) + 2c_{n}^{s}]^{-1}.$$
(33)

How close to the true multiplicities are the numbers P from (33)? For the purpose of comparison we will consider the quantity $|\Delta P|$ which is the modulus of relative deviation of theoretical numbers P from true ones.

For constant s and increasing $n |\Delta P|$ increases, reaches its maximum $|\Delta P|_{max}$ for some n = n' and after that decreases to zero. For some small s we have

S	1	2	3	4
$n' \Delta P^s_{0n} _{\max}$	6	12	20	>20
	17%	7%	4∙6%	<2·5%

For s = 1 the modulus of deviation has a poorly distinguished maximum and the numbers n = 6 and $|\Delta P|_{\text{max}} = 17\%$ are to some extent conditional.

On the other hand, if we increase the index j beginning from zero, we will find that $|\Delta P|$ is smaller than or approximately equal to $|\Delta P|$ for j = 0. This will be true up to $j \approx ns/2$. In the region of $j \approx j_{max}$ (the value of j for which P_j has a maximum) the relative error is particularly small. It is not difficult to find from (33)

$$j_{\max} = [(8n\Delta_s + 1)^{1/2} - 1]/4 \approx n\Delta_s/2.$$

For j > ns/2 (the tail of the distribution curve) and small n, the theoretical numbers apparently exceed the true ones.

As a whole, for small $j(j \le ns/3)$ and for increasing *n* the relative error moves to zero. Figure 1 gives quite good proof of this statement, where the theoretical and true numbers *P* for n = 10 and s = 4 are given.



Figure 1. Angular momentum multiplicities P_i which occur with the addition of ten angular momenta each equal to four. The smooth curve is derived in accordance with formula (27). The discrete points are exact multiplicities.

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