The Application of Symmetry Concepts to Physical Problems II

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1.1 Introduction

This course is a continuation of the previous semester course but it does not assume the subject matter of that course. The course will be given in English. While the concluding examination paper will be set in English students may elect to answer written questions in Polish.

In this semester I will be considering applications of symmetry concepts to and more particularly groups to problems in physics with special emphasis on applications to one- and many-particle systems. Some acquaintance with the basics of finite groups would be useful though not essential. Full notes will be available for each lecture.

I shall be assuming you have had a preliminary course in quantum theory including the rudiments of perturbation theory and the quantum theory of angular momentum. I propose to first give a brief review of atomic structure in order to establish some notationand then move on to a discussion of some relevant properties of finite groups taking the symmetric group as out prime example and give a brief outline of the properties of symmetric functions. I will then introduce you to the subject of Lie groups and algebras using the quantum theory of angular momentum as an example. This will lead to direct applications to the hydrogen atom and the harmonic oscillator and then to the concept of a dynamical group. The remainder of the course will then be devoted to a wide range of applications.

In making quantum calculations it is essential to be able to specify right at the beginning (1). the Hamiltonian appropriate to the system being studied and (2). by what manner we propose to solve the quantum problem. The latter usually requires that we specify a particular perturbation procedure. I would like to strongly emphasise the preceding two remarks. All to often one

reads in the literature papers where neither remark is clearly stated.

■ 1.2 The many-electron Hamiltonian

Only in very special cases can we write down a Hamiltonian for a system and solve the quantum equations exactly. Examples of these special cases include one-electron hydrogenic atoms. Note even when we say "*an exact solution*" we really mean an exact solution of a model system. For any real system our solutions can only be approximate. In some cases the solutions may apply to a system, such as, for example, a relativistic hydrogen atom with astonishing precision while for a rare earth atom with ~ 60 electrons we cannot expect to attain anything like the same precision.

For an $N-$electron atom we may write the Hamil- tonian, **H**, as

$$\mathbf{H} = \sum_{i=1}^{N} \left[\mathbf{p}_i^2 - \frac{Ze^2}{r_i} + \zeta(r_i)(\mathbf{s} \cdot \mathbf{l})_i \right] + \sum_{i>j} \frac{e^2}{r_{ij}} + \ldots \qquad (1-1)$$

The first term represents the kinetic energy of the electrons, the second the Coulomb attraction between the positively charge nucleus of atomic number Z and the $i-th$ electron, the third the spin-orbit coupling, and the fourth term the Coulomb repulsion between pairs of electrons. The $\ldots$ are there to remind us that there may be many other terms such as internal, or external, magnetic or electric fields, hyperfine interactions coupling the nuclear magnetic or electric quadrupole moments to the electrons, crystal fields and a multitude of relativistic effects etc. Furthermore, we are assuming, for the moment that the nucleus is an infinitely massive point object which means that we ignore mass isotope effects and finite nuclear size effects. Given the above Hamiltonian we wish to solve the eigenvalue equation

$$\mathbf{H}\Psi = \mathbf{E}\Psi \qquad (1-2)$$

This deceptively simple equation is incapable of exact solution, or even near exact solution for nearly all atoms. We seek to solve a simpler problem and then proceed to use perturbation theory.

■ 1.3 Central Field approximation

In order to simplify our problem let us assume each electron moves independently of the other electrons in a spherically averaged central field

potential $-\mathbf{U}(r_i)/e$ with a zero-order Hamiltonian, $\mathbf{H}_0$,

$$\mathbf{H}_0 = \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} + \mathbf{U}(r_i) \right] \tag{1-3}$$

with

$$\mathbf{H}' = \sum_i \left[-\frac{Ze^2}{r_i} - \mathbf{U}(r_i) \right] + \sum_{i>j} \frac{e^2}{r_{ij}} + \sum_i \zeta(r_i)(\ \mathbf{s} \cdot\ \mathbf{l})_i + \ldots \tag{1-4}$$

To proceed we first solve the much simpler central field equation

$$\mathbf{H}_0 \Psi_0 = \mathbf{E}_0 \Psi_0 \tag{1-5}$$

This equation can be separated using a set of functions $\psi(\alpha_i)$ such that

$$\Psi_0 = \prod_{i=1}^{N} \psi_i(\alpha_i) \quad \text{and} \quad \mathbf{E}_0 = \sum_{i=1}^{N} \varepsilon_i(\alpha_i) \tag{1-6}$$

leading to equations of the general form

$$\left[\frac{\mathbf{p}^2}{2m} + U(r) \right] \psi(\alpha) = \varepsilon(\alpha)\psi(\alpha) \tag{1-7}$$

This equation may be separated in spherical coordinates (r, θ, ϕ) by writing

$$\psi(\alpha) = \frac{\mathbf{R}_{n\ell}(r)\mathbf{Y}_{\ell m_\ell}(\theta, \phi)}{r} \tag{1-8}$$

with the usual definition of the spherical harmonics as

$$Y_{\ell m_\ell}(\theta, \phi) = (-1)^{m_\ell} \sqrt{\frac{2\ell + 1)(l - m_\ell)!}{4\pi(\ell + m_\ell)!}} \mathbf{P}_\ell^{m_\ell}(cos\theta)\, exp^{im_\ell \phi} \tag{1-9}$$

with

$$P_\ell^{m_\ell}(z) = \frac{(1 - z^2)^{\frac{m_\ell}{2}}}{2^\ell \ell!} \frac{d^{\ell + m_\ell}}{dz^{\ell + m_\ell}} (z^2 - 1)^\ell \tag{1-10}$$

Whereas the radial function $\mathbf{R}_{n\ell}(r)$ depends explicitly upon the central field potential $\mathbf{U}(r)$ the angular part $\mathbf{Y}_{\ell m_\ell}(\theta, \phi)$ is exactly the same as that for a hydrogenic atom. Each electron carries a spin $s = \frac{1}{2}$ with spin projection $m_s = \pm\frac{1}{2}$ and hence we should augment the orbital eigenfunctions of Eq.(1-8) with a two-component spinor $\chi(s, m_s)$ to give a complete spin-orbital eigenfunction

$$\psi(\alpha) = \frac{\mathbf{R}_{n\ell}(r)\mathbf{Y}_{\ell m_\ell}(\theta, \phi)}{r} \chi(s, m_s) \tag{1-11}$$

where now

$$\alpha \equiv (n\ell m_\ell s m_s) \tag{1-12}$$

describes a set of five quantum numbers associated with the state of a particular electron in the central field approximation (for the moment we suspend discussion of the identity of electrons).

■ 1.4 Electron Configurations

Note that the one-electron energies $\varepsilon_{n\ell}$ depend only on the quantum number pair $n\ell$ and hence the sequence of quantum numbers

$$n_1\ell_1, n_2\ell_2, \ldots, n_N\ell_N \qquad (1-13)$$

define an *electron configuration*. Within the central field approximation the states associated with the same sequence of $n\ell$ quantum numbers, and hence electron configuration, are degenerate in energy. Different electron configurations have different energy eigenvalues. As is usual in designating a particular electron configuration we will normally suppress the quantum numbers associated with closed shells and will thus often refer to configurations giving just such as are necessary for clarity e.g. $3d^x$ (the 3d transition ions) or $4f^x$ (the lanthanide ions) with multiple occupation of an orbital being indicated by a superscript.

■ 1.5 Single Configuration Approximation

The lowest energy configuration is the *ground configuration*. In neutral atoms there are often several electron configurations competing for lowest energy. Thus in the neutral $3d$ transition metal atoms the $3d^N$, $3d^{N-1}4s$ and $3d^{N-2}4s^2$ are usually energetically close and strongly interacting. In that case we have *configuration mixing* occurring. A similar situation arises in the neutral lanthanides. As the ionisation of atoms increases the low lying electron configurations tend to become energetically separated from one another and the lowest states of the ion may be well characterised by those of a single configuration. Thus the low lying states of the doubly charged transition ions are well characterised by a single $3d^N$ $(N = 1, 2, \ldots, 10)$ configuration and those of the triply ionised lanthanides by a single $4f^N$ $(N = 1, 2, \ldots, 14)$. In much of our work we shall assume a single configuration approximation though, as we shall see later, there are important phenomena such as intensities of transitions in solid state materials where such an assumption must abandoned.

■ 1.6 Bosons and fermions

The particles we commonly encounter in physics can be divided into two classes *bosons* and *fermions*. Bosons are associated with *integer* spin, examples being photons, gluons and the weak interaction bosons Z^0 and $W^{\pm}$. Fermions are associated with *half-integer* spin, examples being electrons, neutrinos and quarks. Bosons establish the *interactions* between fermions. Thus the *pho-*

ton, a massless spin 1 particle, is the exchange particle associated with electromagnetic interactions. In most of atomic and molecular physics we can restrict our attention to quantum electrodynamics (QED). The weak interactions manifest themselves in atomic and molecular physics in very small parity violations. Bosons and fermions obey different statistics, namely Bose-Einstein and Fermi-Dirac, respectively. That requires us to construct totally symmetric wavefunctions for many-boson systems and totally antisymmetric wavefunctions for many-fermion systems.

■ 1.7 Permutational Symmetry

Bosons and fermions differ with respect to their behaviour under an interchange of their position, or equivalently with respect to a rotation through 2π or 360^o. We shall designate the wavefunction for a single fermion or boson as $\phi(\alpha)$ where α is an appropriate set of single particle quantum numbers associated with some single particle solution of , for example, some central field potential. Thus for a hydrogen atom we might use $\alpha = \{ns\ell m_s m_\ell\}$ or $\alpha = \{ns\ell j m_j\}$. A $N-$particle system will involve $N-$single particle wavefunctions $(\phi_i \qquad i = 1, 2, \ldots, N)$ and $N-$sets of single particle quantum numbers $(\alpha_k \qquad k = 1, 2, \ldots, N)$. The wavefunction , Ψ, for the $N-$particle system will be such that

$$\Psi = \Psi(\phi_1, \phi_2, \ldots, \phi_N) \tag{1.14}$$

For a two-particle system we could write

$$\Psi(\phi_1, \phi_2) = \frac{1}{\sqrt{2}}\{\phi_1(\alpha_1)\phi_2(\alpha_2) \pm \phi_1(\alpha_2)\phi_2(\alpha_1)\} \tag{1.15}$$

The *positive* sign corresponds to a *symmetric* wavefunction and the *minus* sign corresponds to an *antisymmetric* wavefunction. Note that we have permuted the quantum numbers with respect to the coordinates of the particles. The wavefunction of a pair of fermions, unlike a pair of bosons, undergoes a change of sign. If $\alpha_1 = \alpha_2$ then for identical fermions Eq.(1.15) vanishes though not for bosons. That is consistent with the Pauli exclusion principle for identical fermions. Thus permutational symmetry, required by the indistinguishability of identical particles, leads for $N-$fermions to the construction of of *determinantal states* to give totally *antisymmetric* states while for $N-$bosons to the construction of *permanental states* to give totally *symmetric* states. Hence for an $N-$fermion system we have the totally antisymmetric wavefunction

$$\Psi(\phi_1,\phi_2,\ldots,\phi_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\phi_1(\alpha_1) & \phi_1(\alpha_2) & \ldots & \phi_1(\alpha_N)\\ \phi_2(\alpha_1) & \phi_2(\alpha_2) & \ldots & \phi_2(\alpha_N)\\ \vdots & \vdots & \ddots & \vdots\\ \phi_N(\alpha_1) & \phi_N(\alpha_2) & \ldots & \phi_N(\alpha_N)\end{vmatrix}^{\{1^N\}} \tag{1.16}$$

In LS–coupling basis we use $\alpha=\{ns\ell m_s m_\ell\}$ whereas in jj–coupling we would use $\alpha=\{ns\ell jm_j\}$. The information content of the determinantal state may be fully specified by the abbreviated form

$$\{\alpha_1\alpha_2\ldots\alpha_N\} \tag{1.17}$$

In the case of bosons we are required to construct permanental states to yield totally symmetric wavefunctions,

$$\Psi(\phi_1,\phi_2,\ldots,\phi_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\phi_1(\alpha_1) & \phi_1(\alpha_2) & \ldots & \phi_1(\alpha_N)\\ \phi_2(\alpha_1) & \phi_2(\alpha_2) & \ldots & \phi_2(\alpha_N)\\ \vdots & \vdots & \ddots & \vdots\\ \phi_N(\alpha_1) & \phi_N(\alpha_2) & \ldots & \phi_N(\alpha_N)\end{vmatrix}^{\{N\}} \tag{1.18}$$

The information content of the permanental state may be fully specified by the abbreviated form

$$[\alpha_1\alpha_2\ldots\alpha_N] \tag{1.19}$$

We shall use square brackets [] to indicate boson states and curly brackets {} for fermion states. Equations (1.16) and (1.18) look remarkably similar. We have distinguished them by superscripts $\{1^N\}$ and $\{N\}$, respectively. The matrix of the single particle functions are the same in both cases but the action on the matrix is different. In the first case the *determinant* of the matrix is formed and in the second the *permanent* of the matrix is formed. Could we form other objects of interest by other actions on a matrix?

■ 1.8 Many-particle states of Bosons and Fermions

Let us for the moment consider the states of N identical bosons or fermions. Suppose the boson has an angular momentum $j=2$ (i.e. a d–boson) and hence $m_j=0,\pm1,\pm2$ while the fermion has angular momentum $j=5/2$ and hence $m_j=\pm1/2,\pm3/2,\pm5/2$. If $N=2$ in both cases what are the allowed values of J ? We note that

$$M_J=m_{j_1}+m_{j_2}$$

Just considering the non-negative values of M_J we obtain for the fermions the following table of determinantal states:

Table 1.1 Determinantal states for $(5/2)^2$ fermions.

M_J	States		
4	$\{5/2\,3/2\}$		
3	$\{5/2\,1/2\}$		
2	$\{5/2\,-1/2\}$	$\{3/2\,1/2\}$	
1	$\{5/2\,-3/2\}$	$\{3/2\,-1/2\}$	
0	$\{5/2\,-5/2\}$	$\{3/2\,-3/2\}$	$\{1/2\,-1/2\}$

Inspection of the above table leads to the conclusion that the allowed values of J in $(5/2)^2$ are $J = 0, 2, 4$.

The corresponding d^2 boson states for non-negative M_J are given in Table 1.2.

Table 1.2. Permanental states for d^2 bosons

M_J	States		
4	$[2\,2]$		
3	$[2\,1]$		
2	$[2\,0]$	$[1\,1]$	
1	$[2\,-1]$	$[1\,0]$	
0	$[2\,-2]$	$[1\,-1]$	$[0\,0]$

Inspection of the above table leads to the conclusion that the allowed values of J in d^2 are $J = 0, 2, 4$ exactly those [1] found for $(5/2)^2$.

■ 1.9 Ladder Operators and Determinantal States

For the electron configuration f^2 we can enumerate the set of determinantal states for non-negative M_S, M_L as in Table 1.3.

[1] In general the *antisymmetric* states of N identical particles each having angular $j = m/2$ and the *symmetric* states of N particles each having angular momentum $j = (m+n+1)/2$ have the same total angular momentum J values. See B.G.Wybourne, *Hermite's reciprocity Law and the Angular Momentum States of Equivalent Particle Configurations* J.Math.Phys. 10, 467-71 (1969).

Table 1.3. Determinantal states for the Electron Configuration f^2.

M_L	$M_S = 0$						$M_S = 1$		
6	$\{^{+}_{3}\ ^{-}_{3}\}$								
5	$\{^{+}_{3}\ ^{-}_{2}\}$	$\{^{+}_{2}\ ^{-}_{3}\}$					$\{^{+}_{3}\ ^{+}_{2}\}$		
4	$\{^{+}_{3}\ ^{-}_{1}\}$	$\{^{+}_{2}\ ^{-}_{2}\}$	$\{^{+}_{1}\ ^{-}_{3}\}$				$\{^{+}_{3}\ ^{+}_{1}\}$		
3	$\{^{+}_{3}\ ^{-}_{0}\}$	$\{^{+}_{2}\ ^{-}_{1}\}$	$\{^{+}_{1}\ ^{-}_{2}\}$	$\{^{+}_{0}\ ^{-}_{3}\}$			$\{^{+}_{3}\ ^{+}_{0}\}$	$\{^{+}_{2}\ ^{+}_{1}\}$	
2	$\{^{+}_{2}\ ^{-}_{0}\}$	$\{^{+}_{3}\ ^{-}_{-1}\}$	$\{^{+}_{1}\ ^{-}_{1}\}$	$\{^{+}_{0}\ ^{-}_{2}\}$	$\{^{+}_{-1}\ ^{-}_{3}\}$		$\{^{+}_{3}\ ^{+}_{-1}\}$	$\{^{+}_{2}\ ^{+}_{0}\}$	
1	$\{^{+}_{1}\ ^{-}_{0}\}$	$\{^{+}_{2}\ ^{-}_{-1}\}$	$\{^{+}_{3}\ ^{-}_{-2}\}$	$\{^{+}_{0}\ ^{-}_{1}\}$	$\{^{+}_{-1}\ ^{-}_{2}\}$	$\{^{+}_{-2}\ ^{-}_{3}\}$	$\{^{+}_{3}\ ^{+}_{-2}\}$	$\{^{+}_{1}\ ^{+}_{0}\}$	$\{^{+}_{2}\ ^{+}_{-1}\}$
0	$\{^{+}_{0}\ ^{-}_{0}\}$	$\{^{+}_{1}\ ^{-}_{-1}\}$	$\{^{+}_{2}\ ^{-}_{-2}\}$	$\{^{+}_{3}\ ^{-}_{-3}\}$	$\{^{+}_{-1}\ ^{-}_{1}\}$	$\{^{+}_{-3}\ ^{-}_{3}\}$	$\{^{+}_{3}\ ^{+}_{-3}\}$	$\{^{+}_{2}\ ^{+}_{-2}\}$	$\{^{+}_{1}\ ^{+}_{-1}\}$
	$\{^{+}_{-2}\ ^{-}_{2}\}$								

Recall that for an electron in an $f-$orbital $\ell = 3$ and hence $m_\ell = 0, \pm 1, \pm 2, \pm 3$. There are just two values of the spin projection $m_s = \pm 1/2$. Thus it suffices in writing a determinantal state to just display the values of m_ℓ and indicate the value of m_s as a $+$ or $-$ sign placed above m_ℓ. For a given determinantal state we have

$$M_S = \sum_{i=1}^{n} m_{s_i} \qquad \text{and} \qquad M_L = \sum_{i=1}^{n} m_{\ell_i} \tag{1.20}$$

Thus every determinantal state may be associated with definite values of M_S and M_L. That does not mean that they are eigenstates of the total spin S and orbital L angular momentum. To form such eigenstates we must form appropriate linear combinations of the determinantal states to give eigenstates $|SLM_SM_L>$. Following tradition we will normally write such a state as $|^{2S+1}LM_SM_L>$ where $(2S+1)$ is known as the *spin multiplicity*. The quantum number L is usually associated with alphabetical letters

0	1	2	3	4	5	6	7	8
S	P	D	F	G	H	I	K	M

A spectroscopic term will be designated as

$$^{2S+1}L$$

Associated with a given value on S there are $(2S+1)$ values of M_S and with L there are $(2L+1)$ values of M_L where

$$M_S = S, S-1, \ldots, -S+1, -S \quad \text{and} \quad M_L = L, L-1, \ldots, -L+1, -L$$

Inspection of Table 1.3 shows that the spectroscopic terms of the electron configuration f^2 are

$$^3PFH \quad ^1SDGI$$

Choose

$$|^1I06> \equiv \{ \begin{matrix} + & - \\ 3 & 3 \end{matrix} \} \tag{1.22}$$

Let us now determine $|^1I05>$. To do this we use the properties of ladder operators. Recall

$$L_\pm |LM> = \sqrt{L(L+1) - M(M \pm 1)}\,|LM \pm 1> \tag{1.23}$$

and

$$L_\pm = \sum_{i=1}^{n} \ell_{\pm_i} \tag{1.24}$$

Let (1.23) act on the left-hand-side of (1.22) and noting (1.23) act also on the determinantal state to give

$$L_-|^1I06>=\sqrt{6\times 7-6\times 5}|^1I05>=\sqrt{12}|^1I05> \tag{1.25}$$

and

$$L_-\{\begin{smallmatrix}+&-\\3&3\end{smallmatrix}\}=\sqrt{3\times 4-3\times 2}[\{\begin{smallmatrix}+&-\\2&3\end{smallmatrix}\}+\{\begin{smallmatrix}+&-\\3&2\end{smallmatrix}\}] \tag{1.26}$$

Equating (1.25) and (1.26) gives

$$|^1I05>=\frac{\sqrt{2}}{2}[\{\begin{smallmatrix}+&-\\2&3\end{smallmatrix}\}+\{\begin{smallmatrix}+&-\\3&2\end{smallmatrix}\}] \tag{1.27}$$

This state must be orthogonal to the state $|^3H05>$ and hence after fixing a phase we have

$$|^3H05>=\frac{\sqrt{2}}{2}[\{\begin{smallmatrix}+&-\\2&3\end{smallmatrix}\}-\{\begin{smallmatrix}+&-\\3&2\end{smallmatrix}\}] \tag{1.28}$$

Application of the spin raising operator S_+ to (1.28) gives

$$S_+|^3H05>=\sqrt{2}|^3H15>=\frac{\sqrt{2}}{2}[\{\begin{smallmatrix}+&+\\2&3\end{smallmatrix}\}-\{\begin{smallmatrix}+&+\\3&2\end{smallmatrix}\}]$$

and hence

$$|^3H15>=-\{\begin{smallmatrix}+&+\\3&2\end{smallmatrix}\}] \tag{1.29}$$

Note the appearance of the minus sign which comes from our particular choice of enumeration of the determinantal states.

■ Exercises

1.1 Show that the totally antisymmetric orbital angular momentum states of g^3 $(\ell=4)$ (i.e. the states of maximum multiplicity) are the same as for the totally symmetric states of $(5/2)^4$.

1.2 Determine the allowed values of J for the jj–coupled configurations $(5/2)^2, (5/2\,7/2)$ and $(7/2)^2$.

1.3 Determine the allowed values of S and L for the electron configuration f^2.

1.4 Given that for an LS–coupled term ^{2S+1}L we have $\mathbf{J=L+S}$ and

$$J=L+S, L+S-1, \ldots, |L-S| \tag{1.30}$$

Show that the values of J for the list of terms found in Ex 1.3. are the same as those found in Ex 1.2.

1.5 Show that in the configuration j^2 the only allowed values of J are the even integers $0, 2, \ldots, 2j-1$.

1.6 Starting with the angular momentum commutation relations

$$[J_x, J_y] = iJ_z \quad , [J_y, J_z] = iJ_x \quad , [J_z, J_x] = iJ_y \tag{1.31}$$

show that if $J_\pm = J_x \pm iJ_y$ **then**

$$\mathbf{J}^2 = \frac{J_+ J_- + J_- J_+}{2} + J_z^2 \tag{1.32}$$

1.7 If $\mathbf{J = L + S}$ **show that**

$$J(J+1) - L(L+1) - S(S+1) = S_+ L_- + S_- L_+ + 2S_z L_z \tag{1.33}$$

1.8 Determine the eigenstates

$$|^1I04> \quad |^3H04> \quad |^1G04> \quad |^3H14>$$

as linear combinations of determinantal states.

1.9 Discuss how you could determine the eigenstates $|^3HJM>$ **as linear combinations of the states** $|^3HM_SM_L>$. *Hint*: **use the fact that** $J_\pm = L_\pm + S_\pm$.

The Application of Symmetry Concepts to Physical Problems II

B. G. Wybourne

■ **2.1 Introduction** The structure of an electron configuration develops when we include the Coulomb repulsion and spin-orbit terms as a perturbation on our zero-order central field solutions. In this lecture we review the basic structure of d^N and f^N electron configurations.

■ **2.2 Multiplets**

The Coulomb interaction, $\mathbf{H}_C$, commutes with the angular momentum operators $\mathbf{J}^2$, $\mathbf{S}^2$ and $\mathbf{L}^2$ which ensures that the matrix elements of H_C are diagonal in the quantum numbers **SLJ**. Furthermore, H_C commutes with J_z, S_z and L_z leading to the matrix elements being diagonal in M_J, M_S and M_L and independent of the quantum numbers J, M_J, M_S, M_L. Thus the effect of introducing the Coulomb interaction in first order is to partially lift the degeneracies of electron configurations In general a configuration splits into a series of multiplets that are characterised by the total spin $\mathcal{S}$ and orbital $\mathcal{L}$ quantum numbers. Each $\mathcal{SL}$ multiplet is still degernerate with respect to the quantum numbers M_S, M_L or equivalently with respect to the quantum numbers J, M_J. Thus each multiplet involves a set of $(2S+1)(2L+1)$-fold degenerate states.

■ **2.3 Spin-Orbit Splittings**

The spin-orbit interaction term, $\mathbf{H}_{so}$, commutes with $\mathbf{J}^2$ and M_J but neither with $\mathbf{S}^2$ or $\mathbf{L}^2$ and hence the matrix elements of $\mathbf{H}_{so}$ are diagonal in the quantum numbers J, M_J and independent of M_J. Very importantly, The spin-orbit interaction is *not* diagonal in S and L and hence there is the possibility of S and L ceasing to be "good quantum numbers" and a state $|\alpha J M_J\rangle$ becomes some linear combination of $|SLJM_J\rangle$ states

$$|\alpha J M_J\rangle = \sum_{S,L} a(S,L,J)|SLJM_J\rangle \tag{2.1}$$

This mixing of multiplets is often responsible for a breakdown of selection rules and for departures from LS–coupling.

The spin-orbit interaction results in a further lifting of degeneracy, each S, L multiplet splits into a series of sublevels each characterised by the total angular momentum J where

$$J = L + S, L + S - 1, \ldots, |L - S| \tag{2.2}$$

with each level of total angular momentum J being $2J+1$-fold degenerate. This residual degeneracy may be lifted by the application of an external magnetic field as in the case of the Zeeman effect.

■ 2.4 The LS terms of d^N and f^N configurations

We now give in table form the various LS terms that arise in the d^N and f^N configurations. Here I have used the theory of Lie groups to give a full description of the states. In the case of the d^N configuration we have for a single d–orbital a total of 10 states $|dm_s m_\ell\rangle$ which can be regarded as a vector in a 10-dimensional unitary space. The LS multiplets of d^N and $d^{10-N}$are the same and hence we need only list the cases for $N \leq 5$.

■ 2.5 The Hund's rule groundstates for atoms

The groundstate of an atomic configuration of the type ℓ^N may be determined by application of Hund's rules.

1. From the list of LS multiplets select the multiplets of maximal S.
2. From the multiplets of maximal S select the multiplet of largest L.
3. If $N \leq 2\ell + 1$ select the *smallest* value of the total angular momentum J while for $N > 2\ell + 1$ select the *largest* value of J.

Table 2.1 LS multiplets of the d^N (N = 0 to 5) configurations

# of states	U_{10}	$SU_2^S \times SU_5^L$	SO_5	^{2S+1}L
1	$\{0\}$	$\{0\} \times \{0\}$	[00]	^1S
10	$\{1\}$	$\{1\} \times \{1\}$	[10]	^2D
45	$\{1^2\}$	$\{2\} \times \{1^2\}$	[11]	^3PF
		$\{0\} \times \{2\}$	[20]	^1DG
			[00]	^1S
120	$\{1^3\}$	$\{3\} \times \{1^3\}$	[11]	^4PF
		$\{1\} \times \{21\}$	[21]	^2PDFGH
			[10]	^2D
210	$\{1^4\}$	$\{4\} \times \{1^4\}$	[10]	^5D
		$\{2\} \times \{21^2\}$	[21]	^3PDFGH
			[10]	^3D
		$\{0\} \times \{2^2\}$	[22]	^1SDFGI
			[20]	^1DG
			[00]	^1S
252	$\{1^5\}$	$\{5\} \times \{1^5\}$	[00]	^6S
		$\{3\} \times \{21^3\}$	[20]	^4DG
			[11]	^4PF
		$\{1\} \times \{2^21\}$	[22]	^2SDFGI
			[21]	^2PDFGH
			[10]	^2D

Table 2.2 LS multiplets of the f^N (N = 1 to 5) configurations

# of states	U_{14}	$SU_2^S \times SU_7^L$	SO_7	G_2	^{2S+1}L
1	$\{0\}$	$\{0\} \times \{0\}$	[000]	(00)	^1S
14	$\{1\}$	$\{1\} \times \{1\}$	[100]	(10)	^2F
45	$\{1^2\}$	$\{2\} \times \{1^2\}$	[110]	(11)	^3PH
				(10)	^3F
		$\{0\} \times \{2\}$	[200]	(20)	^1DGI
			[000]	(00)	^{S}
364	$\{1^3\}$	$\{3\} \times \{1^3\}$	[111]	(20)	^4DGI
				(10)	^4F
				(00)	^4S
		$\{1\} \times \{21\}$	[210]	(21)	^2DFGHKL
				(20)	^2DGI
				(11)	^2PH
			[100]	(10)	^2F
1001	$\{1^4\}$	$\{4\} \times \{1^4\}$	[111]	(20)	^5DGI
				(10)	^5F
				(00)	^5S
		$\{2\} \times \{211\}$	[211]	(30)	$^3PFGHIKM$
				(21)	^3DFGHKL
				(20)	^3DGI
				(11)	^3PH
				(10)	^3F
		$\{0\} \times \{2^2\}$	[220]	(22)	$^1SDGHILN$
				(21)	^1DFGHKL
				(20)	^1DGI
			[200]	(20)	^1DGI
			[000]	(00)	^1S
2002	$\{1^5\}$	$\{5\} \times \{1^5\}$	[110]	(11)	^6PH
				(10)	^6F
		$\{3\} \times \{21^3\}$	[211]	(30)	$^4PFGHIKM$
				(21)	^4DFGHKL
				(20)	^4DGI
				(11)	^4PH
				(10)	^4F
			[111]	(20)	^4DGI
				(10)	^4F
				(00)	^4S
		$\{1\} \times \{2^21\}$	[221]	(31)	$^2PDFFGHHIIKKLMNO$
				(30)	$^2PFGHIKM$
				(21)	^2DFGHKL
				(20)	^2DGI
				(11)	^2PH
				(10)	^2F
			[210]	(21)	$^2DFGHIKL$
				(20)	^2DGI
				(11)	^2PH
			[100]	(10)	^2F

Table 2.3 LS multiplets of the f^6 configuration

# of states	U_{14}	$SU_7^S \times SU_7^L$	SO_7	G_2	^{2S+1}L
3003	$\{1^6\}$	$\{6\} \times \{1^6\}$	[100]	(10)	^7F
		$\{4\} \times \{21^4\}$	[210]	(21)	$^5DFGHIKL$
				(20)	^5DGI
				(11)	^5PH
			[111]	(20)	^5DGI
				(10)	^5F
				(00)	^5S
		$\{2\} \times \{2^2 1^2\}$	[221]	(31)	$^3PDFFGHHIIKKLMNO$
				(30)	$^3PFGHIKM$
				(21)	^3DFGHKL
				(20)	^3DGI
				(11)	^3PH
				(10)	^3F
			[211]	(30)	$^3PFGHIKM$
				(21)	^3DFGHKL
				(20)	^3DGI
				(11)	^3PH
				(10)	^3F
			[110]	(11)	^3PH
				(10)	^3F
		$\{0\} \times \{2^3\}$	[222]	(40)	$^1SDFGGHIIKLLMNQ$
				(30)	$^1PFGHIKM$
				(20)	^1DGI
				(10)	^1F
				(00)	^1S
			[220]	(22)	$^1SDGHILN$
				(21)	^1DFGHKL
				(20)	^1DGI
			[200]	(20)	^1DGI
			[000]	(00)	^1S

Table 2.4 LS multiplets of the f^7 configuration

# of states	U_{14}	$SU_7^S \times SU_7^L$	SO_7	G_2	^{2S+1}L
3432	$\{1^7\}$	$\{7\} \times \{1^7\}$	[000]	(00)	^8S
		$\{5\} \times \{21^5\}$	[200]	(20)	^6DGI
			[110]	(11)	^6PH
				(10)	^6F
		$\{3\} \times \{2^2 1^3\}$	[220]	(22)	$^4SDGHILN$
				(21)	^4DFGHKL
				(20)	^4DGI
			[211]	(30)	$^4PFGHIKM$
				(21)	^4DFGHKL
				(20)	^4DGI
				(11)	^4PH
				(10)	^4F
			[111]	(20)	^4DGI
				(10)	^4F
				(00)	^4S
		$\{1\} \times \{2^3 1\}$	[222]	(40)	$^2SDFGGHIIKLLMNQ$
				(30)	$^2PFGHIKM$
				(20)	^2DGI
				(10)	^2F
				(00)	^2S
			[221]	(31)	$^2PDFFGHHIIKKLMNO$
				(30)	$^2PFGHIKM$
				(21)	^2DFGHKL
				(20)	^2DGI
				(11)	^2PH
				(10)	^2F
			[210]	(21)	$^2DFGHIKL$
				(20)	^2DGI
				(11)	^2PH
			[100]	(10)	^2F

■ Exercises

2.1 Construct a proof that the matrix elements of $\mathbf{H}_C$ are independent of J, M_J, M_S, M_L.

2.2 Draw up a list of the Hund's rule groundstates for the d^N and f^N configurations.

The Application of Symmetry Concepts to Physical Problems II

B. G. Wybourne

With the odd number five strange natures laws
Plays many freaks nor once mistakes the cause
And in the cowslap peeps this very day
Five spots appear which time neer wears away
Nor once mistakes the counting - look within
Each peep and five nor more nor less is seen
And trailing bindweed with its pinky cup
Five lines of paler hue goes streaking up
And birds a many keep the rule alive
And lay five eggs nor more nor less then five
And flowers how many own that mystic power
With five leaves making up the flower

John Clare ˚ 1821

■ Lecture 3

■ 3.1 Permutations and the Symmetric Group

Permutations play an important role in the physics of identical particles. A permutation leads to a reordering of a sequence of objects. We can place n objects in the natural number ordering $1, 2, \ldots, n$. Any other ordering can be discussed in terms of this ordering and can be specified in a two line notation

$$\begin{matrix} 1 & 2 & \ldots & n \\ \pi(1) & \pi(2) & \ldots & \pi(n) \end{matrix} \tag{3.1}$$

For $n = 3$ we have the six permutations

$$\begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix} \quad \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix} \quad \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix}$$
$$\begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix} \quad \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} \tag{3.2}$$

Permutations can be multiplied working from right to left. Thus

$$\begin{pmatrix}1&2&3\\3&1&2\end{pmatrix}\times\begin{pmatrix}1&2&3\\2&3&1\end{pmatrix}=\begin{pmatrix}1&2&3\\1&2&3\end{pmatrix}$$

The six permutations in (3.2) satisfy the following properties:

1. There is an identity element $\begin{pmatrix}1&2&3\\1&2&3\end{pmatrix}$.
2. Every element has an inverse among the set of elements.
3. The product of any two elements yields elements of the set.
4. The elements satisfy the associativity condition $a(bc)=(ab)c$. These conditions establish that the permutations form a *group*. In general the $n!$ permutations form the elements of the *symmetric group* $\mathcal{S}_n$.

■ Exercise 3.1 Construct a multiplication table (The Cayley Table) for the six permutations given in (3.2) and verify that the set of six permutations form a group.

■ Exercise 3.2 Inspect your Cayley table and see what subsets of the elements satisfy the four group axioms and thus form a *subgroup* of $\mathcal{S}_6$.

■ 3.2 Cycle Structure of Permutations

It is useful to express permutations as a cycle structure. A cycle $(i,j,k,\ldots,l)$ is interpreted as $i\rightarrow j, j\rightarrow k$ and finally $l\rightarrow i$. Thus our six permutations have the cycle structures

$$(1)(2)(3),(1,2)(3),(1)(2,3),(1,3)(2),(1,3,2),(1,2,3) \tag{3.3}$$

The elements within a cycle can be cyclically permuted and the order of the cycles is irrelevant. Thus $(123)(45)\equiv(54)(312)$.

■ A *k-cycle* or *cycle of length k* contains k elements. It is useful to organise cycles into *types* or *classes*. We shall designate the *cycle type* of a permutation π by

$$(1^{m_1}2^{m_2}\ldots,n^{m_n}) \tag{3.4}$$

where m_k is the number of cycles of length k in the cycle representation of the permutation π.

■ For $\mathcal{S}_4$ there are five cycle types

$$(1^4),(1^2\ 2^1),(2^2),(1^1\ 3^1),(4^1) \tag{3.5}$$

Normally exponents of unity are omitted and Eq.(3.5) written as

$$(1^4),(1^2 2),(2^2),(13),(4) \tag{3.6}$$

■ **Cycle types may be equally well labelled by ordered partitions of the integer** n

$$\lambda = (\lambda_1 \lambda_2 \ldots \lambda_\ell) \tag{3.6}$$

where the λ_i **are weakly decreasing and**

$$\sum_{i=1}^{\ell} \lambda_i = n \tag{3.7}$$

The partition is said to be of *length* ℓ_λ **and of** *weight* $w_\lambda = n$**. In terms of partitions the cycle types for** $\mathcal{S}_5$ **are**

$$(1^5), (21^3), (2^2 1), (32), (31^2), (41), (5) \tag{3.8}$$

■ 3.3 Conjugacy Classes of $\mathcal{S}_n$

In any group G **the elements** g **and** h **are** *conjugates* **if**

$$g = khk^{-1} \qquad \text{for some} \qquad k \in G \tag{3.9}$$

The set of all elements conjugate to a given g **is called the** *conjugacy class* **of** g **which we denote as** K_g**.**

■ **Exercises**

3.3 Show that for $\mathcal{S}_4$ **there are five conjugacy classes that may be labelled by the five partitions of the integer** 4**.**

3.4 Show that the permutations, expressed in cycles, with cycles of length one suppressed, divide among the conjugacy classes as

$$\begin{aligned}
(1^4) &\supset e \\
(21^2) &\supset (12), (13), (14), (23), (24), (34) \\
(2^2) &\supset (12)(34), (13)(24), (14)(23) \\
(31) &\supset (123), (124), (132), (134), (142) \\
&\quad\ (143), (234), (243) \\
(4) &\supset (1234), (1243), (1342), (1432)
\end{aligned} \tag{3.10}$$

In general two permutations are in the same conjugacy class if, and only if, they are of the same cycle type. The number of classes of $\mathcal{S}_n$ **is equal the number of partitions of the integer** n**.**

If $\lambda = (1^{m_1} 2^{m_2} \ldots n^{m_n})$ **then the number of permutations** k_λ **in the class** (λ) **of** $\mathcal{S}_n$ **is**

$$k_\lambda = \frac{n!}{1^{m_1} m_1! 2^{m_2} m_2! \ldots n^{m_n} m_n!} \tag{3.11}$$

■ **3.4 The Cayley Table for $\mathcal{S}_3$**

	e	(12)	(13)	(23)	(132)	(123)
e	e	(12)	(13)	(23)	(132)	(123)
(12)	(12)	e	(132)	(123)	(13)	(23)
(13)	(13)	(123)	e	(132)	(23)	(12)
(23)	(23)	(132)	(123)	e	(12)	(13)
(132)	(132)	(23)	(12)	(13)	(123)	e
(123)	(123)	(13)	(23)	(12)	e	(132)

■ **3.5 Transpositions and cycles of $\mathcal{S}_n$**

1. **A cycle of order two is termed a** *transposition*.
2. **A transposition $(i, i+1)$ is termed an** *adjacent transposition*.
3. **The entire symmetric group $\mathcal{S}_n$ can be generated (or given a** *presentation* **in terms of the set of adjacent transpositions**

$$(1\,2),\ (2\,3),\ \ldots,\ (n-1\,n) \tag{3.12}$$

■ **If $\pi = \tau_1\tau_2\ldots\tau_k$, where the τ_i are transpositions then the** *sign* **of π is defined to be**

$$sgn(\pi) = (-1)^k \tag{3.13}$$

If the number of cycles of *even* **order is** *even* **then the permutation is** *even* **or** *positive*; **if it is** *odd* **then the permutation is** *odd* **or** *negative*.

■ **3.6 The Presentation of $\mathcal{S}_n$**

Let us designate an adjacent transposition by

$$s_i = (i, i+1) \qquad \textbf{for} \quad i = 1, 2, \ldots, n-1 \tag{3.14}$$

then we can give a *presentation* **of the symmetric group $\mathcal{S}_n$ in terms of the s_i via the following three relations:-**

$$s_i^2 = 1 \qquad \textbf{for} \quad i = 1, 2, \ldots, n-1 \tag{3.15a}$$

$$s_i s_{i+1} s_i = s_{i+1} s_i s_{i+1} \qquad \textbf{for} \quad i = 1, 2, \ldots, n-2 \tag{3.15b}$$

$$s_i s_j = s_j s_i \qquad \textbf{for} \quad |i-j| \geq 2 \tag{3.15c}$$

Every permutation π in S_n can be expressed as a *reduced word* **of minimal length $\ell(\pi)$ in the s_i.**

■ **Exercise**

3.5 Verify the last sentence in the case of $\mathcal{S}_3$

■ 3.7 Note on Hecke algebra $\mathcal{H}_n(q)$ of type $\mathcal{A}_{n-1}$

We can q–deform the presentation of $\mathcal{S}_n$ to give the complex Hecke algebra $\mathcal{H}_n(q)$, with q an arbitrary but fixed complex parameter, generated by g_i with $i = 1, 2, \ldots, n-1$ subject to the relations:

$$g_i^2 = (q-1)g_i + q \qquad \textbf{for} \quad i = 1, 2, \ldots, n-1 \tag{3.16a}$$

$$g_i g_{i+1} g_i = g_{i+1} g_i g_{i+1} \qquad \textbf{for} \quad i = 1, 2, \ldots, n-2 \tag{3.16b}$$

$$g_i g_j = g_j g_i \qquad \textbf{for} \quad |i-j| \geq 2 \tag{3.16c}$$

For $q = 1$ these relations are exactly those appropriate to the symmetric group $\mathcal{S}_n$. There exists a map h from $\mathcal{S}_n$ to $\mathcal{H}_n(q)$ such that $h(s_i) = g_i$ and $h(\pi) = g_{i_1} g_{i_2} \ldots g_{i_m}$ for any permutation $\pi = s_{i_1} s_{i_2} \ldots s_{i_m} \in \mathcal{S}_n$. The set of reduced words $h(\pi)$ for all $n!$ permutations $\pi \in \mathcal{S}_n$ forms a basis of $\mathcal{H}_n(q)$. For more details see:- R. C. King and B. G. Wybourne, *J. Phys. A: Math. Gen. 23* L1193 (1990).

■ 3.8 The Alternating Group $\mathcal{A}_n$

The set of *even* permutations form a subgroup of $\mathcal{S}_n$ known as the *alternating group* $\mathcal{A}_n$ and has precisely half the elements of $\mathcal{S}_n$ i.e. $(\frac{1}{2})n!$.

■ Exercises

3.6 Show that the set of six matrices

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & -1 \end{bmatrix} \begin{bmatrix} -1 & -1 \\ 1 & 0 \end{bmatrix}$$
$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} -1 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ -1 & -1 \end{bmatrix} \tag{3.17}$$

with the usual rule of matrix multiplication form a group isomorphic to $\mathcal{S}_3$.

3.7 Show that the symmetric group $\mathcal{S}_n$ has two one-dimensional representations, a symmetric representation where every element is mapped onto unity and an antisymmetric representation where the elements are mapped onto the sign defined in Eq. (3.13).

■ 3.9 Partitions

The partition of integers play a key role in much that follows. Here we review some of their properties and establish some notation for later usage.

■ A partition is any finite or infinite sequence of integers

$$\lambda = (\lambda_1 \, \lambda_2 \, \ldots \, \lambda_i \, \ldots) \tag{3.18}$$

Unless otherwise stated we shall assume the sequence involves non-negative integers in non-increasing order;

$$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_i \geq \ldots \tag{3.19}$$

Normally we will omit zeros.

■ The non-zero λ_i form the *parts* of λ. The number of parts is the *length*, $\ell(\lambda)$, of λ while the sum of its parts, \lambda, is the *weight* of λ. If \lambda $= n$ then λ is said to be a *partition* of n.

■ We shall frequently write $\lambda \vdash n$ to indicate that λ is a partition of n. Repeated parts of a partition will frequently be indicated as i^{m_i} where m_i is the number of times the part i occurs in the partition λ.

■ The partitions for $n = 6$ are

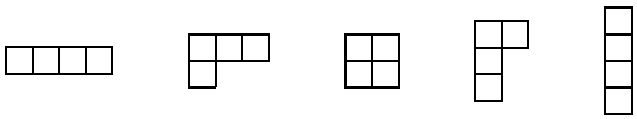
$$(6)\,(51)\,(42)\,(41^2)\,(3^2)\,(321)\,(31^3)\,(2^3)\,(2^21^2)\,(21^4)\,(1^6)$$

■ Note, in the above example the partitions have been listed in *reverse lexicographic order*. The ordering is such that the first non-vanishing difference $\lambda_i - \mu_i$, for successive partitions λ, μ is *positive*.

■ 3.10 The Ferrers-Sylvester diagram

■ Every partition $\lambda \vdash n$ may be associated with a *Ferrers-Sylvester diagram*, *shape* or *frame* involving n cells, dots or boxes in $\ell(\lambda)$ left-adjusted rows with the i-th row containing λ_i cells, dots, or boxes.

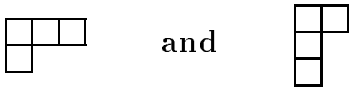
For $n = 4$ we have the five diagrams



■ We will formally designate the frame associated with a partition λ as F^λ.

■ The *conjugate* of a partition λ is a partition λ' whose diagram is the transpose of the diagram of λ. If $\lambda' \equiv \lambda$ then the partition λ is said to be *self-conjugate*.

Thus



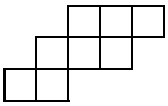
are conjugates while

is self-conjugate.

■ **3.11 Skew frames**

■ **Given two partitions λ and μ such that $\lambda \supset \mu$ implies that the frame F^{λ} contains the frame F^{μ}, i.e. that $\lambda_i \geq \mu_i$ for all $i \geq 1$. The difference $\rho = \lambda - \mu$ forms a *skew* frame $F^{\lambda/\mu}$.**

Thus, for example, the skew frame $F^{542/21}$ has the form



Note that a skew frame may consist of disconnected pieces.

■ **3.12 Frobenius notation for partitions**

■ **There is an alternative notation for partitions due to Frobenius. The *diagonal* of nodes in a Ferrers-Sylvester diagram beginning at the top left-hand corner is called the *leading diagonal*. The number of nodes in the leading diagonal is called the *rank* of the partition.**

■ **If r is the rank of a partition then let a_i be the number of nodes to the right of the leading diagonal in the i–th row and let b_i be the number of nodes below the leading diagonal in the i–th column. The partition is then denoted by Frobenius as**

$$\begin{pmatrix} a_1, & a_2, & \ldots, & a_r \\ b_1, & b_2, & \ldots, & b_r \end{pmatrix} \tag{3.20}$$

We note that

$$a_1 > a_2 > \ldots > a_r$$

$$b_1 > b_2 > \ldots > b_r$$

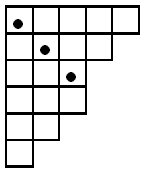
and

$$a_1 + a_2 + \ldots + a_r + b_1 + b_2 + \ldots + b_r + r = n$$

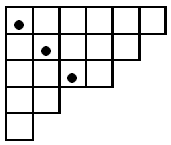
■ **The partition conjugate to that of Eq.(3.20) is just**

$$\begin{pmatrix} b_1, & b_2, & \ldots, & b_r \\ a_1, & a_2, & \ldots, & a_r \end{pmatrix} \tag{3.21}$$

As an example consider the partitions $(5\,4\,3^2\,2\,1)$ and $(6\,5\,4\,2\,1)$. Drawing their diagrams and marking their leading diagonal we have



and



from which we deduce the respective Frobenius designations

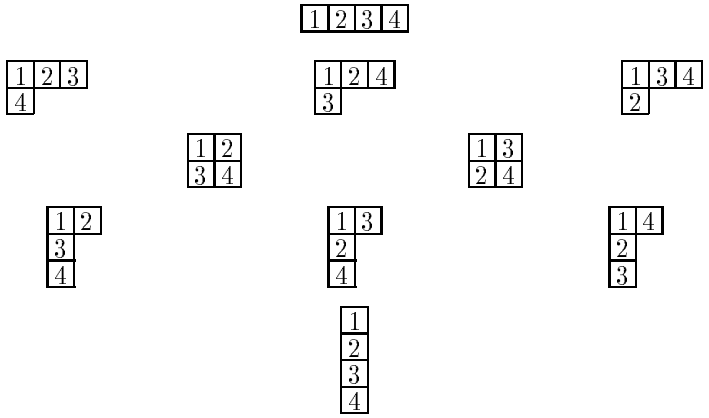
$$\begin{pmatrix} 4 & 2 & 0 \\ 5 & 3 & 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 5 & 3 & 1 \\ 4 & 2 & 0 \end{pmatrix}$$

■ **3.13 Young tableaux**

■ **A Young tableau is an assignment of n numbers to the n cells of a frame F^λ with $\lambda \vdash n$ according to some numbering sequence.**

■ **A tableau is *standard* if the assignment of the numbers $1, 2, \ldots, n$ is such that the numbers are positively increasing from left to right in rows and down columns from top to bottom.**

Thus for the partitions of the integer 4 we have the standard Young tableaux

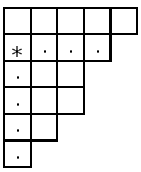


■ **In the above examples the number of standard tableaux for conjugate partitions is the same. Indeed the number of standard tableaux associated with a given frame F^λ is the *dimension* f_n^λ of an irreducible representation $\{\lambda\}$ of the symmetric group $\mathcal{S}_n$.**

■ **3.14 Hook lengths and dimensions for $\mathcal{S}_n$**

■ **The *hook length* of a given box in a frame F^λ is the length of the right-angled path in the frame with that box as the upper left vertex.**

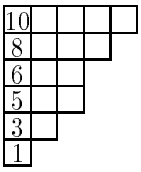
For example, the hook length of the marked box in



is 8.

Theorem 3.1: *To find the dimension of the representation of $\mathcal{S}_n$ corresponding to the frame F^λ, divide $n!$ by the factorial of the hook length of each box in the first column of F^λ and multiply by the difference of each pair of such hook lengths.*

Thus for the partition $(5\,4\,3^2\,2\,1)$ we have the hook lengths



and hence a dimension

$$f_{18}^{543^221} = 18\,! \frac{2\times 4\times 5\times 7\times 9\times 2\times 3\times 5\times 7\times 1\times 3\times 5\times 2\times 4\times 2}{10\,!\times 8\,!\times 6\,!\times 5\,!\times 3\,!\times 1\,!}$$
$$= 10720710$$

It is not suggested that you check the above result by explicit enumeration! This is an example of a combinatorially explosive situation. Thus in $\mathcal{S}_{105}$ one finds for the *staircase* partition $\{14131211109876543 21\}$ the number of standard tableaux is equal to

$$dimension = 513,782,568,580,731,957,367,019,767,803,085,320,396$$
$$632,776,099,975,918,380,865,685,412,418,054,992,691,200$$

■ **Exercise**

Estimate how long it would take a supercomputer to enumerate the number of tableaux and compare your result with the age of the universe. Would any forseeable developments in computer technology allow the enumeration to be completed on the human scale?

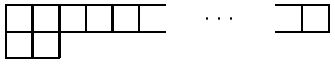
■ The above evaluation can also be equivalently made by computing the hook lengths h_{ij} for every box at position (i,j) and then noting that

$$f_n^\lambda = \frac{n\,!}{\prod_{(i,j)\in\lambda} h_{ij}} \tag{3.22}$$

which is the celebrated result of Frame, Robinson and Thrall.

■ **Exercises**

3.8 Show that the dimension of of the representation

$\{p{+}2,2\} =$ 

is

$$\frac{1}{2}(p{+}4)(p{+}1)$$

3.9 Calculate the dimensions of the irreducible representations of $\mathcal{S}_6$ and show that

$$\sum_{\lambda\vdash 6}(f_6^\lambda)^2 = 6\,!$$

■ **3.15 The Symmetric group and Tensors**

■ Let $T_{\mu_1 \cdots \mu_n}$ be a "generic" n-index tensor, without any special symmetry. (For the moment, "tensor" means just a function of n indices, not necessarily with any geometrical realization. It must be meaningful, however, to *add* (and form linear combinations of) tensors of the same rank.)

■ The entries $1, 2, \ldots n$ in the standard numbering of a tableau indicate the n successive indices of $T_{\mu_1 \cdots \mu_n}$.

■ The tableau defines a certain symmetrization operation on these indices: *symmetrize* on the set of indices indicated by the entries in each row, then *antisymmetrize* the result on the set of indices indicated by the entries in each column.

■ The resulting object is a tensor, T, with certain index symmetries. Now let each permutation in S_n act (separately) upon T. The $n!$ results are not linearly independent; they span a vector space which supports an irreducible representation of S_n.

■ Different tableaux corresponding to the same
frame yield equivalent (but not identical) representations.

Example: The partition $\{2\,2\}$ of 4 has two standard tableaux:

$$\begin{array}{|c|c|}\hline 1&2\\\hline 3&4\\\hline\end{array} \qquad \textit{and} \qquad \begin{array}{|c|c|}\hline 1&3\\\hline 2&4\\\hline\end{array} \tag{3.23}$$

Let us construct the symmetrized tensor T corresponding to the second of these.

■ First symmetrize over the first and third indices, and over the second and fourth:

$$\frac{1}{4}(T_{abcd} + T_{cbad} + T_{adcb} + T_{cdab}).$$

Now antisymmetrize the result over the first and second indices, and the third and fourth; dropping the combinatorial factor $\frac{1}{16}$, we get

$$\begin{aligned} T_{abcd} = {} & T_{abcd} + T_{cbad} + T_{adcb} + T_{cdab} \\ & - T_{bacd} - T_{cabd} - T_{bdca} - T_{cdba} \\ & - T_{abdc} - T_{dbac} - T_{acdb} - T_{dcab} \\ & + T_{badc} + T_{dabc} + T_{bcda} + T_{dcba}\,. \end{aligned} \tag{3.24}$$

It is easy (though tedious) to check that T possesses the symmetries characteristic of the Riemann tensor.

■ **Exercise**

3.10 Construct a set of three 4-index tensors corresponding to the three Young tableaux associated with the partition $\{3\,1\}$.

■ **3.16 Unitary numbering of Young tableaux**

■ Many different prescriptions can be given for injecting numbers into the boxes of a frame.

■ The standard numbering is intimately associated with the symmetric group $\mathcal{S}_n$.

■ Another important numbering prescription is that of *unitary* numbering where now numbers $1, 2, \ldots, d$ are injected into the boxes of a frame F^λ such that:

i. Numbers are non-decreasing across a row going from left to right.

ii. Numbers are positively increasing in columns from top to bottom.

■ The first condition permits repetitions of integers.

Using the numbers $1, 2, 3$ in the frame $F^{2\,1}$ we obtain the 8 tableaux

$$\begin{array}{|c|c|}\hline 1&1\\\hline 2\\\cline{1-1}\end{array}\quad\begin{array}{|c|c|}\hline 1&1\\\hline 3\\\cline{1-1}\end{array}\quad\begin{array}{|c|c|}\hline 1&2\\\hline 2\\\cline{1-1}\end{array}$$

$$\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}\quad\begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}\quad\begin{array}{|c|c|}\hline 1&3\\\hline 3\\\cline{1-1}\end{array}\quad\begin{array}{|c|c|}\hline 2&2\\\hline 3\\\cline{1-1}\end{array}\quad\begin{array}{|c|c|}\hline 2&3\\\hline 3\\\cline{1-1}\end{array}\qquad(3.25)$$

Had we chosen $d = 2$ we would have obtained just two tableaux while $d = 4$ yields twenty tableaux. In general, for a frame F^λ a unitary numbering using the integers $1, 2, \ldots, d$ leads to

$$f^\lambda_d = \frac{G^\lambda_d}{H_\lambda} \qquad (3.26)$$

where H_λ is the product of the hook lengths h_{ij} of the frame and

$$G^\lambda_d = \prod_{(i,j)\in\lambda} (d+i-j) \qquad (3.27)$$

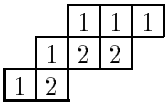
Thus for $d = 5$ and $\lambda = (4\,2\,1)$ we have $H_{(4\,2\,1)} = 144$ and $G^{\{4\,2\,1\}}_5 = 100800$ from which we deduce that

$$f^{\{4\,2\,1\}}_5 = 700$$

which is the dimension of the irreducible representation $\{4\,2\,1\}$ of the general linear group $GL(5)$.

■ In general, f_d^λ is the dimension of the irreducible representation $\{\lambda\}$ of $GL(d)$. Since the representations of $GL(d)$ labelled by partitions λ remain irreducible under restriction to the unitary group $U(d)$ **Eq.(3.26)** is valid for computing the dimensions of the irreducible representations of the unitary group $U(d)$.

■ The same rules for a unitary numbering may be applied to the skew frames $F^{\lambda/\mu}$ introduced in **S3.3**. Thus for $F^{542/21}$ an allowed unitary numbering using just the integers 1 and 2 would be



■ Note that our unitary numbering yields what in the mathematical literature are commonly referred to as *semistandard* Young tableaux. Other numberings are possible and have been developed for all the classical Lie algebras.

■ Exercises

3.11 Draw the frames $F^{2^2/1}$, $F^{43^21/421^2}$, and $F^{321/21}$.

3.12 Use the integers $1, 2, 3$ to construct the complete set of semistandard tableaux for the frame $F^{43^21/421^2}$ and show that the same number of tableaux arise for the frame F^{21}.

3.13 Make a similar unitary numbering for the frame $F^{321/21}$ and show that the same number of semistandard tableaux arise in the set of frames $F^3 + 2F^{21} + F^{1^3}$.

The Application of Symmetry Concepts to Physical Problems II

B. G. Wybourne

For every complex question there is a simple answer
– and it's wrong.
– *H. L. Mencken*

■ Lecture Four

■ 4.1 Young tableaux and monomials

A numbered frame may be associated with a unique monomial by replacing each integer i by a variable x_i. Thus the Young tableau

1	1	2	4	5
3	3	3	5	
4	6	7		
5	7	8		
6	8			
7				

can be associated with the monomial

$x_1^2\, x_2\, x_3^3\, x_4^2\, x_5^3\, x_6^2\, x_7^3\, x_8^2$

■ 4.2 Monomial symmetric functions

Consider a set of variables $(x) = x_1, x_2, \ldots, x_d$. A *symmetric* monomial

$$\boxed{m_\lambda(x) = \sum_\alpha x^\alpha} \tag{4.1}$$

involves a sum over all distinct permutations α of $(\lambda) = (\lambda_1, \lambda_2, \ldots)$. Thus if $(x) = (x_1, x_2, x_3)$ then

$$m_{21}(x) = x_1^2\, x_2 + x_1^2\, x_3 + x_1\, x_2^2 + x_1\, x_3^2 + x_2^2\, x_3$$

$$m_{1^3}(x) = x_1\, x_2\, x_3$$

The unitary numbering of $(\lambda) = (2\,1)$ with $1, 2, 3$ corresponds to the sum of monomials

$$\boxed{m_{21}(x) + 2m_{1^3}(x)}$$

The same linear combination occurs for any number of variables with $d \geq 3$.

The monomials $m_\lambda(x)$ are *symmetric functions*. If $\lambda \vdash n$ then $m_\lambda(x)$ is homogeneous of degree n. Unless otherwise stated we shall henceforth assume that x involves an infinite number of variables x_i.

The *ring of symmetric functions* $\Lambda = \Lambda(x)$ is the vector space spanned by all the $m_\lambda(x)$. This space can be decomposed as

$$\Lambda = \oplus_{n\geq 0}\Lambda^n \tag{4.2}$$

where Λ^n is the space spanned by all m_λ of degree n. Thus the $\{m_\lambda | \lambda \vdash n\}$ form a basis for the space Λ^n which is of dimension $p(n)$ where $p(n)$ is the number of partitions of n. It is of interest to ask if other bases can be constructed for the space Λ^n.

4.3 The classical symmetric functions

Three other classical bases are well-known - some since the time of Newton.

1. The elementary symmetric functions

   The n–th elementary symmetric function e_n is the sum over all products of n distinct variables x_i, with $e_0 = 1$ and generally

$$e_n = m_{1^n} = \sum_{i_1<i_2\cdots<i_n} x_{i_1}\, x_{i_2}\, \cdots\, x_{i_n} \tag{4.3}$$

   The *generating function* for the e_n is

$$E(t) = \sum_{n\geq 0} e_n t^n = \prod_{i\geq 1}(1+x_i t) \tag{4.4}$$

2. The complete symmetric functions

   The n–th complete or *homogeneous* symmetric function h_n is the sum of all monomials of total degree n in the variables $x_1, x_2, \ldots$, with $h_0 = 1$ and generally

$$h_n = \sum_{|\lambda|=n} m_\lambda = \sum_{i_1\leq i_2\cdots\leq i_n} x_{i_1}\, x_{i_2}\, \cdots\, x_{i_n} \tag{4.5}$$

   The generating function for the h_n is

$$H(t) = \sum_{n\geq 0} h_n t^n = \prod_{i\geq 1}(1-x_i t)^{-1} \tag{4.6}$$

3. The power sum symmetric function

   The n–th power sum symmetric function is

$$p_n = m_n = \sum_{i\geq 1} x_i^n \tag{4.7}$$

   The generating function for the p_n is

$$\begin{aligned} P(t) = \sum_{n\geq 1} p_n t^{n-1} &= \sum_{i\geq 1}\sum_{n\geq 1} x_i^n t^{n-1} \\ &= \sum_{i\geq 1} \frac{x_i}{1-x_i t} \end{aligned}$$

$$= \sum_{i \geq 1} \frac{d}{dt} log \frac{1}{1 - x_i t} \tag{4.8}$$

and hence

$$\begin{aligned} P(t) &= \frac{d}{dt} log \prod_{i \geq 1} (1 - x_i t)^{-1} \\ &= \frac{d}{dt} log\, H(t) \\ &= H^{'}(t)/H(t) \end{aligned} \tag{4.9}$$

Similarly,

$$P(-t) = \frac{d}{dt} log\, E(t) = E^{'}(t)/E(t) \tag{4.10}$$

Equation (4.9) leads to the relationship

$$n h_n = \sum_{r=1}^{n} p_r\, h_{n-r} \tag{4.11}$$

It follows from (4.9) that

$$\begin{aligned} H(t) &= exp \sum_{n \geq 1} p_n\, t^n/n \\ &= \prod_{n \geq 1} exp(p_n\, t^n/n) \\ &= \prod_{n \geq 1} \sum_{m_n = 0}^{\infty} (p_n\, t^n)^{m_n}/n^{m_n}.m_n! \end{aligned} \tag{4.12}$$

and hence

$$H(t) = \sum_{\lambda} z_{\lambda}^{-1} p_{\lambda}\, t^{|\lambda|} \tag{4.13}$$

where

$$z_{\lambda} = \prod_{i \geq 1} i^{m_i}.m_i! \tag{4.14}$$

where $m_i = m_i(\lambda)$ is the number of parts of λ equal to i.
Defining

$$\varepsilon_{\lambda} = (-1)^{|\lambda| - \ell(\lambda)} \tag{4.15}$$

we can show in an exactly similar manner to that of Eq.(4.13) that

$$E(t) = \sum_{\lambda} \varepsilon_{\lambda}\, z_{\lambda}^{-1} p_{\lambda}\, t^{|\lambda|} \tag{4.16}$$

It then follows from Eqs.(4.13) and (4.16) that

$$h_n = \sum_{|\lambda| = n} z_{\lambda}^{-1} p_{\lambda} \tag{4.17}$$

and

$$e_n = \sum_{|\lambda| = n} \varepsilon_{\lambda}\, z_{\lambda}^{-1} p_{\lambda} \tag{4.18}$$

■ Exercises

4.1 Show that for $n = 3$

$$\begin{aligned} p_3 &= x_1^3 + x_2^3 + x_3^3 + \ldots \\ e_3 &= x_1\,x_2\,x_3 + x_1\,x_2\,x_4 + x_2\,x_3\,x_4 + \ldots \\ h_3 &= x_1^3 + x_2^3 + \ldots + x_1^2\,x_2 + x_1\,x_2^2 + \ldots + x_1\,x_2\,x_3 + x_1\,x_2\,x_4 + \ldots \end{aligned} \tag{4.19}$$

4.2 Noting Eqs. (4.4) and (4.6) and that $H(t)E(-t) = 1$, show that

$$\sum_{r=0}^{n} (-1)^r h_{n-r}\, e_r = 0 \tag{4.20}$$

for $n \geq 1$.

4.3 Use Eq.(4.20) to show that

$$e_n = det(h_{1-i+j})_{1\leq i,j\leq n} \tag{4.21}$$

and hence

$$h_n = det(e_{1-i+j})_{1\leq i,j\leq n} \tag{4.22}$$

4.4 Use Eq.(4.11) to obtain the determinantal expressions

$$p_n = \begin{vmatrix} e_1 & 1 & 0 & \ldots & 0 \\ 2e_2 & e_1 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \\ ne_n & e_{n-1} & e_{n-2} & \ldots & e_1 \end{vmatrix} \tag{4.23}$$

$$n!e_n = \begin{vmatrix} p_1 & 1 & 0 & \ldots & 0 \\ p_2 & p_1 & 2 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \\ p_{n-1} & p_{n-2} & . & \ldots & n-1 \\ p_n & p_{n-1} & . & \ldots & p_1 \end{vmatrix} \tag{4.24}$$

$$(-1)^{n-1}p_n = \begin{vmatrix} h_1 & 1 & 0 & \ldots & 0 \\ 2h_2 & h_1 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \\ nh_n & h_{n-1} & h_{n-2} & \ldots & h_1 \end{vmatrix} \tag{4.25}$$

$$n!h_n = \begin{vmatrix} p_1 & -1 & 0 & \ldots & 0 \\ p_2 & p_1 & -2 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \\ p_{n-1} & p_{n-2} & . & \ldots & -n+1 \\ p_n & p_{n-1} & . & \ldots & p_1 \end{vmatrix} \tag{4.26}$$

■ 4.4 Multiplicative bases for Λ^n

The three types of symmetric functions, h_n, e_n, p_n, do not have enough elements to form a basis for Λ^n, there must be one function for every partition $\lambda \vdash n$. To

that end in each case we form *multiplicative* functions f_λ so that for each $\lambda \vdash n$

$$f_\lambda = f_{\lambda_1} f_{\lambda_2} \ldots f_{\lambda_\ell} \tag{4.27}$$

where $f = e,\, h,$ or p Thus, for example,

$$e_{21} = e_2 \cdot e_1 = (x_1 x_2 + x_1 x_3 + x_2 x_3 + \ldots)(x_1 + x_2 + x_3 + \ldots)$$

■ 4.5 The Schur functions

The symmetric functions

$$m_\lambda,\, e_\lambda,\, h_\lambda,\, p_\lambda \tag{4.28}$$

where $\lambda \vdash n$ each form a basis for Λ^n. A very important fifth basis is realised in terms of the Schur functions, s_λ, *or for brevity, S–functions* which may be variously defined. Combinatorially they may be defined as

$$s_\lambda(x) = \sum_T x^T \tag{4.29}$$

where the summation is over all semistandard
λ–tableaux T. For example, consider the S–functions s_λ in just three variables $(x_1,\, x_2,\, x_3)$. For $\lambda = (2\,1)$ we have the eight tableaux T found earlier

$$\begin{array}{|c|c|}\hline 1&1\\\hline 2\\\cline{1-1}\end{array}\quad \begin{array}{|c|c|}\hline 1&1\\\hline 3\\\cline{1-1}\end{array}\quad \begin{array}{|c|c|}\hline 1&2\\\hline 2\\\cline{1-1}\end{array}\quad \begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}\quad \begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}\quad \begin{array}{|c|c|}\hline 1&3\\\hline 3\\\cline{1-1}\end{array}\quad \begin{array}{|c|c|}\hline 2&2\\\hline 3\\\cline{1-1}\end{array}\quad \begin{array}{|c|c|}\hline 2&3\\\hline 3\\\cline{1-1}\end{array} \tag{3.8}$$

Each tableaux T corresponds to a monomial x^T to give

$$\begin{aligned} s_{2\,1}(x_1,\, x_2,\, x_3) =& x_1^2 x_2 + x_1^2 x^3 + x_1 x_2^2 + x_1 x_2 x_3 + x_1 x_2 x_3 + x_1 x_3^2 \\ &+ x_2^2 x_3 + x_2 x_3^2 \end{aligned} \tag{4.30}$$

We note that the monomials in Eq.(4.30) can be expressed in terms of just two *symmetric monomials* in the three variables $(x_1,\, x_2,\, x_3)$ to give

$$s_{2\,1}(x_1,\, x_2,\, x_3) = m_{2\,1}(x_1,\, x_2,\, x_3) + 2m_{1^3}(x_1,\, x_2,\, x_3) \tag{4.31}$$

In an arbitrary number of variables

$$s_{2\,1}(x) = m_{2\,1}(x) + 2m_{1^3}(x) \tag{4.32}$$

This is an example of the general result that the
S–function may be expressed as a linear combination of symmetric monomials as indeed would be expected if the S–functions are a basis of Λ^n. In fact

$$s_\lambda(x) = \sum_{\mu \vdash n} K_{\lambda\mu} m_\mu \tag{4.33}$$

where $|\lambda| = n$ and $K_{\lambda\lambda} = 1$. The $K_{\lambda\mu}$ are the elements of an upper triangular matrix K known as the Kostka matrix. K is an example of a *transition matrix* that relates one symmetric function basis to another.

■ **4.6 Calculation of the elements of the Kostka matrix**

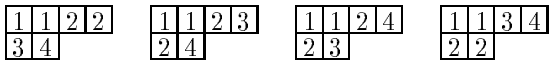
The elements $K_{\lambda\mu}$ of the Kostka matrix may be readily calculated by the following algorithm :

i. Draw the frame F^λ.

ii. Form all possible semistandard tableaux that arise in numbering F^λ with μ_1 ones, μ_2 twos etc.

iii. $K_{\lambda\mu}$ is the number of semistandard tableaux so formed.

Thus calculating $K_{(42)(2^2\,1^2)}$ we obtain the four semistandard tableaux



and hence $K_{(42)(2^2\,1^2)} = 4$.

■ **Exercises**

4.5 Construct the Kostka matrix for $\lambda, \mu \vdash 4$.

4.6 Show that in the variables (x_1, x_2, x_3) the evaluation of the determinantal ratio

$$\frac{\begin{vmatrix} x_1^4 & x_1^2 & 1 \\ x_2^4 & x_2^2 & 1 \\ x_3^4 & x_3^2 & 1 \end{vmatrix}}{\begin{vmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ x_3^2 & x_3 & 1 \end{vmatrix}}$$

yields the monomial content of the S–function s_{21} in three variables as found in Eq.(4.30). N.B. The above exercise is tedious by hand but trivial using MAPLEV.

The last exercise is an example of the classical definition, as opposed to the equivalent combinatorial definition given in Eq.(4.29), given first by Jacobi, namely,

$$s_\lambda = s_\lambda(x_1, x_2, \ldots, x_n) = \frac{a_{\lambda+\delta}}{a_\delta} \tag{4.34}$$

where λ is a partition of length $\leq n$ and
$\delta = (n-1, n-2, \ldots, 1, 0)$ with

$$a_{\lambda+\delta} = det(x_i^{\lambda_j+n-j})_{1\leq i,j\leq n} \tag{4.35}$$

and

$$a_\delta = \prod_{1\leq i,j\leq n} (x_i - x_j) = det(x_i^{n-j}) \tag{4.36}$$

is the *Vandermonde determinant*. Note that the Vandermonde determinant is an *alternating* or *antisymmetric* function. Any *even* power of the Vandermonde

determinant is an *symmetric* function. This has important applications in the interpretation of the quantum Hall effect.

■ 4.7 Non-standard S–functions

The S–functions are symmetric functions indexed by ordered partitions λ. We shall frequently write S–functions $s_\lambda(x)$ as $\{\lambda\}(x)$ or, since we will generally consider the number of variables to be unrestricted, just $\{\lambda\}$. As a matter of notation the partitions will normally be written without spacing or commas separating the parts where $\lambda_i \leq 9$. A space will be left after any part $\lambda_i \geq 10$. Thus we write $\{12,11,9,8,3,2,1\} \equiv \{12\quad 11\quad 98321\}$ While we have defined the S–function in terms of ordered partitions we sometimes encounter S–functions that are not in the standard form and must convert such *non-standard* S–functions into standard S–functions. Inspection of the determinantal
forms of the S–function leads to the establishment of the following *modification rules* :

$$\{\lambda_1,\lambda_2,\ldots,-\lambda_\ell\} = 0 \tag{4.37}$$

$$\{\lambda_1,\ldots,\lambda_i,\lambda_{i+1},\ldots,\lambda_\ell\} = -\{\lambda_1,\ldots,\lambda_{i+1}-1,\lambda_i+1,\ldots,\lambda_\ell\} \tag{4.38}$$

$$\{\lambda\} = 0 \qquad \text{if } \lambda_{i+1} = \lambda_i + 1 \tag{4.39}$$

Repeated application of the above three rules will reduce any non-standard S–function to either zero or to a signed standard S–function. In the process of using the above rules trailing zero parts are omitted

---

■ Exercise

4.7 Show that

$$\{24\} = -\{3^2\}, \quad \{141\} = -\{321\}$$

$$\{14-25-14\} = -\{3^32\}$$

$$\{3042\} = 0, \quad \{3043\} = \{3^22\}$$

■ 4.8 Skew S–functions

The combinatorial definition given for S–functions in Eq.(4.29) is equally valid for skew tableaux and can hence be used to define *skew* S–functions $s_{\lambda/\mu}(x)$ or $\{\lambda/\mu\}$. Since the $s_{\lambda/\mu}(x)$ are symmetric functions they must be expressible in terms of S–functions $s_\nu(x)$ such that

$$s_{\lambda/\mu} = \sum_\nu c^\lambda_{\mu\nu} s_\nu \tag{4.40}$$

It may be shown that the coefficients $c^{\lambda}_{\mu\nu}$ are necessarily non-negative integers and symmetric with respect to μ and ν. The coefficients $c^{\lambda}_{\mu\nu}$ are commonly referred to as *Littlewood-Richardson* coefficients.

■ **4.9 The Littlewood-Richardson rule**

The product of two S–functions can be written as a sum of S–functions, viz.

$$s_{\mu}.s_{\nu} = \sum_{\lambda} c^{\lambda}_{\mu\nu} s_{\lambda} \tag{4.41}$$

The Littlewood-Richardson coefficients $c^{\lambda}_{\mu\nu}$ in
Eqs. (4.40) and (4.41) are identical, though the summations are of course different. In both cases $|\mu| + |\nu| = |\lambda|$. A rule for evaluating the coefficients $c^{\lambda}_{\mu\nu}$ was given by Littlewood and Richardson in 1934 and has played a major role in all subsequent developments. The rule may be stated in various ways. We shall state it first in terms of semistandard tableaux and then also give the rule for evaluating the product given in Eq.(4.41) which is commonly referred to as the *outer multiplication* of S–functions. In each statement the concepts of a *row-word* and of a *lattice permutation* is used.

■ **Definition 4.1 A word**

Let T be a tableau. From T we derive a row-word or sequence $w(T)$ by reading the symbols in T from right to left (i.e. as in Arabic or Hebrew) in successive rows starting at the top row and proceeding to the bottom row

Thus for the tableau

1	1	2	2	3
2	2	3	3	
4	4			
5	6			
7				
8				

we have the word $w(T) = 322113322446578$ and for the skew tableau

		1	1	1
	1	2	2	
1	2			

we have the word $w(T) = 11122121$.

■ **Definition 4.2 A lattice permutation**

A word $w = a_1 a_2 \ldots a_N$ in the symbols $1, 2, \ldots, n$ is said to be a lattice permutation if for $1 \leq r \leq N$ and $1 \leq i \leq n-1$, the number of occurrences of the symbol i in $a_1 a_2 \ldots a_r$ is not less than the number of occurrences of $i+1$.

Thus the word $w(T) = 322113322446578$ is clearly not a lattice permutation whereas

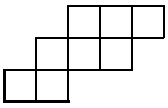
the word $w(T) = 11122121$ is a lattice permutation. The word $w(T) = 12122111$ is not a lattice permutation since the sub-word 12122 has more twos than ones.

■ **Theorem 4.1** *The value of the coefficient $c^{\lambda}_{\mu\nu}$ is equal to the number of semistandard tableaux T of shape $F^{\lambda/\mu}$ and content ν such that $w(T)$ is a lattice permutation.*

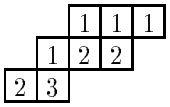
By *content* ν we mean that each tableau T contains ν_1 ones, ν_2 twos, etc.

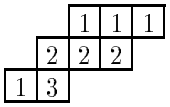
■ **Example**

Let us evaluate the coefficient $c^{\{542\}}_{\{431\}\{21\}}$. We first draw the frame $F^{\{542/21\}}$.

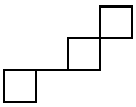


Into this frame we must inject the content of $\{431\}$ i.e. 4 ones, 3 twos and 1 three in such a way that we have a lattice permutation. We find two such numberings

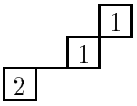


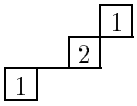


and hence $c^{\{542\}}_{\{431\}\{21\}} = 2$. Note that in the evaluation we had a choice, we could have, and indeed more simply, evaluated $c^{\{542\}}_{\{21\}\{431\}}$. In that case we would have drawn the frame $F^{\{542/431\}}$ to get



Note that in this case the three boxes are disjoint. This skew frame is to be numbered with two ones and one 2 leading to the two tableaux





verifying the previous result. Theorem 4.1 gives a direct method for evaluating the Littlewood-Richardson coefficients. These coefficients can be used to evaluate both skews and products. It is sometimes useful to state a procedure for directly evaluating products.

■ **Theorem 4.2** *to evaluate the S–function product $\{\mu\}.\{\nu\}$*

1. *Draw the frame F^{μ} and place ν_1 ones in the first row, ν_2 twos in the second row etc until the frame is filled with integers.*
2. *Draw the frame F^{ν} and inject positive integers to form a semistandard tableau such that the word formed by reading from right to left starting at the top row of the first frame and moving downwards along successive rows to the bottom row and then continuing through the second frame is a lattice permutation.*

3. Repeat the above process until no further words can be constructed.

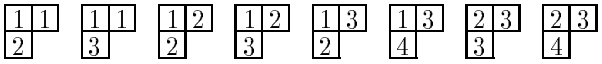
4. Each word corresponds to an S–function $\{\lambda\}$ where λ_1 is the number of ones, λ_2 the number of twos etc.

As an example consider the S–function product

$\{21\}.\{21\}$.

Step 1 gives the tableau

Steps 2 and 3 lead to the eight numbered frames



Step 4 then lead to the eight words

$$112112 \quad 112113 \quad 112212 \quad 112213$$

$$112312 \quad 112314 \quad 112323 \quad 112324$$

from which we conclude that

$$\{21\}.\{21\} = \{42\} + \{41^2\} + \{3^2\} + 2\{321\} + \{31^3\} + \{2^3\} + \{2^2 1^2\}$$

■ **Exercises**

4.8 Show that $c^{\{75321^3\}}_{\{4321\}.\{4321\}} = 8$.

4.9 Show that

$$\begin{aligned}\{31\}.\{31\} =& \{62\} + \{61^2\} + \{53\} + 2\{521\} + \{51^3\} + \{4^2\} \\ &+ 2\{431\} + \{42^2\} + \{421^2\} + \{3^2 2\} + \{3^2 1^2\}\end{aligned}$$

4.10 Show that

$$\{321/21\} = \{3\} + 2\{21\} + \{1^3\}$$

■ **4.10 Relationship to the unitary group**

We have explored various symmetric functions indexed by partitions and defined on sets of variables. The variables can admit many interpretations. In some instances we may choose a set of variables $1, q, q^2, \ldots, q^n$ or we could even use a set of matrices. The link between S–functions and the character theory of groups is such that, if λ is a partition with $\ell(\lambda) \leq N$ and the eigenvalues of a group element, g, of the unitary group U_N are given by $x_j = exp(i\phi_j)$ for $j = 1, 2, \ldots, N$ then the S–function

$$\{\lambda\} = \{\lambda_1 \lambda_2 \ldots \lambda_N\} = s_\lambda(x)$$

$$= s_\lambda(exp(i\phi_1)\, exp(i\phi_2) \ldots exp(i\phi_N))$$

is nothing other than the character of g in the irreducible representation of U_N conventionally designated by $\{\lambda\}$.

The Littlewood-Richardson rule gives the resolution of the Kronecker product $\{\mu\} \times \{\nu\}$ of U_N as

$$\{\mu\} \times \{\nu\} = \sum_{|\lambda|=|\mu|+|\nu|} c^{\{\lambda\}}_{\{\mu\}.\{\nu\}} \{\lambda\} \tag{4.42}$$

where the $c^{\{\lambda\}}_{\{\mu\}.\{\nu\}}$ are the usual Littlewood-Richardson coefficients. Equation (4.42) must be modified for partitions λ involving more than N parts. Here the *modification rule* is very simple. We simply discard all partitions involving more than N parts. We shall return to these matters later in this course when we use our results to discuss the classification of many-electron states, especially for the electronic f–shell.

■ 4.11 S–function series

Infinite series of S–functions play an important role in determining branching rules and furthermore lead to concise symbolic methods well adapted to computer implementation. Consider the infinite series

$$\begin{aligned} L &= \prod_{i=1}^{\infty}(1 - x_i) \\ &= 1 - \sum x_1 + \sum x_1 x_2 - \ldots \end{aligned} \tag{4.43}$$

where the summations are over all distinct terms.

e.g.

$$\sum x_1 x_2 = x_1 x_2 + x_1 x_3 + \ldots + x_2 x_3 + x_2 x_4 + \ldots \tag{4.44}$$

Recalling Eq.(4.3) we see that Eq.(4.43) is simply a signed sum over an infinite set of elementary symmetric functions e_n with

$$e_n = m_{1^n} = s_{1^n} = \{1^n\} \tag{4.45}$$

and hence Eq.(4.43) may be written as an infinite sum of S–functions such that

$$\begin{aligned} L &= 1 - \{1\} + \{1^2\} - \{1^3\} + \ldots \\ &= \sum_{m=0}^{\infty} (-1)^m \{1^m\} \end{aligned} \tag{4.46}$$

We may define a further infinite series of S–functions by taking the inverse of Eq.(4.43) to get

$$M = \prod_{i=1}^{\infty}(1 - x_i)^{-1}$$

$$\begin{aligned} &= 1 + \{1\} + \{2\} + \dots \\ &= \sum_{m=0}^{\infty} \{m\} \end{aligned} \tag{4.47}$$

Clearly

$$LM = 1 \tag{4.48}$$

a result that is by no means obvious by simply looking at the product of the two series.

In practice large numbers of infinite series and their associated generating functions may be constructed. We list a few of them below:

$\mathbf{A} = \sum_\alpha (-1)^{w_\alpha} \{\alpha\}$	$\mathbf{B} = \sum_\beta \{\beta\}$
$\mathbf{C} = \sum_\gamma (-1)^{w_\gamma/2} \{\gamma\}$	$\mathbf{D} = \sum_\delta \{\delta\}$
$\mathbf{E} = \sum_\epsilon (-1)^{(w_\epsilon + r)/2} \{\epsilon\}$	$\mathbf{F} = \sum_\zeta \{\zeta\}$
$\mathbf{G} = \sum_\epsilon (-1)^{(w_\epsilon - r)/2} \{\epsilon\}$	$\mathbf{H} = \sum_\zeta (-1)^{w_\zeta} \{\zeta\}$
$\mathbf{L} = \sum_m (-1)^m \{1^m\}$	$\mathbf{M} = \sum_m \{m\}$
$\mathbf{P} = \sum_m (-1)^m \{m\}$	$\mathbf{Q} = \sum_m \{1^m\}$

(4.49)

where (α) and (γ) are mutually conjugate partitions, which in the Frobenius notation take the form

$$(\alpha) = \begin{pmatrix} a_1 & a_2 & \dots & a_r \\ a_1 + 1 & a_2 + 1 & \dots & a_r + 1 \end{pmatrix} \tag{4.50a}$$

and

$$(\gamma) = \begin{pmatrix} a_1 + 1 & a_2 + 1 & \dots & a_r + 1 \\ a_1 & a_2 & \dots & a_r \end{pmatrix} \tag{4.50b}$$

(δ) is a partition into *even parts* only and (β) is conjugate to (δ). (ζ) is any partition and (ϵ) is any self-conjugate partition. r is the Frobenius rank of (α), (γ) and (ϵ).

These series occur in mutually inverse pairs:

$$AB = CD = EF = GH = LM = PQ = \{0\} = 1 \tag{4.51}$$

Furthermore,

$$\begin{aligned} LA = PC = E \quad & MB = QD = F \\ MC = AQ = G \quad & LD = PB = H \end{aligned} \tag{4.52}$$

We also note the series

$$R = \{0\} - 2\sum_{a,b} (-1)^{a+b+1} \binom{a}{b} \qquad S = \{0\} + 2\sum_{a,b} \binom{a}{b} \tag{4.53}$$

where we have again used the Frobenius notation, and

$$V = \sum_{\omega}(-1)^q\{\tilde{\omega}\} \qquad W = \sum_{\omega}(-1)^q\{\omega\}$$
$$X = \sum_{\omega}\{\tilde{\omega}\} \qquad Y = \sum_{\omega}\{\omega\} \tag{4.54}$$

where (ω) is a partition of an even number into at most two parts, the second of which is q, and $\tilde{\omega}$ is the conjugate of ω. We have the further relations

$$RS = VW = \{0\} = 1 \tag{4.55}$$

and

$$PM = AD = W \qquad LQ = BC = V$$
$$MQ = FG = S \qquad LP = HE = R \tag{4.56}$$

■ 4.12 Symbolic manipulation

The above relations lead to a method of describing many of the properties of groups via symbolic manipulation of infinite series of S–functions. Thus if $\{\lambda\}$ is an S–function then we may symbolically write, for example,

$$\{\lambda/M\} = \sum_{m}\{\lambda/m\} \tag{4.57}$$

We can construct quite remarkable identities such as:

$$BD = \sum_{\zeta}\{\zeta\}\cdot\{\zeta\} \tag{4.58}$$

or for an arbitrary S–function $\{\epsilon\}$

$$BD\cdot\{\epsilon\} = \sum_{\zeta}\{\zeta\}\cdot\{\zeta/\epsilon\} \tag{4.59}$$

Equally remarkably we can find identities such as

$$\{\sigma\cdot\tau\}/Z = \{\sigma/Z\}\cdot\{\tau/Z\} \quad \textbf{for} \quad Z = L, M, P, Q, R, S, V, W \tag{4.60a}$$

$$\{\sigma\cdot\tau\}/Z = \sum_{\zeta}\{\sigma/\zeta Z\}\cdot\{\tau/\zeta Z\} \quad \textbf{for} \quad Z = B, D, F, H \tag{4.60b}$$

$$\{\sigma\cdot\tau\}/Z = \sum_{\zeta}(-1)^{w_\zeta}\{\sigma/\zeta Z\}\cdot\{\tau/\tilde{\zeta}Z\} \quad \textbf{for} \quad Z = A, C, E, G \tag{4.60c}$$

These various identities can lead to a symbolic method of treating properties of groups particulary amenable to computer implementation.

■ 4.13 The $U_n \to U_{n-1}$ branching rule

As an illustration of the preceding remarks we apply the properties of S–functions to the determination of the $U_n \to U_{n-1}$ branching rules. The vector irrep $\{1\}$ of U_n can be taken as decomposing under $U_n \to U_{n-1}$ as

$$\{1\} \to \{1\} + \{0\} \tag{4.61}$$

that is into a vector $\{1\}$ and scalar $\{0\}$ of U_{n-1}. In general, the spaces corresponding to tensors for which a particular number of indices, say m, take on the value n, define invariant subspaces. Such indices must be mutually symmetrised. The irreducible representations specified by the quotient $\{\lambda/m\}$ are those corresponding to tensors obtained by contracting the indices of the tensor corresponding to $\{\lambda\}$ with an m–th rank symmetric tensor. Thus we may symbolically write the general branching rule as simply

$$\{\lambda\} \rightarrow \{\lambda/M\} \tag{4.62}$$

Thus for example under $U_3 \rightarrow U_2$ we have

$$\begin{aligned} \{21\} &\rightarrow \{21/M\} \\ &\rightarrow \{21/0\} + \{21/1\} + \{21/2\} \\ &\rightarrow \{21\} + \{2\} + \{11\} + \{1\} \end{aligned} \tag{4.63}$$

■ 4.14 The Gel'fand states and the betweenness condition

The so-called Gel'fand states play an important role in the Unitary Group Approach (UGA) to many-electron theory. This comes about from considering the canonical chain of groups

$$U_n \supset U_{n-1} \supset \ldots U_2 \supset U_1 \tag{4.64}$$

The states of such a chain follow directly from consideration of Eq.(4.62). Each state may be represented by a triangular array having n rows. There are n entries $m_{i,n}$ with $i = 1, 2, \ldots, n$ corresponding to the usual partition (λ) padded out with zeroes to fill the row if need be. The second row contains $n-1$ entries $m_{i,n-1}$ placed below the first row so that the entry $m_{1,n-1}$ occurs between the entries $m_{1,n}$ and $m_{2,n}$ etc. Each successive row contains one less entry with the bottom row containing just one entry $m_{1,1}$. The number of such states is just the dimension of the irrep $\{\lambda\}$ of U_n.

Consider the irrep of U_3 labelled as $\{21\}$. We find the eight Gel'fand states

$$\begin{pmatrix} 2 & & 1 & & 0 \\ & 2 & & 1 & \\ & & 2 & & \end{pmatrix} \qquad \begin{pmatrix} 2 & & 1 & & 0 \\ & 2 & & 1 & \\ & & 1 & & \end{pmatrix}$$

$$\begin{pmatrix} 2 & & 1 & & 0 \\ & 2 & & 0 & \\ & & 2 & & \end{pmatrix} \qquad \begin{pmatrix} 2 & & 1 & & 0 \\ & 2 & & 0 & \\ & & 1 & & \end{pmatrix}$$

$$\begin{pmatrix} 2 & & 1 & & 0 \\ & 2 & & 0 & \\ & & 0 & & \end{pmatrix} \qquad \begin{pmatrix} 2 & & 1 & & 0 \\ & 1 & & 1 & \\ & & 1 & & \end{pmatrix}$$

$$\begin{pmatrix} 2 & & 1 & & 0 \\ & 1 & & 0 & \\ & & 1 & & \end{pmatrix} \qquad \begin{pmatrix} 2 & & 1 & & 0 \\ & 1 & & 0 & \\ & & 0 & & \end{pmatrix}$$

$\mathcal{S}_2$

Class	(1^2)	(2)
Order	1	1
$\{2\}$	1	1
$\{1^2\}$	1	-1

$\mathcal{S}_3$

Class	(1^3)	(21)	(3)
Order	1	3	2
$\{3\}$	1	1	1
$\{21\}$	2	0	-1
$\{1^3\}$	1	-1	1

$\mathcal{S}_4$

Class	(1^4)	(21^2)	(31)	(4)	(2^2)
Order	1	6	8	6	3
$\{4\}$	1	1	1	1	1
$\{31\}$	3	1	0	-1	-1
$\{2^2\}$	2	0	-1	0	2
$\{21^2\}$	3	-1	0	1	-1
$\{1^4\}$	1	-1	1	-1	1

$\mathcal{S}_5$

Class	(1^5)	(21^3)	(31^2)	(41)	$(2^2 1)$	(32)	(5)
Order	1	10	20	30	15	20	24
$\{5\}$	1	1	1	1	1	1	1
$\{41\}$	4	2	1	0	1	-1	-1
$\{32\}$	5	1	-1	-1	1	1	0
$\{31^2\}$	6	0	0	0	-2	0	1
$\{2^2 1\}$	5	-1	-1	1	1	-1	0
$\{21^3\}$	4	-2	1	0	0	1	-1
$\{1^5\}$	1	-1	1	-1	1	-1	1

■ 5.7 Orthogonality Properties of Characters

The *rows* of a character table satisfy the orthogonality relation

$$\sum_{\rho} h_\rho \chi_\rho^{(i)} \chi_\rho^{(j)} = h\delta_{ij} \tag{5.5}$$

while the *columns* satisfy

$$\sum_{i} h_\rho \chi_\rho^{(i)} \chi_\sigma^{(i)} = h\delta_{\sigma\rho'} \tag{5.6}$$

■ 5.8 Compound Characters

A group character may be *simple* or *compound*. If the representation is *irreducible* the character is *simple*. A fully reducible representation has a *compound* character. A compound character ϕ with a set of characteristics ϕ_ρ may be expressed as a sum of simple characters by use of the orthogonality relations. Suppose

$$\phi = \sum_k c_k \chi^{(k)} \tag{5.7}$$

then the coefficients c_k may be found as follows:-

$$\begin{aligned}\sum_{\rho} h_\rho \phi_\rho \chi^{(k)}_{\rho'} &= \sum_{\rho,j} c_k h_\rho \chi^{(j)}_\rho \chi_r ho^{(k)} \\ &= hc_k\end{aligned}$$

Thus

$$c_k = \frac{1}{h}\sum_{\rho} h_\rho \phi_\rho \chi^{(k)}_{\rho'} \tag{5.8}$$

If ϕ is a simple or compound character, then

$$\begin{aligned}\sum_{\rho} h_\rho \phi_\rho \phi_{\rho'} &= \sum_{\rho,i,j} c_i c_j h_\rho \chi^{(i)}_\rho \chi^{(j)}_{\rho'} \\ &= h\sum_{i} c_i^2 \end{aligned} \tag{5.9}$$

and hence the condition that a character ϕ should be simple is that

$$\sum_{\rho} h_\rho \phi_\rho \phi_{\rho'} = h \tag{5.10}$$

■ 5.9 Calculation of $\mathcal{S}_n$ Characters

The characteristics of the symmetric group $\mathcal{S}_n$ are the elements of the transition matrix relating the power sum symmetric functions to the Schur functions. In fact

$$p_\sigma = \sum_{\lambda \vdash n} \chi^\lambda_\sigma s_\lambda \tag{5.11}$$

For a one part partition (r) Eq. (5.11) specializes to

$$p_r = \sum_{\substack{a,b=0 \\ a+b+1=r}}^{r-1} (-1)^b s_{(a+1,1^b)} \tag{5.12}$$

Note that the partitions $(a+1,1^b)$ associated with the S–functions appearing in Eq. (5.12) are all of the form of single hooks. Thus

$$\begin{aligned} p_3 &= s_3 - s_{21} + s_{1^3} \\ p_2 &= s_2 - s_{1^2} \\ p_1 &= s_1 \end{aligned} \tag{5.13}$$

Recalling the multiplicative property of the power sum symmetric functions we have

$$\begin{aligned} p_{21} &= p_2 \times p_1 \\ &= (s_2 - s_{1^2}) \times s_1 \\ &= s_3 - s_{1^3} \end{aligned}$$

which gives us the column of the character table for $\mathcal{S}_3$ for the class (21) where the Littlewood-Richardson rule has been used to multiply out the S–function products.

■ Exercise

5.1 Calculate the character table for $\mathcal{S}_4$ using Eqs. (5.11) and (5.12) together with the Littlewood-Richardson rule.

■ 5.10 Character Table for $\mathcal{S}_6$

Continuing the above procedure we can compute the characters of $\mathcal{S}_6$. We note that these calculations can be rapidly calculated using SCHUR and the command p_to_s or using MAPLE V.

σ	(1^4)	(21^4)	(31^3)	(41^2)	(2^21^2)	(321)	(51)	(6)	(42)	(2^3)
h_σ	1	15	40	90	45	120	144	120	90	15
$\{6\}$	1	1	1	1	1	1	1	1	1	1
$\{51\}$	5	3	2	1	1	0	0	−1	−1	−1
$\{42\}$	9	3	0	−1	1	0	−1	0	1	3
$\{41^2\}$	10	2	1	0	−2	−1	0	1	0	−2
$\{3^2\}$	5	1	−1	−1	1	1	0	0	−1	−3
$\{321\}$	16	0	−2	0	0	0	1	0	0	0
$\{2^3\}$	5	−1	−1	1	1	−1	0	0	−1	3
$\{31^3\}$	10	−2	1	0	−2	1	0	−1	0	2
$\{2^21^2\}$	9	−3	0	1	1	0	−1	0	1	−3
$\{21^4\}$	5	−3	2	−1	1	0	0	1	−1	1
$\{1^6\}$	1	−1	1	−1	1	−1	1	−1	1	−1

■ 5.11 Kronecker Products of Representations

Let us consider two sets of functions $\phi_1, \phi_2, \ldots, \phi_n$ and $\xi_1, \xi_2, \ldots, \xi_m$ which respectively form bases for the n–dimensional irreducible representation Γ_P and the m–dimensional irreducible representation Γ_Q of the group $\mathcal{G}$. Under the operations of the group $\mathcal{G}$ the mn functions $\phi_i\xi_k$ transform into linear combinations of themselves forming a basis for a representation Γ_T of $\mathcal{G}$. This representation is known as the *Kronecker product* (or *direct product*) of the representations Γ_P and Γ_Q and designated as $\Gamma_P \times \Gamma_Q$. Recall

$$g_i\phi_j = \sum_k p_{kj}(i)\phi_k$$

$$g_i\xi_\ell = \sum_s q_{s\ell}(i)\xi_s$$

and hence

$$g_i(\phi_j\xi_e ll) = \sum_{k,s} p_{kj}(i)q_{s\ell}(i)(\phi_k\xi_s)$$

Since

$$\sum_{j,\ell} p_{jj}(i) q_{\ell\ell}(i) = \left(\sum_j p_{jj}(i) \right) \left(\sum_s q_{\ell\ell}(i) \right)$$

we have for the characters of the representations

$$\chi^T(i) = \chi^P(i) \chi^Q(i) \tag{5.13}$$

■ 5.12 Worked Example of a Compound Character of $\mathcal{S}_6$

Let us review the preceding notes by first resolving a compound character for $\mathcal{S}_6$ and at the same time introducing *permutation matrices*. There is a class for every ordered partition of the integer 6. The orders h_ρ of the eleven classes can be computed via Eq. (3.11) to give

σ	(1^4)	(21^4)	(31^3)	(41^2)	(2^21^2)	(321)	(51)	(6)	(42)	(2^3)	$(3^2$
h_σ	1	15	40	90	45	120	144	120	90	15	40

We can construct a typical permutation matrix for each class:-

$$(1^6): \begin{bmatrix} 1&0&0&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&1&0&0&0 \\ 0&0&0&1&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \end{bmatrix} \qquad (21^4): \begin{bmatrix} 1&0&0&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&1&0&0&0 \\ 0&0&0&1&0&0 \\ 0&0&0&0&0&1 \\ 0&0&0&0&1&0 \end{bmatrix}$$

$$(31^3): \begin{bmatrix} 1&0&0&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&1&0&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \\ 0&0&0&1&0&0 \end{bmatrix} \qquad (41^2): \begin{bmatrix} 1&0&0&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&0&1&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \\ 0&0&1&0&0&0 \end{bmatrix}$$

$$(2^21^2): \begin{bmatrix} 1&0&0&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&0&1&0&0 \\ 0&0&1&0&0&0 \\ 0&0&0&0&0&1 \\ 0&0&0&0&1&0 \end{bmatrix} \qquad (321): \begin{bmatrix} 1&0&0&0&0&0 \\ 0&0&1&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \\ 0&0&0&1&0&0 \end{bmatrix}$$

$$(42): \begin{bmatrix} 0&1&0&0&0&0 \\ 1&0&0&0&0&0 \\ 0&0&0&1&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \\ 0&0&1&0&0&0 \end{bmatrix} \qquad (2^3): \begin{bmatrix} 0&1&0&0&0&0 \\ 1&0&0&0&0&0 \\ 0&0&0&1&0&0 \\ 0&0&1&0&0&0 \\ 0&0&0&0&0&1 \\ 0&0&0&0&1&0 \end{bmatrix}$$

$$(3^2): \begin{bmatrix} 0&1&0&0&0&0 \\ 0&0&1&0&0&0 \\ 1&0&0&0&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \\ 0&0&0&1&0&0 \end{bmatrix} \qquad (51): \begin{bmatrix} 1&0&0&0&0&0 \\ 0&0&0&0&0&1 \\ 0&1&0&0&0&0 \\ 0&0&0&0&1&0 \\ 0&0&1&0&0&0 \\ 0&0&0&1&0&0 \end{bmatrix}$$

$$(6): \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

If we take the traces of these matrices we obtain a compound character of $\mathcal{S}_6$

$$\phi = 6, 4, 3.2, 2, 1, 1, 0, 0, 0 \tag{5.14}$$

Recall Eq. (5.8)

$$c_k = \frac{1}{h}\sum_{\rho} h_\rho \phi_\rho \chi^{(k)}_{\rho'} \tag{5.8}$$

We have $h = 6! = 720$. Let us compute the number of times the simple character $\chi^{\{6\}}$ occurs in Eq. (5.14). Each of the characteristics $\chi^{\{6\}}_\sigma = 1$ leading to

$$c_{\{6\}} = \frac{1}{720}(1x6 + 15x4 + 40x3 + 90x2 + 45x2 + 120x1 + 144x1) = 1$$

and hence Eq. (5.14) contains the simple character $\chi^{\{6\}}$ once. Subtracting the simple character from ϕ leaves the residue

$$\phi' = 5, 3, 1, 1, 0, 0, -1, -1, -1 \tag{5.15}$$

Inspection of the character table of $\mathcal{S}_6$ shows that ϕ' corresponds to the simple character $\chi^{\{51\}}$ and hence

$$\phi = \chi^{\{6\}} + \chi^{\{51\}}$$

■ 5.13 Example of a Kronecker Product in $\mathcal{S}_4$

Let us resolve the Kronecker product of the representation labelled by the partition (31) with that labelled by (2^2). Let us write this product as $\{31\} \circ \{2^2\}$ and we wish to determine the coefficients $c^{\{\lambda\}}_{\{31\}\circ\{2^2\}}$ where

$$\{31\} \circ \{2^2\} = \sum_{\lambda \vdash 4} c^{\{\lambda\}}_{\{31\}\circ\{2^2\}} \{\lambda\}$$

We first calculate the characteristics for the Kronecker product using Eq. (5.13) to obtain the compound character

$$\phi = 9,\ -1,\ 0,\ -1,\ 1$$

We must now resolve the compound character ϕ into a sum of simple characters using Eq. (5.8) and the character table for $\mathcal{S}_4$

$$c_k = \frac{1}{h}\sum_{\rho} h_\rho \phi_\rho \chi^{(k)}_{\rho'} \tag{5.8}$$

to obtain

$$c^{\{4\}}_{\{31\}\circ\{21^2\}} = \frac{1}{24}[9-6+0-6+3] = 0$$
$$c^{\{31\}}_{\{31\}\circ\{21^2\}} = \frac{1}{24}[27-6+0+6-3] = 1$$
$$c^{\{2^2\}}_{\{31\}\circ\{21^2\}} = \frac{1}{24}[18+0+0+0+6] = 1$$
$$c^{\{21^2\}}_{\{31\}\circ\{21^2\}} = \frac{1}{24}[27+6+0-6-3] = 1$$

and hence we conclude that

$$\phi = \chi^{\{31\}} + \chi^{\{2^2\}} + \chi^{\{21^2\}} + \chi^{\{1^4\}}$$

The calculation of Kronecker products for the symmetric group is equivalent to calculating the *inner product* of the corresponding S–functions. Thus in SCHUR one finds:-

```
DP>

->sfn

Schur Function Mode

SFN>

->i31,21^2

      {31} + {2^2 } + {21^2 } + {1^4 }

SFN>
```

The resolution of Kronecker products plays an important role in solid state physics in determining the splitting of levels in crystal fields and in selection rules for transitions between crystal field levels. In the next lecture we will examine such problems in relationship to the octahedral group $\mathcal{O}$

The Application of Symmetry Concepts to Physical Problems II

B. G. Wybourne

To do research you don't have to know everything
All you have to know is one thing that is not known
–Art Schawlow *Nobel Laureate*

- Lecture 6
- 6.1 Example of the Octahedral Group $\mathcal{O}$

We now illustrate much of the material of the previous lecture by a detailed consideration of the octahedral group $\mathcal{O}$. The octahedral group involves the 24 symmetry operations corresponding to the proper rotations that send a cube into itself. These operations comprise:

1. The identity operation E.
2. The eight rotations $8C_3$ through $\pm 120°$ about the four body diagonals.
3. The three rotations $3C_2$ through $180°$ about axes passing through the centres of opposite faces of the cube.
4. The 6 rotations $6C_2$ through $180°$ about axes joining the midpoints of opposite edges of the cube.
5. The 6 rotations $6C_4$ through $\pm 90°$ about axes passing through the centres of opposite faces of the cube.

The octahedral group $\mathcal{O}$ is isomorphic to the symmetric group $\mathcal{S}_4$. There are five classes (E, C_3, C_2, C_4, C_2') which are in one-to-one correspondence with the five classes $(e, (31), (2^2), (21^2), (4))$ of $\mathcal{S}_4$. The group $\mathcal{O}$ has five inequivalent irreducible representations designated in Mulliken's notation as A_1, A_2, E, T_1, T_2 or in Bethe's Γ notation as $\Gamma_1, \ldots, \Gamma_5$. These irreducible representations respectively correspond to the irreducible representations $\{4\}, \{1^4\}, \{2^2\}, \{21^2\}, \{31\}$ of $\mathcal{S}_4$. The character table for the group $\mathcal{O}$ is given below:-

$\mathcal{O}$

$Class$	E	C_3	C_2	C_4	C_2'
$Order$	1	8	3	6	6
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

■ 6.2 Kronecker Products for $\mathcal{O}$

The Kronecker products of the irreducible representations of $\mathcal{O}$ can be readily evaluated by using the character table for $\mathcal{O}$ to produce a compound character and then using Eq. (5.8) to resolve the compound character into simple characters of $\mathcal{O}$. We give a table of Kronecker products for $\mathcal{O}$.

Kronecker products for $\mathcal{O}$

	A_1	A_2	E	T_1	T_2
A_1	A_1	A_2	E	T_1	T_2
A_2	A_2	A_1	E	T_2	T_1
E	E	E	A_1+A_2+E	T_1+T_2	T_1+T_2
T_1	T_1	T_2	T_1+T_2	$A_1+E+T_1+T_2$	$A_2+E+T_1+T_2$
T_2	T_2	T_1	T_1+T_2	$A_2+E+T_1+T_2$	$A_1+E+T_1+T_2$

■ 6.3 Some Basis Functions for $\mathcal{O}$

Let us choose a set of axes x, y, z parallel to the edges of the cube and passing through the centres of its faces and consider the action of a typical member of each class on x, y, z. Typically we find:-

$$E(x,y,z) \rightarrow (x,y,z), \quad C_2(x,y,z) \rightarrow (y,x,-z), \quad C_2'(x,y,z) \rightarrow (x,-y,-z), \quad C_3(x,y,z) \rightarrow (z,x,y)$$
$$C_4(x,y,z) \rightarrow (x,-z,y) \tag{6.1}$$

Each of the transformations can be represented by a rank three permutation matrix to give respectively the typical matrices:-

$$E: \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad C_2: \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad C_2': \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$
$$C_3: \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \quad C_4: \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \tag{6.2}$$

Taking the traces of these matrices gives the character:

$$3,\ 0,\ -1,\ 1,\ -1$$

which corresponds to the simple character χ^{T_1} of $\mathcal{O}$ thus we may conclude that the functions x, y, z form a basis for the irreducible representation T_1 of the group $\mathcal{O}$.

Let us now consider the transformation properties of the functions x^2, y^2, z^2. Noting Eq. (6.1) we obtain

$$E(x^2,y^2,z^2) \rightarrow (x^2,y^2,z^2), \quad C_2(x^2,y^2,z^2) \rightarrow (y^2,x^2,z^2), \quad C_2'(x^2,y^2,z^2) \rightarrow (x^2,y^2,z^2),$$
$$C_3 : (x^2,y^2,z^2) \rightarrow (z^2,x^2,y^2), \quad C_4(x^2,y^2,z^2) \rightarrow (x^2,z^2,y^2) \tag{6.3}$$

Againg these transformations can be represented by rank three permutation matrices and taking their traces we obtain the compound character

$$\phi = 3,\ 1,\ 3,\ 0,\ 1 \tag{6.4}$$

Using the character table for $\mathcal{O}$ we resolve the compound character ϕ as

$$\phi = \chi^{A_1} + \chi^{E} \tag{6.5}$$

We need three linear combinations of the functions x^2, y^2, z^2 to span these two irreducible representations of $\mathcal{O}$. One of these must be an invariant that transforms as A_1 and may be taken as $x^2 + y^2 + z^2 = r^2$. The two linearly independent combinations $x^2 - y^2$ and $3z^2 - r^2$ can be taken as a basis for the E irreducible representation of $\mathcal{O}$.

■ 6.4 Example of a Kronecker Product

Take the functions x_1, y_1, z_1 and x_2, y_2, z_2 as representing the coordinates of two electrons. Each set of functions forms a basis for a T_1 irreducible representation of $\mathcal{O}$. From these we can form a set of nine functions $x_1x_2, x_1y_2, x_1z_2, \ldots, z_1z_2$ which will span the Kronecker product $T_1 \times T_1$ with a compound character

$$\phi = 9,\ 0,\ 1,\ 1,\ 1 \tag{6.6}$$

Either using the Kronecker product table or using the character table of $\mathcal{O}$ together with Eq. (5.8) we find

$$\phi = \chi^{A_1} + \chi^{E} + \chi^{T_1} + \chi^{T_2} \tag{6.7}$$

Noting Eq. (6.7) we can produce an orthonormal set of basis functions as

$$A_1 : \phi_1 = \sqrt{\frac{1}{3}}(x_1x_2 + y_1y_2 + z_1z_2) \tag{6.8a}$$
$$E : \phi_2 = \sqrt{\frac{1}{2}}(x_1x_2 - y_1y_2)$$
$$\phi_3 = \sqrt{\frac{1}{6}}(2z_1z_2 - x_1x_2 - y_1y_2) \tag{6.8b}$$

$$
\begin{aligned}
T_1 : \phi_4 &= \sqrt{\frac{1}{2}}(y_1 z_2 + z_1 y_2) \\
\phi_5 &= \sqrt{\frac{1}{2}}(z_1 x_2 + x_1 z_2) \\
\phi_6 &= \sqrt{\frac{1}{2}}(x_1 y_2 + y_1 x_2) \qquad (6.8c) \\
T_2 : \phi_7 &= \sqrt{\frac{1}{2}}(y_1 z_2 - z_1 y_2) \\
\phi_8 &= \sqrt{\frac{1}{2}}(z_1 x_2 - x_1 z_2) \\
\phi_9 &= \sqrt{\frac{1}{2}}(x_1 y_2 - y_1 x_2) \qquad (6.8d)
\end{aligned}
$$

■ 6.5 Characters of SO_3

The group of continuous rotations that turn a sphere into itself is designated as SO_3. The octahedral group $\mathcal{O}$ is a subgroup of SO_3 as indeed are all the **32** point groups associated with crystals. The $2\ell+1$ spherical harmonics $Y_{\ell m}(\theta,\phi)$ of rank ℓ form a basis for a $2\ell+1$ dimensional irreducible representation $\mathcal{D}_\ell$ of SO_3. All rotations through the same angle α belong to the same class of SO_3 irrespective of the axis of rotation. For a rotation through an angle α about the z–axis

$$Y_{\ell m}(\theta, \phi + \alpha) = e^{im\alpha} Y_{\ell m}(\theta, \phi) \qquad (6.9)$$

Such a rotation can be represented by a rank $(2\ell+1)$ diagonal matrix with diagonal matrix elements $e^{im\alpha}$ and hence of trace, or character,

$$
\begin{aligned}
\chi^\ell_\alpha &= \sum_{m=-\ell}^{\ell} e^{im\alpha} \\
&= \frac{e^{i(\ell+\frac{1}{2})\alpha} - e^{-i(\ell+\frac{1}{2})\alpha}}{e^{i\frac{\alpha}{2}} - e^{-i\frac{\alpha}{2}}} \\
&= \frac{sin\,\frac{1}{2}(2\ell+1)\alpha}{sin\,\frac{1}{2}\alpha} \qquad (6.10)
\end{aligned}
$$

It is worth noting that the identity element of SO_3 corresponds to a rotation through $\alpha = 0°$ and hence

$$\chi^\ell_0 = (2\ell+1) \qquad (6.11)$$

At this point we also note that the Kronecker products for SO_3 give

$$\mathcal{D}_{\ell_1} \times \mathcal{D}_{\ell_2} = \sum_{L=|\ell_1-\ell_2|}^{\ell_1+\ell_2} \mathcal{D}_L \qquad (6.12)$$

as commonly encountered in the quantum theory of the addition of angular momentum.

■ 6.6 The $SO_3 \rightarrow \mathcal{O}$ Branching Rules

The octahedral group $\mathcal{O}$ is a subgroup of SO_3, i.e. $SO_3 \in \mathcal{O}$. The spherical harmonics $Y_{\ell m}(\theta, \phi)$ for a basis for the SO_3 irreducible representation $\mathcal{D}_\ell$. However this irreducible representation will normally be a reducible representation of the octahedral subgroup and simple character of SO_3 will become a compound character ϕ for $\mathcal{O}$. To obtain the compound character ϕ we calculate the characteristics χ^ℓ_α of SO_3 for the angles of rotation associated with each class of $\mathcal{O}$ using Eqns. (6.10) and (6.11). For $\mathcal{O}$ we note particularly the characteristics

$$\chi^\ell_0 = (2\ell+1), \quad \chi^\ell_\pi = (-1)^\ell, \quad \chi^\ell_{\frac{2\pi}{3}} = (-1)^{[\ell/2]}(1+(-1)^\ell)/2, \quad \chi^\ell_{\frac{\pi}{2}} = (-1)^{[\ell/2]} \tag{6.13}$$

Note the characteristics for the classes C_2 and C_2' are the same. Thus for $\ell = 4$ we obtain the compound character

$$\phi = 9,\ 0,\ 1,\ 1,\ 1 \tag{6.14}$$

which we may resolve into simple characters of $\mathcal{O}$ as

$$\phi = \chi^{A_1} + \chi^E + \chi^{T_1} + \chi^{T_2} \tag{6.15}$$

or as a *branching rule*

$$D_4 \rightarrow A_1 + E + T_1 + T_2 \tag{6.16}$$

Continuing in this way we can establish the $SO_3 \rightarrow \mathcal{O}$ branching rules

$$\begin{aligned}
D_0 &\rightarrow A_1 \\
D_1 &\rightarrow T_1 \\
D_2 &\rightarrow E + T_2 \\
D_3 &\rightarrow A_2 + T_1 + T_2 \\
D_4 &\rightarrow A_1 + E + T_1 + T_2 \\
D_5 &\rightarrow E + 2T_1 + T_2 \\
D_6 &\rightarrow A_1 + A_2 + E + T_1 + 2T_2
\end{aligned} \tag{6.17}$$

■ 6.7 The $\mathcal{C}_4$ Subgroup of $\mathcal{O}$

The group $\mathcal{C}_4$ corresponds to the rotational symmetry of a square and involves four elements, the identity $E,\ C_4,\ C_2,\ C_4^{-1}$. These are a subset of those of the octahedral group $\mathcal{O}$. Whereas in the octahedral group C_4 and C_4^{-1} occur in the same class in going to $\mathcal{C}_4$ the class splits. Likewise only one of the C_2 elements in $\mathcal{O}$ survives and comes from the class C_2 of $\mathcal{O}$. The character table of the group $\mathcal{C}_4$ is given below

$\mathcal{C}_4$	E	C_4	C_2	C_4^{-1}
A	1	1	1	1
B	1	−1	1	−1
E	1	i	−1	$-i$
	1	$-i$	−1	i

Note that the character E involves a *pair* of characters that are complex conjugates of each other.

■ Exercises

6.1 Show that the group comprising the identity permutation e and the three permutations

(1234), (1432), (13)(24) form a group that is isomorphic to $\mathcal{C}_4$.

6.2 Show that for the group $\mathcal{C}_4$ the function z transforms as A while the functions x, y span the E irreducible representation.

■ 6.8 The $\mathcal{O} \rightarrow \mathcal{C}_\triangle$ Branching Rules

The $\mathcal{O} \rightarrow \mathcal{C}_\triangle$ branching rules may be determined listing the characteristics of the octahedral group $\mathcal{O}$ for the elements that are in common with those of the group $\mathcal{C}_4$. Thus we obtain the following compound characters

$$\phi^{A_1} = 1,\ 1,\ 1,\ 1$$

$$\phi^{A_2} = 1,\ -1,\ 1,\ -1$$

$$\phi^{E} = 2,\ 0,\ 2,\ 0$$

$$\phi^{T_1} = 3,\ 1,\ -1,\ 1$$

$$\phi^{T_2} = 3,\ -1,\ -1,\ -1$$

These compound characters may be resolved into simple characters of $\mathcal{C}_4$ using Eq. (5.8) together with the character table of $\mathcal{C}_4$ to yield the branching rules given below:-

$\mathcal{O} \rightarrow \mathcal{C}_\triangle$ Branching Rules

$$\begin{aligned} A_1 &\rightarrow A \\ A_2 &\rightarrow B \\ E &\rightarrow A + B \\ T_1 &\rightarrow A + E \\ T_2 &\rightarrow B + E \end{aligned} \tag{6.18}$$

■ 6.9 Application to a d–orbital

Let us now apply some of our preceding results to a d–orbital. Under spherical symmetry the d–orbital forms a basis for the $\mathcal{D}_2$ irreducible representation of SO_3 and has 5–fold degeneracy (we ignore spin at the moment). If the d–orbital is place in a crystal field having octahedral symmetry then the 5–fold orbital degeneracy will be partially lifted since under $SO_3 \to \mathcal{O}$ we found that

$$\mathcal{D}_2 \to E + T_2$$

and thus we conclude that the energy levels will involve a 3–fold degenerate level (T_2) and a 2–fold degenerate level (E). If we were to distort the octahedral symmetry so as to leave the rotational symmetry of a square we would deduce from Eq. (6.18) that the E level of $\mathcal{O}$ would split into a pair of sublevels belonging to the A and B levels of $\mathcal{C}_4$ while the T_2 level of $\mathcal{O}$ would split into a non-degenerate level B and a 2–fold degenerate level E of $\mathcal{C}_4$.

■ Exercise

6.3 Repeat the above analysis for a f–orbital.

■ 6.10 Half-Integer Angular Momentum

So far we have neglected spin and the possibility of half-integer angular momentum. We recall from the quantum theory of angular momentum that

$$J_\pm |JM\rangle = \sqrt{J(J+1) - M(M \pm 1)}\,|JM \pm 1\rangle \tag{6.19a}$$

$$J_z |JM\rangle = M|JM\rangle \tag{6.19b}$$

which is valid for both integer *and* half-integer values of J. These operators produce states with the *same* value of J and the states $|JM\rangle$ produce a basis for a $(2J+1)$–dimensional irreducible representation $\mathcal{D}_J$ of SO_3. Since

$$e^{-i\alpha J_z}|JM\rangle = e^{-i\alpha M}|JM\rangle \tag{6.20}$$

it follows that the characteristics χ^J_α of SO_3 will be exactly given as in Eq. (6.10) except for the replacement of ℓ by J. Note that for half-integer values of J the factor $e^{-2\pi i M} = -1$ and hence for a rotation about a z–axis through $\alpha = 2\pi$ $|JM\rangle \to -|JM\rangle$. Under the group $\mathcal{O}$ rotations through 0 and 2π are equivalent and hence it is impossible to form, for half-integer J, linear combinations of $|JM\rangle$ that possess octahedral symmetry. The solution was given by Bethe in 1929 with the introduction of *double groups* or perhaps more accurately *extended groups*. The finite group is augmented with an element $\bar{E}$ which commutes

with all the elements of the group and is such that $\bar{E}^2 = E$. This results in additional group elements $\bar{g}$ when $\bar{g} = \bar{E} \times g = g \times \bar{E}$ if $\bar{g} \not\equiv g$. This may lead to a doubling of the number of elements to form the extended group (and hence the name *double group*) except classes containing rotations through π are often not doubled. Technically these extended groups are associated with the fact that they are subgroups of SU_2 the *covering group* of SO_3.

In the case of the octahedral group $\mathcal{O}$ we are led to the extended group $\bar{\mathcal{O}}$ whose character table is given below:-

$\bar{\mathcal{O}}$	E	$\bar{E}$	$8C_3$	$8\bar{C}_3$	$3\bar{C}_2$ $3C_2$	$6C_4$	$6\bar{C}_4$	$6\bar{C}_2'$ $6C_2''$
A_1	1	1	1	1	1	1	1	1
A_2	1	1	1	1	1	−1	−1	−1
E	2	2	−1	−1	2	0	0	0
T_1	3	3	0	0	−1	1	1	−1
T_2	3	3	0	0	−1	−1	−1	1
E'	2	−2	1	−1	0	$\sqrt{2}$	$-\sqrt{2}$	0
E''	2	−2	1	−1	0	$-\sqrt{2}$	$\sqrt{2}$	0
U'	4	−4	−1	1	0	0	0	0

■ 6.11 The $SO_3 \rightarrow \bar{O}$ Branching Rules

The $SO_3 \rightarrow \bar{O}$ branching rules may be evaluated in the same manner as previous examples, namely using Eq. (5.8) and the character table for $\bar{\mathcal{O}}$. There is no change in the branching rules for the integer values of J. For the half-integer values of J we obtain the branching rules given below.

$$\begin{aligned}
\mathcal{D}_{\frac{1}{2}} &\rightarrow E' \\
\mathcal{D}_{\frac{3}{2}} &\rightarrow U' \\
\mathcal{D}_{\frac{5}{2}} &\rightarrow E'' + U' \\
\mathcal{D}_{\frac{7}{2}} &\rightarrow E' + E'' + U' \\
\mathcal{D}_{\frac{9}{2}} &\rightarrow E' + 2U'
\end{aligned} \tag{6.19}$$

Note that for an octahedral symmetry states with $J \leq \frac{3}{2}$ remain degenerate.

■ Exercise

6.4 Enlarge the Kronecker product table given earlier for the octahedral group $\mathcal{O}$ to cover the case for the extended group $\bar{\mathcal{O}}$.

■ 6.12 The Wigner-Eckart Theorem

So far we have used group theory to obtain largely qualitative information for physical systems and have made no attempt to calculate matrix elements,

the key to obtaining quantitative results. A typical matrix element may be written in the form

$$\langle \phi_i | h_j | \chi_k \rangle = \int \phi_i^* h_j \chi_k d\tau \tag{6.21}$$

We will choose the states ϕ, χ and the interaction term h to span the irreducible representations $\Gamma_\phi, \Gamma_\chi, \Gamma_h$ of the group $\mathcal{G}$. Thus the states ϕ_i with $i = 1, 2, \ldots, p$ will be chosen to form an orthonormal basis for the p–dimensional irreducible representation Γ_ϕ, those of χ_j with $k = 1, 2, \ldots, q$ an orthonormal basis for the q–dimensional irreducible representation Γ_χ. The operators h_j representing an interaction term with $j = 1, 2, \ldots, r$ and forming an orthonormal basis for a r–dimensional irreducible representation Γ_h of $\mathcal{G}$. The Wigner-Eckart theorem then leads to the result that:-

$$\langle \phi_i | h_j | \chi_k \rangle = \sum_\alpha (\Gamma_\phi \alpha i | \Gamma_h j; \Gamma_\chi k) R_\alpha \tag{6.22}$$

Where the first term on the right-hand-side is a *coupling coefficient* that contains completely the dependence of the matrix element on the components of the group irreducible representations while the final quantity R_α is a *reduced matrix element* that is totally independent of the components of the irreducible representations appearing in the matrix element.

■ 6.13 Selection Rules

The sum over α involves c_ϕ terms where c_ϕ is the number of times the irreducible representation Γ_ϕ occurs in the Kronecker product $\Gamma_h \times \Gamma_\chi$. It follows that if $c_\phi = 0$ then the matrix element necessarily vanishes and we have a *selection rule*. In the case of the octahedral group the angular momentum operators (L_x, L_y, L_z) form a basis for the T_1 irreducible representation of $\mathcal{O}$. The Kronecker product

$$T_1 \times E = T_1 + T_2 \tag{6.23}$$

from which we may conclude that the matrix elements of the angular momentum operators evaluated between states transforming as the irreducible representation E are necessarily null. This corresponds to the common statement that orbital angular momentum is *quenched* in E levels.

The Application of Symmetry Concepts to Physical Problems II

B. G. Wybourne

No man is wise enough to think of all the ideas
that can occur to a fool
– Rudolph Peierls *Bird of Passage, Princeton 1985*

- **Lecture 8**
- **8.1 The Infinitesimal Operators of $SO(3)$**

The group SO_3 plays a central role in the quantum theory of angular momentum. It is associated with the group of transformations that send a sphere in three-dimensions into itself. The transformation matrices are degree three orthogonal matrices, A, of determinant $|A| = +1$. The orthogonality requirement requires that

$$^tAA = \mathcal{I}_3 \tag{8.1}$$

where $\mathcal{I}_3$ is the three dimensional unit matrix. For infinitesimal rotations we have

$$A = \mathcal{I}_3 + B \tag{8.2}$$

where B is a matrix that has all its elements in the neighbourhood of zero. For the transformation to preserve the orthogonality we must have

$$\mathcal{I}_3 =^t AA = (\mathcal{I}_3 +^t B)(\mathcal{I}_3 + B) \approx \mathcal{I}_3 +^t B + B \tag{8.2}$$

i.e

$$^tB + B = 0 \tag{8.3}$$

Thus B must be a *skew-symmetric* matrix with three independent components, say

$$B = \begin{pmatrix} 0 & a & -b \\ -a & 0 & c \\ b & -c & 0 \end{pmatrix} \tag{8.4}$$

But $x' = (\mathcal{I}_3 + \epsilon)x$, i.e.

$$\begin{pmatrix} x + dx \\ y + dy \\ z + dz \end{pmatrix} = \left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & a & -b \\ -a & 0 & c \\ b & -c & 0 \end{pmatrix} \right] \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{8.5}$$

Thus

$$dx = ay - bx$$
$$dy = ax + cz$$
$$dz = bx - cy \tag{8.6}$$

Hence the infinitesimal operators of $SO(3)$ are

$$\begin{aligned} X_1 &= \frac{\partial(cz)}{\partial c}\frac{\partial}{\partial y} + \frac{\partial(-cy)}{\partial c}\frac{\partial}{\partial z} = z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z} \\ X_2 &= \frac{\partial(-bz)}{\partial c}\frac{\partial}{\partial x} + \frac{\partial(bx)}{\partial b}\frac{\partial}{\partial z} = x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x} \\ X_3 &= \frac{\partial(ay)}{\partial a}\frac{\partial}{\partial x} + \frac{\partial(-ax)}{\partial a}\frac{\partial}{\partial y} = y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y} \end{aligned} \tag{8.7}$$

The above infinitesimal operators of $SO(3)$ close under commutation:

$$[X_1, X_2] = X_3 \quad [X_2, X_3] = X_1 \quad [X_3, X_1] = X_2 \tag{8.8}$$

The normal operators associated with the quantum theory of angular momentum are $J_k = -iX_k \quad k = 1, 2, 3$ and the corresponding commutation relations are

$$[J_1, J_2] = iJ_3 \quad [J_2, J_3] = iJ_1 \quad [J_3, J_1] = iJ_2 \tag{8.9}$$

where we have chosen our units so that $\hbar = 1$.

■ 8.2 Irreducible representations of $SO(3)$

We now seek to find a basis for the irreducible representations of $SO(3)$ obtaining results familiar in the quantum theory of angular momentum. We will identify J_3 as the generator of infinitesimal rotations in two-dimensions and hence associated with the subgroup of $SO(3)$, namely, $SO(2)$. Let us write

$$J_\pm = \frac{1}{\sqrt{2}}(J_1 \pm iJ_2) \tag{8.10}$$

leading to the commutation relations

$$[J_+, J_-] = J_3 \quad \text{and} \quad [J_3, J_\pm] = \pm J_\pm \tag{8.11}$$

The operator

$$J^2 = J_1^2 + J_2^2 + J_3^2 = J_+J_- + J_+J_- + J_3^2 \tag{8.12}$$

has the special property of commuting with the set of operators (J_1, J_2, J_3) and is termed the *Casimir operator* associated with the *Lie algebra* $so(3)$ of the *Lie group* $SO(3)$. Of course we recognise it as the familiar square of the total angular momentum J. Noting Eqn.(8.11) we have

$$2J_+J_- = J^2 - J_3(J_3 - 1) \quad \text{and} \quad 2J_-J_+ = J^2 - J_3(J_3 + 1) \tag{8.13}$$

We seek the eigenvalue spectra of J^2 and J_3. Let us label the representations of SO_3 by the eigenvalues X of J^2. We shall construct the eigenvectors $|Xa\rangle$ spanning the space of a particular representation to be simultaneous eigenvectors of J^2 and J_3 and label them by their associated eigenvalues X and a.

Since J^2 is a sum of positive-definite Hermitian operators it must itself be a Hermitian operator and hence for a *unitary* representation must have *real* and *positive* eigenvalues. Likewise, J_3, is a Hermitian operator and must have real eigenvalues. Hence

$$J^2|Xa\rangle = X|Xa\rangle \quad (X \geq 0, X \in R) \tag{8.14}$$

and

$$J_3|Xa\rangle = a|Xa\rangle \quad (a \in R) \tag{8.15}$$

Use of Eqn.(8.13) leads to

$$2J_+J_-|Xa\rangle = [X - a(a-1)]|Xa\rangle \tag{8.16a}$$

$$2J_-J_+|Xa\rangle = [X - a(a+1)]|Xa\rangle \tag{8.16b}$$

In a unitary representation we must have

$$J_+^\dagger = J_- \tag{8.17}$$

and hence the eigenvalues of J_-J_+ or J_+J_- must be positive definite. Thus Eqns. (8.16a) and (8.16b) imply that for a unitary representation we necessarily have

$$X - a(a \pm 1) \geq 0 \tag{8.18}$$

Using Eqn (8.11) we obtain

$$\langle Xa'|[J_3, J_+]|Xa\rangle = (a - a')\langle Xa'|J_+|Xa\rangle = \langle Xa'|J_+|Xa\rangle \tag{8.19}$$

leading to

$$a' - a = 1 \tag{8.20}$$

For a given finite nonnegative value of X, it is possible to satisfy Eq. (8.15) with real values of X and a only if a has an upper positive bound a_+ and a lower negative bound a_-, with $a_+ - a_-$ an integer. Solving Eq. (8.18) f0 $a_\pm$ gives

$$a_\pm = -\frac{1}{2} \mp \frac{1}{2}\sqrt{1+4X} \tag{8.21}$$

and hence

$$X = a_+(a_+ + 1) \quad \text{and} \quad a_- = -a_+ - 1 \tag{8.22}$$

Since a_+ and a_- differ by an integer, $2a_+$ must be a positive integer and hence a_+ is limited to the field of positive integers or half odd integers.

Let us put $j = a_+$ and replace a by m. It follows that a given unitary irreducible representation of $SO(3)$ may be labelled by the upper bound j with the eigenvectors designated as $|jm\rangle$ where for a given value of j there are $2j+1$ values of m

$$m = j, j-1, \ldots, -j+1, -j \tag{8.23}$$

The range of m is *bounded above and below* and hence the unitary irreducible representations of $SO(3)$ are all of *finite* dimension equal to $2j+1$. It follows from Eqns. (8.16a),(8.16b) and Eqn. (8.17) that

$$J_\pm |jm\rangle = \frac{1}{\sqrt{2}} \sqrt{j(j+1) - m(m \pm 1)} |jm \pm 1\rangle \tag{8.24}$$

where the arbitrary phase factor has been chosen as positive. The *ladder operators* $J_\pm$ allow us to step the value of m in steps of ± 1 with

$$J_\pm |j, \pm m\rangle = 0 \tag{8.24}$$

Note that the preceding equations are invariant under the substitution

$$j \rightarrow -j-1 \quad \text{and} \quad m \rightarrow m \tag{8.25}$$

with D^j and D^{-j-1} being *equivalent* representations of $SO(3)$.

■ 8.3 Lie Algebras

In the preceding section we have been discussing the properties of a particular example of a *Lie algebra*. Formally we may define a Lie algebra as follows: Let A be a r-dimensional vector space over a field K in which the law of composition for vectors is such that to each pair of vectors X and Y there corresponds a vector $Z = [X, Y]$ in such a way that

$$[\alpha X + \beta Y, Z] = \alpha [X, Z] + \beta [Y, Z] \tag{8.26}$$

$$[X, Y] + [Y, X] = 0 \tag{8.27}$$

$$[X, [Y, Z]] + [Y, [Z, X]] + [Z, [X, Y]] = 0 \tag{8.28}$$

for all $\alpha, \beta, \ldots, \in K$ and all $X, Y, Z, \ldots, \in A$. A vector space satisfying the above relationships is said to constitute a Lie algebra. A given Lie algebra is said to be *real* if K is the field of real numbers and *complex* if K is the field of complex numbers.

■ 8.4 Structure Constants

The formation of a Lie algebra requires that the r elements of the Lie algebra, X_ρ satisfy the closure condition

$$[X_\rho, X_\sigma] = c^\tau_{\rho\sigma} X_\tau \tag{8.29}$$

where the $c^{\tau}_{\rho\sigma} = -c^{\tau}_{\sigma\rho}$ are known as the *structure constants* of the Lie algebra.

■ 8.5 The Killing Form

We may form a symmetrical tensor from the structure constants by writing

$$g_{\sigma\lambda} = g_{\lambda\sigma} = c^{\tau}_{\sigma\rho} c^{\rho}_{\lambda\tau} \tag{8.30}$$

which is known as the *metric tensor* or *Killing form*. Every Lie algebra may be associated with a particular metric tensor. A Lie algebra A is said to be *semisimple* if and only if A can be written as a sum of simple Lie algebras. A Lie algebra A will be semisimple if and only if

$$det|g_{\sigma\lambda}| \not\emptyset \tag{8.31}$$

As an example consider the Lie algebra of $so(3)$

$$[X_1, X_2] = X_3, \quad [X_2, X_3] = X_1, \quad [X_3, X_1] = X_2 \tag{8.32}$$

We have from Eqn. (8.30)

$$g_{11} = c^{\tau}_{1\rho} c^{\rho}_{1\tau} = c^{3}_{12} c^{2}_{13} + c^{2}_{13} c^{3}_{12} = (1)(-1) + (-1)(1) = -2$$

Continuing we find

$$g_{\sigma\lambda} = -2\delta_{\sigma\lambda}$$

and hence $so(3)$ is semisimple and its metric tensor is *negative definite*

Now let us consider a Lie algebra whose elements satisfy

$$[X_1, X_2] = X_3, \quad [X_2, X_3] = -X_1, \quad [X_3, X_1] = X_2 \tag{8.33}$$

We now find

$$g_{\sigma\lambda} = \begin{pmatrix} -2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{8.34}$$

that is

$$det|g_{\sigma\lambda}| = -8$$

and hence we have a semisimple Lie algebra but the metric is indefinite.

■ 8.6 Lie Algebra of the Euclidean Plane

The Euclidean group of the plane, E_2, relates a point (x, y) to a point (x', y') in a plane by the transformation

$$\begin{aligned} x' &= x\,cos\,\theta - y\,sin\,\theta + a \\ y' &= x\,sin\,\theta + y\,cos\,\theta + b \end{aligned} \tag{8.35}$$

where θ is an angle of rotation in the plane about the origin and a and b are the x and y components of a translation in the plane. Each point (x, y) in the

plane may be associated with a vector $(x, y, 1)$ which is transformed into $(x', y', 1)$ by the matrix

$$\begin{pmatrix} cos\,\theta & -sin\,\theta & a \\ sin\,\theta & cos\,\theta & b \\ 0 & 0 & 1 \end{pmatrix} \tag{8.36}$$

From that we may obtain three infinitesmal operators

$$X_\theta = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad X_a = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad X_b == \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \tag{8.37}$$

which satisfy the commutation relations

$$[X_\theta, X_a] = X_b, \quad [X_\theta, X_b] = -X_a, \quad [X_a, X_b] = 0 \tag{8.38}$$

The metric tensor is now found to be

$$g_{\sigma\lambda} = \begin{pmatrix} -2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{8.39}$$

which is obviously non-singular and hence E_2 is *not* semisimple. The two elements X_2, X_3 form a non-trivial Abelian subalgebra. This Lie algebra cannot be reduced to a direct sum of simple Lie algebras but is rather a *semidirect sum*

$$E_2 = T_2 \oplus_s X_1 \tag{8.40}$$

■ Exercise

8.1 Show that the Euclidean group in three dimensions, E_3, is not associated with a semisimple Lie algebra and that it may be written as a semidirect sum of an Abelian Lie algebra associated with the group of translations T_3 and of the Lie algebra $so(3)$.

■ 8.7 Antisymmetric Tensors

Let us define a new tensor

$$c_{\sigma\mu\nu} = g_{\sigma\lambda} c^\lambda_{\mu\nu} \tag{8.41}$$

Recalling Eqn. (8.30) we have

$$c_{\sigma\mu\nu} = c^\tau_{\sigma\rho} c^\rho_{\lambda\tau} c^\lambda_{\mu\nu} = c^\tau_{\sigma\rho} c^\lambda_{\mu\nu} c^\rho_{\lambda\tau} \tag{8.42}$$

Use of the Jacobi identity, Eqn. (8.28), we have

$$\begin{aligned} c_{\sigma\mu\nu} &= -c^\tau_{\sigma\rho} c^\lambda_{\nu\tau} c^\rho_{\mu\lambda} - c^\tau_{\sigma\rho} c^\lambda_{\tau\mu} c^\rho_{\lambda\nu} \\ &= c^\tau_{\rho\sigma} c^\lambda_{\nu\tau} c^\rho_{\mu\lambda} + c^\tau_{\rho\sigma} c^\lambda_{\tau\mu} c^\rho_{\lambda\nu} \end{aligned} \tag{8.43}$$

The right-hand-side is invariant under any cyclic permutation of the indices. Since $g_{\sigma\lambda}$ is a symmetric tensor and $c^\lambda_{\mu\nu}$ is antisymmetric in μ and ν it follows that $c_{\sigma\mu\nu}$ is a totally antisymmetric tensor under any interchange of its indices.

■ 8.8 The Casimir Operators

Let X_τ stand for an element of a Lie algebra A and define

$$C = g^{\rho\sigma} X_\rho X_\sigma \tag{8.44}$$

The operator C is known as the *Casimir operator* and has the very important property of commuting with all the elements of a semisimple Lie algebra.

■ Exercises

8.2 Given the Lie algebra for $so(3)$ defined by the commutation relations given in Eqn. (8.8) show that its Casimir operator is given by

$$C = -\frac{1}{2}(X_1^2 + X_2^2 + X_3^2) \tag{8.45}$$

8.3 The commutation relations given in Eqn. (8.33), which are those of the *non-compact* Lie algebra $so(2,1)$ has the Casimir operator

$$C = -\frac{1}{2}(X_1^2 - X_2^2 - X_3^2) \tag{8.46}$$

■ Concluding Remarks

The Casimir operators play an important role in applications to physical problems whereas the Lie algebra $so(2,1)$ will lead us to simple solutions to a wide range of problems in physics involving second-order differential equations, the subject of Lecture 9.

The Application of Symmetry Concepts to Physical Problems II

B. G. Wybourne

People have now a-days, got a strange opinion that everything should be taught by lectures. Now, I cannot see that lectures can do so much good as as reading the books from which the lectures are taken. I know nothing that can best be taught by lectures, except where experiments are to be shewn. You may teach chymistry by lectures. You might teach the making of shoes by lectures!
– Samuel Johnson 1766

■ Lecture 10

■ 10.1 Spectrum Generating Lie Algebras based upon $so(2,1)$

Most of the analytically solvable second-order differential equations involving a single variable that are of interest in electromagnetic and quantum theory can be transformed into the standard form:-

$$\frac{d^2Y}{dy^2} + f(y)Y = 0 \tag{10.1}$$

where $Y = Y(y)$.

Many of the differential equations can be expressed in terms of the elements of the Lie algebra $so(2,1) \sim su(1,1)$. If we know the spectral properties of these elements we can immediately generate the spectrum associated with the relevant second-order differential equation.

■ 10.2 A realisation of $so(2,1)$

The Lie algebra associated with the group $SO(2,1)$ is characterised by the commutation relationships

$$[\Gamma_1, \Gamma_2] = -i\Gamma_3, \qquad [\Gamma_2, \Gamma_3] = i\Gamma_1, \qquad [\Gamma_3, \Gamma_1] = i\Gamma_2 \tag{10.2}$$

A realisation in terms of a single dimensionless variable y may be obtained by writing

$$\begin{aligned}
\Gamma_1 &= \frac{\partial^2}{\partial y^2} + a_1(y) \\
\Gamma_2 &= i\left[k(y)\frac{\partial}{\partial y} + a_2(y)\right] \\
\Gamma_3 &= \frac{\partial^2}{\partial y^2} + a_3(y)
\end{aligned} \tag{10.3}$$

Making use of Eqn. (10.2) then gives

$$\begin{aligned} a_1 &= \frac{\alpha}{(\beta - y)^2} + \frac{(\beta - y)^2}{16} \\ a_2 &= -\frac{3}{4} \\ a_3 &= \frac{\alpha}{(\beta - y)^2} + \frac{(\beta - y)^2}{16} + \gamma \\ k &= \frac{\beta - y}{2} \end{aligned} \tag{10.4}$$

where α, β and γ are integration constants.

The existence of the Casimir invariant

$$\Gamma^2 = \Gamma_3^2 - \Gamma_1^2 - \Gamma_2^2 \tag{10.5}$$

requires that $\gamma = 0$ and hence

$$\Gamma^2 = -\frac{\alpha}{4} - \frac{3}{16} \tag{10.6}$$

If we choose $\beta = 0$ we obtain the standard form for $so(2,1)$ in terms of a single variable y as

$$\begin{aligned} \Gamma_1 &= \frac{\partial^2}{\partial y^2} + \frac{\alpha}{y^2} + \frac{y^2}{16} \\ \Gamma_2 &= -\frac{i}{2}\left(y\frac{\partial}{\partial y} + \frac{1}{2}\right) \\ \Gamma_3 &= \frac{\partial^2}{\partial y^2} + \frac{\alpha}{y^2} - \frac{y^2}{16} \end{aligned} \tag{10.7}$$

■ 10.3 The Second-Order Differential Equation

Recall the standard form

$$\frac{d^2Y}{dy^2} + f(y)Y = 0 \tag{10.1}$$

and let us put

$$f(y) = \frac{a}{y^2} + by^2 + c \tag{10.8}$$

We may now rewrite Eqn. (10.1) in the form

$$\frac{\partial^2}{\partial y^2} + \frac{a}{y^2} + by^2 + c = (\frac{1}{2} + 8b)\Gamma_1 + (\frac{1}{2} - 8b)\Gamma_3 + c \tag{10.9}$$

Making the identification

$$a = -4\Gamma^2 - \frac{1}{4} \tag{10.10}$$

yielding

$$\left[(\frac{1}{2} + 8b)\Gamma_1 + (\frac{1}{2} - 8b)\Gamma_3 + c\right] Y = 0 \tag{10.11}$$

■ 10.4 The Tilting Angle

Equation (10.11) can be greatly simplified by performing a rotation through an arbitrary *tilting angle* θ such that

$$e^{-i\theta\Gamma_2}\Gamma_1 e^{i\theta\Gamma_2} = \Gamma_1 \cosh\theta + \Gamma_3 \sinh\theta$$

and

$$e^{-i\theta\Gamma_2}\Gamma_3 e^{i\theta\Gamma_2} = \Gamma_1 \sinh\theta + \Gamma_3 \cosh\theta \tag{10.12}$$

giving

$$\left(\left[(\frac{1}{2}+8b)\sinh\theta + (\frac{1}{2}-8b)\cosh\theta\right]\Gamma_1 + \left[(\frac{1}{2}+8b)\sinh\theta + (\frac{1}{2}-8b)\cosh\theta\right]\Gamma_3 + c\right)\tilde{Y} = 0 \tag{10.13}$$

where

$$\tilde{Y} = e^{-i\theta\Gamma_2}Y \tag{10.14}$$

The tilting angle θ may be chosen to either diagonalise Γ_3 to yield the *discrete* spectrum or diagonalise Γ_1 yielding the continuous part of the spectrum.

■ 10.5 The Discrete Spectrum

If we put

$$\tanh\theta = -\frac{\frac{1}{2}+8b}{\frac{1}{2}-8b} \tag{10.15}$$

equation (10.13) reduces to just

$$\Gamma_3\tilde{Y} = \frac{c}{4\sqrt{-b}}\tilde{Y} \tag{10.16}$$

where $\tilde{Y}$ is a simultaneous eigenvector of Γ^2 and Γ_3 and hence the eigenvectors must span one of the discrete infinite unitary irreducible representations $\mathcal{D}^+(\Phi)$ or $\mathcal{D}^-(\Phi)$ of $so(2,1)$. In the case of $\mathcal{D}^+(\Phi)$ the eigenvalues of Γ_3 will have a lower bound Φ which increases in steps of unity with no upper bound and conversely for $\mathcal{D}^-(\Phi)$. Thus we may write the eigenvalue solution of Eqn. (10.16) as

$$\begin{aligned}\Gamma_3\tilde{Y}^+_{\Phi x} &= (-\Phi + x)\tilde{Y}^+_{\Phi x} \\ &= \frac{c}{4\sqrt{-b}}\tilde{Y}^+_{\Phi x} \quad (x = 0, 1, 2, \ldots)\end{aligned} \tag{10.17}$$

with

$$\Gamma^2\tilde{Y}^+_{\Phi x} = \Phi(\Phi+1)\tilde{Y}^+_{\Phi x} \quad (\Phi < 0) \tag{10.18}$$

Noting Eqn. (10.17) we conclude that the existence of a discrete eigenvalue solution associated with the second-order differential equation

$$\left(\frac{\partial^2}{\partial y^2} + \frac{a}{y^2} + by^2 + c\right)Y = 0 \tag{10.19}$$

requires that

$$4(-\Phi + x) = \frac{c}{\sqrt{-c}} \tag{10.20}$$

This equation may be put into a more direct form by noting from Eqn. (10.6) that

$$\Phi(\Phi+1) = -\frac{\alpha}{4} - \frac{3}{16} \tag{10.21}$$

and $a = \alpha$ and hence

$$\Phi = -\frac{1}{2}(1 + \sqrt{\frac{1}{4} - a}) \quad (\frac{1}{4} - a \geq 0) \tag{10.22}$$

where, since $\Phi < 0$ we keep only the negative root. Using this result in Eqn. (10.20) yields the key result

$$4x + 2 + \sqrt{1 - 4a} = \frac{c}{\sqrt{-b}} \qquad x = 0, 1, 2, \ldots \tag{10.23}$$

■ 10.6 The Continuous Eigenvalue Spectrum

In this case we diagonalise the non-compact generator Γ_1 using the tilting angle

$$tanh\,\theta = \frac{\frac{1}{2} - 8b}{\frac{1}{2} + 8b} \tag{10.24}$$

Eqn. (10.13) then reduces to

$$\Gamma_1 \tilde{Y} = \frac{-c}{4\sqrt{-b}} \tilde{Y} \tag{10.25}$$

The eigenvalue spectrum is characterised by a continuous spectrum λ where

$$\lambda = \frac{-c}{4\sqrt{-b}} \tag{10.26}$$

Note that the continuous part of the spectrum only exists where $tanh\,\theta$ exists.

■ 10.7 The Three-Dimensional Harmonic Oscillator

The three-dimensional isotropic harmonic oscillator is of great importance in nuclear shell theory, vibrational states in molecules and solids and in the theory of quantum dots. The appropriate radial differential equation is

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - r^2 + 2E\right) R(r) = 0 \tag{10.27}$$

Comparison with Eqn. (10.19) requires

$$a = -\ell(\ell+1), \quad b = -1, \quad \text{and} \quad c = 2E$$

Using these values in Eqn. (10.23) gives

$$E = 2x + \ell + \frac{3}{2} \qquad (x = 0, 1, 2, \ldots)$$

Putting $n = 2x + \ell$ yields the familiar result

$$E_n = (n + \frac{3}{2}) \tag{10.28}$$

If we add a perturbing term $\frac{\epsilon}{r^2}$ $(\epsilon \geq 0)$ to the Hamiltonian Eqn. (10.27) becomes

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)+\epsilon}{r^2} - r^2 + 2E\right) R(r) = 0$$

leading to

$$E = 2x + 1 + \sqrt{(\ell + \frac{1}{2})^2 + \epsilon} \tag{10.29}$$

Note there is no continuous spectrum for the harmonic oscillator since putting $b = -1$ in Eqn. (10.24) leads to a tilting angle that falls outside of the allowed limits of $tanh\,\theta$.

■ 10.8 The Kepler Problem

Consider the differential equation

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{t}{r} + \frac{u}{r^2} + v\right) R(r) = 0 \tag{10.30}$$

We can transform it into standard form by putting

$$r = y^2 \quad \text{and} \quad R(r) = y^{-\frac{3}{\lambda}}\mathcal{R}(y) \tag{10.31}$$

to give

$$\left(\frac{d^2}{dy^2} + \frac{4u - \frac{3}{4}}{y^2} + 4vy^2 + 4t\right) \mathcal{R}(y) = 0 \tag{10.32}$$

Using Eqns. (10.10) and (10.23) gives for the discrete spectrum

$$2x + 1 + \sqrt{1 - 4u} = \frac{t}{\sqrt{-v}} \qquad (x = 0, 1, 2, \ldots) \tag{10.33}$$

For a non-relativistic hydrogen atom we have $t = -2Z$, $u = -\ell(\ell+1)$ and $v = 2E$ which in Eqn. (10.33) yields the bound state spectrum as

$$E_n = -\frac{Z^2}{2n^2} \tag{10.34}$$

with $n = x + \ell + 1$.

Adding an inverse-cube potential to the Hamiltonian puts $u = -\ell(\ell+1) - \epsilon$ to yield the discrete spectrum

$$E = \frac{-Z^2}{2\left[x + \frac{1}{2} + \sqrt{(\ell + \frac{1}{2})^2 + 2\epsilon}\right]^2} \qquad (x = 0, 1, 2, \ldots) \tag{10.35}$$

which lifts the degeneracy of the H-atom in a manner similar to the normal fine structure.

■ 10.9 Klien-Gordon H-atom

The case of the Klien-Gordon equation for an H-atom leads to $t = -2Z\alpha^2 E$, $u = Z^2\alpha^2 - \ell(\ell+1)$, and $v = \frac{(\alpha^4 E^2 - 1)}{\alpha^2}$ in Eqn. (10.33) to yield the spectrum

$$\alpha^2 E = \frac{1}{\sqrt{1 + \frac{Z^2\alpha^2}{n^2}}} \tag{10.36}$$

where $n = x + \frac{1}{2} + \sqrt{(\ell + \frac{1}{2})^2 - Z^2\alpha^2}$ and α is the fine structure constant.

■ 10.10 The Morse Potential

The differential equation

$$\left(\frac{d^2}{dz^2} + p\, exp^{2\tau z} + q\, exp^{\tau z} + r\right) R(z) = 0 \tag{10.37}$$

arises in certain physical problems and may be transformed into the standard form by putting

$$z = ln\, y^2 \quad \text{and} \quad R(z) = \frac{\mathcal{R}(y)}{\sqrt{y}}$$

to give

$$\left(\frac{d^2}{dy^2} + \frac{16r + \tau^2}{4\tau^2 y^2} + \frac{4p}{\tau^2}y^2 + \frac{4q}{\tau^2}\right) \mathcal{R}(y) = 0 \tag{10.38}$$

Morse has considered the energy eigenvalue spectrum associated with the differential equation

$$\left(\frac{d^2}{dr^2} - 2D\, exp^{-2\tau z} + 4D\, exp^{-\tau z} + 2E\right) R(r) = 0 \tag{10.39}$$

Noting Eqns. (10.37) and (10.38) we obtain the standard form

$$\left(\frac{d^2}{dy^2} + \frac{32E + \tau^2}{4\tau^2 y^2} - \frac{8D}{\tau^2}y^2 + \frac{16D}{\tau^2}\right) \mathcal{R}(y) = 0 \tag{10.40}$$

Use of Eqn. (10.23) leads to

$$E = \frac{-\tau^2}{2}\left(\frac{\sqrt{2}D}{\tau} - (x + \frac{1}{2})\right)^2 \qquad (x = 0, 1, 2, \ldots, x_{max}) \tag{10.41}$$

where

$$x_{max} + \frac{1}{2} < \frac{\sqrt{2}D}{\tau} \tag{10.42}$$

■ 10.11 Concluding Remark

In this lecture we have seen a few examples of the application of a non-compact Lie algebra to solving differential equations in physics. This is just a beginning. The subject of Lie symmetries and the differential equations of physics has developed into an important research area in theoretical physics. We have looked so far at just the three-parameter Lie groups. However, there is a vast range of possible Lie groups, their associated Lie algebras and their applications as will be discussed in subsequent lectures.

The Application of Symmetry Concepts to Physical Problems II

B. G. Wybourne

- Lecture 11
- 11.1 Quantum Dots and Symmetry Physics

The subject of quantum dots involves the confinement of N electrons in two or three dimensions, commonly by electrostatic fields, over a nano-metre scale. The confining potential is, to a good approximation parabolic. The quantum dot behaves as an N–electron atom without a nuclear core. One may add or subtract a single electron from a quantum dot giving rise to the possibility of nano-metre scale devices such as transitors etc.

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 making normal perturbative methods difficult. 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. We shall first review some of the properties of the isotropic harmonic oscillator, the unitary group $U(3)$ and the special unitary group $SU(3)$.

- 11.2 The Isotropic harmonic oscillator

The Hamiltonian H of a normalised isotropic harmonic oscillator (i.e. with $m = \hbar = \omega = 1$) in three-dimensions may be written as

$$H = \frac{1}{2}(p^2 + r^2) \tag{11.1}$$

From Heisenberg's quantisation postulate the coordinates q_i and momenta p_i satisfy the commutation relations

$$[q_i, q_j] = [p_i, p_j] = 0, \qquad [q_i, p_j] = i\delta_{ij} \tag{11.2}$$

Now introduce boson annihilation and creation operators (a and $a^\dagger$ respec-

tively)

$$a = \frac{1}{\sqrt{2}}(r + ip), \qquad a^\dagger = \frac{1}{\sqrt{2}}(r - ip) \tag{11.3}$$

which satisfy the bosonic commutation relation

$$[a_i, a_j^\dagger] = \delta_{ij} \tag{11.4}$$

The Hamiltonian can now be written as

$$H = a^\dagger \cdot a + \frac{3}{2} \tag{11.5}$$

Use of Eqn. (11.4) then leads to

$$[H, a_j^\dagger] = a_j^\dagger, \qquad [H, a_j] = -a_j \tag{11.6}$$

Thus we deduce that $a_j^\dagger$ creates and a_j annihilates a quantum in the j direction. We recognise $a^\dagger \cdot a$ as being the *number operator* with eigenvalues of

$$n = n_1 + n_2 + n_3 \tag{11.7}$$

and hence the energy eigenvalues of H are

$$E_n = n + \frac{3}{2} \quad (n = 0, 1, 2, \ldots) \tag{11.8}$$

with normalised state vectors

$$|n_1 n_2 n_3\rangle = \prod_{i=1}^{3} \frac{a_i^{\dagger n_i}}{\sqrt{n_i!}} |000\rangle \tag{11.9}$$

with $|000\rangle$ being the vacuum state with

$$a_j |000\rangle = 0 \tag{11.10}$$

Noting that $\mathbf{a}^\dagger = \mathbf{a}^*$ we have

$$\langle n_1 n_2 n_3| = \langle 000| \prod_{i=1}^{3} \frac{a_i^{n_i}}{\sqrt{n_i!}} \tag{11.11}$$

with

$$\langle 000| a_j^\dagger = 0 \tag{11.12}$$

■ 11.3 The Full Linear Group $GL(n)$

Consider a vector space V_n and linear transformations of *contravariant* vectors with components $x^1, \ldots, x^n$ such that

$$x^i \rightarrow x'^i = \alpha_j^i x^j \tag{11.13}$$

The coefficients α_j^i are complex numbers and we assume the Einstein summation convention over repeated upper and lower indices. We restrict ourselves to transformations which have an inverse and hence to non-singular matrices $[a_j^i]$. The set of all such transformations in V_n form the full linear group $GL(n)$

The set of matrix transformations of $GL(n)$ involving unitary matrices of rank n form the elements of the unitary group $U(n)$. Transformations with the property

$$det[a_j^i] = +1 \tag{11.14}$$

are called *unimodular*; the special unitary group, $SU(n)$, is the subgroup of unimodular transformations in $U(3)$.

We can define *covariant* vectors with components $x_1, \ldots, x_n$ which undergo linear transformations

$$x_i \rightarrow x_i' = x_j b_i^j \tag{11.15}$$

such that

$$x_i' x'^i = x_i x^i$$

implying that

$$a_j^i b_i^k = \delta_j^k \tag{11.16}$$

Restricting transformations to those of $U(n)$ the relationship between covariant and contravariant transformations is that of *complex conjugation*.

■ 11.4 Note on Tensors

Tensors with covariant and contravariant indices are defined by their transformation properties:-

$$T_{kl\ldots}^{ij\ldots} \rightarrow a_m^i a_n^j \ldots T_{pq\ldots}^{mn\ldots} b_k^p b_l^q \ldots \tag{11.17}$$

A tensor with m upper suffixes and n lower indices is said to be of *order* $m+n$. The upper and lower indices of a tensor may be separately *symmetrised* and *antisymmetrised*; in general an *irreducible* tensor must be such that on separate permutation of its upper and lower indices it transforms according to an irreducible representation of the group of permutations on the indices concerned. In addition it must be separated into its irreducible parts by successive contractions of upper and lower indices.

■ 11.5 Irreducible representations of the Unitary group $U(n)$

There is a close relation between the properties of tensors as bases for the irreducible representations of $GL(n)$ and as bases for the irreducible representations of the groups of permutations acting on their indices. For the moment let us restrict our attention to tensors that are purely covariant or contravariant. For $GL(n)$ (or $U(n)$) the irreducible tensors may be described by partitions $\lambda \vdash m$ where m is the order of the tensor (i.e. the number of upper (or lower) indices) and

$$\lambda_1 \geq \lambda_2 \geq \ldots \lambda_p \tag{11.18}$$

A *symmetric* tensor of rank three would correspond to the partition (3) while an *antisymmetric* tensor of rank 3 would correspond to the partition (1^3). Likewise, there is an irreducible representation of the group $U(n)$ for every partition into not more than n parts. Note that there is an infinite number of irreducible representations for a given $U(n)$. For example, in the case of $U(3)$ $\{100\}, \{210\}, \{321\}, \ldots$ all label distinct irreducible representations of $U(3)$.

■ 11.6 Irreducible representations of the Special Unitary group $SU(n)$

Under the restriction from $U(n) \rightarrow SU(n)$ the representations

$$\{\lambda_1, \lambda_2, \ldots, \lambda_n\} \equiv \{\lambda_1 + x, \lambda_2 + x, \ldots, \lambda_n + x\} \tag{11.19}$$

become equivalent for x a positive or negative integer. We can always choose x to give $\lambda_n = 0$ and hence it suffices for $SU(n)$ to label inequivalent irreducible representations of $SU(n)$ by partitions into at most $n-1$ non-zero parts. Thus under $U(3) \rightarrow SU(3)$ we have $\{321\} \rightarrow \{21\}$.

■ 11.7 Characters of $U(n)$

The character of an irreducible representation $\{\lambda\}$ may be shown to be the S–function $s_\lambda(\epsilon_1, \ldots, \epsilon_n)$ where the $\epsilon_1, \ldots, \epsilon_n$ are the eigenvalues of the unitary transformation matrices. Note that the characters satisfy

$$\{\lambda_1 + x, \lambda_2 + x, \ldots, \lambda_n + x\} = (\epsilon_1 \ldots \epsilon_n)^x \{\lambda_1, \lambda_2, \ldots, \lambda_n\} \tag{11.20}$$

■ 11.8 Degeneracy Group of the Isotropic Harmonic Oscillator

Let us introduce nine operators

$$T_{ij} = \frac{1}{2}\{a_i^\dagger, a_j\} \qquad (i, j = 1, 2, 3) \tag{11.21}$$

where $\{a, b\} \equiv ab + ba$. Using the basic boson commutation relations of Eqn. (11.4) we find

$$[T_{ij}, T_{rs}] = \delta_{jr} T_{is} - \delta_{is} T_{rj} \tag{11.22}$$

Thus the nine operators T_{ij} close under commutation and generate a Lie algebra. Putting $H_i \equiv T_{ii}$ (do not confuse this with the Hamiltonian) we find the three H_i form a self-commuting set and

$$[H_i, T_{jr}] = (\delta_{ij} - \delta_{ir})T_{jr} \tag{11.23}$$

all the roots are of the form $e_i - e_j$ where the e are mutually orthogonal unit vectors.

The set of nine operators T_{ij} may be identified as the generators of the unitary group in three dimensions, $U(3)$. The Hamiltonian H is related to the H_i of Eqn. (11.23) via

$$H = H_1 + H_2 + H_3 \tag{11.24}$$

commutes with all T_{ij}. The three operators

$$H' = H_i - \frac{H}{3} \tag{11.25}$$

taken with the $T_{ij} \quad (i \neq j)$ can be taken as the generators of the special unitary group $SU(3)$ if we remember that since $\sum_i H_i' = 0$ the H_i' are not linearly independent. For reasons that will become apparent shortly we refer to $U(3)$ as the degeneracy group of the isotropic harmonic oscillator.

■ 11.9 Labelling Representations and Weights

In the case of the angular momentum group $SO(3)$ we label the angular momentum states as $|JM\rangle$ where M is the eigenvalue of J_z with J being the *highest weight* of M. This idea carries over to Lie groups in general. We recall that in the case of $SO(3)$ we can write the defining commutation relations as

$$[J_z, J_\pm] = \pm L_\pm \qquad [J_+, J_-] = J_z \tag{11.26}$$

with

$$J_\pm = \frac{1}{\sqrt{(2)}}(J_x \pm iJ_y) \tag{11.27}$$

For a general semisimple Lie algebra of rank ℓ we have ℓ operators ,$H_i \quad (i = 1, \ldots, \ell)$, that commute among themselves. The Lie algebra can be cast into the standard Cartan-Weyl form as

$$\begin{aligned}
[H_i, H_j] &= 0 \qquad (i, j = 1, \ldots \ell) \\
[H_i, E_\alpha] &= \alpha_i E_\alpha \\
[E_\alpha, E_\beta] &= N_{\alpha\beta} E_{\alpha+\beta} \\
[E_\alpha, E_{-\alpha}] &= \alpha^i H_i
\end{aligned} \tag{11.28}$$

where the E_α are the analogues of the ladder operators $J_\pm$ of SO_3.

Just as in SO_3 we distinguish the components of a representation by the eigenvalues of J_z for a Lie group we may label the components of a representation by the eigenvalues of the ℓ self-commuting operators H_i. For any compact Lie algebra the *highest* weight vector is unique and hence can be used to specify the representation. Consider for example, the group $U(3)$ which has three self-commuting operators H_i. Suppose we wish to determine the representation of $U(3)$ whose components are the annihilation a and creation operators $a^\dagger$, we have

$$[H_i, a_j^\dagger] = \delta_{ij} a_j^\dagger \quad \text{and} \quad [H_i, a_j] = -\delta_{ij} a_j \tag{11.29}$$

Thus the components of $a^\dagger$ give rise to the set of weight vectors $(100), (010), (001)$. The highest weight vector is (100) and hence we can label the representation as $\{100\}$ of $U(3)$. Likewise, the components of a give rise to the weight vectors $(-100), (0-10), (00-1)$. We say that a weight vector w is higher than a weight vector w' if the first component of their difference $w - w'$ is *positive*. Thus the highest weight for a is $(00-1)$ and the representation of $U(3)$ spanned by the components of a may be labelled as $\{00-1\}$ which is *contragredient* to $\{100\}$.

■ Exercises

11.1 Noting Eqn(11.22) show that the nine operators T_{ij} are associated with the nine weight vectors (000), (000), (000), (1-10), (10-1), (01-1), (-110), (-101), (0-11).

11.2 Determine the highest weight vector in the above set of weight vectors.

11.3 Repeat the above analysis for a two-dimensional isotropic harmonic oscillator and show that the relevant symmetry group is $U(2)$.

■ 11.10 Rotational Symmetry and the Isotropic Harmonic Oscillator

The harmonic oscillator Hamiltonian, Eqn. (11.1), commutes with all the components of the angular momentum operator

$$L = rxp = iaxa^\dagger \tag{11.30}$$

and hence H is rotationally invariant. The components of L form under commutation the Lie algebra associated with the group $SO(3)$. Noting the definition of the operators T_{ij}, Eqn.(11.21), and Eqn. (11.30) we have

$$L_1 = -i(T_{23} - T32), \quad L_2 = -i(T_{31} - T_{13}), \quad L_3 = -i(T_{12} - T_{21}) \tag{11.31}$$

We may choose L_3 as the generator of the group $SO(2)$ and hence for the three-dimensional isotropic harmonic oscillator we have the group structure

$$U(3) \supset SU(3) \supset SO(3) \supset SO(2) \tag{11.32}$$

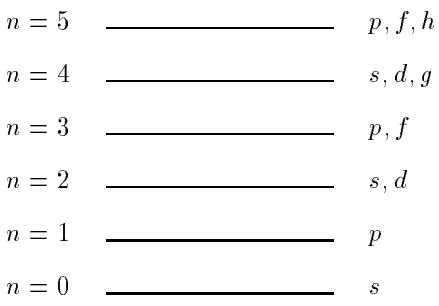
It is convenient to label the oscillator states in a basis $|n\ell m\rangle$ where $n = 0, 1, 2, \ldots$. From Lecture 10 we have

$$n = 2x + \ell \qquad \text{with} \quad x = 0, 1, 2, \ldots \tag{11.33}$$

and hence the values of ℓ associated with a given value of n are

$$\begin{aligned} \ell &= 1, 3, 5, \ldots, n \qquad n \quad odd \\ &= 0, 2, 4, \ldots, n \qquad n \quad even \end{aligned} \tag{11.34}$$

and thus for a given n there is a set of $\frac{(n+1)(n+2)}{2}$-fold degenerate states $|n\ell m\rangle$. This is precisely the dimension of the symmetric representation of $U(3)$ designated by the partition $\{n, 0, 0\}$ and hence the statement that the group $U(3)$ is the *degeneracy group* of the three-dimensional isotropic harmonic oscillator.



The first six levels of the isotropic harmonic oscillator

In the preceding we have developed the theory for a *single* particle in a harmonic oscillator potential. This particle could equally well be a nucleon as in nuclear physics or an electron in a quantum dot. The degeneracies are exactly the same as is the form of the energy spectrum. To proceed further requires we develop a many-particle model for particles interacting in a harmonic oscillator potential. To that end we may seek to develop a *dynamical group* which is the subject of the next lecture.

The Application of Symmetry Concepts to Physical Problems II

B. G. Wybourne

Ah, he thought, the truth bursting on him suddenly, nobody grows up. Everyone carries around all the selves that they have ever been, intact, waiting to be activated in moments of pain, of fear, of danger. Everything is retrievable, every shock, every hurt. But perhaps it becomes a duty to abandon the stock of time that carries within oneself, to discard it in favour of the present, so that one's embrace may be turned outwards to the world in which one has made one's home (page 210)

— Anita Brookner, *Latecomers*

- **Lecture 12**
- **12.1 A Hamiltonian for Quantum Dots**

Experimentally the electrons of a quantum dot are contained in a parabolic potential and hence we expect a close relationship with a many-electron system subject to a harmonic oscillator potential. The interaction potential $V(r_i, r_j)$ between particles i and j moving in a two-dimensional confining potential in the $x-y$ plane is taken to saturate at small particle separations and to decrease quadratically with increasing separation. In free space we would expect the interaction between two electrons to vary as $|r_i - r_j|^{-1}$. In a quantum dot the form of $V(r_i, r_j)$ is modified by the presence of image charges. The wavefunctions of the electrons confined in the quantum dots have a small but finite extent in the z–direction perpendicular to the $x-y$ plane. This results in a smearing of the electron charges along the z–direction. As a result the interparticle repulsion tends to saturate at small distances. This suggests choosing the interaction as

$$V(r_i, r_j) = 2V_0 - \frac{1}{2}m^*\Omega^2|r_i - r_j|^2 \tag{12.1}$$

where m^* is the electron effective mass and V_0 and Ω are positive parameters. Consider an N–electron quantum dot each with a charge $-e$, a g–factor g^*, spatial coordinates r_i and spin components $s_{z,i}$ along the z–axis. Suppose there

is a magnetic field B along the z–axis. The spatial part of the Hamiltonian can be written as

$$H_{space} = \frac{1}{2m^*}\sum_i \left[p_i + \frac{eA_i}{c}\right]^2 + \frac{1}{2}m^*\omega_0^2 \sum_i |r_i|^2 + \sum_{i<j} V(r_i, r_j) \tag{12.2}$$

and the spin part as

$$H_{spin} = -g^*\mu_B B \sum_i s_{z,i} \tag{12.3}$$

where the momentum and vector potential associated with the $i-th$ electron are given by

$$p_i = (p_{x,i}, p_{y,i}) \qquad A_i = (A_{x,i}, A_{y,i}) \tag{12.4}$$

and μ_B is the Bohr magneton.

The eigenstates of H will involve the product of the spatial and spin eigenstates obtained from $H_{spatial}$ and H_{spin}. The total spin projection $S_Z = \sum_i s_{z,i}$ will be a good quantum number. Choosing a circular gauge $A_i = B(-y_i/2, x_i/2, 0)$ Eqn. (12.2) becomes

$$H_{space} = \frac{1}{2m^*}\sum_i p_i^2 + \frac{1}{2}m^*\omega_0^2(B)\sum_i |r_i|^2 + \sum_{i<j}\left[2V_0 - \frac{1}{2}m^*\Omega^2|r_i, r_j|^2\right] + \frac{\omega_c}{2}\sum_i L_{z,i} \tag{12.5}$$

where $\omega_0^2(B) = \omega_0^2 + \omega_c^2/4$ and $\omega_c = eB/m^*c$.

■ 12.2 Note on Commutators and Second-quantisation

In much that follows we will need to be able to manipulate bosonic annihilation (a_i) and creation operators ($a_i^\dagger$). The basic bosonic commutation relations are

$$[a_i, a_j] = 0, \qquad [a_i^\dagger, a_j^\dagger] = 0, \qquad [a_i, a_j^\dagger] = \delta_{i,j} \tag{12.6}$$

These can be used to simplify expressions. As an example, consider the anti-commutator $\{a_i^\dagger, a_j\} = a_i^\dagger a_j + a_j a_i^\dagger$ and let us evaluate the commutator $[\{a_i^\dagger, a_j\}, a_k]$. Expanding out we have

$$[a_i^\dagger a_j + a_j a_i^\dagger, a_k] = [a_i^\dagger a_j\,, a_k] + [a_j a_i^\dagger, a_k] \tag{12.7}$$

Expanding out the first commutator we have

$$[a_i^\dagger a_j\,, a_k] = a_i^\dagger a_j a_k - a_k a_i^\dagger a_j \tag{12.8}$$

To simplify this commutator we want to try to rearrange the first term on the right-hand-side to cancel the second term. Using the first commutator in

Eqno. (12.6) we can rearrange the first term as

$$a_i^\dagger a_j a_k \rightarrow a_i^\dagger a_k a_j \tag{12.9}$$

and hence the right-hand-side of Eqn. (12.9) becomes

$$\begin{aligned} a_i^\dagger a_j a_k - a_k a_i^\dagger a_j &\rightarrow a_i^\dagger a_k a_j - a_k a_i^\dagger a_j \\ &= [a_i^\dagger, a_k] a_j \\ &= -[a_k, a_i^\dagger] a_j \\ &= -\delta_{i,k} a_j \end{aligned}$$

■ Exercise

Show that if

$$T_{ij} = \frac{1}{2}\{a_i^\dagger, a_j\}$$

then

$$[T_{ij}, T_{rs}] = \delta_{j,r} T_{is} - \delta_{i,s} T_{rj}$$

■ 12.3 The Degeneracy Group for Mesoscopic Systems

In this lecture we enlarge the concept of a *degeneracy* group to a *dynamical* group. The degeneracy group for the isotropic harmonic oscillator was found to be $SU(3)$. Each irreducible representation $\{n00\}$ is spanned by a set of $\frac{(n+1)(n+2)}{2}$ eigenstates of the Hamiltonian and associated with the *same* energy eigenvalue E_n of the harmonic oscillator. There is one weight vector for every eigenstate. The algebra of the degeneracy group contains a set of operators that allow us to start from any eigenstate and ladder through the entire set of degenerate eigenstates associated with a given degenerate eigenvalue. Thus the angular momentum ladder operators $L_\pm$ take us from one $|\alpha LM\rangle$ eigenstate to another $|\alpha LM \pm 1\rangle$ but leaving L fixed. The operators $L_z, L_\pm$ that generate the angular momentum group SO_3 but cannot take us from states belonging to one irreducible representation of SO_3 to another. To do that we must use the operators contained in the degeneracy algebra that lie outside of those of the angular momentum algebra. In addition the algebra of the degeneracy group contains operators that allow us to ladder between states of a given $SU(3)$ multiplet changing *both* L and M quantum numbers but *not* n. These additional operators reflect the fact that the isotropic harmonic oscillator has, like the H–atom, symmetry higher that just rotational symmetry.

■ 12.4 A Dynamical Group

We seek a *dynamical* group that contains the degeneracy group as a subgroup and has the energy eigenstates belonging to a single irreducible representation. Such a group contains among its generators operators that allow one to ladder between different irreducible representations of the degeneracy group. The degeneracy group contains an infinite set of finite dimensional unitary irreducible representations and hence the dynamical group must necessarily be a non-compact group with infinite dimensional unitary irreducible representations . We now construct the dynamical group for mesoscopic quantum systems.

■ 12.5 The Dynamical Group for Mesoscopic Quantum Systems

1. Assume the Hamiltonian of the $N-$particle system is a function of coordinate and momentum operators of the individual particles.
2. Designate the coordinates of the $r-$th particle by x_{ri} with $r = 1, \ldots, N$ and the momentum by p_{ri} with $i = 1, \ldots, d$.
3. The associated operators X_{ri} and P_{ri} obey the usual Heisenberg commutation relations (We choose units such that $\hbar = 1$)

$$[X_{ri}, X_{sj}] = 0, [X_{ri}, P_{sj}] = i\delta_{rs}\delta_{ij}, [P_{ri}, P_{sj}] = 0 \tag{12.10}$$

4. The $(2Nd)^2$ bilinear operators

$$\{X_{ri}X_{sj}, X_{ri}P_{sj}, P_{ri}X_{sj}, P_{ri}P_{sj}\} \tag{12.11}$$

close under commutation. However, only
$(2Nd+1)Nd$ of these operators are independent since

$$P_{ri}X_{sj} = X_{sj}P_{ri} - i\delta_{rs}\delta_{ij} \tag{12.12}$$

5. Consider the $(2Nd+1)Nd$ independent operators

$$Q_{risj} = \frac{1}{2}\{X_{ri}, X_{sj}\}, \quad V_{risj} = \frac{1}{2}\{X_{ri}, P_{sj}\},$$
$$K_{risj} = \frac{1}{2}\{P_{ri}, P_{sj}\} \tag{12.13}$$

They close under commutation on the non-
compact Lie algebra $Sp(2Nd, R)$ which we can take as the dynamical algebra of our mesoscopic $N-$ electron system.

■ 12.6 Subalgebras of the Dynamical Algebra

1. **We can construct subalgebras of $Sp(2Nd,R$ by forming subsets of the defining generators that close under commutation. Thus, for example, the V's close under commutation forming the elements of the $GL(Nd,R)$ algebra.**

2. **Contracting on particle or spatial indices can yield further Lie subalgebras. Thus the two sets of operators (summing on repeated indices)**

$$\begin{aligned} Q_{ij} &= X_{ri}X_{rj}, \quad L_{ij} = X_{ri}P_{rj} - X_{rj}P_{ri}, \\ K_{ij} &= P_{ri}P_{rj} \\ T_{ij} &= \frac{1}{2}(X_{ri}P_{rj} + X_{rj}P_{ri} + P_{ri}X_{rj} + P_{rj}X_{ri}) \end{aligned} \tag{12.14}$$

and

$$\begin{aligned} Q_{rs} &= X_{ri}X_{si}, \quad L_{rs} = X_{ri}P_{si} - X_{si}P_{ri}, \\ K_{rs} &= P_{ri}P_{si} \\ T_{rs} &= \frac{1}{2}(X_{ri}P_{si} + X_{si}P_{ri} + P_{ri}X_{si} + P_{si}X_{ri}) \end{aligned} \tag{12.15}$$

close under commutation and separately generate the Lie algebras $Sp(2d,R)$ and $Sp(2N,R)$.

3. **The above two algebras do not commute but the subsets $\{L_{ij}\}$ and $\{L_{rs}\}$ do separately close under commutation with**

$$\begin{aligned} [L_{ij}\,, L_{kl}] &= i(L_{ik}\delta_{jl} - L_{il}\delta_{jk} + L_{jk}\delta_{il} + L_{jk}\delta_{il} - L_{jl}\delta_{ik}) \\ [L_{rs}\,, L_{tu}] &= i(L_{rt}\delta_{su} - L_{ru}\delta_{st} + L_{st}\delta_{ru} - L_{su}\delta_{rt}) \end{aligned} \tag{12.16}$$

and form the generators of the subalgebras $O(d)$ and $O(N)$.

4. **Continuing we are led to the following possible Lie subalgebras of $Sp(2Nd,R)$:-**

$$\begin{aligned} Sp(2,R) \times O(Nd) &\supset Sp(2,R) \times O(N) \times O(d) \\ &\supset U(1) \times O(N) \times O(d) \end{aligned} \tag{12.17}$$

$$Sp(2N,R) \times O(d) \supset U(N) \times O(d) \supset U(1) \times O(N) \times O(d) \tag{12.18}$$

$$Sp(2d) \times O(N) \supset U(d) \times O(N) \supset U(1) \times O(d) \times O(N) \tag{12.19}$$

$$U(Nd) \supset U(N) \times U(d) \supset U(1) \times O(N) \times O(d) \tag{12.20}$$

Note the separation of the spatial and particle dependencies.

■ 12.7 Identification of the $Sp(2,R)$ Subgroup

Let us introduce three operators defined by

$$Q = X_{ri}X_{ri}, \quad T = X_{ri}P_{ri} + P_{ri}X_{ri}, \quad K = P_{ri}P_{ri} \tag{12.21}$$

and having the non-zero commutation relations

$$[Q, K] = 2iT, \quad [Q, T] = 4iQ, \quad [K, T] = -4iK \tag{12.21}$$

These commutation relations are those of a three element Lie algebra. Let us first decide if the algebra is compact or non-compact. This we may do by calculating the metric tensor

$$g_{ij} = c^t_{ik}c^k_{jt} \tag{12.22}$$

where the c^t_{ik} are the structure constants of the Lie algebra. Noting Eqn. (12.21) we have

$$c^T_{QK} = 2i, \quad c^Q_{QT} = 4i, \quad c^K_{KT} = -4i \tag{12.23}$$

Recall that the structure constants are antisymmetric. We now find for the diagonal elements of the metric tensor

$$\begin{aligned} g_{QQ} &= g_{KK} = 0 \\ g_{TT} &= c^Q_{TQ}c^Q_{TQ} + c^K_{TK}c^K_{TK} = -4i \times -4i + 4i \times 4i = -32 \end{aligned} \tag{12.24}$$

In addition we have the off-diagonal elements

$$g_{QK} = g_{KQ} = c^Q_{QT}c^T_{KQ} + c^T_{QK}c^K_{KT} = 4i \times -2i + 2i \times -4i = 16 \tag{12.25}$$

and thus the complete metric tensor is represented by the matrix

$$[g_{ij}] = \begin{array}{c} \\ Q \\ K \\ T \end{array} \begin{array}{c} \begin{array}{ccc} Q & K & T \end{array} \\ \begin{pmatrix} 0 & 16 & 0 \\ 16 & 0 & 0 \\ 0 & 0 & -32 \end{pmatrix} \end{array} \tag{12.26}$$

We can produce a diagonal metric tensor by putting

$$A_\pm = \frac{1}{\sqrt{2}}(Q \pm K) \tag{12.27}$$

to give the Lie algebra as

$$[A_\pm, T] = 4iA_\mp, \qquad [A_+, A_-] = 2iT \tag{12.28}$$

and the metric tensor as

$$[g_{ij}] = \begin{array}{c} \\ A_+ \\ A_- \\ T \end{array} \begin{array}{c} \begin{array}{ccc} A_+ & A_- & T \end{array} \\ \begin{pmatrix} -16 & 0 & 0 \\ 0 & +16 & 0 \\ 0 & 0 & -32 \end{pmatrix} \end{array} \tag{12.29}$$

We first note that the metric tensor has $det\,|g_{ij}|\ \not 0$ and hence we can conclude that the Lie algebra is semisimple. Furthermore the metric tensor is indefinite as required for the algebra to correspond to be non-compact. and hence our Lie algebra is necessarily

$$SO(2,1) \sim Sp(2,R) \tag{12.30}$$

■ 12.8 Back to the Quantum Dot Hamiltonian

We can express terms in the Hamiltonian of an isotropic harmonic oscillator

$$H_o = \frac{1}{2m} P_{ri} P_{ri} + \frac{m\omega^2}{2} X_{ri} X_{ri} \tag{12.31}$$

in terms of the group generators of $Sp(2,R)$ by noting that

$$\frac{1}{2m} P_{ri} P_{ri} = \frac{1}{2m} K \tag{12.31}$$

and

$$\frac{m\omega^2}{2} X_{ri} X_{ri} = \frac{m\omega^2}{2} Q \tag{12.32}$$

to give

$$H_o = \frac{1}{2m} K + \frac{m\omega^2}{2} Q \tag{12.33}$$

Now consider our earlier Hamiltonian

$$H_{space} = \frac{1}{2m^*} \sum_i p_i^2 + \frac{1}{2} m^* \omega_0^2(B) \sum_i |r_i|^2 + \sum_{i<j} \left[2V_0 - \frac{1}{2} m^* \Omega^2 |r_i, r_j|^2 \right] + \frac{\omega_c}{2} \sum_i L_{z,i} \tag{12.5}$$

We can write the electron-electron interaction term for an $N-$electron quantum dot as

$$N(N-1)V_0 - \frac{m\Omega^2}{4} \sum_{rsi} (X_{ri} - X_{si})(X_{ri} - X_{si})$$

leading to

$$H_{space} = \frac{1}{2m} K + \frac{m\Omega_0^2}{2} Q - \frac{eB}{4mc} L_{12} + N(N-1)V_0 + \frac{m\Omega^2}{2} \sum_{rs} Q_{rs} \tag{12.34}$$

with

$$\Omega_0^2 = \omega^2 + (\frac{eB}{2mc})^2 - N\Omega^2 \tag{12.35}$$

The significance of these results is that the first three terms in Eqno. **(12.34)** have been expressed in terms of the generators of $Sp(2,R)$ (K,Q) and $O(d)$ (L_{12})

and the last term in terms of generators of the group $Sp(2N, R)$. A practical calculation then involves the evaluation of matrix elements of the group generators in a harmonic oscillator basis.

The Application of Symmetry Concepts to Physical Problems II

B. G. Wybourne

I prefer the open landscape under a clear sky with its depth of perspective, where the wealth of sharply defined nearby details gradually fades away towards the horizon.
— H. Weyl, Classical Groups 1938

Lecture 13

13.1 Introduction

Today is the last lecture in this semester and I propose to first review where we have travelled this semester and outline where we will travel in the next semester. Our journey through symmetry physics is a journey without end. In this semester we have been looking at some of the tools required to exploit symmetry in physical problems. In the subject of finite groups we looked in some detail at the symmetric group leading into the theory of symmetric functions indexed by partitions of integers. The introduction of the pictorial representation of partitions in terms of Young frames led to the numbering of frames and a combinatorial definition of the Schur functions and the remarkable Littlewood-Richardson rule for multiplying Schur functions. These functions provided a link between the finite symmetric groups and the unitary groups, the Schur functions being the characters of the representations of the unitary group.

The representations and characters of the symmetric group, and other finite groups introduced the idea of the Kronecker product and its resolution into its irreducible components. The octahedral group $\mathcal{O}$, isomorphic to the symmetric group S_4 introduced the idea of broken symmetry and branching rules. Thus the symmetry of the sphere was broken down to the symmetry of the octahedron. The Wigner-Eckart theorem introduced the idea of *coupling coefficients* that contain completely the dependence of matrix elements on the

components of irreducible representations and the *reduced matrix elements* that are totally independent of the components of the irreducible representations appearing in the matrix elements. This is a powerful theorem that leads to practical results, a subject to be explored in more detail next semester.

The Lie algebras were defined and some of their properties explored. In particular we looked at their expression in terms of infinitesimal transformation operators introducing us to Lie groups. We looked at examples of both *compact* and *non-compact* Lie algebras with particular emphasis on the algebras associated with $so(3)$ and $so(2,1)$. Unitary representations in the former were found to be finite dimensional and in the latter infinite dimensional. This led us to the idea of spectrum generating Lie algebras and thence to degeneracy and dynamical groups culminating in and introduction to quantum dot applications.

■ 13.2 The Continuing Journey

To proceed further and to be able to get into practical applications we need to develop our subject further. Firstly we must be able to recognise particular varieties of Lie algebras. This requires that we make a systematic classification of the Lie algebras casting them into a standard form. We then need to look at the systematic description of the representations of Lie algebras and how one reduces from an algebra to a subalgebra in terms of branching rules. We can then return to the Wigner-Eckart theorem and introduce tensor operators which are the key to practical calculations. It is only then that we can expect to make applications to physical problems.

■ 13.3 The standard form of a Lie algebra

It is important to be able to transform a Lie algebra into some standard and recognisable form. To that end we seek a standard form for the commutators of the elements, X_τ, of a semisimple Lie algebra. Suppose A is an arbitrary linear combination of the X_τ such that

$$A = a^\mu X_\mu \tag{13.1}$$

Let X be another linear combination such that

$$X = b^\nu X_\nu \tag{13.2}$$

and

$$[A, X] = \rho X \tag{13.3}$$

This is the form of an eigenvalue equation with eigenvalue ρ and eigenvector X. In detail

$$a^\mu b^\nu c^\tau_{\mu\nu} X_\tau = \rho b^\tau X_\tau \tag{13.4}$$

The linear independence of X_τ requires that

$$(a^\mu c^\tau_{\mu\nu} - \rho\delta^\tau_\nu) b^\nu = 0 \tag{13.5}$$

and hence

$$det\,|a^\mu c^\tau_{\mu\nu} - \rho\delta^\tau_\nu| = 0 \tag{13.6}$$

For a lie algebra having r elements Eqno. (13.6) cannot have more than r roots. If A is chosen so that Eqno. (13.6) has the maximum number of distinct roots then Cartan has shown that for semisimple Lie algebras only $\rho = 0$ is degenerate. If the degeneracy is ℓ-fold then ℓ is called the *rank* of the semisimple Lie algebra.

The roots corresponding to $\rho = 0$ will be associated with ℓ linearly independent eigenvectors H_i spanning an ℓ-dimensional subspace of the r-dimensional root vector space. Thus

$$[A, H_i] = 0 \qquad (i = 1, \ldots, \ell) \tag{13.7}$$

The eigenvectors E_α associated with the remaining $r - \ell$ distinct roots will span a $(r - \ell)$-dimensional subspace of the r-dimensional root vector space and thus

$$[A, E_\alpha] = \alpha E_\alpha \tag{13.8}$$

Since A commutes with H_i we may write

$$A = \lambda^i H_i \tag{13.9}$$

Different Lie algebras are characterised by different root structures so we need to examine the properties of root vectors. to that end consider the commutator

$$\begin{aligned}
[A, [H_i, E_\alpha] &= [A, H E_\alpha] - [A, E_\alpha H_i] \\
&= [A, H]E_\alpha + H_i[A, E_\alpha] - [A, E_\alpha]H_i - E_\alpha[A, H_i] \\
&= \alpha[H_i, E_\alpha]
\end{aligned} \tag{13.10}$$

Thus if E_α is an eigenvector associated with the eigenvalue α there must be ℓ eigenvectors $[H_i, E_\alpha]$ belonging to the same eigenvalue. But the α are non-degenerate and hence the eigenvectors E_α must each be proportional to E_α

implying that

$$[H_i, E_\alpha] = \alpha_i E_\alpha \tag{13.11}$$

and hence that

$$c^\tau_{i\alpha} = \alpha_i \delta^\tau_\alpha \tag{13.12}$$

Noting Eqnos.(13.8), (13.9) and (13.11) we have

$$\alpha = \lambda^i \alpha_i \qquad (i = 1, \ldots, \ell) \tag{13.13}$$

and hence the α_i may be regarded as the covariant components of a vector α in an ℓ-dimensional space.

Consider the Jacobi identity

$$[A, [E_\alpha, E_\beta]] + [E_\alpha, [E_\beta, A]] + [E_\beta, [A, E_\alpha]] \tag{13.14}$$

Use of Eqno. (13.8) then gives

$$[A, [E_\alpha, E_\beta]] = (\alpha + \beta)[E_\alpha, E_\beta] \tag{13.15}$$

showing that the eigenvector $[E_\alpha, E_\beta]$ is associated with the root $\alpha + \beta$ if $\alpha + \beta$ is non-vanishing. If $\alpha = -\beta$ then $[E_\alpha, E_\beta]$ must be a linear combination of the H_i

$$[E_\alpha, E_{-\alpha}] = c^i_{\alpha,-\alpha} H_i \tag{13.16}$$

with $c^\tau_{\alpha\beta} = 0$ if $\tau \not= \alpha + \beta$. If $\alpha + \beta$ is a non-vanishing root then

$$\begin{aligned} [E_\alpha, E_\beta] &= N_{\alpha\beta} E_{\alpha+\beta} \\ &= c^{\alpha+\beta}_{\alpha\beta} E_{\alpha+\beta} \end{aligned} \tag{13.17}$$

We now establish an important property of roots:

Theorem 13.1

For every non-vanishing root α of a semisimple Lie algebra there is a root $-\alpha$

Proof

Recall the metric tensor

$$g_{\alpha\tau} = c^\mu_{\alpha\eta} c^\eta_{\tau\mu} \tag{13.18}$$

The summation over μ and η is restricted by Eqno. (13.12) and (13.16) and hence

$$g_{\alpha\tau} = c^\alpha_{\alpha\eta} c^\eta_{\tau\alpha} + c^\mu_{\alpha-\alpha} c^{-\alpha}_{\tau\mu} + \sum_{\beta\not=\alpha} c^{\alpha+\beta}_{\alpha\beta} c^\beta_{\alpha+\beta\tau} \tag{13.19}$$

But it follows from Eqno. (13.12) and (13.16) that each term can only exist if $\tau = -\alpha$ and hence

$$g_{\alpha\tau} = 0 \qquad \text{if} \quad \tau \not= -\alpha \tag{13.20}$$

Thus if $-\alpha$ is not a root then $det\,|g_{\alpha\tau}| = 0$ and Cartan's criterion for a semisimple Lie algebra is not satisfied.

■ 13.4 The Standard Cartan-Weyl Form

We are free to normalise the E_α of Eqno. (13.8) so that

$$g_{\alpha -\alpha} = 1 \tag{13.21}$$

We can order our basis so that

$$g_{ab} = \begin{pmatrix} g_{ik} & \vdots & & & & & & & & \\ - - - & - & - & - & - & - & - & - & - & - \\ & \vdots & 0 & & 1 & & & & & \\ & \vdots & 1 & & 0 & & & & & \\ & \vdots & & & & \cdots & & & & \\ & \vdots & & & & & & 0 & & 1 \\ & \vdots & & & & & & 1 & & 0 \end{pmatrix} \tag{13.21}$$

For a semisimple Lie algebra $det\,|g_{ab}| \not= 0$. Noting Eqno. (13.11) and (13.12) we have

$$g_{ik} = \sum_\alpha c^\alpha_{i\alpha} c^\alpha_{k\alpha} = \sum_\alpha \alpha_i \alpha_k \tag{13.22}$$

and hence g_{ik} may be used as a metric tensor for the ℓ-dimensional space spanned by the vectors α.

Recalling the antisymmetric tensor

$$c_{\sigma\mu\nu} = g_{\sigma\lambda} c^\lambda_{\mu\nu} \tag{13.23}$$

and

$$c^\lambda_{\sigma\tau} = g^{\lambda\rho} c_{\nu\sigma\tau} \tag{13.24}$$

we have

$$\begin{aligned} c^i_{\alpha -\alpha} &= g^{ik} c_{\alpha -\alpha k} \\ &= g^{ik} c_{k\alpha -\alpha} \\ &= g^{ik} c^\alpha_{k\alpha} \\ &= g^{ik} \alpha_k = \alpha^i \end{aligned} \tag{13.25}$$

since

$$c_{k\alpha-\alpha} = c^{\tau}_{k\alpha} g_{\tau-\alpha} \quad \text{and} \quad g_{\alpha-\alpha} = 1$$

and hence

$$[E_\alpha, E_{-\alpha}] = \alpha^i H_i \tag{13.26}$$

with the α^i being the contravariant components of the root vector α.

We can now write out the standard Cartan-Weyl form of a semisimple algebra as

$$[H_i, H_j] = 0 \quad (i, j = 1, \ldots, \ell) \tag{13.27a}$$

$$[H_i, E_\alpha] = \alpha_i E_\alpha \tag{13.27b}$$

$$[E_\alpha, E_\beta] = N_{\alpha\beta} E_{\alpha+\beta} \quad \text{(if } \alpha + \beta \not\emptyset) \tag{13.27c}$$

$$[E_\alpha, E_{-\alpha}] = \alpha^i H_i \tag{13.27d}$$

Note that Eqno(13.27a) amounts to constructing from the elements ■ **13.5 Example of so_3**

The Lie algebra of the rotation group, SO_3, may be defined in terms of the standard commutation relation

$$[L_i, L_j] = i\varepsilon_{ijk} L_k \tag{13.28}$$

Or in terms of the ladder operators $L_1 \pm iL_2$ as

$$[L_3, L_\pm] = \pm L_\pm, \quad [L_+, L_-] = 2L_3 \tag{13.29}$$

To place the algebra in the Cartan-Weyl form we choose

$$H_1 = L_3, \quad E_\pm = \frac{1}{\sqrt{2}} L_\pm \tag{13.30}$$

to give

$$[H_1, H_1] = 0, \quad [H_1, E_\pm] = \pm E_, \quad [E_+, E_-] = H_1 \tag{13.31}$$

To proceed to the classification of the semisimple Lie Algebras we need to first consider some further properties of root vectors and then develop a graphical representation of root vectors to finally a complete classification in terms of Coxeter-Dynkin diagrams, but that must await future lectures.