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Rapid calculation of exact spin distributions of multilevel configurations

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A simple extension of a previously derived result allows one to efficiently calculate the spin distribution of an arbitrary combination of fermionic and bosonic levels with a fixed number of particles per level. The calculation time is approximately linear in the maximum total angular momentum and depends very little on the actual complexity of the configuration. The method is recursive and easy to use even without going into the details of its derivation.

Spin distributions of multilevel configurations are of interest for a variety of reasons. Their calculation can present an important practical problem, especially in the shell model with its very large configuration space. For low-lying configurations, one can resort to published tabulations.[1,2] For extensive calculations, such as that of Hillman and Grover,[3] one has to make one's own program, and the usual method is an odometer that scans systematically all single-particle distributions searching for those compatible with the Pauli principle.[3,4] The inefficiency of this procedure has apparently been one of the real limitations of the combinatorial approach to the calculation of nuclear level densities.[5] For high-lying configurations, the approximate expression of Bethe[6] is most often used.[5] Its modified Gaussian form (13) has been shown by Cleary and Wybourne[7] to be the asymptotic limit of an exact approach.

I wish to report on a recursive algorithm that efficiently generates the exact spin distribution of any multilevel configuration, even one including bosonic levels, as encountered in composite models. The report is self-contained in the sense that the extension may be understood without the references, if the previous result is taken for granted.

It has been shown[8] that the multiplicity of states with a given total angular momentum projection M for n particles of spin j is equal to the coefficient of q^M in

$$q^{-J_{max}}\begin{bmatrix} r \\ n \end{bmatrix}_q , \tag{1}$$

where the square brackets denote a Gaussian polynomial,[9] having powers of q from zero to $2J_{max} = n(r-n)$, and

$$r = 2j+1 \text{ (fermions)} ,$$
$$r = 2j+n \text{ (bosons)} . \tag{2}$$

The coefficients of the polynomial in (1) are best calculated by use of the property of any formal series in q with $c_0 = 1$, that if coefficients p_k are defined by

$$\sum_{m \geq 0} c_m q^m = \exp\left(\sum_{k \geq 1} \frac{1}{k} p_k q^k\right) , \tag{3}$$

then the c's are generated by a recursion with use of the p's:

$$mc_m = p_1 c_{m-1} + p_2 c_{m-2} + \cdots + p_{m-1} c_1 + p_m . \tag{4}$$

For the particular case of a Gaussian polynomial,

$$p_k = \sum_{\substack{s=1 \\ s|k}}^{\min(n,r-n)} s - \sum_{\substack{s=\max(n,r-n)+1 \\ s|k}}^{r} s , \tag{5}$$

where r and n appear in (1), and $s|k$ means that s must divide k in order to contribute to (5).

Once the coefficients are calculated through (4), the multiplicity of a given $J = M$ is obtained by subtracting two successive M-state multiplicities [coefficients of q^M and q^{M+1} in (1)], as described in any textbook.[4]

I shall now extend the method for the case of more than one level. If two particles which differ by some quantum number are coupled, the resulting angular momentum is restricted only by the triangle relation

$$|j_1 - j_2| \leq J \leq j_1 + j_2 . \tag{6}$$

I now make the simple but essential observation that all the projection states of the composite system are obtained by addition of the two single-particle projections in all possible ways. This corresponds to a multiplication of two generating functions (1) with $n = 1$,

$$(q^{-j_1} + q^{-j_1+1} + \cdots + q^{j_1-1} + q^{j_1})$$
$$\times (q^{-j_2} + q^{-j_2+1} + \cdots + q^{j_2-1} + q^{j_2}) . \tag{7}$$

So (7) is the generating function for the M-state multiplicities of the composite system. A third particle may be added by multiplying (7) with the appropriate generating function, and so on, up to any number of particles. Since the multiplication of polynomials is commutative and associative, the result does not depend on the order of the couplings, and an extended expression of the type (7) may be expressed as the product of "clusters," each cluster representing a subsystem. A special cluster is given by (1). It contains all the information on symmetry restrictions of angular momentum couplings within one level. Since the angular momenta of different levels couple without such restrictions, the generating function of the M-state multiplicities of a configuration of z levels with n_i particles per level is the product of the generating functions (1) of individual levels,

$$q^{-J_{max}^{tot}} \prod_{i=1}^{z} \begin{bmatrix} r_i \\ n_i \end{bmatrix}_q , \tag{8}$$

with

$$J_{max}^{tot} = \sum_{i=1}^{z} J_{max}^{(i)} ,$$

and $J_{max}^{(i)}$ is given below (1).

To calculate the coefficients appearing in (8), expression (3) may be used to advantage. Since a product of the series corresponds to summation in the exponent, we have the

expression

$$p_k = \sum_{i=1}^{z} p_k^{(i)} \qquad (9)$$

for the p coefficient of the product in (8). The numbers $p_k^{(i)}$ are of course given by (5) with $r = r_i$ and $n = n_i$. Now (4), which is valid for any formal series, may be used to obtain the M-state multiplicities of the multilevel configuration.

I shall now illustrate the method with a concrete example, and at the same time provide a recipe for its implementation.

Suppose there are ten particles in the $f_{7/2}$ shell, in the configuration $(\tfrac{7}{2})^3(\tfrac{3}{2})^2(\tfrac{5}{2})^2(\tfrac{1}{2})^1(\tfrac{9}{2})^2$. The generating function (8) is

$$q^{-22} \begin{bmatrix} 8 \\ 3 \end{bmatrix}_q \begin{bmatrix} 4 \\ 2 \end{bmatrix}_q \begin{bmatrix} 6 \\ 2 \end{bmatrix}_q \begin{bmatrix} 2 \\ 1 \end{bmatrix}_q \begin{bmatrix} 10 \\ 2 \end{bmatrix}_q . \qquad (10)$$

According to (9), the p's for the product in (10) are given by

$$p_k = \sum_{\substack{s=1 \\ s|k}}^{3} s - \sum_{\substack{s=6 \\ s|k}}^{8} s + \sum_{\substack{s=1 \\ s|k}}^{2} s - \sum_{\substack{s=3 \\ s|k}}^{4} s + \sum_{\substack{s=1 \\ s|k}}^{2} s$$

$$- \sum_{\substack{s=5 \\ s|k}}^{6} s + \sum_{\substack{s=1 \\ s|k}}^{1} s - \sum_{\substack{s=2 \\ s|k}}^{2} s + \sum_{\substack{s=1 \\ s|k}}^{2} s - \sum_{\substack{s=9 \\ s|k}}^{10} s , \qquad (11)$$

which is easily arranged to read

$$p_k = 5 + 3 \times \{2;2|k\} - \{6;6|k\} - \sum_{\substack{s=4 \\ s|k}}^{10} s , \qquad (12)$$

where the curly brackets mean that the number inside contributes if it divides k. Since $J_{max}^{tot} = 22$, we need the first 23 c coefficients, corresponding to all nonpositive projections, beginning with $c_0 = 1$. Thus we need the p's up to p_{22}. They are given in Table I, which also shows a good way to implement the recursion (4). The reader is urged to complete Table I himself.

The J multiplicites are differences of successive c's, and are shown in Table II. If a four-function calculator is used, it takes about an hour to complete Table II, beginning with writing (10).

The procedure is self-checking. Once (12) is written correctly, any error in the p's will show up as a noninteger c when the erroneous p is first introduced. The final result may be checked dimensionally, since the total number of M states is equal to the product of binomial coefficients corresponding to (10), and also to

$$\sum_J n_J(2J+1) .$$

The calculation time depends linearly on the number of p's and c's which need to be calculated, and this is equal to J_{max}^{tot} (or $J_{max}^{tot} - \tfrac{1}{2}$ for half-integer J's). The complexity of the configuration enters only in the expression for the p's (11), but this is easily reduced to expressions of the type (12), where the complexity shows up mostly through factors multiplying the various entries. Thus one is justified in saying that the calculation time depends "very little" on the complexity of a configuration producing a given total maximum angular momentum.

One promising application of the method is to upgrade

TABLE I. Values of p_k (12) for the configuration $(\tfrac{7}{2})^3(\tfrac{3}{2})^2(\tfrac{5}{2})^2(\tfrac{1}{2})^1(\tfrac{9}{2})^2$ are shown together with some M-state multiplicities c_m. The sum of products of the superposed coefficients is 125 320, which divided by 13 gives 9640 for c_{13}. The lower two rows (c_m, m) may then be moved one step to the left, and the process repeated. See (4).

k		0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
p_k			5	11	5	7	0	-1	-2	-1	-4	-4	5	-5	5	4	0	-1	5	-10	5	-8	-2	11
c_m		9640	7222	5207	3602	2381	1497	889	495	255	120	50	18	5	1									
m	14	13	12	11	10	9	8	7	6	5	4	3	2	1	0									

TABLE II. Spin distribution for the configuration $(\tfrac{7}{2})^3(\tfrac{3}{2})^2(\tfrac{5}{2})^2(\tfrac{1}{2})^1(\tfrac{9}{2})^2$. The multiplicities are differences of successive c's in Table I.

J	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
n_J	422	1236	1956	2536	2939	3153	3180	3043	2775	2418	2015	1605	1221	884	608	394	240	135	70	32	13	4	1

the combinatorial approach to the calculation of nuclear level densities, extending it to heavier nuclei and higher energies. It is also possible to investigate the spin distributions in composite models at high excitations, and thus take into account shape effects[10] in a semimicroscopic way. [Some of the r_i's in (8) would then be of the "bosonic" type (2).]

Another application would be to attempt to justify from a shell-model point of view the published empirical values of A and σ in the expression[5,6]

$$\rho_J = A(J + \tfrac{1}{2})\exp[-(J + \tfrac{1}{2})^2/\sigma^2] \, , \tag{13}$$

such as those given by Gilbert and Cameron.[11]

While one may find A and σ to fit a concrete distribution such as the one in Table II, general statements about A and σ as functions of r_i and n_i in (8) are difficult to obtain. This is because any such statement contains, through (5), some general statement about the divisibility of numbers, and that is a notoriously difficult problem of number theory. This observation ties in nicely with a comment by Cleary and Wybourne,[7] who noted that expressing A and σ in this fashion "is closely akin to the elusive problem of solving the Clebsch-Gordan series in an analytic sense." It seems,

then, that the latter problem is also connected with the divisibility problem.

We have shown in this report how to calculate *efficiently* the spin distribution of an arbitrary multilevel configuration. The problem of determining which configurations contribute at a given energy and to what extent has not been touched upon. In order to solve it, some specific model has to be invoked. As far as the concept of single-particle levels labeled by angular momentum can be considered model independent, we may reasonably conclude that we have solved the model-independent part of the microscopic level-density problem.

Note added in proof. The author recently received a copy of an article by M. G. Hirst and B. G. Wybourne, J. Phys. A (to be published), where A and G are expressed through r and n in a way that avoids both problems mentioned above. Its implications for them remain to be investigated.

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