Recent Extensions and Developments in SCHUR

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The sublime and the ridiculous are often so nearly related, that it is difficult to class them separately. One step above the sublime makes the ridiculous, and one step above the ridiculous makes the sublime again
—Thomas Paine. 1737-1809

ABSTRACT

The programme SCHUR is an interactive C package for computing properties of Lie groups and symmetric functions. We illustrate a number of examples where the use of SCHUR has led to a several interesting conjectures and to their ultimate establishment as hitherto unknown theorems. A number of examples related to the non-compact group $Sp(2n, R)$ and its subgroups are discussed. The potential of SCHUR as a self-teaching tool is briefly considered.

1. Introduction

The range of problems requiring a detailed knowledge of the properties of Lie groups, compact and non-compact, is well illustrated by the group-subgroup structure relevant to N particles in a $d-$dimensional isotropic harmonic oscillator shown in Fig. 1. The practical implementation of such a structure requires a knowledge of a host of group-subgroup decompositions (or branching rules), Kronecker products and plethysms for both compact and non-compact Lie groups as well as properties such as the dimensions and Casimir operator eigenvalues of of irreducible representations . The non-trivial unitary irreducible representations of non-compact Lie group $Sp(2Nd, R)$ are infinite dimensional and hence one must be able to determine properties up to a user chosen cutoff. In determining the permutational symmetry of states one also needs to know decompositions such as $O(N) \Rightarrow S(N)$ where $S(N)$ is the finite symmetric group acting on N particles. This latter problem requires a knowledge of so-called *inner plethysms* which in turn requires a knowledge of symmetric functions such as the Schur functions ($S-$functions for brevity). Symmetric functions find many applications in chemistry and physics quite apart from their intrinsic interest in mathematics.

Practioners find that whereas in simple cases it is possible to proceed with hand calculations they rapidly achieve a state of mental exhaustion and doubts as to whether their results are error free. The algorithms for carrying out calculations are often very complex and frequently beyond the applicators knowledge. In making practical calculations, while understanding the basic physics of a given problem, the practioner should not require a simultaneous detailed knowledge of the mathematics behind the calculations.

The objective of **SCHUR**[1]has been to supply results with the complex algorithms fortunately hidden from view with the user able to obtain specific results and to be able to use these results in a fully interactive manner, effectively using **SCHUR** as a scratch pad. The development of **SCHUR** has occurred over many years and has been driven by response to specific research problems and in the need to make available to students a tool for learning about Lie groups by student creation of examples of practical examples.

In what follows I will first outline the tools included in **SCHUR** for carrying out

[1] The SCHUR package is available as a compiled C code for UNIX and DOS operating systems for IBM PC compatibles and work stations such as SUN, Hewlett-Packard and Silicon Graphics. The distribution is through S. Christensen, PO Box 16175, Chapel Hill, NC 27516 USA. Email: steve@smc.vnet.net . Additional details are available on the WEB at http://smc.vnet.net/Christensen.html and at the authors WEB site at http://www.phys.torun.pl/~bgw which contains downloadable versions of some of the papers referenced below as well as further examples of the use of SCHUR.

the computations required to analyse group-subgroup structures such as displayed in Fig. 1 and then show how **SCHUR** has led to various conjectures that in turn have led to new theorems. Finally I will briefly discuss the use of **SCHUR** as a self-instructing teaching tool.

2. Labelling irreducible representations of Lie Groups

The basic object in **SCHUR** is the partition of an integer into integers. The irreducible representations of the compact Lie groups[1-3], and certain of the unitary irreducible representations of the non-compact Lie groups such as $Sp(2n, R)$[4,5], may be uniquely by certain constrained partitions of integers, as for tensor representations, or as half-integers for spinor representations. Such a notation is familiar to physicists in the use of Young tableaux in describing tensors. The standard and spin irreducible representations of the symmetric group may be similarly labelled. These labels are encased in brackets according to the particular type of group being considered: curly brackets $\{,\}$ for $U(n), U(p,q), SU(n), S(n)$; angular brackets $<,>$ for $Sp(2n), Sp(2n, R)$; square brackets $[,]$ for $O(n), SO(n), SO^*(2n)$; curved brackets for the exceptional groups G_2, F_4, E_6, E_7, E_8. **SCHUR** automatically chooses the brackets appropriate to the set groups. **SCHUR** is significantly different from programmes involving weight space constructions and Dynkin diagrams though **SCHUR** will give translations of partition labels into Dynkin labels and vice versa.

In certain calculations non-standard partition labels may arise. **SCHUR** will automatically apply modification rules[1,6] to yield either signed standard labelled irreducible representations or null results as appropriate as may be seen in the following **SCHUR** fragment

```
DP>
->gr6u4so5sp6e8spr6osp5,6
Groups are   U(4) * SO(5) * Sp(6) * E(8) * Sp(6,R) * OSp(5/6)
DP>
->[21*s1^4*321*21^7*s1;21*431]
      {21}[s;1^4]<321>(21^7 )<s1;(21)>[431>
DP>
->std last
       - {21}[s;1^2 ]<321>(21^7 )<s1;(21)>[431>
DP>
```

where the input is distinguished by an arrow $->$. Note that the $SO(5)$ irreducible representation labelled $[s;1^4]$ is non-standard and in the final line of output has been converted into the standard irreducible representation $[s;1^2]$ with a negative sign.

3. Properties of irreducible representations

In practical applications one often needs to know the dimension of an irreducible representationor a list of irreducible representations. Thus for the staircase partition of weight 153 of $S(153)$ we have the **SCHUR** fragment

```
REP>
->gr s153
Group is S(153)
REP>
->conv_s wt-153 ser 153,t
      {17 16 15 14 13 12 11 10 987654321}
REP>
->dim last
dimension=12671579865747532750746781433923532863503681425492319766
          50253430956950626708285103360378018562189941581034579401
          4793141889217331200
REP>
```

where in the second line of input we obtained the relevant partition from the t series of staircase $S-$functions.

The eigenvalues of the Casimir invariants are useful in the study of model Hamiltonians[7,8]. **SCHUR** can present a number of properties upon invoking the command <<prop>> as shown below:-

```
REP>
->gr e8
Group is E(8)
REP>
->prop42
<dynkin label>(00000020)
dimension=4881384   60*2nd-casimir=200
2nd-dynkin=65610
```

In the case of the group $Sp(2n,R)$ the non-trivial unitary irreducible representations are of infinite dimension and just the eigenvalue of the second-order Casimir operator is evaluated. Thus

```
REP>
->gr spr8
Group is Sp(8,R)
REP>
->prop s1;21
   4*2nd-casimir=300
REP>
```

where for $Sp(2n,R)$ we have

$$C_2(<\frac{k}{2};(\lambda)>) = \sum_{i=1}^{n} \lambda_i(\lambda_i - 2i) + \frac{(k+2n+2)(nk+4\omega_\lambda)}{4} \tag{1}$$

The eigenvalues of higher order Casimir invariants may be evaluated for the compact Lie groups.

4. Kronecker products of irreducible representations

SCHUR readily handles Kronecker products for the compact Lie groups. The non-compact groups $Sp(2n,R)$ require special consideration since the non-trivial unitary irreducible representations are all of infinite dimension and results must be truncated to a finite cutoff. Consider the two fundamental irreducible representations $<s;(0)>$ and $<s;(1)>$ where $s=\frac{1}{2}$. **SCHUR** readily yields the terms of the three possible Kronecker products for $Sp(6,R)$, to weight 15, as

```
REP>
p s;0,s;0
      <1;(14 )> + <1;(12 )> + <1;(10 )> + <1;(8)> + <1;(6)> + <1;(4)>
       + <1;(2)> + <1;(0)>
REP>
p s;0,s;1
      <1;(15 )> + <1;(13 )> + <1;(11 )> + <1;(9)> + <1;(7)> + <1;(5)>
       + <1;(3)> + <1;(1)>
REP>
p s;1,s;1
      <1;(14 )> + <1;(12 )> + <1;(10 )> + <1;(8)> + <1;(6)> + <1;(4)>
       + <1;(2)> + <1;(1^2 )>
REP>
```

The above results lead to the conjecture that

$$<s;(0)> \times <s;(0)> = \sum_{i=0}^{\infty} <1;(2i)> \tag{2a}$$

$$< s; (0) > \times < s; (1) > = \sum_{i=0}^{\infty} < 1; (2i+1) > \qquad (2b)$$

$$< s; (1) > \times < s; (1) > =< 1; (1^2) > + \sum_{i=0}^{\infty} < 1; (2i) > \qquad (2c)$$

Examination of $Sp(2n, R)$ for $n > 3$ shows the result to continue to hold. Such results imply the existence of certain $S-$function identities which play an essential part in proving the conjectures which we shall not give here[9]. This gives us our first example of the way in which **SCHUR** can uncover, hitherto unknown, general results.

As a further example, consider the group $SU(4)$ whose adjoint irreducible representation is $\{21^2\}$. Suppose $\{\lambda\}$ is a real irreducible representation of $SU(4)$. We can ask ourselves "How many times does the adjoint irreducible representation occur in the Kronecker square of $\{\lambda\}$?". Consider the following results from **SCHUR**:-

```
REP>
gr su4
Group is SU(4)
REP>
p22,22
      {4^2 } + {431} + {42^2 } + {2^2 } + {21^2 } + {0}
REP>
p211,211
      {42^2 } + {3^2 2} + {31} + {2^2 } + 2{21^2 } + {0}
REP>
p321,321
      {642} + {63^2 } + {5^2 2} + 2{543} + {53}
   + 2{521} + {4^3 } + {4^2 } + 4{431} + 3{42^2 }
    + {4} + 3{3^2 2} + 3{31} + 2{2^2 } + 3{21^2 } + {0}
REP>
```

Note that in the above three products the $SU(4)$ irreducible representation $\{21^2\}$ occurs with multiplicities 1, 2, and 3 respectively. Is it a coincidence that those numbers correspond to the number of distinct steps in the Young diagrams of the partitions associated with the partitions $(2^2), (21^2), (321)$ respectively? For $SU(5)$ the adjoint irreducible representation is $\{21^3\}$ and using **SCHUR** we find that $\{4321\} \supset 4\{21^3\}$. This leads us to conject that the number of times the square of a real irreducible representation $\{\lambda\}$ of $SU(n)$ contains the adjoint irreducible representation is equal to the number of distinct steps in the Young diagram of the partition (λ). Formal proofs of this conjecture are given elsewhere[10,11]. The original inspiration came from use of **SCHUR**.

5. Symmetrized Kronecker powers

Plethysms for the classical compact Lie groups and the exceptional group G_2 can be evaluated in **SCHUR**. **SCHUR** can also resolve Kronecker powers of irreducible representations of

$Sp(2n,R)$ into their symmetrized components which amounts to evaluating plethysms. Again such resolutions are given up to a user defined limit. Thus we find for the two fundamental irreducible representations of $Sp(6,R)$ to weight 15

```
REP>
pl s;0,2
      <1;(12 )> + <1;(8)> + <1;(4)> + <1;(0)>
REP>
pl s;0,11
      <1;(14 )> + <1;(10 )> + <1;(6)> + <1;(2)>
REP>
pl s;1,2
      <1;(14 )> + <1;(10 )> + <1;(6)> + <1;(2)>
REP>
pl s;1,11
      <1;(12 )> + <1;(8)> + <1;(4)> + <1;(1^2 )>
REP>
```

The above results suggest that for general $Sp(2n,R)$ we have

$$< s;(0) > \otimes\{2\} = \sum_{i=0}^{\infty} < 1;(4i) > \tag{3a}$$

$$< s;(0) > \otimes\{1^2\} = \sum_{i=0}^{\infty} < 1;(4i+2) > \tag{3b}$$

$$< s;(1) > \otimes\{2\} = \sum_{i=0}^{\infty} < 1;(4i+2) > \tag{3c}$$

$$< s;(1) > \otimes\{1^2\} = < 1;(1^2) > + \sum_{i=0}^{\infty} < 1;(4i+4) > \tag{3d}$$

Notice that the irreducible representations contained in Eq. (3b) and (3c) are identical and implies the existence of hitherto unknown S−function identities[9].

Plethysms can play an important role in establishing selection rules. We alluded to the problem of determining the number of times the adjoint irreducible representation of a Lie group can occur in the Kronecker square of a real irreducible representation. The natural extension is to ask "How many times does the adjoint irreducible representation occur in each of the symmetrized Kronecker power of a real irreducible representation".

This question has been answered elsewhere[10,11].

6. Group-subgroup decompositions

Figure 1 displays a very rich group-subgroup structure. To be of practical use one must be able to make group-subgroup decompositions for every group-subgroup pair displayed in Fig. 1. Recent extensions of **SCHUR** make it possible to determine all such decompositions in a systematic and self-consistent manner. In the case of the group being a non-compact group the decompositions are determined up to a user defined limit. If the group is compact then the decomposition is complete. Most of the relevant calculations are well beyond the possibilities of hand calculations. Nearly 60 generic types of group-subgroup decompositions are available in **SCHUR**. By way of example we give the following $Sp(12,R) \Rightarrow Sp(4,R) \times O(3)$ decomposition for the fundamental irreducible representation $< s;(0) >$ of $Sp(12,R)$ where terms to weight 12 have been evaluated:-

```
DP>
->gr spr12
DP>
->br38,4,3gr1[s;0]
Groups are   Sp(4,R) * O(3)
      <s1;(12 )>[12 ] + <s1;(11 1)>[11 ]# + <s1;(10 )>[10 ] + <s1;(91)>[9]#
       + <s1;(8)>[8] + <s1;(71)>[7]# + <s1;(6)>[6] + <s1;(51)>[5]#
       + <s1;(4)>[4] + <s1;(31)>[3]# + <s1;(2)>[2] + <s1;(1^2 )>[1]#
       + <s1;(0)>[0]
DP>
```

The hash sign # is used to distinguish associated irreducible representations of $O(3)$.

7. The $O(n) \Rightarrow S(n)$ decompositions and inner plethysms

The $O(n) \Rightarrow S(n)$ decompositions play an important role in determining the spin states that arise in symplectic models of nuclei and mesoscopic systems such as quantum dots[12-15]. The relevant branching rule can be succinctly written for tensor irreducible representations $[\lambda]$ of $O(n)$ as[16]

$$[\lambda] \Rightarrow < 1 > \otimes \{\lambda/G\} \tag{4}$$

where

$$G = \sum_{\varepsilon} (-1)^{\frac{(\omega_\varepsilon - r)}{2}} \{\varepsilon\}$$

The term, $<1> \otimes\{\lambda/G\}$, is an example of a *reduced inner plethysm*[17]. Such objects defy description here, suffice to say that **SCHUR** automatically evalutes Eq. (4) and reduced inner plethysms of the generic type $<1> \otimes\{\lambda\}$ and can systematically build up the more general reduced inner plethysms $<\mu> \otimes\{\lambda\}$. As an example we obtain the result for $<21> \otimes\{21\}$ as

$$\begin{array}{llllll}
<71> & +\,2<7> & +\,<621> & +\,5<62> & +\,5<61^2> & +\,17<61> \\
+\,14<6> & +\,<54> & +\,2<531> & +\,9<53> & +\,<52^2> & +\,2<521^2> \\
+\,20<521> & +\,45<52> & +\,<51^4> & +\,10<51^3> & +\,47<51^2> & +\,81<51> \\
+\,45<5> & +\,<4^21> & +\,5<4^2> & +\,3<432> & +\,3<431^2> & +\,25<431> \\
+\,47<43> & +\,3<42^21> & +\,20<42^2> & +\,2<421^3> & +\,30<421^2> & +\,118<421> \\
+\,149<42> & +\,10<41^4> & +\,64<41^3> & +\,163<41^2> & +\,185<41> & +\,78<4> \\
+\,3<3^221> & +\,16<3^22> & +\,<3^21^3> & +\,20<3^21^2> & +\,73<3^21> & +\,82<3^2> \\
+\,<32^3> & +\,2<32^21^2> & +\,25<32^21> & +\,73<32^2> & +\,<321^4> & +\,20<321^3> \\
+\,118<321^2> & +\,270<321> & +\,235<32> & +\,5<31^5> & +\,47<31^4> & +\,163<31^3> \\
+\,280<31^2> & +\,240<31> & +\,83<3> & +\,<2^41> & +\,5<2^4> & +\,9<2^31^2> \\
+\,47<2^31> & +\,82<2^3> & +\,5<2^21^4> & +\,45<2^21^3> & +\,149<2^21^2> & +\,235<2^21> \\
+\,162<2^2> & +\,<21^6> & +\,17<21^5> & +\,81<21^4> & +\,185<21^3> & +\,240<21^2> \\
+\,173<21> & +\,55<2> & +\,2<1^7> & +\,14<1^6> & +\,45<1^5> & +\,78<1^4> \\
+\,83<1^3> & +\,55<1^2> & +\,19<1> & +\,2<0> & &
\end{array}$$

where **SCHUR**'s ability to produce TEX output has been exploited. Inspecting the above result one is immediately struck by the observation that the complete set of partitions is self-associated as may be verified by the **SCHUR** fragment

```
SFN>
->sets1last
SFN>
->sub sv1,conj sv1
      zero
SFN>
```

Furthermore, the partition (21) is a staircase partition. Could it be that *if* $<\mu> \otimes\{\lambda\} =<H>$, *where* (μ) *and* (λ) *are staircase partitions, then* H *is self-associated*?

If we try $< 21 > \otimes\{321\}$ we find the conjecture holds! This motivates us to see if the conjecture can be proved, as indeed it can[17]. This is but another of many examples of the application of **SCHUR** being used to establish a conjecture and leading to a hitherto unknown theorem.

8. SCHUR as a teaching tool

The above results have emphasized the use of **SCHUR** as a research tool. It can also be useful as a teaching tool in the areas of group theory and in the theory of symmetric groups. Here one can exploit the interactive nature of **SCHUR** to allow the student to develop simple examples, such as computing the dimensions of simple irreducible representations of $S(n)$, drawing a Young frame, constructing the hook length graph of a Young frame, computing Kronecker products in $U(n)$ etc. A large array of help files can be brought to screen describing every command with examples of its use.

9. Concluding remarks

In the preceding I have tried to illustrate a few applications of **SCHUR**. Many other applications such as, to Riemann tensor polynomials[18], automorphisms of $SO(8)$ and the electronic $f-$shell[19], expansion of powers of the Vandermonde determinant in $S-$functions[20], or the various aspects of the exceptional Lie groups in atomic physics [21,22], have been omitted for reasons of space-time and are left to you to explore in the literature.

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References

[1]. B. G. Wybourne and M. J. Bowick, Basic properties of the exceptional Lie groups, *Austr. J. Phys.* **30** (1977) 259-86.

[2]. R. C. King and A. H. A. Al-Qubanchi, Natural labelling schemes for simple roots and irreducible representations of exceptional Lie algebras, *J. Phys. A:Math.Gen.* **14** (1981) 15-49.

[3] G. R. E. Black, R. C. King and B. G. Wybourne, Kronecker products for compact semisimple Lie groups, *J. Phys. A:Math.Gen.* **16** (1983) 1553-89.

[4]. D. J. Rowe, B. G. Wybourne and P. H. Butler, Unitary representations, branching rules and matrix elements for the non-compact symplectic groups, *J. Phys. A:Math.Gen.* **18** (1985) 939-53.

[5]. R. C. King and B. G. Wybourne, Holomorphic discrete series and harmonic series unitary irreducible representations of non-compact Lie groups: $Sp(2n, R), U(p, q)$ and $SO^*(2n)$, *J. Phys. A:Math.Gen.* **18** (1985) 3113-39.

[6]. R. C. King, Branching rules for classical Lie groups using temnsor and spinor methods, *J. Phys. A:Math.Gen.* **8** (1975) 429-49.

[7]. B. G. Wybourne, Orbit-orbit Interactions and the 'Linear Theory' of configuration interaction, *J. Chem. Phys.* **40** (1964) 1457-1458.

[8]. I. Morrison, P. W. Pieruschka and B. G. Wybourne, The interacting boson model with the exceptional groups G_2 and E_6, *J. Math. Phys.* **32** (1991) 356-372.

[9]. K. Grudzinski and B. G. Wybourne, Plethysm for the noncompact group $Sp(2n, R)$ and new S–function identities, *J. Phys. A:Math.Gen.* **29** (1996) In Press.

[10]. M. Yang and B. G. Wybourne, Squares of S–functions of special shapes, *J. Phys. A:Math.Gen.* **28** (1995) 7011-17.

[11]. R. C. King and B. G. Wybourne, The place of the adjoint representation in the Kronecker square of irreducible representations of simple Lie groups, *J. Phys.*

A:Math.Gen. **29** (1996) 5059-77.

[12] R. W. Haase and N. F. Johnson, Classification of $N-$electron states in a quantum dot, *Phys. Rev.* **B48** (1993) 1583-94.

[13]. B. G. Wybourne, Applications of $S-$functions to the quantum Hall effect and quantum dots, *Rept. Math. Phys.* **34** (1994) 9-16.

[14] K. Grudzinski and B. G. Wybourne, Computing properties of the non-compact groups $Mp(2n)$ and $Sp(2n,R)$ using SCHUR, in T. Lulek, W. Florek and S. Wałcerz, *Symmetry and Structural Properties of Condensed Matter* (World Sci., Singapore, 1995) 469-93.

[15]. K. Grudzinski and B. G. Wybourne, Symplectic models of $n-$particle systems, *Rept. Math. Phys.* (1996) .

[16]. M. A. Salam and B. G. Wybourne, $Q-$functions and $O(n) \to S(n)$ branching rules for ordinary and spin irreps, *J. Phys. A:Math.Gen.* **22** (1989) 3770-78.

[17] Thomas Scharf, Jean-Yves Thibon and Brian G. Wybourne, Reduced notation, inner plethysm and the symmetric group, *J. Phys. A:Math.Gen.* **26** (1993) 7461-78.

[18]. S. A. Fulling, R. C. King, B. G. Wybourne and C. J. Cummins, Normal forms for tensor polynomials: I. The Riemann tensor, *Class. Quantum Grav.* **9** (1992) 1151-97.

[19]. B. G. Wybourne, The eight-fold way of the electronic $f-$shell, *J. Phys. B: At. Mol. Opt. Phys.* **25** (1992) 1683-96.

[20] T. Scharf, J-Y Thibon and B. G. Wybourne, Powers of the Vandermonde determinant and the quantum Hall effect, *J. Phys. A:Math.Gen.* **27** (1994) 4211-19.

[21] B. R. Judd, Applicability of the Lie group F_4 to the atomic f shell, *J. Phys. B: At. Mol. Opt. Phys.* **28** (1995) L203-7.

[22]. B. G. Wybourne, Exceptional Lie groups in physics, *Lithuanian J. Phys.* **35** (1995) 123-31.