Computing Properties of the Non-Compact Groups $Mp(2n)$ and $Sp(2n,R)$ using SCHUR

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Abstract

The problems of computing properties of the non-compact groups $Sp(2n,R)$ and $Mp(2n)$ are considered. The implementation of algorithms for calculating branching rules applicable to quantum dots are illustrated by a number of examples. The question of the elimination of spurious states is considered.

1. Introduction

A knowledge of the properties of compact Lie groups, and their associated Lie algebras, is essential in many areas of physics. Witness the application of $SU(3)$ in quantum chromodynamics and in the nuclear shell-model, $SO(4)$ as the degeneracy group of the H-atom, $SO(10)$ and $E(8)$ in string theory etc. The unitary irreducible representations of the compact Lie groups are all of finite dimension and hence it is possible to compute complete results even though at times the dimensions may be very large. Much less is known of the non-compact Lie groups and yet they too find applications in physics. The non-compact symplectic Lie group $Sp(2n,R)$, and its metaplectic covering group, $Mp(2n)$, occur in the theory of three-dimensional harmonic oscillator ($n=3$) and more generally in symplectic models of nuclei, quantum dots and quantum optics. A fundamental difference between the non-compact and compact Lie groups is that the non-trivial unitary irreducible representations of the former are all of infinite dimension. Thus in most cases it is only possible to compute such things as tensor products and branching rules up to some prescribed cutoff.

The program SCHUR* was initially designed to compute properties such as the dimensions of irreducible representations , Kronecker products and branching rules for compact Lie groups. In this paper we outline extensions to SCHUR that permit the calculation of Kronecker products and branching rules involving irreducible representations of the non-compact symplectic group $Sp(2n,R)$ and important subgroups thereof. We shall first review the labelling of representations of the classical Lie groups and then consider the labelling of the representations of $Sp(2n,R)$ in terms of the partition labels used for its maximal compact subgroup, $U(n)$. We then briefly outline some of the features of SCHUR in computing properties of the classical Lie groups and then consider the problems, and their solutions, in extending SCHUR to $Sp(2n,R)$. Specific attention is next given to the implementation of the branching rules and Kronecker products that arise in the classification of the states of a many-electron quantum dot, a problem closely related to the corresponding many-nucleon symplectic model of the nucleus. We give a number of examples of specific calculations done with the new version of SCHUR.

2. Labelling Irreducible representations of the Classical Lie Groups

The irreducible representations of the classical Lie groups, $SU(n)$, $SO(2k+1)$, $Sp(2k)$ and $SO(2k)$ may be unequivocally labelled by ordered partitions of integers, or in the case of spin representations half-odd-integers, subject to certain constraints[1]. The irreducible representations of the full orthogonal groups, $O(2k+1)$ and $O(2k)$, may likewise be labelled by integers and half-odd-integers. In those cases we extend the labels by an additional

* SCHUR is an interactive program for calculating the properties of Lie groups and symmetric functions distributed by S. Christensen, PO Box 16175, Chapel Hill, NC 27516 USA. E-mail stevec@wri.com

'#' to distinguish associated pairs of irreducible representations. The standard partition labels are summarised in Table 1 and their relationship to the Dynkin labels in Table 2.

Table 1 Standard labels for representations of the classical Lie groups of rank k.

Group	Label	Constraints
U_n	$\{\overline{\mu};\lambda\}$	$\ell_\lambda + \ell_\mu \leq k = n$
SU_n	$\{\lambda\}$	$\ell_\lambda \leq k = n-1$
O_{2k+1}	$[\lambda],[\lambda]\#$	$\ell_\lambda \leq k$
	$[\Delta;\lambda],[\Delta;\lambda]\#$	$\ell_\lambda \leq k$
SO_{2k+1}	$[\lambda],[\Delta;\lambda]$	$\ell_\lambda \leq k$
Sp_{2k}	$<\lambda>$	$\ell_\lambda \leq k$
O_{2k}	$[\lambda],[\lambda]\#$	$\ell_\lambda < k$
	$[\lambda]$	$\ell_\lambda = k$
	$[\Delta;\lambda]$	$\ell_\lambda \leq k$
SO_{2k}	$[\lambda]$	$\ell_\lambda < k$
	$[\lambda]\pm$	$\ell_\lambda = k$
	$[\Delta;\lambda]\pm$	$\ell_\lambda \leq k$

In specific calculations non-standard partitions may arise and these must be converted into either standard partition labels appropriate to the group being considered or become null objects. For the classical Lie groups these modification rules normally involve drawing the Young frame of the non-standard partition λ and removing a continuous strip of boxes of length h, starting at the foot of the first column and working up along the right edge. This strip removal is symbolised as $\lambda - h$. A phase factor also occurs which is dependent upon the column c in which the removal ends. If the resulting Young diagram corresponds to an ordered partition then $\lambda \rightarrow \lambda - h$, otherwise λ is discarded. In practice the procedure is repeated until either a standard label results or a null result is obtained. The modification rules appropriate to the classical Lie groups are summarised in Table 3. These modification rules are automatically implemented in SCHUR as well as the possibility

Table 2 Relationship between standard SCHUR labels and the corresponding Dynkin labels for the classical Lie groups.

Group	Dynkin label	Standard Label
SU_{k+1}	$a_1 = l_1 - l_2$	$l_1 = a_1 + a_2 + \ldots + a_{k-1} + a_k$
	$a_2 = l_2 - l_3$	$l_2 = a_2 + \ldots + a_{k-1} + a_k$
	$\vdots$	$\vdots$
	$a_{k-1} = l_{k-1} - l_k$	$l_{k-1} = a_{k-1} + a_k$
	$a_k = l_k$	$l_k = a_k$
SO_{2k+1}	$a_1 = l_1 - l_2$	$l_1 = a_1 + a_2 + \ldots + a_{k-1} + \frac{a_k}{2}$
	$a_2 = l_2 - l_3$	$l_2 = a_2 + \ldots + a_{k-1} + \frac{a_k}{2}$
	$\vdots$	$\vdots$
	$a_{k-1} = l_{k-1} - l_k$	$l_{k-1} = a_{k-1} + \frac{a_k}{2}$
	$a_k = 2\ l_k$	$l_k = \frac{a_k}{2}$
Sp_{2k}	$a_1 = l_1 - l_2$	$l_1 = a_1 + a_2 + \ldots + a_{k-1} + a_k$
	$a_2 = l_2 - l_3$	$l_2 = a_2 + \ldots + a_{k-1} + a_k$
	$\vdots$	$\vdots$
	$a_{k-1} = l_{k-1} - l_k$	$l_{k-1} = a_{k-1} + a_k$
	$a_k = l_k$	$l_k = a_k$
SO_{2k}	$a_1 = l_1 - l_2$	$l_1 = a_1 + a_2 + \ldots + a_{k-2} + \frac{a_{k-1}}{2} + \frac{a_k}{2}$
	$a_2 = l_2 - l_3$	$l_2 = a_2 + \ldots + a_{k-2} + \frac{a_{k-1}}{2} + \frac{a_k}{2}$
	$\vdots$	$\vdots$
	$a_{k-2} = l_{k-2} - l_{k-1}$	$l_{k-2} = a_{k-2} + \frac{a_{k-1}}{2} + \frac{a_k}{2}$
	$a_{k-1} = l_{k-1} - l_k$	$l_{k-1} = \frac{a_{k-1}}{2} + \frac{a_k}{2}$
	$a_k = l_{k-1} + l_k$	$l_k = \frac{a_{k-1}}{2} - \frac{a_k}{2}$

of transforming standard partition labels into Dynkin labels and vice versa.

Table 3 The modification rules appropriate to the classical Lie groups.

Group	**modification rule**	**h**
U_n, SU_n	$\{\overline{\mu};\lambda\} = (-1)^{c+d-1}\{\overline{\mu-h};\lambda-h\}$	$h = \ell_\mu + \ell_\lambda - n - 1 \geq 0$
O_{2k+1}	$[\lambda] = (-1)^{c-1}[\lambda-h]\#$	$h = 2\ell_\lambda - 2k - 1 > 0$
	$[\lambda]\# = (-1)^{c-1}[\lambda-h]$	$h = 2\ell_\lambda - 2k - 1 > 0$
	$[\Delta;\lambda] = (-1)^{c}[\Delta;\lambda-h]\#$	$h = 2\ell_\lambda - 2k - 2 \geq 0$
	$[\Delta;\lambda]\# = (-1)^{c}[\Delta;\lambda-h]$	$h = 2\ell_\lambda - 2k - 2 \geq 0$
SO_{2k+1}	$[\lambda] = (-1)^{c-1}[\lambda-h]$	$h = 2\ell_\lambda - 2k - 1 > 0$
	$[\Delta;\lambda] = (-1)^{c}[\Delta;\lambda-h]$	$h = 2\ell_\lambda - 2k - 2 \geq 0$
Sp_{2k}	$< \lambda >= (-1)^{c} < \lambda-h >$	$h = 2\ell_\lambda - 2k - 2 \geq 0$
O_{2k}	$[\lambda] = (-1)^{c-1}[\lambda-h]\#$	$h = 2\ell_\lambda - 2k > 0$
	$[\lambda]\# = (-1)^{c-1}[\lambda-h]$	$h = 2\ell_\lambda - 2k > 0$
	$[\Delta;\lambda] = (-1)^{c}[\Delta;\lambda-h]$	$h = 2\ell_\lambda - 2k - 1 \geq 0$
SO_{2k}	$[\lambda] = (-1)^{c-1}[\lambda-h]$	$h = 2\ell_\lambda - 2k > 0$
	$[\lambda]_\pm = (-1)^{c-1}[\lambda-h]_\mp$	$h = 2\ell_\lambda - 2k > 0$
	$[\Delta;\lambda]\pm = (-1)^{c}[\Delta;\lambda-h]\mp$	$h = 2\ell_\lambda - 2k - 1 \geq 0$

A considerable advantage in using partition labels acrues when it is realised that the characters of the classical Lie groups can be represented in terms of finite sequences of the symmetric Schur functions[2,3] ($S-$functions), themselves indexed by partitions, allowing the calculation of Kronecker products and branching rules to be made in terms of simple manipulations of $S-$functions [1]. In practice well defined infinite series of $S-$functions are involved with the number of terms being limited by the fact that the unitary irreducible representations of the compact Lie groups are all finite dimensional[4]. SCHUR is able to automatically determine the content of the appropriate $S-$series, make the truncation of the infinite series, and carry out the necessary $S-$function computations rapidly. The irreducible representations of the compact exceptional Lie groups may also be labelled in terms of constrained partitions based upon the corresponding labels of their maximal classical Lie subgroups[1,5–7]. A similar procedure may be used for the discrete series of irreducible representations of non-compact groups[8,9].

3. Labelling the Irreducible representations of Non-compact Lie Groups

Here we shall limit ourselves to discussion of the so-called positive discrete unitary irreducible representations of the group $Sp(2n,R)$ and its double covering group, $Mp(2n)$, drawing heavily upon references [8] and [9]. These irreducible representations are all infinite dimensional and are characterised by a *lowest weight* with respect to the ordering of weights of the maximal compact subgroup $U(n)$. There exists a harmonic representation, $\tilde{\Delta}$, associated with the Heisenberg algebra. This is a true, unitary, infinite dimensional irreducible representation of the double covering group $Mp(2n)$ of $Sp(2n,R)$, the so-called *metaplectic group*. This representation is reducible into the sum of two irreducible representations $\tilde{\Delta}_+$ and $\tilde{\Delta}_-$ whose leading weights are $(\frac{1}{2}\frac{1}{2}\ldots\frac{1}{2})$ and $(\frac{3}{2}\frac{1}{2}\ldots\frac{1}{2})$ corresponding to the highest weights of the representations $\varepsilon^{\frac{1}{2}}\{0\}$ and $\varepsilon^{\frac{1}{2}}\{1\}$ which appear in the restriction of $Sp(2n,R)$ to its maximal compact subgroup $U(n)$.

The tensor powers $\tilde{\Delta}^k$ all decompose into a direct sum of unitary irreducible representations of $Mp(2n)$. All those irreducible representations which derive from $\tilde{\Delta}^k$ for some k will be referred to as *harmonic series representaions*. All those irreducible representations that appear in $\tilde{\Delta}^k$ will be labelled by the symbols $\langle\frac{k}{2}(\lambda)\rangle$. The harmonic series representations appearing in $\tilde{\Delta}^k$ are in one-to-one correspondence with the terms arising in the branching rule appropriate to the restriction from $Mp(2nk)$ to $Sp(2n,R)\times O(k)$

$$\tilde{\Delta} \to \sum_{\lambda}\langle\frac{k}{2}(\lambda)\rangle \times [\lambda] \tag{1}$$

where the summation is carried out over all partitions $(\lambda)=(\lambda_1,\lambda_2,\ldots)$ for which the conjugate partition $(\tilde{\lambda})=(\tilde{\lambda}_1,\tilde{\lambda}_2,\ldots)$ satisfies the constraints

$$\tilde{\lambda}_1+\tilde{\lambda}_2 \le k \tag{2a}$$

and

$$\tilde{\lambda}_1 \leq n \tag{2b}$$

Irreducible representations of $Sp(2n,R)$ $\langle \frac{1}{2}k(\lambda)\rangle$ satisfying Eq.(2) will be said to be *standard* and we may limit our attention to these irreducible representations of $Sp(2n,R)$.

The value of $\frac{k}{2}$ maybe an integer (k *even*) or a half-odd-integer (k *odd*). In terms of inputting and outputting $Sp(2n,R)$ labelled irreducible representations into SCHUR it is useful to introduce the equivalent notation

$$\langle s\kappa;(\lambda)\rangle \equiv \langle \frac{k}{2}(\lambda)\rangle \tag{3}$$

where

$$\frac{k}{2} = s + \kappa \tag{4}$$

with κ being the integer part of $\frac{k}{2}$ and the residue part is $s = 0$ or $\frac{1}{2}$. Thus we have the typical notational equivalences

$$\langle s1;(\lambda)\rangle \equiv \langle \frac{3}{2}(\lambda)\rangle, k = 3 \quad \langle 1;(\lambda)\rangle \equiv \langle 1(\lambda)\rangle \quad k = 2$$

SCHUR accepts irreducible representation labels in the form of lists of $\langle s\kappa;\lambda\rangle$ and standardises the input in accordance with the constraints of Eq.(2) making null all non-standard $Sp(2n,R)$ irreducible representations. As an example taken from SCHUR with the inputs marked $->$ we have

```
->gr spr8

Group is Sp(8,R)

REP>

->2;211 + 2;31 + 2;2211 + s1;21 + s2;32

      <2;(21^2) > + <2;(31)> + <2;(2^2 1^2) > + <s1;(21)> + <s2;(32)>

REP>

->std last

       <s2;(32)> + <2;(31)> + <2;(21^2)> + <s1;(21)>
```

The second instruction has applied Eq.(2) to the list and eliminated the non-standard $< 2; (2211) >$ label.

4. Branching Rules for subgroups of $Mp(2n)$ and $Sp(2n, R)$

The branching rule for the group-subgroup decomposition $Sp(2n, R) \rightarrow U(n)$ has been shown to be[8,9]

$$\langle \frac{k}{2}(\lambda) \rangle \rightarrow \varepsilon^{\frac{k}{2}} \cdot \{\{\lambda_s\}_N^k \cdot D_N\}_N \tag{5}$$

with $N = min(n, k)$. The infinite $S-$function series

$$D = \sum_{\delta} \{\delta\} \tag{6}$$

involves a sum over all partitions (δ) whose parts are even. This series is restricted to D_N in Eq. (6) involving members (δ) of the $D-$series having not more than N parts. Nevertheless, the series D_N remains as an infinite series of $S-$functions.

The *signed sequence*[8,9] $\{\lambda_s\}_N^k$ is the set of terms $\pm\{\rho\}$ such that $\pm[\rho]$ is equivalent to $[\lambda]$ under the modification rules of the group $O(k)$. The signed sequence is rendered finite by restriction to terms $\{\rho\}$ involving not more than N parts.

The first $\cdot$ indicates a product in $U(n)$ and the second $\cdot$ a product in $U(N)$ as implied by the final subscript N.

The harmonic discrete series irreducible representations of $Sp(2n, R)$ are all of infinite dimension and hence there are an infinite number of $U(n)$ irreducible representations arising on the right-hand-side of Eq. (5). Clearly, in practical implementations of the branching rule a user definable cutoff must be introduced to produce a manageablely finite number of terms. In SCHUR we solve this problem by introducing a user defined integer constant that results in the computation of all terms up to a chosen maximal weight partition. SCHUR possesses procedures to generate the necessary signed sequences and $S-$function series, as well as carrying out the relevant Kronecker products and modification rules. A typical example of verbatim SCHUR input and output is given below:

```
->gr spr8

Group is Sp(8,R)

DP>

->br44,8gr1[s1;21]

Group is U(4)

      {s;11 21^2 } + {s;10 31^2 } + {s;10 2^2 1} + {s;941^2 } + {s;9321}

       + {s;921^2 } + {s;851^2 } + 2{s;8421} + {s;831^2 } + {s;82^2 1}

       + {s;761^2 } + {s;7521} + {s;7431} + {s;741^2 } + {s;7321}

       + {s;721^2 } + {s;6^2 21} + {s;6531} + {s;651^2 } + {s;64^2 1}

       + 2{s;6421} + {s;631^2 } + {s;62^2 1} + {s;5431} + {s;541^2 }

       + {s;5321} + {s;521^2 } + {s;4^2 21} + {s;431^2 } + {s;42^2 1}

       + {s;321^2 }
```

The branching rule for the decomposition of the irreducible representation $\tilde{\Delta} \equiv \langle s;(0)\rangle$ of the metaplectic group $Mp(2nk)$ upon restriction to the subgroup $Sp(2n,R)\times O(k)$ follows from implementation of Eq. (1) into SCHUR.

We find for example:

```
DP>

->sb_tex true

DP>

->columns4

DP>

->gr mp24

Group is Mp(24)

DP>

->br46,6,4gr1[s;0]
```

```
Groups are   Sp(6,R) * O(4)
```

$< 2;(12\ ) > [12\ ]$ $+ < 2;(11\ 1) > [11\ 1]$ $+ < 2;(11\ ) > [11\ ]$ $+ < 2;(10\ 2) > [10\ 2]$
$+ < 2;(10\ 1^2) > [10\ ]\#$ $+ < 2;(10\ 1) > [10\ 1]$ $+ < 2;(10\ ) > [10\ ]$ $+ < 2;(93) > [93]$
$+ < 2;(92) > [92]$ $+ < 2;(91^2) > [9]\#$ $+ < 2;(91) > [91]$ $+ < 2;(9) > [9]$
$+ < 2;(84) > [84]$ $+ < 2;(83) > [83]$ $+ < 2;(82) > [82]$ $+ < 2;(81^2) > [8]\#$
$+ < 2;(81) > [81]$ $+ < 2;(8) > [8]$ $+ < 2;(75) > [75]$ $+ < 2;(74) > [74]$
$+ < 2;(73) > [73]$ $+ < 2;(72) > [72]$ $+ < 2;(71^2) > [7]\#$ $+ < 2;(71) > [71]$
$+ < 2;(7) > [7]$ $+ < 2;(6^2) > [6^2]$ $+ < 2;(65) > [65]$ $+ < 2;(64) > [64]$
$+ < 2;(63) > [63]$ $+ < 2;(62) > [62]$ $+ < 2;(61^2) > [6]\#$ $+ < 2;(61) > [61]$
$+ < 2;(6) > [6]$ $+ < 2;(5^2) > [5^2]$ $+ < 2;(54) > [54]$ $+ < 2;(53) > [53]$
$+ < 2;(52) > [52]$ $+ < 2;(51^2) > [5]\#$ $+ < 2;(51) > [51]$ $+ < 2;(5) > [5]$
$+ < 2;(4^2) > [4^2]$ $+ < 2;(43) > [43]$ $+ < 2;(42) > [42]$ $+ < 2;(41^2) > [4]\#$
$+ < 2;(41) > [41]$ $+ < 2;(4) > [4]$ $+ < 2;(3^2) > [3^2]$ $+ < 2;(32) > [32]$
$+ < 2;(31^2) > [3]\#$ $+ < 2;(31) > [31]$ $+ < 2;(3) > [3]$ $+ < 2;(2^2) > [2^2]$
$+ < 2;(21^2) > [2]\#$ $+ < 2;(21) > [21]$ $+ < 2;(2) > [2]$ $+ < 2;(1^3) > [1]\#$
$+ < 2;(1^2) > [1^2]$ $+ < 2;(1) > [1]$ $+ < 2;(0) > [0]$

Note that in this case SCHUR has been requested to produce TEX output in four columns forming a setbox with the appropriate settabs and TEX commands automatically inserted.

Under the restriction $Mp(2n) \to Sp(2n,R)$ we have

$$\langle s;(0)\rangle \to \langle s;(0)\rangle + \langle s;(1)\rangle \tag{7}$$

It the case of the harmonic oscillator this corresponds to separating the odd and even states. The appropriate branching rules for these two irreducible representations have been given by Haase and Johnson[10,11] and have been implemented in SCHUR. For example,

```
->gr spr24
Group is Sp(24,R)
DP>
->br47,6,4gr1[s;0]
Groups are   Sp(6,R) * O(4)
```

$< 2;(12\ ) > [12\ ]$ $+ < 2;(11\ 1) > [11\ 1]$ $+ < 2;(10\ 2) > [10\ 2]$ $+ < 2;(10\ 1^2) > [10\ ]\#$
$+ < 2;(10\ ) > [10\ ]$ $+ < 2;(93) > [93]$ $+ < 2;(91) > [91]$ $+ < 2;(84) > [84]$
$+ < 2;(82) > [82]$ $+ < 2;(81^2) > [8]\#$ $+ < 2;(8) > [8]$ $+ < 2;(75) > [75]$
$+ < 2;(73) > [73]$ $+ < 2;(71) > [71]$ $+ < 2;(6^2) > [6^2]$ $+ < 2;(64) > [64]$
$+ < 2;(62) > [62]$ $+ < 2;(61^2) > [6]\#$ $+ < 2;(6) > [6]$ $+ < 2;(5^2) > [5^2]$
$+ < 2;(53) > [53]$ $+ < 2;(51) > [51]$ $+ < 2;(4^2) > [4^2]$ $+ < 2;(42) > [42]$
$+ < 2;(41^2) > [4]\#$ $+ < 2;(4) > [4]$ $+ < 2;(3^2) > [3^2]$ $+ < 2;(31) > [31]$
$+ < 2;(2^2) > [2^2]$ $+ < 2;(21^2) > [2]\#$ $+ < 2;(2) > [2]$ $+ < 2;(1^2) > [1^2]$
$+ < 2;(0) > [0]$

```
->gr spr24
Group is Sp(24,R)
DP>
->br47,6,4gr1[s;1]
Groups are   Sp(6,R) * O(4)
```

$< 2;(11\ ) > [11\ ]$ $+ < 2;(10\ 1) > [10\ 1]$ $+ < 2;(92) > [92]$ $+ < 2;(91^2) > [9]\#$
$+ < 2;(9) > [9]$ $+ < 2;(83) > [83]$ $+ < 2;(81) > [81]$ $+ < 2;(74) > [74]$
$+ < 2;(72) > [72]$ $+ < 2;(71^2) > [7]\#$ $+ < 2;(7) > [7]$ $+ < 2;(65) > [65]$
$+ < 2;(63) > [63]$ $+ < 2;(61) > [61]$ $+ < 2;(54) > [54]$ $+ < 2;(52) > [52]$
$+ < 2;(51^2) > [5]\#$ $+ < 2;(5) > [5]$ $+ < 2;(43) > [43]$ $+ < 2;(41) > [41]$
$+ < 2;(32) > [32]$ $+ < 2;(31^2) > [3]\#$ $+ < 2;(3) > [3]$ $+ < 2;(21) > [21]$
$+ < 2;(1^3) > [1]\#$ $+ < 2;(1) > [1]$

Not surprisingly the sum of the above two results coincides with those for the $Mp(24) \to Sp(6,R) \times O(4)$ decomposition given earlier.

The final branching rule we require is the general reduction for $Sp(2n,R) \to Sp(2,R) \times O(n)$. Again the relevant result is available and has been added to SCHUR. As a typical example we have:-

```
->gr spr8

Group is Sp(8,R)

DP>

->br45,8gr1[s1;21]

Groups are   Sp(2,R) * O(4)
```

$<6;(11\ )>[10\ 1]$	$+\ <6;(11\ )>[92]$	$+\ <6;(11\ )>[9]\#$	$+\ 2<6;(11\ )>[9]$
$+\ <6;(11\ )>[83]$	$+\ 4<6;(11\ )>[81]$	$+\ <6;(11\ )>[74]$	$+\ 5<6;(11\ )>[72]$
$+\ 3<6;(11\ )>[7]\#$	$+\ 4<6;(11\ )>[7]$	$+\ <6;(11\ )>[65]$	$+\ 5<6;(11\ )>[63]$
$+\ 10<6;(11\ )>[61]$	$+\ 3<6;(11\ )>[54]$	$+\ 9<6;(11\ )>[52]$	$+\ 6<6;(11\ )>[5]\#$
$+\ 8<6;(11\ )>[5]$	$+\ 6<6;(11\ )>[43]$	$+\ 13<6;(11\ )>[41]$	$+\ 8<6;(11\ )>[32]$
$+\ 5<6;(11\ )>[3]\#$	$+\ 7<6;(11\ )>[3]$	$+\ 7<6;(11\ )>[21]$	$+\ 2<6;(11\ )>[1]\#$
$+\ 3<6;(11\ )>[1]$	$+\ <6;(9)>[81]$	$+\ <6;(9)>[72]$	$+\ <6;(9)>[7]\#$
$+\ 2<6;(9)>[7]$	$+\ <6;(9)>[63]$	$+\ 4<6;(9)>[61]$	$+\ <6;(9)>[54]$
$+\ 5<6;(9)>[52]$	$+\ 3<6;(9)>[5]\#$	$+\ 4<6;(9)>[5]$	$+\ 3<6;(9)>[43]$
$+\ 8<6;(9)>[41]$	$+\ 5<6;(9)>[32]$	$+\ 4<6;(9)>[3]\#$	$+\ 5<6;(9)>[3]$
$+\ 6<6;(9)>[21]$	$+\ <6;(9)>[1]\#$	$+\ 2<6;(9)>[1]$	$+\ <6;(7)>[61]$
$+\ <6;(7)>[52]$	$+\ <6;(7)>[5]\#$	$+\ 2<6;(7)>[5]$	$+\ <6;(7)>[43]$
$+\ 4<6;(7)>[41]$	$+\ 3<6;(7)>[32]$	$+\ 2<6;(7)>[3]\#$	$+\ 3<6;(7)>[3]$
$+\ 4<6;(7)>[21]$	$+\ <6;(7)>[1]\#$	$+\ 2<6;(7)>[1]$	$+\ <6;(5)>[41]$
$+\ <6;(5)>[32]$	$+\ <6;(5)>[3]\#$	$+\ 2<6;(5)>[3]$	$+\ 2<6;(5)>[21]$
$+\ <6;(5)>[1]\#$	$+\ <6;(5)>[1]$	$+\ <6;(3)>[21]$	$+\ <6;(3)>[1]$

The above results give an indication of the application of SCHUR to branching rules involving non-compact groups. The examples have been kept quite small but SCHUR can evaluate terms almost without limit if required. The application of these results to quantum dots will be considered shortly but first we digress to consider the Kronecker products of irreducible representations of the harmonic series of the non-compact group $Sp(2n,R)$

5. Kronecker Products for $Sp(2n,R)$

The evaluation of Kronecker products of harmonic series irreducible representations of the non-compact group $Sp(2n,R)$ have been considered by King and Wybourne[9]. They establish the complete result

$$\langle\frac{k}{2}(\mu)\rangle \times \langle\frac{\ell}{2}(\nu)\rangle = \langle\frac{k+\ell}{2}((\{\mu_s\}^k \cdot \{\nu_s\}^\ell \cdot D))_{k+\ell,n}\rangle \tag{8}$$

where $((\lambda))_{k+\ell,n}$ is interpreted as null unless the constraints of Eq.(2) are satisfied. This method requires the use of two signed sequences and as a consequence there is considerable overcounting.

They have conjectured the validity of a somehat simpler formula

$$\begin{aligned}
&\langle\frac{k}{2}(\mu)\rangle \times \langle\frac{\ell}{2}(\nu)\rangle \\
&\qquad = \langle\frac{k+\ell}{2}((\{\mu\} \cdot \{\nu_s\}_N^\ell \cdot D_N)_N\rangle_n \quad \text{with } N = min(n,\ell) && (9a)\\
&\qquad = \langle\frac{k+\ell}{2}((\{\nu\} \cdot \{\mu_s\}_N^\ell \cdot D_M)_M\rangle_n \quad \text{with } M = min(n,k) && (9b)
\end{aligned}$$

The symbol $\langle\frac{k+\ell}{2}(\lambda)\rangle_n$ is interpreted as a harmonic series irreducible representation subject to a two stage modification that first modifies (λ) in $O(k+\ell)$ and then modifies in $U(n)$. These modifications are automatically done in SCHUR.

To date no counter-example to Eq.(9) is known in spite of much searching. King and Wybourne[9] have presented arguments in favour of the plausibility of their conjecture but to date no formal proof has been offered. Currently there is implementation of both Eq. (8) and (9) in SCHUR but only when a complete proof is obtained can one consider the results with certainty from Eq. (9). As an example of the implementation of Eq. (9) we have

```
REP>
->gr spr8
Group is Sp(8,R)
->p s1;21,2;31
```

$$< 3;(92) > + < 3;(91^2) > + 2 < 3;(83) > + 4 < 3;(821) > + 2 < 3;(81^3) >$$
$$+ 3 < 3;(74) > + 7 < 3;(731) > + 4 < 3;(72^2) > + 5 < 3;(721^2) > + < 3;(72) >$$
$$+ < 3;(71^2) > + 2 < 3;(65) > + 8 < 3;(641) > + 8 < 3;(632) > + 8 < 3;(631^2) >$$
$$+ 2 < 3;(63) > + 4 < 3;(62^21) > + 4 < 3;(621) > + 2 < 3;(61^3) > + 3 < 3;(5^21) >$$
$$+ 7 < 3;(542) > + 6 < 3;(541^2) > + 2 < 3;(54) > + 4 < 3;(53^2) > + 8 < 3;(5321) >$$
$$+ 5 < 3;(531) > + 3 < 3;(52^2) > + 4 < 3;(521^2) > + < 3;(52) > + < 3;(51^2) >$$
$$+ 3 < 3;(4^23) > + 4 < 3;(4^221) > + 3 < 3;(4^21) > + 4 < 3;(43^21) > + 4 < 3;(432) >$$
$$+ 4 < 3;(431^2) > + < 3;(43) > + 2 < 3;(42^21) > + 2 < 3;(421) > + < 3;(41^3) >$$
$$+ < 3;(3^3) > + 2 < 3;(3^221) > + < 3;(3^21) > + < 3;(32^2) > + < 3;(321^2) >$$

also in agreement with Eq. (8). A boolean has been added to SCHUR to permit the user to toggle between the two equations.

6. Application to Quantum Dots

The development of SCHUR has always been motivated by specific applications. Thus the extension to the non-compact groups $Mp(2n)$ and $Sp(2n,R)$ has been driven by a need to develop systematic methods for calculating the relevant branching rules required for the classification of the states quantum dots and of nuclei. A quantum dot involves the confinement of N electrons in $d = 2\mathrm{or}3$ dimensions over a nanometre scale[12]. The confining potential is, to a good approximation, parabolic. The quantum dot behaves like an $N-$electron atom without a nuclear core. In an atom the kinetic energy tends to dominate over the potential energy (the confinement length is small) whereas in a quantum dot the two contributions are roughly of the same order. A closely analogous problem is that of nucleons confined in a harmonic oscillator potential with quantised motion occuring about the centre-of-mass of the $N-$nucleon system. Indeed the formal group structure is identical to that proposed by Haase and Johnson[10,11] for a quantum dot confined in three dimensions. A quantum dot may involve anything from a single electron to sixty or more electrons.

The symmetry, or degeneracy, group of the isotropic harmonic oscillator is $SU(3)$. A dynamical group[13], containing the degeneracy group as a subgroup, with a single irreducible representation that can be spanned by the complete set of states maybe found[10,11] by consideration of the commutation relations satisfied by the coordinate and momentum operators of the individual particles. Such an irreducible representation is necessarily infinite dimensional and the dynamical group is necessarily non-compact. For our case of $N-$particles confined in d dimensions the appropriate dynamical group[10,11] is $Sp(2Nd,R)$ with its covering group being the metaplectic group $Mp(2Nd)$. More accurately, we have a Lie algebra, but by the customary physicists abuse of notation we shall discuss them as groups.

The group $Mp(2Nd)$ possesses a very rich subgroup structure[10,11] which we portray in Fig. 1. The group $Mp(2Nd)$ sits at the top and involves the single irreducible representation $\tilde{\Delta} \sim \langle s;(0)\rangle$. Upon restriction to $Sp(2Nd,R)$ the irreducible representation splits into two irreducible representations as in Eq. (7). Continuing down Fig. 1. we pass through various group-subgroup chains each involning branchings that may be determined using SCHUR . The various subgroups reflect different ways of separating the spatial and particle number dependencies. The group $O(d)$ describes the angular momentum states of the system while the group $O(N)$ gives information on the permutational symmetries[14–16] of the states via the $S(N)$ symmetric subgroup of $O(N)$.

7. Permutational Symmetries and Spurious States

The role of permutational symmetries and the removal of spurious states is best illustrated by a specific example of six electrons ($N=6$) in an isotropic three-dimensional space ($d=3$). The dynamical group is $Mp(36)$ and upon restriction to $Sp(36,R)$ we have

$$\langle s;(0)\rangle \to \langle s;(0)\rangle + \langle s;(1)\rangle \tag{10}$$

Looking at Fig. 1 let us choose the subgroup $Sp(6,R) \times O(6)$. The group $O(6)$ gives the spatial symmetries of the six-electron states. Using SCHUR we have $\langle s;(0)\rangle \rightarrow$

```
DP>
->gr spr36
Group is Sp(36,R)
DP>
->br47,6,6gr1[s;0]
Groups are Sp(6,R) * O(6)
       ......................................+ <3;(6)>[6]
       + <3;(5^2 2)>[5^2 2] + <3;(5^2 )>[5^2 ] + <3;(543)>[543]
       + <3;(541)>[541] + <3;(532)>[532] + <3;(53)>[53] + <3;(521)>[521]
       + <3;(51)>[51] + <3;(4^3 )>[4^3 ] + <3;(4^2 2)>[4^2 2]
       + <3;(4^2 )>[4^2 ] + <3;(43^2 )>[43^2 ] + <3;(431)>[431]
       + <3;(42^2 )>[42^2 ] + <3;(42)>[42] + <3;(41^2 )>[41^2 ]
       + <3;(4)>[4] + <3;(3^2 2)>[3^2 2] + <3;(3^2 )>[3^2 ]
       + <3;(321)>[321] + <3;(31)>[31] + <3;(2^3 )>[2^3 ]
       + <3;(2^2 )>[2^2 ] + <3;(21^2 )>[21^2 ] + <3;(2)>[2]
       + <3;(1^2 )>[1^2 ] + <3;(0)>[0]
DP>
```

and

```
->gr spr36
Group is Sp(36,R)
DP>
->br47,6,6gr1[s;1]
```

```
Groups are   Sp(6,R) * O(6)

       ......................................+ <3;(61)>[61]

       + <3;(5^2 1)>[5^2 1] + <3;(542)>[542] + <3;(54)>[54]

       + <3;(53^2 )>[53^2 ] + <3;(531)>[531] + <3;(52^2 )>[52^2 ]

       + <3;(52)>[52] + <3;(51^2 )>[51^2 ] + <3;(5)>[5]

       + <3;(4^2 3)>[4^2 3] + <3;(4^2 1)>[4^2 1] + <3;(432)>[432]

       + <3;(43)>[43] + <3;(421)>[421] + <3;(41)>[41] + <3;(3^3 )>[3^3 ]

       + <3;(3^2 1)>[3^2 1] + <3;(32^2 )>[32^2 ] + <3;(32)>[32]

       + <3;(31^2 )>[31^2 ] + <3;(3)>[3] + <3;(2^2 1)>[2^2 1]

       + <3;(21)>[21] + <3;(1^3 )>[1^3 ] + <3;(1)>[1]

DP>
```

The permutational symmetries associated with each $O(6)$ irreducible representation $[\lambda]$ is determined by an examination of its decomposition under $O(6) \to S(6)$. Thus for example we have from SCHUR

```
DP>

->brm

Branch Mode

->4,6

O(6) to S(6)

BRM>

0    ->  {6}

1^2  ->  {51} + {41^2 }

2    ->  {6} + 2{51} + {42}

21^2 ->  {42} + 2{41^2 } + 2{321} + 2{31^3 } + {2^2 1^2 }

2^2  ->  {51} + 3{42} + {41^2 } + {3^2 } + 2{321} + {2^3 }
```

```
2^3  ->  {42} + 2{3^2 } + 2{321} + 2{2^3 } + {2^2 1^2 }

31   ->  {6} + 4{51} + 4{42} + 5{41^2 } + 2{3^2 } + 3{321} + {31^3 }

321  -> 2{51} + 6{42} + 6{41^2 } + 4{3^2 } + 14{321} + 6{31^3 }

      + 4{2^3 } + 6{2^2 1^2 } + 2{21^4 }

BRM>
```

Only permutational states involving partitions of the form $[2^r1^s]$, where $r = \frac{N}{2} - S$ and $s = 2S$, can give rise to totally antisymmetric states as required for N identical spin $\frac{1}{2}$ fermions. Inspection of the above $O(6) \rightarrow S(6)$ decompositions shows that the states associated with the $Sp(6,R)$ irreducible representations

$$\langle 3;(0)\rangle, \langle 3;(11)\rangle, \langle 3;(2)\rangle, \langle 3;(31)\rangle$$

are spurious and must be discarded. Likewise for other $Sp(6,R)$ irreducible representations only certain spin states are admissible.

As a second example consider the alternative group-subgroup chain

$$Sp(36,R) \rightarrow U(18) \rightarrow U(3) \times U(6) \rightarrow U(3) \times O(6)$$

Here the group $U(3)$ involves the angular momentum states associated with its subgroup $O(3)$ while $U(6)$ involves the permutational symmetries associated with the $O(6) \supset S(6)$ subgroup. The irreducible representations of $U(18)$ all involve partitions (m) where m is an even integer for $\langle s;(0)\rangle$ and an odd integer for $\langle s;(1)\rangle$. Let us restrict our attention to the $U(18)$ representations with $m = 0,2,4,6$. From SCHUR we have

```
DP>

->gr u18

Group is U(18)

DP>

->br9,3,6gr1[0+2+4]

Groups are   U(3) * U(6)
```

```
      {4}{4} + {31}{31} + {2^2 }{2^2 } + {21^2 }{21^2 }

       + {2}{2} + {1^2 }{1^2 } + {0}{0}

DP>

->br1,6gr2last

Groups are   U(3) * O(6)

      {4}[4] + {4}[2] + {4}[0] + {31}[31] + {31}[2]

       + {31}[1^2 ] + {2^2 }[2^2 ] + {2^2 }[2] + {2^2 }[0]

       + {21^2 }[21^2 ] + {21^2 }[1^2 ] + {2}[2] + {2}[0]

       + {1^2 }[1^2 ] + {0}[0]

DP>
```

Inspection of the $O(6) \to S(6)$ branching rules show that the $U(3)$ irreducible representations $\{0\}, \{1^2\}, \{2\}, \{31\}, \{4\}$ are all associated with spurious states and may be eliminated. This leaves just two irreducible representations of $U(3) \times O(6)$, $\{2^2\} \times [2^2]$ and $\{21^2\} \times [21^2]$, as survivors, the first having spin $S = 0$ and the second with $S = 1$.

Under $U(3) \to O(3)$ we have

$$\{22\} \to [2] + [0] \quad \{21^2\} \to [1]$$

and thus we have the states ${}^1SD$ and ${}^3P$. These are precisely the states that are expected from putting two electrons in the lowest $s-$orbital and four electrons in the lowest $p-$orbital of a three-dimensional isotropic harmonic oscillator potential, that is the states of a s^2p^4 electron configuration. Going to higher values of m for irreducible representations of $U(18)$ we of course obtain a larger portion of the spectrum of states. Similar analyses can be made for the odd m cases that arise in the reduction of the $\langle s; (1) \rangle$ irreducible representation of $Sp(36, R)$ and again with the elimination of spurious states.

8. Concluding Remark

SCHUR has in the past being able to handle many problems associated with compact

Lie groups. Here we have outlined how SCHUR has been extended to include the generation of information on the non-compact group $Sp(2n,R)$ and its covering group $Mp(2n)$ and illustrated these extensions by their application to the classification of the states of quantum dots.

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