Plethysm in Physics and Chemistry Applications

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I have yet to see any problem, however complicated, which, when you looked at it in the right way, did not become still more complicated.
—Poul Anderson

ABSTRACT

The relevance of the mathematical concept of plethysm to physical problems is considered. The role of plethysm in symplectic many-body models is outlined with particular emphasis on the case of the isotropic harmonic oscillator.

1. Introduction

The symmetrization postulate that the wavefunction for n identical fermions must be totally antisymmetric with respect to positional permutations of the particles and that for n identical bosons must be totally symmetric has a strong experimental underpinning (See [1-3] and references therein). The construction of wavefunctions according to the symmetrization postulate is central to many quantum physics applications. Note that the symmetrization postulate refers to the *total* wavefunction. The total space of the wavefunction may factor into the product of two, or more, subspaces as for example into the product of a spin and an orbital space. The functions spanning these subspaces need not be symmetric or antisymmetric with respect to permutations but may be of mixed permutational symmetry. The only requirement is that the total space be symmetric or antisymmetric. This means that the various subspaces will be symmetrized according to particular irreducible representations of the symmetric group $\mathcal{S}_N$ in the case of an $N-$particle system.

A common problem in physics is to have a set of functions that span an irreducible representation λ of some group $\mathcal{G}$ and to form an $N-$fold product of these functions. The resulting set of functions will span the irreducible representations contained in the $N-th$ Kronecker power of the irreducible representation λ. This Kronecker power may be resolved into parts of definite permutation symmetry according to

$$\lambda^{\times N} = \sum_{\rho \vdash N} f_N^{\rho} \lambda \otimes \{\rho\} \tag{1}$$

where f_N^{ρ} is the dimension of the irreducible representation $\{\rho\}$ of the symmetric group $\mathcal{S}_N$ and the summation is over all standard partitions (ρ) of the integer N. The terms $\lambda \otimes \{\rho\}$ represent the terms in the $N-th$ Kronecker power of λ that are symmetrized with respect to permutations and transforming under the $\{\rho\}$ irreducible representations of $\mathcal{S}_N$. $\lambda \otimes \{\rho\}$ will normally correspond to a *reducible* representation of the group $\mathcal{G}$. The process of resolving $\lambda \otimes \{\rho\}$ into irreducible representations of the group $\mathcal{G}$ is commonly referred to as a *plethysm*, a term coined by D. E. Littlewood in connection with his "new multiplication of $S-$functions".

The group $\mathcal{G}$ may be a finite group, such as the octahedral $\mathcal{O} \sim \mathcal{S}_4$ or icosahedral $\mathcal{I} \sim \mathcal{A}_5$ groups, or a compact Lie group or a non-compact Lie group. The group $\mathcal{G}$ may be a simple group or a product of several groups of various types depending on the nature of the physical problem being considered. The Schur functions[4-8] ($S-$functions for brevity) play a key role in the practical resolution of plethysms[4,5,9-11]. The basic ideas of symmetric functions and $S-$function plethysm are sketched in the proceedings of an earlier school[12] and will not be repeated here. The key idea here is that if one knows how to expand the characters of the group $\mathcal{G}$ as a sum of $S-$functions and inversely express $S-$functions as characters of the group $\mathcal{G}$[5,13-16] then the evaluation of plethysms for the group $\mathcal{G}$ reduces to an evaluation of S–function plethysms.

2. Boson and fermion $N-$ particle states

In many cases one needs to know what are the possible states for N identical bosons or fermions. If λ is a finite dimensional representation , not necessarily irreducible, of the group $\mathcal{G}$ which is spanned by a finite set of single particle states then the relevant plethysms are

$$\lambda \otimes \{1^N\} \qquad \text{For } N \text{ fermions} \tag{2a}$$

$$\lambda \otimes \{N\} \qquad \text{For } N \text{ bosons} \tag{2b}$$

The symmetry postulate limits N in the case of fermions to $dim(\lambda)_{\mathcal{G}}$ whereas for bosons there is no limit.

In the case of fermions or bosons having an angular momentum $j = m/2$ we have, from Hermite's reciprocity principle[17] for the binary full linear group,

$$\{m\} \otimes \{1^N\} = \{m+1-N\} \otimes \{N\}, \quad m+1 \geq N \tag{3a}$$

$$\{m\} \otimes \{1^N\} = \{N\} \otimes \{m+1-N\}, \quad m+1 \geq N \tag{3b}$$

$$\{m\} \otimes \{1^N\} = \{m\} \otimes \{1^{m+1-N}\}, \quad m+1 \geq N \tag{3c}$$

The above results give a direct link between totally antisymmetric and totally symmetric states. Thus from Eq.(3a) we see that the totally antisymmetric orbital states of g^3 are in one-to-one correspondence with the totally symmetric orbital states of f^3. From Eq.(3b) we see there is a similar correspondence between the antisymmetric states of g^4 and the symmetric states of d^5. Finally the last equation, for jj-coupled states, exhibits the well-known particle-hole symmetry or in the case of LS-coupled states the so-called quarter-shell symmetry for states of maximum multiplicity.

The above examples all involve finite dimensional irreducible representations of a compact Lie group. However, even for a single fermion or boson the total set of states is infinite. In the well-known case of the isotropic three-dimensional harmonic oscillator the states are all discrete whereas in the corresponding Coulomb problem there are both discrete and continuum states. The enumeration of the states for $N-$particles in a harmonic or Coulomb problem raise new aspects of plethysm involving infinite dimensional irreducible representations of non-compact Lie groups. Here we shall restrict discussion to the problem of $n-$particles in an isotropic harmonic oscillator potential, the first step in symplectic models of nuclei and certain mesoscopic systems.

3. The harmonic oscillator dynamical group for a single particle

The dynamical group for a single particle in an isotropic three-dimensional harmonic oscillator is the non-compact symplectic group $Sp(6,R)$. The associated Lie algebra is readily constructed from bilinear products of boson annihilation and creation operators defined in terms of the coordinates and momenta of the oscillator[18]. The complete set of states span two infinite dimensional unitary irreducible representations of the group $Sp(6,R)$ which I shall designate as $<\frac{1}{2};(0)>$ and $<\frac{1}{2};(1)>$[19-22]. These two irreducible representations belong to a single irreducible representation of the metaplectic group $Mp(6)$ which is the covering group of $Sp(6,R)$.

The group $Sp(6,R)$ has the group $U(3)$ as a maximal compact Lie subgroup and under the reduction $Sp(6,R) \Rightarrow U(3)$[15,16]

$$
\begin{aligned}
<\frac{1}{2};(0)> &\Rightarrow \varepsilon^{\frac{1}{2}}(\{0\}+\{2\}+\{4\}+\ldots) \\
&= \varepsilon^{\frac{1}{2}}M_{+} \qquad (4a) \\
<\frac{1}{2};(1)> &\Rightarrow \varepsilon^{\frac{1}{2}}(\{1\}+\{3\}+\{5\}+\ldots) \\
&= \varepsilon^{\frac{1}{2}}M_{-} \qquad (4b)
\end{aligned}
$$

where M_+ and M_- are respectively the *even* and *odd* terms of the infinite $S-$ function series indexed by the one part partitions (m) with $m = 0,1,\ldots,\infty$. Thus for a single particle the $<\frac{1}{2};(0)>$ and $<\frac{1}{2};(1)>$ irreducible representations of $Sp(6,R)$ are spanned by the *even* and *odd* parity states respectively.

4. Symplectic many-particle models and plethysms

Generalisation of the dynamical group approach for N identical non-interacting particles in a $d-$dimensional isotropic harmonic oscillator potential is straightforward[20-24]. The complete set of states span a single irreducible representation of the metaplectic group $Mp(2Nd)$, the covering group of $Sp(2ND,R)$. The metaplectic group $Mp(2Nd)$ has a very rich subgroup structure[20,21,23] as shown in Fig.1. These subgroup structures can be determined by contracting on particle or spatial indices. The diversity of the subgroup structures reflect different ways of separating the spatial and particle number dependencies. This topic has been discussed in the proceedings of our last school[20] and will not be explored further here. The *even* parity $N-$particle states span the $<\frac{1}{2};(0)>$ irreducible representation of $Sp(2Nd)$ and those of *odd* parity that of $<\frac{1}{2};(1)>$. These irreducible representations may be decomposed using the typical group chain

$$Sp(2ND,R)\supset Sp(2N,R)\times O(d)\supset Sp(2N,R)\times S(d) \tag{5}$$

with the $O(d)\Rightarrow S(d)$ leading to a determination of the spins of the various states. Such symplectic models for $N-$particles are important in the description of certain nuclear[25-28] and mesoscopic models[21]. These problems involve infinite dimensional unitary irreducible representations and the resolution of the Kronecker powers of the basic irreducible representations $<\frac{1}{2};(0)>$ and $<\frac{1}{2};(1)>$ for groups of the generic type $Sp(2n,R)$ and hence the evaluation of plethysms for these irreducible representations arises. Plethysms for the *reducible* representation $<\frac{1}{2};(0)>+<\frac{1}{2};(1)>$ have already been considered in the literature[27,28]. If one wishes to maintain close contact with configurations of particles in the usual shell model presentations it is desirable to be able to compute separately the plethysms

$$<\frac{1}{2};(0)>\otimes\{\nu\} \qquad \text{and} \qquad <\frac{1}{2};(1)>\otimes\{\nu\} \tag{6}$$

More generally, one may wish to compute plethysms of the generic type

$$<\frac{k}{2};(\lambda)>\otimes\{\nu\} \tag{7}$$

where under $Sp(2n,R)\Rightarrow U(n)$[16]

$$<\frac{k}{2};(\lambda)>\Rightarrow \varepsilon^{\frac{k}{2}}\cdot\{\{\lambda_s\}_N^k\cdot D_N\}_N \qquad N=min(n,k) \tag{8}$$

with $\{\lambda_s\}^k$ being a *signed sequence*[15,16] of terms $\pm\{\rho\}$ such that $\pm[\rho]$ is equivalent to $[\lambda]$ under the modification rules[13,14] for the group $O(k)$ and D_N the infinite $S-$function series indexed by even partitions into not more than N parts. The first $\cdot$ indicates a product in $U(n)$ and the second $\cdot$ a product in $U(N)$. Specific examples of this branching rule are given elsewhere[15,16]. The decomposition in Eq.(8) will normally involve an infinite series of $U(n$ irreducible representations and hence in practical applications the series must be truncated.

Likewise, the plethysms typified by Eqs. (6) and (7) will also involve an infinite series of $Sp(2n, R)$ irreducible representations and must be truncated in practical applications. In general

$$< \frac{k}{2}; (\lambda) > \otimes\{\nu\} = \sum_{\tau} c_{\nu}^{\tau} < \frac{\ell}{2}; (\tau) > \tag{9}$$

where

$$\ell = k \times |\nu| \tag{10}$$

where the c_{ν}^{τ} are non-negative integers.

A practical, though far from optimal, way of evaluating $Sp(2n, R)$ plethysms for the irreducible representation $< \frac{k}{2}; (\lambda) >$ is to first use Eq.(8) to express $< \frac{k}{2}; (\lambda) >$ in terms of list of $U(n)$ irreducible representations up to a chosen cutoff. Then select from the list the $U(n)$ irreducible representation of lowest weight, say $\{\rho_m\}$. Noting Eq. (8), this implies that at the $Sp(2n, R)$ level the plethysm necessarily contains the $Sp(2n, R)$ irreducible representation $< \frac{\ell}{2}; (\rho_m) >$. Thus we may remove from the list of $U(n)$ irreducible representations all those derived from $< \frac{\ell}{2}; (\rho_m) >$. The lowest weight irreducible representation contained in the residue of the $U(n)$ list is identified and the $U(n)$ content of the next $Sp(2n, R)$ irreducible representation removed. This process is continued up to the chosen cutoff.

Clearly the above method is completely impossible for hand calculations but has been implemented in the current version of **SCHUR**[29] which is the topic of my second lecture.

The plethysms of the irreps $< s; (0) >$ and $< s; (1) >$ are of particular interest in physics applications. The resolution of their Kronecker squares is straightforward. The terms, to weight 16, for plethysms for up to power 4 are relevant to the description of the states of two to four particles in an isotropic three-dimensional harmonic oscillator and have been evaluated. The tabulated results are available at the WEB site http://www.phys.uni.torun.pl/~bgw/.

5. Properties of $Sp(2n, R)$ plethysms

The advantage of having available even limited tables of $Sp(2n, R)$ plethysms is that they can be a source of clues for a deeper understanding of such plethysms and to suggest new identities[30]. Our detailed understanding of even plethysms for $S-$functions remains as very limited and does not encourage the search for properties of more general plethysms. Nevertheless some progress has been made[19,21,22,30] which we now briefly review. In the particular case of the Kronecker squares of $< s; (0) >$ and $< s; (1) >$ one is able to establish the complete results:-

$$< s; (0) > \otimes \{2\} = \sum_{i=0}^{\infty} < 1; (0 + 4i) > \tag{11}$$

$$< s; (0) > \otimes \{1^2\} = \sum_{i=0}^{\infty} < 1; (2 + 4i) > \tag{12}$$

$$< s; (1) > \otimes \{2\} = \sum_{i=0}^{\infty} < 1; (2 + 4i) > \tag{13}$$

$$< s; (1) > \otimes \{1^2\} =< 1; (1^2) > + \sum_{i=0}^{\infty} < 1; (4 + 4i) > \tag{14}$$

which hold for all $Sp(2n, R)$ with $n \geq 2$. For $n = 1$ the irrep $< 1; (1^2) >$ in Eq.(14) must be deleted. Further, one notices that the right-hand sides of Eqs. (12) and (13) are identical showing that

$$< s; (0) > \otimes \{1^2\} \equiv < s; (1) > \otimes \{2\} \tag{15}$$

Even more surprising is the equivalence

$$< s; (0) > \otimes \{21^2\} \equiv < s; (1) > \otimes \{31\} \tag{16}$$

These equivalences are associated with hitherto unknown S–function identities such as[22]

$$M_+ \otimes \{1^2\} \equiv M_- \otimes \{2\} \tag{17}$$

and

$$M_+ \otimes \{21^2\} \equiv M_- \otimes \{31\} \tag{18}$$

There are many hints that much remains to be discovered about the properties of $Sp(2n, R)$ plethysms. Inspection of tables for the plethyms $< s; (0) > \otimes \{\lambda\}$ and $< s; (1) > \otimes \{\tilde{\lambda}\}$ where $\tilde{\lambda}$ is the conjugate of λ suggests that the two plethysms are remarkably related by one-to-one mappings such that if

$$< s; (0) > \otimes \{\lambda\} = \sum_{\mu} g^{\mu} < k; (\mu) > \tag{19}$$

where $k = |\lambda|/2$ and g^{μ} is the multiplicity, then the terms $g^{\mu} < k; (\mu) >$ in $< s; (1) > \otimes \{\tilde{\lambda}\}$ are identical to those in Eq. (19) apart from those that are related by the following simple (μ) one-to-one mappings

$$\begin{array}{llllll}
\lambda \vdash 2 & (0) \to (1^2) & & & & \\
\lambda \vdash 3 & (0) \to (1^3) & (a) \to (a1) & (a1) \to (a) & & \\
\lambda \vdash 4 & (0) \to (1^4) & (a) \to (a1^2) & (a1^2) \to (a) & & \\
\lambda \vdash 5 & (0) \to (1^5) & (a) \to (a1^3) & (a1^3) \to (a) & (ab) \to (ab1) & (ab1) \to (ab) \\
\lambda \vdash 6 & (0) \to (1^6) & (a) \to (a1^4) & (a1^4) \to (a) & (ab) \to (ab1^2) & (ab1^2) \to (ab)
\end{array} \tag{20}$$

That such simple relationships seem to exist is by no means evident from the methods used to establish the plethysms and hints at an underlying simplicity that remains to be discovered and a conjugacy theorem still to be exposed.

6. Back to the harmonic oscillator

The above remarks give an increased understanding of even the case of two particles. It follows from the plethysm identity, Eq. (15), that for the even-parity two-particle states there is a one-to-one correspondence between the spin triplet states formed by two-particles in even-parity orbitals with the spin singlet states formed by two particles in odd-parity orbitals, a feature of the much studied isotropic three-dimensional harmonic oscillator potential that does not seem to have been hitherto observed. One finds that the plethysms exhibit stability properties[22] and hence certain plethysms for $Sp(2n,R)$ become independent of n and this must in turn be reflected in relating systems having different numbers of particles. It is now possible to systematically establish the $Sp(2n,R)$ irreducible representations relevant to a particular many-particle symplectic model. The evaluation of the decompositions for all the group-subgroup combinations exhibited in Fig. 1 are, in principle known, and readily computable. Nevertheless much remains to be done. Problems relating to multiplicity separation remain to be considered. Already enough is known to be able to discuss model Hamiltonians for explicit systems and much such work has been done in the case of nuclear symplectic models[25,26].

7 The Coulomb many-particle problem

As in the case of the harmonic oscillator it is possible to construct a dynamical group for a single charged particle in a spherically symmetric Coulomb field such as for the hydrogen atom[18]. The situation is complicated by the existence of an energy spectrum involving a discrete and a continuous part. The relevant dynamical group is $SO(4,2) \sim SU(2,2)$. Virtually nothing is known about plethysms for these groups and relatively little of their general group-subgroup decompositions. I know of no construction of a dynamical group structure similar to that shown in Fig. 1 for the harmonic oscillator.

8. Concluding remarks

The concept of plethysm developed originally as a part of the theory of symmetric functions but now finds wide application in many areas of physics and chemistry. Here we have merely sketched a few areas having said nothing about applications to selection rules, enumeration of effective operators, determination of normal forms for tensor polynomials of objects such as the Riemann tensor, explicit determination of the place of the adjoint representation in the Kronecker square of irreducible representations of simple Lie groups etc. Many of the results draw on developments in mathematics while others raise new problems in mathematics.

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