Continuous Symmetries in Physics

This course is a monographic series of lectures discussing examples of continuous symmetries in physics as opposed to discrete symmetries. The course will consist of one hour lectures in English with accompanying notes. The level will be appropriate to fifth year and graduate students and will assume a prior course in quantum mechanics. Among the subjects to be covered will be:-

1. Symmetries of the classical one-dimensional harmonic oscillator.
2. Second quantisation representation of the Lie groups $SO(3)$ and $SO(2,1)$.
3. Application to the calculation of the energy levels of hydrogenic atoms and harmonic oscillators.
4. Solutions for other potential forms. (eg. Morse, Davidson potentials etc.)
5. Non-compact groups and the n-dimensional harmonic oscillator.
6. $SO(4)$ models of doubly excited states of atoms.

I anticipate a maximum of eight students in which case the classes will take place in my office. The time of the initial meeting will be posted and will be subject to change if required to avoid clashes with other lectures. If you are interested in this course please see me in my office (Room 485) for further details.

B. G. Wybourne

Continuous Symmetries I.

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It has been rumoured that the "group pest" is gradually being cut out of quantum physics

—H. Weyl *The Theory of Groups and Quantum Mechanics, 1930*

We wish finally to make a few remarks concerning the place of the theory of groups in the study of the quantum mechanics of atomic spectra. The reader will have heard that this mathematical discipline is of great importance for the subject. We manage to get along without it.

— E. U. Condon and G. H. Shortley *Theory of Atomic Spectra, 1935*

Disclaimer

These notes are intended only as a guide and a summary of class discussions. They reflect my view that lectures should outline a path but that ultimately the student's main task is to learn to teach themselves and to become independent of the teacher. References are given to encourage independent study.

Symmetries of the Classical One-Dimensional Harmonic Oscillator

Introduction

These notes largely follow Wulfman and Wybourne[1] and references therein. The classical harmonic oscillator in one-dimension is a feature of most elementary physics courses. The motion is governed by one of the simplest differential equations encountered in physics courses. In appropriate units the Newtonian of Lagrange equation of motion is

$$\frac{d^2x}{dt^2} + x = 0, \quad or \quad \ddot{x} + x = 0 \tag{1}$$

Such a simple equation hides many symmetries associated with the one-dimensional harmonic oscillator(HO). If I translate the HO in time I find the form of the equation of motion is unchanged even though (x,t) have changed. View the HO though a magnifying glass and the period of the motion is unchanged, likewise make a movie of the HO filming on an appropriate curved surface and again the form of the motion is unchanged.

Clearly we need some procedure that will expose all the possible symmetries that leave the equation of motion *form invariant*. To that end we seek those infinitesimal transformations of the variables x,t that leave the equation of motion form invariant and hence interconvert its solutions. A general method was developed by Sophus Lie over a century ago[2] and takes us into the theory of group transformations. The key concept is that of *infinitesimal transformations* and in particular *point transformations*.

Infinitesimal Transformations

Here we are interested in transformations that carry a point (x,t) into a point (x',t') such that

$$x' = \Phi(x,t,a_0+\delta a) \qquad t' = \Psi(x,t,a_0+\delta a) \tag{2}$$

The quantity a is a *parameter* such that for the identity transformation $x = \Phi(x,t,a_0)$ and $t = \Psi(x,t,a_0)$. An infinitesimal transformation corresponds to a transformation that is infinitesimally close to to the identity. Thus the infinitesimal change in x and t due to an infinitesimal change δa in the parameter a is given by

$$\delta x = \xi \delta a \qquad \delta t = \eta \delta a \tag{3}$$

where

$$\xi = \xi(x,t) = \left(\frac{\partial \Phi}{\partial a}\right)_{a_0} \qquad \eta = \eta(x,t) = \left(\frac{\partial \Psi}{\partial a}\right)_{a_0} \tag{4}$$

If $f(x,t)$ is an analytic function of x,t then under an infinitesimal transformation

$$\delta f = U f \delta a \tag{5}$$

where

$$U = \xi \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial t} \tag{6}$$

The particular differential equation of interest, Eq.(1), is of second order and it is necessary to consider the second extension of the point transformation of Eq.(2). The infinitesimal operator U'' of the second extended transformation has been given by Lie[2] as

$$U'' = U + \xi' \frac{\partial}{\partial \dot{x}} + \xi'' \frac{\partial}{\partial \ddot{x}} \tag{7}$$

where

$$\xi' = \frac{\delta \dot{x}}{\delta a} = \frac{\partial \xi}{\partial t} + \left(\frac{\partial \xi}{\partial x} - \frac{\partial \eta}{\partial t}\right)\dot{x} - \left(\frac{\partial \eta}{\partial x}\right)\dot{x}^2 \tag{8}$$

and

$$\begin{aligned} \xi'' &= \frac{\delta \ddot{x}}{\delta a} \\ &= \frac{\partial^2 \xi}{\partial t^2} + \left(2\frac{\partial^2 \xi}{\partial x \partial t} - \frac{\partial^2 \eta}{\partial t^2}\right)\dot{x} + \left(\frac{\partial^2 \xi}{\partial x^2} - 2\frac{\partial^2 \eta}{\partial x \partial t}\right)\dot{x}^2 - \left(\frac{\partial^2 \eta}{\partial x^2}\right)\dot{x}^3 + \left(\frac{\partial \xi}{\partial x} - 2\frac{\partial \eta}{\partial t} - 3\dot{x}\frac{\partial \eta}{\partial x}\right)\ddot{x} \end{aligned} \tag{9}$$

Equations (7) to (9) look somewhat formidable, particularly as we are looking at one of the simplest of differential equations. This has lead to the development of many algebraic programmes for studying more complex differential equations[3].

Invariance of the Equation of Motion

The equation of motion (1) will be form invariant if and only if

$$U''(\ddot{x} + x) = 0 \qquad \text{whenever} \qquad \ddot{x} + x = 0 \tag{10}$$

which leads to the condition

$$\xi + \frac{\partial^2 \xi}{\partial t^2} - \left(\frac{\partial \xi}{\partial x} - 2\frac{\partial \eta}{\partial t}\right)x + \left(2\frac{\partial^2 \xi}{\partial x \partial t} - \frac{\partial^2 \eta}{\partial t^2} + 3x\frac{\partial \eta}{\partial x}\right)\dot{x} + \left(\frac{\partial^2 \xi}{\partial x^2} - 2\frac{\partial^2 \eta}{\partial x \partial t}\right)\dot{x}^2 - \left(\frac{\partial^2 \eta}{\partial x^2}\right)\dot{x}^3 = 0 \tag{11}$$

Our conditional equation must be satisfied for all values of the variables. This means that the following four equations must be satisfied:-

$$\frac{\partial^2 \eta}{\partial x^2} = 0 \tag{12a}$$

$$\frac{\partial^2 \xi}{\partial x^2} - 2\frac{\partial^2 \eta}{\partial x \partial t} = 0 \tag{12b}$$

$$2\frac{\partial^2 \xi}{\partial x \partial t} - \frac{\partial^2 \eta}{\partial t^2} + 3x\frac{\partial \eta}{\partial x} = 0 \tag{12c}$$

$$\xi + \frac{\partial^2 \xi}{\partial t^2} - x\frac{\partial \xi}{\partial x} + 2x\frac{\partial \eta}{\partial t} = 0 \tag{12d}$$

The above four equations can be integrated to give

$$U = \sum_{i=1}^{8} b_i X_i \tag{13}$$

where the b_i are integration constants and the X_i are a set of eight operators which we may take as

$$\begin{aligned}
X_1 &= (1+x^2)\sin t\frac{\partial}{\partial x} - x\cos t\frac{\partial}{\partial t}\\
X_2 &= (1-x^2)\sin t\frac{\partial}{\partial x} + x\cos t\frac{\partial}{\partial t}\\
X_3 &= (1+x^2)\cos t\frac{\partial}{\partial x} + x\sin t\frac{\partial}{\partial t}\\
X_4 &= (1-x^2)\cos t\frac{\partial}{\partial x} - x\sin t\frac{\partial}{\partial t}\\
X_5 &= \frac{\partial}{\partial t}\\
X_6 &= x\frac{\partial}{\partial x}\\
X_7 &= x\cos 2t\frac{\partial}{\partial x} + \sin 2t\frac{\partial}{\partial t}\\
X_8 &= -x\sin 2t\frac{\partial}{\partial x} + \cos 2t\frac{\partial}{\partial t}
\end{aligned} \tag{14}$$

Note that the above operators may be replaced by any linearly independent linear combination of them. We can exploit this freedom to choose a linear combination leading to a set of 8 operators that close under commutation to form a particular Lie algebra which we shall shortly identify.

The Commutators $[X_i, X_j]$

The eight infinitesimal operators close under commutation and thus should be associated with some Lie algebra. We have

$$[X_i, X_j] = c_{ij}^k X_k \quad i,j,k = 1,\ldots,8 \tag{15}$$

where the c_{ij}^k are known as the *structure constants* of the algebra.

Commutation relations of the Infinitesimal Operators X_i

X_i	X_j							
	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8
X_1	0	$X_7 - 3X_6$	X_5	X_8	$-X_3$	X_2	$-X_2$	$-X_8$
X_2	$-X_7 + 3X_6$	0	$-X_8$	$-X_5$	$-X_4$	X_1	$-X_1$	$-X_3$
X_3	$-X_5$	X_8	0	$-X_7 - 3X_6$	X_1	X_4	X_4	$-X_2$
X_4	$-X_8$	X_5	$X_7 + 3X_6$	0	X_2	X_3	X_3	$-X_1$
X_5	X_3	X_4	$-X_1$	$-X_2$	0	0	$2X_8$	$-2X_7$
X_6	$-X_2$	$-X_1$	$-X_4$	$-X_3$	0	0	0	0
X_7	X_2	X_1	$-X_4$	$-X_3$	$-2X_8$	0	0	$-2X_8$
X_8	X_4	X_3	X_2	X_1	$2X_7$	0	$2X_5$	0

(16)

Inspection of the above table of commutators shows that there is a non-trivial subalgebra involving the three infinitesimal operators $\{X_1, X_3, X_5\}$. **Commutation relations of the Three-paramter**

subalgebra

X_i		X_j	
	X_1	X_3	X_5
X_1	0	X_5	$-X_3$
X_3	$-X_5$	0	X_1
X_5	X_3	$-X_1$	0

(17)

Identification of the Lie Algebra

Let us define a *metric tensor*[4,5]

$$g_{ij} = c^m_{jk} c^k_{jm} \tag{18}$$

Using the structure constants given in Eq.(16) we find that g_{ij} is diagonal with

$$g_{ii} = \begin{cases} +12 & i = 2,4,7,8 \\ +\ 4 & i = 6 \\ -12 & i = 1,3,5 \end{cases} \tag{19}$$

Note that the metric tensor is indefinite allowing us to conclude that the Lie algebra is that of a Lie group that is *non-compact*[6]. Furthermore det g_ij $\emptyset$ and hence the algebra satisfies Cartan's requirement for a Lie algebra to be *semisimple*. To identify the algebra more closely we may cast the algebra into standard Cartan-Weyl form[4-6] by forming appropriate linear combinations of the X_i leading to the eight operators:-

$$\begin{aligned} H_1 &= (i/2)\tfrac{\partial}{\partial t} & H_2 &= \tfrac{1}{2}\sqrt{3}x\tfrac{\partial}{\partial x} \\ E_\alpha &= e^{-2it}\left(i\tfrac{\partial}{\partial t} + x\tfrac{\partial}{\partial x}\right) & E_{-\alpha} &= e^{2it}\left(i\tfrac{\partial}{\partial t} - x\tfrac{\partial}{\partial x}\right) \\ E_\beta &= e^{-it}\left(x^2\tfrac{\partial}{\partial x} + ix\tfrac{\partial}{\partial t}\right) & E_{-\beta} &= e^{it}\tfrac{\partial}{\partial x} \\ E_\gamma &= \tfrac{\partial}{\partial x} & E_{-\gamma} &= e^{it}\left(x^2\tfrac{\partial}{\partial x} - ix\tfrac{\partial}{\partial t}\right) \end{aligned} \tag{20}$$

The two $\{H_1, H_2\}$ form a maximal self-commuting set known as the Cartan subalgebra and verifies that the Lie algebra is of *rank* 2. The six *shift operators* are indexed by the *roots* $\pm\alpha, \pm\beta, \pm\gamma$ which are respectively

$$(\pm 1, 0), (\pm\frac{1}{2}, \pm\frac{1}{2}\sqrt{3}), (\pm\frac{1}{2}, \mp\frac{1}{2}\sqrt{3}) \tag{21}$$

This is precisely the root structure expected for the non-compact *real* form of Cartan's $\mathbf{A}_2$ algebra. In terms of Lie groups this gives two possible non-compact candidates, $SU(2,1)$ or $SL(3,R)$. Of these only $SL(3,R)$ contains the compact subgroup $SO(3)$.

The three operators $\{X_1, X_3, X_5\}$ form a compact subalgebra with a negative definite metric

$$g_{ij} = -2\delta_{ij} (i,j = 1,3,5) \tag{22}$$

which indeed may be identified with the Lie group $SO(3)$. Note that the complete identification requires consideration of the relevant parameter space [1].

Exercise

Evaluate the commutators $[H_i, E_m]$ and $[E_m, E_n]$ and verify Eq.(21).

Finite Transformations

Different linear combinations of the generators X_i are generators of different infinitesimal and finite transformations. The effect of a finite transformation may be determined either by exponentiation of the infinitesimal operaotrs or by integration of the system of differential equations

$$\frac{dx'}{\xi(x',t')} = \frac{dt'}{\eta(x',t')} = da \tag{23}$$

Thus we readily obtain for X_5

$$x' = x \qquad t' = t + a \tag{24}$$

allowing us to interpret X_5 as involving the invariance of the equation of motion, Eq.(1), with respect to time translations. This implies that if $f(t)$ is any solution of the equation of motion then

$$f(t - \pi) = f(t + \pi) \tag{25}$$

for any choice of t. The motion is cyclic with a period 2π and as far as the oscillator is concerned $t+2\pi = t$ which is why oscillators are used as clocks!

Likewise for X_6 we find for a finite transformation

$$x' = xe^a \qquad t' = t \tag{26}$$

involving the invariance of the equation of motion, Eq.(1), with respect to a change of spatial scale.

The remaining six operators lead to rather more obscure symmetries and we refer to[1] for details.

Concluding Remarks

Differential equations of many different forms occur in physics, such as in Maxwell's equations, Schrodinger's equation, Dirac's equation etc. It can be important to develop systematic methods for fully exploiting their symmetries. Here we have given a relatively simple example. Within the literature you should be able to find many other examples. The basic ideas are to first determine systematically the infinitesimal operators and then to investigate their commutation relations. Note that while in our example the number of operators was finite this need not always be the case. We next endeavour to cast the operators into a standard Cartan-Weyl form and identify the Lie algebra. We can then start to study the effects of finite transformations identifying possible Lie groups and bounds of the group parameters.

> *there are "far better prizes than taking away other people's provinces or lands, or grinding them down in exploitation. The empires of the future are the Empires of the Mind"*
> – Part of an address by Winston Churchill to Harvard University (1943)

References

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Continuous Symmetries II.

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You have heard it said no doubt about extremes resembling one another, certainly the North Pole and the South Pole are very far apart. But if you woke up to-morrow morning at one or the other you would not know which it was. There might be more penguins at one end of the world, and more polar bears at the other. But all around you would be ice and snow and the blast of freezing winds over vast dreary spaces.
—Winston Churchill *UNITED EUROPE May 9, 1948 Open-air Meeting in the Square, Amsterdam*

The Three-Parameter Lie Groups

Introduction

The three-parameter Lie groups and their associated Lie algebras are of considerable interest in physical application and form the prototype of more general Lie groups and algebras. The three-parameter group $SO(3)$ is well-known in the quantum theory of angular momentum, the covering group $SU(2)$ is of importance in discussing spin while the little Lorentz group $SO(2,1)$ is an example of an important class of non-compact Lie groups.

The Casimir Operator of $SO(3)$

The Lie algebra associated with $SO(3)$ involves the familiar three infinitesimal angular momentum operators $\{J_1, J_2, J_3\}$ which satisfies the commutation relations

$$[J_1, J_2] = iJ_3, \quad [J_2, J_3] = iJ_1, \quad [J_3, J_1] = iJ_2 \tag{1}$$

In terms of the traditional ladder operators we write

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

to yield the standard commutation relations

$$[J_+, J_-] = J_3 \quad \text{and} \quad [J_3, J_\pm] = \pm J_\pm \tag{3}$$

Note our ladder operators $J_\pm$ differ by a normalisation factor from the usual ladder operators of standard quantum theory of angular momentum. This has been done to cast the commutation relations in the standard Cartan-Weyl form.

The operator

$$\mathbf{J}^2 = J_1^2 + J_2^2 + J_3^2 = J_+J_- + J_-J_+ + J_3^2 \tag{4}$$

commutes with all the operators $\{J_\pm, J_3\}$ and is known as the *Casimir operator* for the group $SO(3)$. Our task now is to determine the eigenvalues of the operators $\{\mathbf{J}^2, J_3\}$. Let us label the *representations* of $SO(3)$ by the *eigenvalues* X of the Casimir operator $\mathbf{J}^2$. The *eigenvectors* $|Xa\rangle$ will be chosen to be simultaneous eigenvectors of $\{\mathbf{J}^2, J_3\}$ and will span the space of a particular representation. The eigenvalue pair $\{X, a\}$ label a particular eigenvector with a being referred to as its *weight*.

Since $\mathbf{J}^2$ is a sum of positive-definite Hermitian operators, it must itself be a positive-definite Hermitean operator. Thus for a *unitary* representation the eigenvalues of $\mathbf{J}^2$ must be real and positive. Thus

$$\mathbf{J}^2|Xa\rangle = X|Xa\rangle \quad (X \geq 0, X \in \Re) \tag{5}$$

$$J_3|Xa\rangle = a|Xa\rangle \quad (a \in \Re) \tag{6}$$

Noting Eq.(4) and Eq.(5) we can write

$$2J_+J_- = \mathbf{J}^2 - J_3(J_3-1) \quad \text{and} \quad 2J_-J_+ = \mathbf{J}^2 - J_3(J_3+1) \tag{7}$$

and hence

$$2J_+J_-|Xa\rangle = [X - a(a+1)]\,|Xa\rangle \tag{8}$$
$$2J_-J_+|Xa\rangle = [X - a(a-1)]\,|Xa\rangle \tag{9}$$

For a unitary representation we must have

$$J_+^\dagger = J_- \tag{10}$$

and hence the eigenvalues of J_+J_- or J_-J_+ must be positive definite and hence from (8) and (9) we must have for a unitary representation

$$X - a(a \pm 1) \geq 0 \tag{11}$$

The commutation relations in (3) then lead to

$$\langle Xa'|[J_3, J_+]|Xa\rangle = (a'-a)\langle Xa'|J_+|Xa\rangle = \langle Xa'|J_+|Xa\rangle \tag{12}$$

and hence successive eigenvalues a of J_3 must differ by unity, that is

$$a' - a = 1 \tag{13}$$

We now determine the range of a. Eq.(11) will only be satisfied with real values of X and a if a has an upper positive bound a_+ and a lower negative bound a_-, with $a_+ - a_-$ an integer. Solving for a_+ and a_- in Eq. (11) gives

$$a_\pm = -\frac{1}{2} \mp \frac{1}{2}\sqrt{1+4X} \tag{14}$$

and hence

$$X = a_+(a_+ + 1) \quad \text{and} \quad a_- = -a_+ - 1 \tag{15}$$

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

To establish contact with the usual angular momentum notation let us put $j = a_+$ and replace a by m and label our eigenvectors as $|jm\rangle$ where

$$m = j, j-1, \ldots, -j+1, -j \tag{16}$$

The range of m is bounded from above *and* below and hence the unitary representations of $SO(3)$ are of finite dimension $(2j+1)$. Then

$$\mathbf{J}^2|jm\rangle = j(j+1)|jm\rangle \tag{17a}$$
$$J_3|jm\rangle = m|jm\rangle \tag{17b}$$
$$J_\pm|jm\rangle = \frac{1}{\sqrt{2}}\sqrt{j(j+1) - m(m\pm 1)}|jm\pm 1\rangle \tag{17c}$$

Note that the arbitrary phase factor in (17c) has been chosen to be positive. The representations with integer j are the commonly termed the *true* or *ordinary* representations of $SO(3)$ while those involving half odd integer values of j are termed *spin* representations.

The non-compact Lie group $SO(2,1)$

By changing just the sign of one of the commutators in Eq. (1) we obtain a dramatic change in the properties of the Lie algebra. Thus we write

$$[J_1, J_2] = -J_3, \quad [J_2, J_3] = iJ_1, \quad [J_3, J_1] = iJ_2 \tag{18}$$

and again write

$$J_\pm = \frac{1}{\sqrt{2}}(J_1 \pm iJ_2) \tag{19}$$

to yield

$$[J_+, J_-] = J_3 \quad \text{and} \quad [J_3, J_\pm] = \pm J_\pm \tag{20}$$

which is precisely the form of Eq. (3). However, the Casimir operator is now

$$\mathbf{J}^2 = J_1^2 + J_2^2 - J_3^2 = -J_+J_- - J_-J_+ - J_3^2 \tag{21}$$

Note that the Casimir operator is no longer a sum of positive definite Hermitian operators and hence its eigenvalues X may range over the domain of real positive and negative numbers. Again we write

$$\mathbf{J}^2|Xa\rangle = X|Xa\rangle \quad (X \geq 0, X \in \Re) \tag{5}$$

$$J_3|Xa\rangle = a|Xa\rangle \quad (a \in \Re) \tag{22}$$

where $|Xa\rangle$ is a simultaneous eigenvector of $\mathbf{J}^2$ and J_3. Since for unitary representations of $SO(2,1)$ we must have

$$J_+^\dagger = -J_- \tag{23}$$

it follows that the eigenvalues of J_+J_- and J_-J_+ must be real and negative definite it follows from (22) that necessarily

$$X + a(a \pm 1) \geq 0 \tag{24}$$

A complete classification of the unitary representations of $SO(2,1)$ follows from a determination of the real values of X and a that satisfy (24). The representations may be divided into two distinct series, a *continuous series* C associated with continuous eigenvalues of $\mathbf{J}^2$ and a *discrete series* D associated with discrete eigenvalues of $\mathbf{J}^2$. The $SO(2)$ content of these representations follows directly from consideration of (24) to yield:-

The Continuous Series

(a) $0 < X < \infty$. Here we have $X + a(a \pm 1) \geq 0$ for all

$$a = 0, \pm 1, \pm 2, \ldots \tag{25a}$$

and the representations C_X^0 are unbounded from above and below.

(b) $\frac{1}{4} < X < \infty$. Here we have $X + (a(a \pm 1) > 0$ for all

$$a = \pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}, \ldots \tag{25b}$$

and the representations $C_X^{\frac{1}{2}}$ are unbounded from above and below.

Discrete Series

In these cases the eigenvalues of X may all be written in the form $k(1-k)$ where k is a positive integer or half odd integer. Eq. (24) then shows that a has either an upper bound with no lower bound or a lower bound with no upper bound. Thus we have the following two cases:-

(1) D_k^+. Here $X = k(1-k)$ with

$$k = \frac{1}{2}, 1, \frac{3}{2}, \ldots$$

and

$$a = k, k+1, k+2, \ldots \tag{26b}$$

(2) D_k^-. Again $X = k(1-k)$ with

$$k = \frac{1}{2}, 1, \frac{3}{2}, \ldots$$

but now

$$a = -k, -(k+1), -(k+2), \ldots \tag{26b}$$

Note that whereas for $SO(3)$ every unitary irreducible representation is uniquely labelled by an eigenvalue of the Casimir operator, in the case of $SO(2,1)$ different unitary irreducible representations may have the same Casimir operator eigenvalue. These representations are distinguished by their different J_3 eigenvalue spectrum. Whereas the unitary irreducible representations of $SO(3)$ are all of finite dimension those of $SO(2,1)$ are all of infinite dimension. In the preceding we chose to diagonalise the *compact* operator J_3 which generates an $SO(2)$ subgroup. Had we chosen to diagonalise one of the *non-compact* generators J_1 or J_2 that correspond to the non-compact group $SO(1,1)$ we would be led to a continuous, rather than discrete, basis.

The discrete series can be regarded as forming infinite towers of states with each tower being characterised by either a lower bound and no upper bound, the positive discrete series, or an upper bound and no lower bound, the negative discrete series. The complete set of states of a given discrete series or tower is associated with a single Casimir operator eigenvalue whereas the eigenvalues of the generator J_3 change in steps of unity. The ladder operators allow us to move up or down a tower in steps of unity, either terminating with the upper or lower bound or advancing along the series without limit.

In the next lecture we shall apply our knowledge of the eigenvalues of the Casimir operator and the spectrum of the generators of the locally isomorphic $su(1,1) \sim so(2,1) \sim sp(2,R)$ Lie algebras to solve the energy eigenvalues of a number of traditional problems in quantum physics.

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Continuous Symmetries III.

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Some Applications of $SO(2,1) \sim SU(1,1)$

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*

Introduction

The Lie algebras associated with the non-compact groups give a simple method for generating the energy eigenvalues associated with a number of solvable problems in quantum mechanics. Here we outline some of the ideas of *spectrum generating algebras* for second-order differential equations. This is closely related to the shift operator method of Infeld and Hull[1].

$su(1,1)$ and Second-Order Differential Equations

Many of the textbook problems in courses in quantum physics can be cast as a second-order differential equation

$$\frac{d^2Y}{dy^2} + f(y)Y = 0 \tag{1}$$

where $Y = Y(y)$. The key idea is to try to represent the equation in terms of the generators of a Lie group and then to determine the spectrum associated with the equation in terms of the known spectrum of the group generators.

The Lie algebra associated with the non-compact locally isomorphic Lie groups $SO(2,1) \sim SU(1,1)$ is characterised by the commutator relations

$$[\Gamma_1, \Gamma_2] = -i\Gamma_3; \quad [\Gamma_2, \Gamma_3] = i\Gamma_1; \quad [\Gamma_3, \Gamma_1] = i\Gamma_2 \tag{2}$$

We may obtain a *realisation* of the Lie algebra in terms of a single variable y by writing

$$\begin{aligned}
\Gamma_1 &= \frac{\partial^2}{\partial y^2} + a_1(y) \\
\Gamma_2 &= i\left[k(y)\frac{\partial}{\partial y} + a_2(y)\right] \\
\Gamma_3 &= \frac{\partial^2}{\partial u^2} + a_3(y)
\end{aligned} \tag{3}$$

Equation (2) will be satisfied if we choose

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

where α, β and γ are constants of integration.

The requirement that the Casimir invariant of $su(1,1)$

$$\mathbf{\Gamma}^2 = \Gamma_3^2 - \Gamma_1^2 - \Gamma_2^2 \tag{5}$$

must commute with $\{\Gamma_1, \Gamma_2, \Gamma_3\}$ forces $\gamma = 0$ leading to the Casimir eigenvalues

$$\mathbf{\Gamma}^2 = -\frac{\alpha}{4} - \frac{3}{16} \tag{6}$$

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

$$\begin{aligned}
\Gamma_1 &= \frac{\partial^2}{\partial y^2} + \frac{\alpha}{y^2} + \frac{y^2}{16} \\
\Gamma_2 &= -\frac{i}{2}\left(y\frac{\partial}{\partial y} + \frac{1}{2}\right) \\
\Gamma_3 &= \frac{\partial^2}{\partial y^2} + \frac{\alpha}{y^2} - \frac{y^2}{16}
\end{aligned} \tag{7}$$

Let us choose to consider those second-order differential equations with

$$f(y) = \frac{a}{y^2} + by^2 + c \tag{8}$$

Now we can write Eq. (1) in terms of the $su(1,1)$ generators as

$$\frac{\partial^2}{\partial y^2} + \frac{a}{y^2} + by^2 + c = (\frac{1}{2} + 8b)\Gamma_1 + (\frac{1}{2} - 8b)\Gamma_3 + c \tag{9}$$

Let us put

$$a = -4\mathbf{\Gamma}^2 - \frac{3}{4} = \alpha \tag{10}$$

Now Eq.(1) is, in terms of $su(1,1)$ generators,

$$\left[(\frac{1}{2} + 8b)\Gamma_1 + (\frac{1}{2} - 8b)\Gamma_3 + c\right] Y = 0 \tag{11}$$

Recall that Γ_1 is a non-compact generator whereas Γ_3 is a compact generator. We can choose to diagonalise one or the other of these two generators by performing a rotation through a *tilting angle* θ such that

$$\begin{aligned}
e^{-i\theta\Gamma_2}\Gamma_1 e^{i\theta\Gamma_2} &= \Gamma_1\cosh\theta + \Gamma_3\sinh\theta \\
e^{-i\theta\Gamma_2}\Gamma_3 e^{i\theta\Gamma_2} &= \Gamma_1\sinh\theta + \Gamma_3\cosh\theta
\end{aligned} \tag{12}$$

to give

$$\left\{\left[(\frac{1}{2} + 8b)\cosh\theta + (\frac{1}{2} - 8b)\sinh\theta\right]\Gamma_1 + \left[(\frac{1}{2} + 8b)\sinh\theta + (\frac{1}{2} - 8b)\cosh\theta\right]\Gamma_3 + c\right\}\hat{Y} = 0 \tag{13}$$

where

$$\hat{Y} = e^{-i\theta\Gamma_2}Y \tag{14}$$

The Discrete Eigenvalue Spectrum

To diagonalise the compact generator Γ_3 we put

$$\tanh\theta = -\frac{\frac{1}{2} + 8b}{\frac{1}{2} - 8b} \tag{15}$$

leading to

$$\Gamma_3\hat{Y} = \frac{c}{4\sqrt{-b}}\hat{Y} \tag{16}$$

The eigenvector $\hat{Y}$ must be a simultaneous eigenvector of $\mathbf{\Gamma}^2$ and Γ_3 and span one of the infinite-dimensional discrete representations, say $D^+(\Phi)$ or $D^-(\Phi)$ of $su(1,1)$. Note that $SU(1,1)$ is the covering group of $SO(2,1)$ $\{cf.\mathrm{SU}(2) and \mathrm{SO}(3)\}$.

We can now rewrite Eq. (16) as

$$\Gamma_3 \hat{Y}^+_{\phi,x} = (-\Phi + x)\hat{Y}^+_{\phi,x} = \frac{c}{4\sqrt{-b}}\hat{Y}^+_{\phi,x} \quad (x = 0, 1, 2, \ldots) \tag{17}$$

with

$$\mathbf{\Gamma}^2 \hat{Y}^+_{\phi,x} = \Phi(\Phi + 1)\hat{Y}^+_{\phi,x} \quad (\Phi < 0) \tag{18}$$

Thus the existence of a discrete eigenvalue spectrum associated with the second-order differential equation

$$\left(\frac{d^2}{dy^2} + \frac{a}{y^2} + by^2 + c\right) \hat{Y}^+_{\phi,x} = 0 \tag{19}$$

requires that

$$4(-\Phi + x) = \frac{2}{\sqrt{-b}} \tag{20}$$

But from Eq. (6)

$$\Phi(\Phi + 1) = -\frac{\alpha}{4} - \frac{3}{16} \tag{21}$$

and hence

$$\Phi = -\frac{1}{2}\left(1 + \sqrt{\frac{1}{4} - \alpha}\right) \quad (\frac{1}{4} - \alpha) \geq 0 \tag{22}$$

where since $\Phi < 0$ we have kept only the negative root. Thus returning to Eq. (20) we have the key result

$$4x + 2 + \sqrt{\frac{1}{4} - \alpha}) = \frac{c}{\sqrt{-b}} \tag{23}$$

The Continuous Eigenvalue Spectrum

To obtain the continuous eigenvalue spectrum one must diagonalise the non-compact generator Γ_1. This may be done by choosing the tilting angle such that

$$\tanh\theta = -\frac{\frac{1}{2} - 8b}{\frac{1}{2} - 8b} \tag{24}$$

and thus Eq. (13) becomes

$$\Gamma_1 \bar{Y} = \frac{-c}{4\sqrt{-b}}\bar{Y} \tag{25}$$

The eigenvectors $\bar{Y}$ form a continuous basis. The eigenvalue spectrum is characterised by a continuous spectrum λ, where

$$\lambda = \frac{-c}{4\sqrt{-b}} \tag{26}$$

NB. The continuous part of the spectrum will exist only where $\tanh\theta$ exists.

Example:- The Three-Dimensional Isotropic Harmonic Oscillator

For the three-dimensional isotropic harmonic oscillator we have the radial differential equation

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - r^2 + 2E\right) R(r) = 0 \tag{27}$$

We can put this differential equation into the standard form of Eq. (19) by putting

$$a = -\ell(\ell + 1),\ b = -1 \quad and\ c = 2E \tag{28}$$

in Eq.(23)

$$4x + 2 + \sqrt{\frac{1}{4} - \alpha}) = \frac{c}{\sqrt{-b}} \tag{23}$$

gives

$$E = 2x + \ell + \frac{3}{2} \quad (x = 0, 1, 2, \ldots) \tag{29}$$

Putting

$$n = 2x + \ell \tag{30}$$

gives (in atomic units)

$$E_n = (n + \frac{3}{2}) \quad (n = 0, 1, 2, \ldots) \tag{31}$$

Degeneracy

The quantum number n defined in Eq. (31) depends on the values of the integer x and the orbital angular momentum ℓ. The rotational invariance of the isotropic harmonic oscillator ensures that for a given ℓ there will be $2\ell + 1$-eigenfunctions yielding the same energy eigenvalue. However, the degeneracy will often be higher than $2\ell + 1$ since several values of (x, ℓ) may correspond to the same value of n and hence to the same energy eigenvalue E_n as seen in the table below:-

n	x	ℓ	$2\ell + 1$	$n(n+1)/2$	E_n
0	0	0	1	1	$\frac{3}{2}$
1	0	1	3	3	$\frac{5}{2}$
2	1	0	1	6	$\frac{7}{2}$
	0	2	5		
3	1	1	3	10	$\frac{9}{2}$
	0	3	7		
4	2	0	1	15	$\frac{11}{2}$
	1	2	5		
	0	4	9		

In general the total degeneracy D_n associated with a given value of n is

$$D_n = \frac{(n+1)(n+2)}{2} \tag{32}$$

These numbers are in fact just the dimensions of the irreducible representations $\{n\}$ of the *degeneracy group* $SU(3)$.

Note that the *parity* of the degenerate states for a given value of n are all *even* or *odd* as n is *even* or *odd*. Furthermore, the spacings between consecutive energy eigenvalues are equal.

A Perturbing form ϵ/r^2 with $\epsilon \geq 0$

If we add a perturbing form ϵ/r^2 with $\epsilon \geq 0$ our differential equation becomes

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1) + \epsilon}{r^2} - r^2 + 2E \right) R(r) = 0 \tag{33}$$

leading to

$$E = 2x + 1 + \sqrt{(\ell + \frac{1}{2})^2 + \epsilon} \tag{34}$$

Note that adding the perturbing term has partially lifted the degeneracy of the unperturbed oscillator. The $(2\ell + 1)$-fold rotational degeneracy remains.

There is no continuous spectrum for the harmonic oscillator since putting $b = -1$ in Eqn. (24) leads to a tilting angle that falls outside of the allowed limits of $\tanh\theta$.

The Kepler Problem

Consider the differential equation

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{t}{r} + \frac{u}{r^2} + v \right) R(r) = 0 \tag{35}$$

We can transform it into standard form by putting

$$r = y^2 \quad \text{and} \quad R(r) = y^{-\frac{3}{2}} R(y) \tag{36}$$

to give

$$\left(\frac{d^2}{dy^2} + \frac{4u - \frac{3}{4}}{y^2} + 4vy^2 + 4t \right) R(y) = 0 \tag{37}$$

Using Eqns. (10) and (23) gives for the discrete spectrum

$$2x + 1 + \sqrt{1 - 4u} = \frac{t}{\sqrt{-v}} \quad (x = 0, 1, 2, \ldots) \tag{38}$$

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

$$E_n = -\frac{Z^2}{2n^2} \tag{39}$$

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

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

$$E = \frac{-Z^2}{2\left[x + \frac{1}{2} + \sqrt{(\ell + \frac{1}{2})^2 + 2\epsilon}\right]^2} \quad (x = 0, 1, 2, \ldots) \tag{40}$$

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

Klein-Gordon H-atom

The case of the Klein-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. (35) to yield the spectrum

$$\alpha^2 E = \frac{1}{\sqrt{1 + \frac{Z^2\alpha^2}{n^2}}} \tag{41}$$

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

The Morse Potential

The differential equation

$$\left(\frac{d^2}{dz^2} + p \exp^{2\tau z} + q \exp^{\tau z} + r \right) R(z) = 0 \tag{42}$$

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

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

to give

$$\left(\frac{d^2}{dy^2} + \frac{16r + \tau^2}{4\tau^2 y^2} + \frac{4p}{\tau^2} y^2 + \frac{4q}{\tau^2} \right) R(y) = 0 \tag{43}$$

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

$$\left(\frac{d^2}{dr^2} - 2D \exp^{-2\tau z} + 4D \exp^{-\tau z} + 2E \right) R(r) = 0 \tag{44}$$

Noting Eqns. (42) and (43) we obtain the standard form

$$\left(\frac{d^2}{dy^2} + \frac{32E + \tau^2}{4\tau^2 y^2} - \frac{8D}{\tau^2} y^2 + \frac{16D}{\tau^2} \right) \Rightarrow (y) = 0 \tag{45}$$

Use of Eqn. (23) leads to

$$E = \frac{-\tau^2}{2} \left(\frac{\sqrt{2}D}{\tau} - (x + \frac{1}{2}) \right)^2 \quad (x = 0, 1, 2, \ldots, x_{max}) \tag{46}$$

where

$$x_{max} + \frac{1}{2} < \frac{\sqrt{2}D}{\tau} \tag{47}$$

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.

References

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T'is a common proof,
That lowliness is young ambition's ladder,
Whereto the climber-upward turns his face;
But when he once attains the upmost 1 round,
He then unto the ladder turns his back,
Looks in the clouds, scorning the base degrees
By which he did ascend.
– William Shakespeare. Julius Cæsar.

Continuous Symmetries IV.

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A mass enormous! which in modern days
No two of earth's degenerate sons could raise.

—Alexander Pope. 1688-1744

The Degeneracy Group of the Isotropic Harmonic Oscillator

Introduction

I the next few lectures I want to introduce the non-compact Lie group $Sp(2n,\Re)$ as a dynamical group for many particles in an isotropic harmonic oscillator potential. This group crops up in many physical situations such as in nuclear models[1], quantum optics[2] and quantum dots[3]. In this lecture we identify the degeneracy group of the isotropic harmonic oscillator in three dimensions.

Notes on Lie Algebras

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

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

$$[X,Y]+[Y,X]=0 \tag{1}$$

$$[X,[Y,Z]]+[Y,[Z,X]]+[Z,[X,Y]]=0 \tag{2}$$

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.

Structure Constants

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

$$[X_\rho,X_\sigma]=c^\tau_{\rho\sigma}X_\tau \tag{3}$$

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

The Killing Form

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

$$g_{\sigma\lambda}=g_{\lambda\sigma}=c^\tau_{\sigma\rho}c^\rho_{\lambda\tau} \tag{4}$$

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

$$det|g_{\sigma\lambda}|\neq 0 \tag{5}$$

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

$$[X_1,X_2]=X_3,\quad [X_2,X_3]=X_1,\quad [X_3,X_1]=X_2 \tag{6}$$

We have from Eqn. (3)

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

Continuing we find

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

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

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

$$\begin{aligned} x' &= x\cos\theta - y\sin\theta + a \\ y' &= x\sin\theta + y\cos\theta + b \end{aligned} \tag{7}$$

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

$$\begin{pmatrix} \cos\theta & -\sin\theta & a \\ \sin\theta & \cos\theta & b \\ 0 & 0 & 1 \end{pmatrix} \tag{8}$$

From that we may obtain three infinitesmal operators

$$X_\theta = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad X_a = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad X_b == \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \tag{9}$$

which satisfy the commutation relations

$$[X_\theta, X_a] = X_b, \quad [X_\theta, X_b] = -X_a, \quad [X_a, X_b] = 0 \tag{10}$$

The metric tensor is now found to be

$$g_{\sigma\lambda} = \begin{pmatrix} -2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{11}$$

which is obviously singular and hence E_2 is *not* semisimple. The two elements X_a, X_b form a non-trivial Abelian subalgebra T_2. The Lie algebracannot be reduced to a direct sum of simple Lie algebras but is rather a *semidirect sum*

$$E_2 = T_2 \oplus_s X_\theta \tag{12}$$

Exercise

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 $so(3)$.

Antisymmetric Tensors

Let us define a new tensor

$$c_{\sigma\mu\nu} = g_{\sigma\lambda} c^\lambda_{\mu\nu} \tag{13}$$

Recalling Eqn. (3) we have

$$c_{\sigma\mu\nu} = c^\tau_{\sigma\rho} c^\rho_{\lambda\tau} c^\lambda_{\mu\nu} = c^\tau_{\sigma\rho} c^\lambda_{\mu\nu} c^\rho_{\lambda\tau} \tag{14}$$

Use of the Jacobi identity, Eqn. (6), we have

$$\begin{aligned} c_{\sigma\mu\nu} &= -c^\tau_{\sigma\rho} c^\lambda_{\nu\tau} c^\rho_{\mu\lambda} - c^\tau_{\sigma\rho} c^\lambda_{\tau\mu} c^\rho_{\lambda\nu} \\ &= c^\tau_{\rho\sigma} c^\lambda_{\nu\tau} c^\rho_{\mu\lambda} + c^\tau_{\rho\sigma} c^\lambda_{\tau\mu} c^\rho_{\lambda\nu} \end{aligned} \tag{15}$$

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.

The Casimir Operators

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

$$C = g^{\rho\sigma} X_\rho X_\sigma \tag{16}$$

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.

Back to the 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

$$H = \frac{1}{2}(\mathbf{p}^2 + \mathbf{r}^2) \tag{17}$$

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

$$[q_i, q_j] = [p_i, p_j] = 0, \qquad [q_i, p_j] = i\delta_{ij} \tag{18}$$

Now introduce boson annihilation and creation operators ($\mathbf{a}$ and $\mathbf{a}^\dagger$ respectively)

$$\mathbf{a} = \frac{1}{\sqrt{2}}(\mathbf{r} + i\mathbf{p}), \qquad \mathbf{a}^\dagger = \frac{1}{\sqrt{2}}(\mathbf{r} - i\mathbf{p}) \tag{19}$$

which satisfy the bosonic commutation relation

$$[a_i, a_j^\dagger] = \delta_{ij} \tag{20}$$

The Hamiltonian can now be written as

$$H = \mathbf{a}^\dagger \cdot \mathbf{a} + \frac{3}{2} \tag{21}$$

Use of Eqn. (20) then leads to

$$[H, a_j^\dagger] = a_j^\dagger, \qquad [H, a_j] = -a_j \tag{22}$$

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

$$n = n_1 + n_2 + n_3 \tag{23}$$

and hence the energy eigenvalues of H are

$$E_n = n + \frac{3}{2} \quad (n = 0, 1, 2, \ldots) \tag{24}$$

(the same result as obtained in Lecture III) with normalised state vectors

$$|n_1 n_2 n_3\rangle = \prod_{i=1}^{3} \frac{a_i^{\dagger n_i}}{\sqrt{n_i!}} |000\rangle \tag{25}$$

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

$$a_j |000\rangle = 0 \tag{26}$$

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

$$\langle n_1 n_2 n_3| = \langle 000| \prod_{i=1}^{3} \frac{a_i^{n_i}}{\sqrt{n_i!}} \tag{27}$$

with

$$\langle 000| a_j^\dagger = 0 \tag{28}$$

To proceed further we need some remarks about the general linear group $GL(n)$ and the unitary group $U(n)$.

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

$$x^i \to x'^i = \alpha_j^i x^j \tag{29}$$

The coefficients α^i_j 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 $[a^i_j]$. 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

$$\det[a^i_j] = +1 \tag{30}$$

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

$$x_i \rightarrow x'_i = x_j b^j_i \tag{31}$$

such that

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

implying that

$$a^i_j b^k_i = \delta^k_j \tag{32}$$

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

Note on Tensors

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

$$T^{ij\ldots}_{kl\ldots} \rightarrow a^i_m a^j_n \ldots T^{mn\ldots}_{pq\ldots} b^p_k b^q_l \ldots \tag{33}$$

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.

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

$$\lambda_1 \geq \lambda_2 \geq \ldots \lambda_p \tag{34}$$

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 $U(3)$.

Irreducible representations of the Special Unitary group $SU(n)$

Under the restriction from $U(n) \rightarrow SU(n)$ the representations

$$\{\lambda_1, \lambda_2, \ldots, \lambda_n\} \equiv \{\lambda_1 + x, \lambda_2 + x, \ldots, \lambda_n + x\} \tag{35}$$

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 $\{321\} \rightarrow \{21\}$.

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

$$\{\lambda_1 + x, \lambda_2 + x, \ldots, \lambda_n + x\} = (\epsilon_1 \ldots \epsilon_n)^x \{\lambda_1, \lambda_2, \ldots, \lambda_n\} \tag{36}$$

Degeneracy Group of the Isotropic Harmonic Oscillator

Let us introduce nine operators

$$T_{ij} = \frac{1}{2}\{a_i^\dagger, a_j\} \qquad (i,j = 1,2,3) \tag{37}$$

where $\{a,b\} \equiv ab + ba$. Using the basic boson commutation relations of Eqn. (20) we find

$$[T_{ij}\,, T_{rs}] = \delta_{jr} T_{is} - \delta_{is} T_{rj} \tag{38}$$

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

$$[H_i, T_{jr}] = (\delta_{ij} - \delta_{ir}) T_{jr} \tag{39}$$

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. (39) via

$$H = H_1 + H_2 + H_3 \tag{40}$$

commutes with all T_{ij}. The three operators

$$H' = H_i - \frac{H}{3} \tag{41}$$

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.

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

$$[J_z, J_\pm] = \pm J_\pm \qquad [J_+, J_-] = J_z \tag{42}$$

with

$$J_\pm = \frac{1}{\sqrt{(2)}}(J_x \pm i J_y) \tag{43}$$

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

$$\begin{aligned} [H_i, H_j] &= 0 \qquad (i,j = 1, \ldots \ell) \\ [H_i, E_\alpha] &= \alpha_i E_\alpha \\ [E_\alpha, E_\beta] &= N_{\alpha\beta} E_{\alpha+\beta} \\ [E_\alpha, E_{-\alpha}] &= \alpha^i H_i \end{aligned} \tag{44}$$

where the E_α are the analogues of the ladder operators $J_\pm$ of SO_3.

Just as in SO_3 where 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

$$[H_i, a_j^\dagger] = \delta_{ij} a_j^\dagger \quad \text{and} \quad [H_i, a_j] = -\delta_{ij} a_j \tag{45}$$

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

1 Noting Eqn(38) 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).

2 Determine the highest weight vector in the above set of weight vectors.

3 Repeat the above analysis for a two-dimensional isotropic harmonic oscillator and show that the relevant symmetry group is $U(2)$.

Rotational Symmetry and the Isotropic Harmonic Oscillator

The harmonic oscillator Hamiltonian, Eqn. (17), commutes with all the components of the angular momentum operator

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = i\mathbf{a} \times \mathbf{a}^{\dagger} \tag{46}$$

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}, Eqns. (37)to (39) we have

$$L_1 = -i(T_{23} - T32), \quad L_2 = -i(T_{31} - T_{13}), \quad L_3 = -i(T_{12} - T_{21}) \tag{47}$$

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

$$U(3) \supset SU(3) \supset SO(3) \supset SO(2) \tag{48}$$

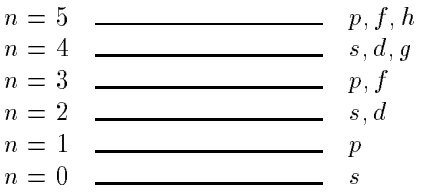
It is convenient to label the oscillator states in a basis $|n\ell m\rangle$ where $n = 0, 1, 2, \ldots$. From Lecture II we have

$$n = 2x + \ell \qquad \text{with} \quad x = 0, 1, 2, \ldots \tag{49}$$

and hence the values of ℓ associated with a given value of n are

$$\begin{aligned} \ell &= 1, 3, 5, \ldots, n \qquad n \quad odd \\ &= 0, 2, 4, \ldots, n \qquad n \quad even \end{aligned} \tag{50}$$

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.

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Gods! How the son degenerates from the sire!

—Alexander Pope. 1688-1744

Continuous Symmetries V.

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The Dynamical Group of the Isotropic Harmonic Oscillator

Symmetry denotes that sort of concordance of several parts by which they integrate into a whole. Beauty is bound up with symmetry.
— H. Weyl, *Symmetry*, Princeton University Press 1952

Introduction

Having established the *degeneracy group* for a three-dimensional isotropic harmonic oscillator we now seek a larger group that contains the degeneracy group as a subgroup and has among its generators operators that will ladder between different degeneracy multiplets. Such a group will be said to be a *dynamical group*. We shall first remark about quantum dots and then say something further about degeneracy groups to then lead up to the dynamical group concept.

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

$$V(r_i, r_j) = 2V_0 - \frac{1}{2} m^* \Omega^2 |r_i - r_j|^2 \tag{1}$$

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

$$H_{space} = \frac{1}{2m^*} \sum_i \left[p_i + \frac{eA_i}{c} \right]^2 + \frac{1}{2} m^* \omega_0^2 \sum_i |r_i|^2 + \sum_{i<j} V(r_i, r_j) \tag{2}$$

and the spin part as

$$H_{spin} = -g^* \mu_B B \sum_i s_{z,i} \tag{3}$$

where the momentum and vector potential associated with the $i-th$ electron are given by

$$p_i = (p_{x,i}, p_{y,i}) \qquad A_i = (A_{x,i}, A_{y,i}) \tag{4}$$

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. (2) becomes

$$H_{space} = \frac{1}{2m^*}\sum_i p_i^2 + \frac{1}{2}m^*\omega_0^2(B)\sum_i |r_i|^2 + \sum_{i<j}\left[2V_0 - \frac{1}{2}m^*\Omega^2|r_i, r_j|^2\right] + \frac{\omega_c}{2}\sum_i L_{z,i} \tag{5}$$

where $\omega_0^2(B) = \omega_0^2 + \omega_c^2/4$ and $\omega_c = eB/m^*c$. We shall return to quantum dots later.

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

$$[a_i, a_j] = 0, \quad [a_i^\dagger, a_j^\dagger] = 0, \quad [a_i, a_j^\dagger] = \delta_{i,j} \tag{6}$$

These can be used to simplify expressions. As an example, consider the anticommutator $\{a_i^\dagger, a_j\} = a_i^\dagger a_j + a_j a_i^\dagger$ and let us evaluate the commutator $[\{a_i^\dagger, a_j\}, a_k]$. Expanding out we have

$$[a_i^\dagger a_j + a_j a_i^\dagger, a_k] = [a_i^\dagger a_j\,, a_k] + [a_j a_i^\dagger, a_k] \tag{7}$$

Expanding out the first commutator we have

$$[a_i^\dagger a_j\,, a_k] = a_i^\dagger a_j a_k - a_k a_i^\dagger a_j \tag{8}$$

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. (6) we can rearrange the first term as

$$a_i^\dagger a_j a_k \rightharpoonup a_i^\dagger a_k a_j \tag{9}$$

and hence the right-hand-side of Eqn. (9) becomes

$$\begin{aligned} a_i^\dagger a_j a_k - a_k a_i^\dagger a_j &\rightharpoonup a_i^\dagger a_k a_j - a_k a_i^\dagger a_j \\ &= [a_i^\dagger, a_k]a_j \\ &= -[a_k, a_i^\dagger]a_j \\ &= -\delta_{i,k}a_j \end{aligned}$$

Exercises

1. Show that if

$$T_{ij} = \frac{1}{2}\{a_i^\dagger, a_j\}$$

then

$$[T_{ij}, T_{rs}] = \delta_{j,r}T_{is} - \delta_{i,s}T_{rj}$$

2. Use the result of the above exercise to show that the degeneracy group of an isotropic harmonic oscillator in $d-$dimensions is $U(d)$.

The Degeneracy Group for Mesoscopic Systems

We start to 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. We might note here that the Lie algebra A_2 associated with the Lie group $SU(3)$ is of rank 2 and hence contains two self-commuting generators $\{H_1, H_2\}$ and hence there exists two constants of the motion, that is there is a constant of the motion additional to that of the angular momentum Casimir invariant $\mathbf{L}^2$.

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.

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 $\hbar = 1$)
$$[X_{ri}, X_{sj}] = 0, [X_{ri}, P_{sj}] = i\delta_{rs}\delta_{ij}, [P_{ri}, P_{sj}] = 0 \tag{10}$$
4. The $(2Nd)^2$ bilinear operators
$$\{X_{ri}X_{sj}, X_{ri}P_{sj}, P_{ri}X_{sj}, P_{ri}P_{sj}\} \tag{11}$$
close under commutation. However, only
$(2Nd+1)Nd$ of these operators are independent since
$$P_{ri}X_{sj} = X_{sj}P_{ri} - i\delta_{rs}\delta_{ij} \tag{12}$$
5. Consider the $(2Nd+1)Nd$ independent operators
$$Q_{risj} = \frac{1}{2}\{X_{ri}, X_{sj}\}, \quad V_{risj} = \frac{1}{2}\{X_{ri}, P_{sj}\},$$
$$K_{risj} = \frac{1}{2}\{P_{ri}, P_{sj}\} \tag{13}$$
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 having $N-$electrons in a $d-$dimensional isotropic harmonic oscillator potential. We now seek possible subalgebras of $Sp(2Nd, R)$.

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)
$$Q_{ij} = X_{ri}X_{rj}, \quad L_{ij} = X_{ri}P_{rj} - X_{rj}P_{ri},$$
$$K_{ij} = P_{ri}P_{rj}$$
$$T_{ij} = \frac{1}{2}(X_{ri}P_{rj} + X_{rj}P_{ri} + P_{ri}X_{rj} + P_{rj}X_{ri}) \tag{14}$$
and
$$Q_{rs} = X_{ri}X_{si}, \quad L_{rs} = X_{ri}P_{si} - X_{si}P_{ri},$$
$$K_{rs} = P_{ri}P_{si}$$

$$T_{rs} = \frac{1}{2}(X_{ri}P_{si} + X_{si}P_{ri} + P_{ri}X_{si} + P_{si}X_{ri}) \tag{15}$$

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

$$\begin{aligned}[L_{ij}, L_{kl}] &= i(L_{ik}\delta_{jl} - L_{il}\delta_{jk} + L_{jk}\delta_{il} + L_{jk}\delta_{il} - L_{jl}\delta_{ik}) \\ [L_{rs}, L_{tu}] &= i(L_{rt}\delta_{su} - L_{ru}\delta_{st} + L_{st}\delta_{ru} - L_{su}\delta_{rt})\end{aligned} \tag{16}$$

and form the generators of the subalgebras $O(d)$ and $O(N)$.

4. Continuing we are led to the following possible Lie subalgebras of $Sp(2Nd, R)$:-

$$\begin{aligned}Sp(2,R) \times O(Nd) \supset Sp(2,R) \times O(N) \times O(d) \\ \supset U(1) \times O(N) \times O(d)\end{aligned} \tag{17}$$

$$Sp(2N,R) \times O(d) \supset U(N) \times O(d) \supset U(1) \times O(N) \times O(d) \tag{18}$$

$$Sp(2d) \times O(N) \supset U(d) \times O(N) \supset U(1) \times O(d) \times O(N) \tag{19}$$

$$U(Nd) \supset U(N) \times U(d) \supset U(1) \times O(N) \times O(d) \tag{20}$$

Note the separation of the spatial and particle dependencies.

Identification of the $Sp(2, R)$ Subgroup

Let us introduce three operators defined by

$$Q = X_{ri}X_{ri}, \quad T = X_{ri}P_{ri} + P_{ri}X_{ri}, \quad K = P_{ri}P_{ri} \tag{21}$$

and having the non-zero commutation relations

$$[Q, K] = 2iT, \quad [Q, T] = 4iQ, \quad [K, T] = -4iK \tag{22}$$

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

$$g_{ij} = c^t_{ik}c^k_{jt} \tag{23}$$

where the c^t_{ik} are the structure constants of the Lie algebra. Noting Eqn. (22) we have

$$c^T_{QK} = 2i, \quad c^Q_{QT} = 4i, \quad c^K_{KT} = -4i \tag{24}$$

Recall that the structure constants are antisymmetric. We now find for the diagonal elements of the metric tensor

$$\begin{aligned}g_{QQ} &= g_{KK} = 0 \\ g_{TT} &= c^Q_{TQ}c^Q_{TQ} + c^K_{TK}c^K_{TK} = -4i \times -4i + 4i \times 4i = -32\end{aligned} \tag{25}$$

In addition we have the off-diagonal elements

$$g_{QK} = g_{KQ} = c^Q_{QT}c^T_{KQ} + c^T_{QK}c^K_{KT} = 4i \times -2i + 2i \times -4i = 16 \tag{26}$$

and thus the complete metric tensor is represented by the matrix

$$[g_{ij}] = \begin{array}{c} \\ Q \\ K \\ T \end{array} \begin{array}{c} \begin{array}{ccc} Q & K & T \end{array} \\ \begin{pmatrix} 0 & 16 & 0 \\ 16 & 0 & 0 \\ 0 & 0 & -32 \end{pmatrix} \end{array} \tag{27}$$

We can produce a diagonal metric tensor by putting

$$A_{\pm} = \frac{1}{\sqrt{2}}(Q \pm K) \tag{28}$$

to give the Lie algebra as

$$[A_{\pm}, T] = 4iA_{\mp}, \qquad [A_{+}, A_{-}] = 2iT \tag{29}$$

and the metric tensor as

$$[g_{ij}] = \begin{array}{c} \\ A_+ \\ A_- \\ T \end{array} \begin{array}{c} \begin{array}{ccc} A_+ & A_- & T \end{array} \\ \begin{pmatrix} -16 & 0 & 0 \\ 0 & +16 & 0 \\ 0 & 0 & -32 \end{pmatrix} \end{array} \tag{30}$$

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

$$SO(2,1) \sim Sp(2,R) \tag{31}$$

The Quantum Dot Hamiltonian (again)

We can express terms in the Hamiltonian of an isotropic harmonic oscillator

$$H_o = \frac{1}{2m} P_{ri} P_{ri} + \frac{m\omega^2}{2} X_{ri} X_{ri} \tag{32}$$

in terms of the group generators of $Sp(2,R)$ by noting that

$$\frac{1}{2m} P_{ri} P_{ri} = \frac{1}{2m} K \tag{33}$$

and

$$\frac{m\omega^2}{2} X_{ri} X_{ri} = \frac{m\omega^2}{2} Q \tag{34}$$

to give

$$H_o = \frac{1}{2m} K + \frac{m\omega^2}{2} Q \tag{35}$$

Now consider our earlier Hamiltonian

$$H_{space} = \frac{1}{2m^*} \sum_i p_i^2 + \frac{1}{2} m^* \omega_0^2(B) \sum_i |r_i|^2 + \sum_{i<j} \left[2V_0 - \frac{1}{2} m^* \Omega^2 |r_i, r_j|^2 \right] + \frac{\omega_c}{2} \sum_i L_{z,i} \tag{5}$$

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

$$H_{space} = \frac{1}{2m} K + \frac{m\Omega_0^2}{2} Q - \frac{eB}{4mc} L_{12} + N(N-1)V_0 + \frac{m\Omega^2}{2} \sum_{rs} Q_{rs} \tag{36}$$

with

$$\Omega_0^2 = \omega^2 + (\frac{eB}{2mc})^2 - N\Omega^2 \tag{37}$$

The significance of these results is that the first three terms in Eqno. (37) 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.

Concluding Remarks

We have now established an extensive group-subgroup structure and must next explore some of its structure. To do that we will need to determine the relevant irreducible representations , branching rules etc.

The perfection of mathematical beauty is such that whatever is most beautiful and regular is also found to be most useful and excellent.

— D'Arcy W. Thompson, *"On Growth and Form"*, Cambridge 1917

Continuous Symmetries VI.

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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

The $SO(4)$ Symmetry of Hydrogenic Atoms

Introduction

In this lecture we establish the rotation group in four spatial dimensions, $SO(4)$ as the degeneracy group for hydrogen-like atoms.

$SO(4)$ and Hydrogen-like Atoms

The Hamiltonian for a non-relativistic spinless hydogenic-like atom of atomic number Z may be written as

$$H = \frac{\mathbf{p}^2}{2m} - \frac{k}{r} \tag{1}$$

where $k = Ze^2$.

Clearly,

$$[H, \mathbf{L}^2] = 0 \qquad and \qquad [H, L_z] = 0 \tag{2}$$

showing that the energy levels are degenerate with respect to M_L for a given L and hence we expect a degeneracy of $2L+1$ for each value of L and yet we know from Bohr's result that, in atomic units,

$$E_n = -\frac{Z^2}{2n^2} \qquad n = 1, 2, \ldots \tag{3}$$

with the actual degeneracy being n^2.

In 1926 Pauli showed that the classical Runge-Lenz vector

$$\mathbf{A}' = \frac{\mathbf{p} \times \mathbf{L}}{m} - \frac{k\mathbf{r}}{r} \tag{4}$$

which occurs as a constant of motion in the Kepler problem can be written as a Hermitian quantum operator as

$$\mathbf{A}'' = \frac{1}{2m}(\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}) - \frac{k\mathbf{r}}{r} \tag{5}$$

We then find the commuation relationships

$$\begin{aligned} [H, L_i] &= [H, A_i''] = 0 \\ [L_i, L_j] &= i\varepsilon_{ijk}L_k, \qquad [L_i, A_j''] = i\varepsilon_{ijk}A_k'' \\ [A_i'', A_j''] &= -\frac{2i}{m}\varepsilon_{ijk}L_k H \end{aligned} \tag{6}$$

Let us put (for bound states with $E < 0$)

$$\mathbf{A} = \sqrt{\frac{-m}{2E}}\mathbf{A}'' \tag{7}$$

and introduce two more vector operators

$$\mathbf{M} = \frac{1}{2}(\mathbf{L} + \mathbf{A}) \qquad and \qquad \mathbf{N} = \frac{1}{2}(\mathbf{L} - \mathbf{A}) \tag{8}$$

to yield

$$[M_i, M_j] = i\varepsilon_{ijk}M_k \quad [N_i, N_j] = i\varepsilon_{ijk}N_k \quad [M_i, N_j] = 0 \tag{9}$$

Note the two vector operators each separately generate the Lie algebra of a rotation group $SO(3)$. Furthermore the components of the two vector operators commute and hence they generate the *direct product* group $SO(3) \times SO(3) \sim SU(2) \times SU(2)$ which is locally isomorphic to the rotation group $SO(4)$. Thus it appears that the symmetry of a hydrogenic atom is higher than that of $SO(3)$. Indeed the degeneracy group is $SO(4)$.

The Sophisticate's derivation of Bohr's Formula

The operators $\mathbf{M}^2$ and $\mathbf{N}^2$ are the Casimir operators of the two commuting $SO(3)$ groups with eigenvalues

$$\mathbf{M}^2 = j(j+1) \qquad and \qquad \mathbf{N}^2 = j'(j'+1) \quad with \quad (j, j' = 0, \frac{1}{2}, 1, \ldots) \tag{10}$$

The group $SO(4)$ is of rank 2 and we may form two Casimir operators

$$F = \mathbf{M}^2 + \mathbf{N}^2 = \frac{1}{2}(\mathbf{L}^2 + \mathbf{A}^2) \tag{11}$$

and

$$G = \mathbf{L} \cdot \mathbf{A} = \mathbf{M}^2 - \mathbf{N}^2 \tag{12}$$

For a hydrogenic atom, BUT not for a many-electron atom, we have $\mathbf{L} \cdot \mathbf{A} = 0$ which forces the equality $j = j'$ and hence $G = 0$ for a hydrogenic atom. Thus for a hydrogenic atom

$$F = 2j(j+1) \qquad (j = 0, \frac{1}{2}, 1, \ldots) \tag{13}$$

But from (7) and (11) we have

$$F = \frac{1}{2}\left(\mathbf{L}^2 - \frac{1}{2E}\mathbf{A}''^2\right) = -\frac{Z^2}{4E} - \frac{1}{2} \tag{14}$$

leading to the familiar Bohr result

$$E_n = -\frac{Z^2}{2n^2} \qquad (n = 2j + 1 = 0, 1, 2, \ldots \tag{15}$$

The Degeneracy Group $SO(4) \sim SO(3) \times SO(3)$

The representations of $SO(3) \times SO(3)$ are of degree $(2j+1) \times (2j'+1)$ and since for a hydrogenic atom $j = j'$ we conclude that the levels are n^2-fold degenerate with an additional factor of 2 required to accommodate the two-fold spin degeneracy of the levels. Thus the degeneracy group of the hydrogen-like atoms is $SO(4) \sim SO(3) \times SO(3)$.

Infinitesimal Operators and Spherical Tensor Operators for $SO(4)$

The group $SO(4)$ may be generated by six infinitesimal rotation operators that leave invariant the quadratic form $x_1^2 + x_2^2 + x_3^2 + x_4^2$ and may be written as

$$J_{\lambda\mu} = i\left(x_\mu \frac{\partial}{\partial x_\lambda} - x_\lambda \frac{\partial}{\partial x_\mu}\right) \quad (\lambda \neq \mu = 1, 2, 3, 4) \tag{16}$$

where $J_{\lambda\mu} = -J_{\mu\lambda}$

We may write the six infinitesimal rotation operators as components of two spherical rank-one tensor operators $\mathbf{L}^{(1)}$ and $\mathbf{A}^{(1)}$ by putting

$$L_0^{(1)} = J_{23} \qquad L_{\pm 1}^{(1)} = \pm\frac{1}{\sqrt{2}}(J_{31} \pm J_{12}) \tag{17a}$$

$$A_0^{(1)} = J_{41} \qquad A_{\pm 1}^{(1)} = \pm\frac{1}{\sqrt{2}}(J_{42} \pm J_{43}) \tag{17b}$$

to yield the commutation algebra

$$[L_i^{(1)}, L_j^{(1)}] = -\varepsilon_{ijk} L_k^{(1)} = [A_i^{(1)}, A_j^{(1)}]$$
$$[L_i^{(1)}, A_j^{(1)}] = -\varepsilon_{ijk} A_k^{(1)} \tag{18}$$

Labelling Irreducible representations of $SO(4)$

The six components of $\mathbf{L}^{(1)}$ and $\mathbf{A}^{(1)}$ may be divided into two sets. The first set contains two operators H_1 and H_2 that commute with one another and are constructed from suitable linear combinations of $L_0^{(1)}$ and $A_0^{(1)}$. The second set comprises the operators E_α which are simultaneous eigenfunctions of H_1 and H_2,

$$[H_1, E_\alpha] = \alpha_1 E_\alpha \qquad and \qquad [H_2, E_\alpha] = \alpha_2 E_\alpha \tag{19}$$

obtained from linear combinations of $L_{\pm 1}^{(1)}$ and $A_{\pm 1}^{(1)}$. The eigenvalues α_1 and α_2 define a two-dimensional weight space. In defining the weight space we are faced with two rather obvious choices:

(1)

$$H_1 = L_0^{(1)} \qquad and \qquad H_2 = A_0^{(1)} \tag{20a}$$

with

$$E_{\pm 1}^{+} = L_{\pm 1}^{(1)} + A_{\pm 1}^{(1)} \qquad and \qquad E_{\pm 1}^{+} = L_{\pm 1}^{(1)} - A_{\pm 1}^{(1)} \tag{20b}$$

(2)

$$H_1 = \frac{1}{2}(L_0^{(1)} + A_0^{(1)}) \qquad and \qquad H_2 = \frac{1}{2}(L_0^{(1)} - A_0^{(1)}) \tag{21a}$$

with

$$E_{\pm 1}^{+} = \frac{1}{2}(L_{\pm 1}^{(1)} + A_{\pm 1}^{(1)}) \qquad and \qquad E_{\pm 1}^{+} = \frac{1}{2}(L_{\pm 1}^{(1)} - A_{\pm 1}^{(1)} \tag{21b}$$

We may choose either Eqn.(20) or (21) to establish a systematic labelling of the irreducible representations of $SO(4)$. Use of Eqn.(21) leads to labelling the irreducible representations in terms of a pair of integers or half-integers $[pq]$ which at the same time label the irreducible representations $\mathrm{D}^{[p]}$ and $\mathrm{D}^{[q]}$ of $SO(3)$ contained in the direct product representation $\mathrm{D}^{[p]} \times \mathrm{D}^{[q]}$ of $SO(3) \times SO(3)$. Note that in this scheme $[pq]$ and $[qp]$ $(p \neq q)$ are distinct irreducible representations but under $SO(4) \rightarrow SO(3)$ they decompose in the same manner.

$$[pq] \rightarrow [p+q] + [p+q-1] + \ldots + [|p-q|] \tag{22}$$

The choice of Eqn.(20) leads to labels $[pq]$ where p and q are both integers or half-integers with $p \geq q$ and although p is necessarily positive, q may be positive or negative. In that case

$$[pq] \rightarrow [p] + [p-1] + \ldots + [|q|] \tag{23}$$

Henceforth I will use this scheme for labelling the irreducible representations of $SO(4)$ and write

$$[p, \pm q] \equiv [pq]_{\pm} \tag{24}$$

$SO(4)$ Coupled States and Coupling Coefficients

The group chain

$$SO(4) \supset SO(3) \supset SO(2) \tag{25}$$

may be used to label symmetrised basis states in the form

$$|[pq]jm\rangle \tag{26}$$

where j labels the $SO(3)$ representations obtained from Eqn.(23) amd m labels the $SO(2)$ representations arising from $SO(3) \rightarrow SO(2)$. These basis states can be related to those of the $SO(3) \times SO(3)$ scheme $|j_1 m_1, j_2 m_2\rangle$ by writing

$$|[pq]jm\rangle = |[j_1 + j_2, j_1 - j_2]jm\rangle = \sum_{m_1, m_2} \langle m_1 m_2 | jm \rangle | j_1 m_1 j_2 m_2 \rangle \tag{27}$$

where the $\langle m_1 m_2 | jm \rangle$ are the usual $SO(3)$ jm coefficients.

The Kronecker product $[p_1 q_1] \times [p_2 q_2]$ may be resolved by noting Eqn.(26) to give

$$[p_1 q_1] \times [p_2 q_2] = \sum_{\alpha=0}^{t} \sum_{\beta=0}^{u} [p_1 + p_2 - \alpha - \beta, q_1 + q_2 - \alpha + \beta] \tag{28}$$

where t is the lesser of $p_1 + q_1$ and $p_2 + q_2$ while u is the lesser of $p_1 - q_1$ and $p_2 - q_2$.

$$[31] \times [21]_- = [52]_- + [5] + [43]_- + [41]_+ + 2[41]_- + [32]_+ + [32]_- + 2[3] + 2[21]_+ + [21]_- + [1]$$

The $SO(4)$ coupling coefficients may be defined as the coefficients $\langle [p_1 q_1][p_2 q_2]; [p_{12} q_{12}] J_{12} M_{12} | [p_1 q_1] j_1 m_1 [p_2 q_2] j_2 m_2 \rangle$ that effect the unitary transformation

$$\begin{aligned} |[p_1 q_1] j_1 m_1 [p_2 q_2] j_2 m_2 \rangle = & \sum_{[p_{12} q_{12}] J_{12} M_{12}} \langle [p_1 q_1][p_2 q_2]; [p_{12} q_{12}] J_{12} M_{12} | [p_1 q_1] j_1 m_1 [p_2 q_2] j_2 m_2 \rangle \\ & \times |[p_1 q_1][p_2 q_2]; [p_{12} q_{12}] J_{12} M_{12} \rangle \end{aligned} \tag{29}$$

This coupling coefficient may be expressed in terms of the $3nj-$symbols of $SO(3)$ angular momentum theory by first making use of Eqn. (27) to yield

$$\begin{aligned} & \langle [p_1 q_1] j_1 m_1 [p_2 q_2] j_2 m_2 | [p_1 q_1][p_2 q_2]; [p_{12} q_{12}] J_{12} M_{12} \rangle \\ & = [(2j_1+1)(2j_2+1)(2J_{12}+1)(p_{12}+q_{12}+1)(p_{12}-q_{12}+1)]^{\frac{1}{2}} \\ & \times (-1)^{J_{12}-M_{12}} \begin{pmatrix} j_1 & J_{12} & j_2 \\ m_1 & -M_{12} & m_2 \end{pmatrix} \\ & \times \begin{Bmatrix} \frac{1}{2}(p_1+q_1) & \frac{1}{2}(p_2+q_2) & \frac{1}{2}(p_{12}+q_{12}) \\ \frac{1}{2}(p_1-q_1) & \frac{1}{2}(p_2-q_2) & \frac{1}{2}(p_{12}-q_{12}) \\ j_1 & j_2 & J_{12} \end{Bmatrix} \end{aligned} \tag{30}$$

This result essentially consists of two factors, the first equivalent to a Clebsch-Gordan coefficient $\langle j_1 m_1 j_2 m_2 | j_1 j_2; J_{12} M_{12} \rangle$ and the second to a coupling coefficient working at the $SO(4) \supset SO(3)$ level. Thus the coupling coefficient defined in Eqn. (30) can be factorised as

$$\begin{aligned} & \langle [p_1 q_1] j_1 m_1 [p_2 q_2] j_2 m_2 | [p_1 q_1][p_2 q_2]; [p_{12} q_{12}] J_{12} M_{12} \rangle \\ & = \langle j_1 m_1 j_2 m_2 | j_1 j_2; J_{12} M_{12} \rangle \langle [p_1 q_1] j_1 [p_2 q_2] j_2 | [p_1 q_1][p_2 q_2]; [p_{12} q_{12}] J_{12} \rangle \end{aligned} \tag{31}$$

with

$$\begin{aligned} & \langle [p_1 q_1] j_1 [p_2 q_2] j_2 | [p_1 q_1][p_2 q_2]; [p_{12} q_{12}] J_{12} \rangle \\ & = [(2j_1+1)(2j_2+1)(p_{12}+q_{12}+1)(p_{12}-q_{12}+1)]^{\frac{1}{2}} \\ & \times \begin{Bmatrix} \frac{1}{2}(p_1+q_1) & \frac{1}{2}(p_2+q_2) & \frac{1}{2}(p_{12}+q_{12}) \\ \frac{1}{2}(p_1-q_1) & \frac{1}{2}(p_2-q_2) & \frac{1}{2}(p_{12}-q_{12}) \\ j_1 & j_2 & J_{12} \end{Bmatrix} \end{aligned} \tag{32}$$

The Wigner-Eckart Theorem for $SO(4)$

Eqn.(30) allows us to construct a basis defined through the group chain $SO(4) \supset SO(3) \supset SO(2)$ and to construct tensor operators $\mathbf{T}^{[pq]K}$ exhibit well-defined transformation properties with respect to the same chain of groups. It then follows from the Wigner-Eckart theorem that

$$\begin{aligned} & \langle \alpha_1 [p_1 q_1] J_1 M_1 | T^{[pq]K}_Q | \alpha_2 [p_2 q_2] J_2 M_2 \rangle \\ & = (-1)^{J_1 - M_1} \begin{pmatrix} J_1 & K & J_2 \\ -M_1 & Q & M_2 \end{pmatrix} \langle \alpha_1 [p_1 q_1] J_1 \| T^{[pq]K} \| \alpha_2 [p_2 q_2] J_2 \rangle \end{aligned} \tag{33}$$

where we have factored off the dependence of the matrix element on the $SO(2)$ representations leaving the reduced matrix element

$$\langle \alpha_1 [p_1 q_1] J_1 \| T^{[pq]K} \| \alpha_2 [p_2 q_2] J_2 \rangle$$

$$= [(2K+1)(2J_1+1)(2J_2+1)]^{\frac{1}{2}} \left\{ \begin{array}{ccc} \frac{1}{2}(p_1+q_1) & \frac{1}{2}(p_2+q_2) & \frac{1}{2}(p+q) \\ \frac{1}{2}(p_1-q_1) & \frac{1}{2}(p_2-q_2) & \frac{1}{2}(p-q) \\ J_1 & J_2 & K \end{array} \right\}$$

$$\times \langle \alpha_1 [p_1 q_1] || T^{[pq]} || \alpha_2 [p_2 q_2] \rangle \tag{34}$$

where a factor $[(p_1+q_1+1)(p_1-q_1+1)]^{\frac{1}{2}}$ has been absorbed in our definition of the reduced matrix element on the right-hand-side. Thus Eqn. (34) allows us to completely encase the dependence of the matrix elements on the quantum numbers associated with the subgroups $SO(3) \supset SO(2)$ in familiar $3nj-$symbols that may be readily computed.

We can use the above tensor operator results to compute the matrix elements of the generators of $SO(4)$.

Eigenvalues of the Casimir Operators of $SO(4)$

Recall

$$F = \mathbf{M}^2 + \mathbf{N}^2 = \frac{1}{2}(\mathbf{L}^2 + \mathbf{A}^2) \tag{11}$$

and

$$G = \mathbf{L} \cdot \mathbf{A} = \mathbf{M}^2 - \mathbf{N}^2 \tag{12}$$

Acting on an $SO(4)$ symmetrised ket and recalling from Eqn.(27) that

$$|[pq]jm\rangle \equiv |[j_1+j_2, j_1-j_2]jm\rangle \tag{35}$$

We readily find the eigenvalues for the two $SO(4)$ Casimir operators as

$$F|\alpha[pq]LM\rangle = \frac{1}{2}(p^2+2p+q^2)^2 |\alpha[pq]LM\rangle \tag{36a}$$

$$G|\alpha[pq]LM\rangle = q(p+1)|\alpha[pq]LM\rangle \tag{36b}$$

Recall that for a hydrogenic-like atom the eigenvalues of G are null and the relevant $SO(4)$ irreducible representations necessarily have $q=0$. Furthermore, from Eqn.(22) under $SO(4) \rightarrow SO(3)$

$$[n-1,0] \rightarrow [n-1] + [n-2] + \ldots [0] \tag{37}$$

and hence the states of a hydrogen-like atom may be described by the basis states

$$|[n-1,0]\ell m\rangle \qquad \ell = 0, 1, \ldots, n-1 \tag{38}$$

The $SO(4)$ irreducible representation $[n-1,0]$ is of dimension n^2 and we may identify n with the usual principal quantum number.

Two-electron $SO(4)$ **Symmetrised States**

Let us now do a worked example and construct the $SO(4)$ symmetrised states for two electrons in $n=2$ orbitals, that is for the three 2-electron configurations $2s^2$, $2s2p$ and $2p^2$. First we note that for a single electron in a $n=2$ orbital the complete set of the four orbital states span the 4-dimensional $SO(4)$ irreducible representation $[1,0]$ (for convenience I will henceforth omit the comma and just write [10] etc.). Thus we have the four states

$$|[10]2s0\rangle, \quad |[10]2p0\rangle, \quad |[10]2p1\rangle, \quad |[10]2p-1\rangle \tag{39}$$

Starting with these four orbitals we wish to form a complete set of states for two-electrons in $n=2$ orbitals.

We evaluate the Kronecker product $[10] \times [10]$ using Eqn.(28) to get

$$[10] \times [10] = [20] + [11]_+ + [11]_- + [00] \tag{40}$$

We then determine the $SO(3)$ content of each $SO(4)$ irreducible representation appearing in the right-hand-side of Eqn. (40) using Eqn. (23) to give the total orbital quantum number L as

$$[20]SPD, \quad [11]_+ P, \quad [11]_- P, [00]S \tag{41}$$

We must also remember that these states will correspond to either spin triplet states with $S = 1$ or spin singlet states with $S = 0$. The triplets will come from the antisymmetric part of Eqn.(40) ($[11]_+ + [11]_-$) and the singlets from the symmetric part ($[20] + [00]$). Thus we could rewrite Eqn.(41) as

$$[20]^1SPD, \quad [11]^3_+P, \quad [11]^3_-P, \quad [00]^1S \tag{42}$$

We note that Eqn. (42) has two ^1S states, presumably associated with those of the configurations $2s^2$ and $2p^2$ so evidently

$$|[20]^1S\rangle = a|2s^{2\ 1}S\rangle + b|2p^{2\ 1}S\rangle \tag{43a}$$
$$|[00]^1S\rangle = -b|2s^{2\ 1}S\rangle + a|2p^{2\ 1}S\rangle \tag{43b}$$

Now our problem is to determine the coefficients of the expansion. This may be done by noting from Eqn. (32) that

$$\begin{aligned}
&|[p_1q_1][p_2q_2]; [p_{12}q_{12}]J_{12}\rangle \\
&= \sum_{j_1,j_2} \langle [p_1q_1]j_1[p_2q_2]j_2|[p_1q_1][p_2q_2]; [p_{12}q_{12}]J_{12}\rangle |[p_1q_1]j_1[p_2q_2]j_2\rangle \\
&= \sum_{j_1,j_2} [(2j_1+1)(2j_2+1)(p_{12}+q_{12}+1)(p_{12}-q_{12}+1)]^{\frac{1}{2}} \left\{ \begin{array}{ccc} \frac{1}{2}(p_1+q_1) & \frac{1}{2}(p_2+q_2) & \frac{1}{2}(p_{12}+q_{12}) \\ \frac{1}{2}(p_1-q_1) & \frac{1}{2}(p_2-q_2) & \frac{1}{2}(p_{12}-q_{12}) \\ j_1 & j_2 & J_{12} \end{array} \right\} \\
&\times |[p_1q_1]j_1[p_2q_2]j_2\rangle
\end{aligned} \tag{44}$$

Thus

$$|[00]^1S\rangle = \sum_{\ell_1,\ell_2} [(2\ell_1+1)(2\ell_2+1)]^{\frac{1}{2}} \left\{ \begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \ell_1 & \ell_2 & 0 \end{array} \right\} |[10]\ell_1[10]\ell_2;^1S\rangle \tag{45}$$

The only permissible values of $\{\ell_1, \ell_2\}$ are $\ell_1 = \ell_2 = 0, 1$. Evaluation of the $9j-$symbols leads immediately to

$$|[00]^1S\rangle = \frac{1}{2}|2s^{2\ 1}S\rangle + \frac{\sqrt{3}}{2}|2p^{2\ 1}S\rangle \tag{46}$$

One may likewise determine the expansion coefficients for the other $SO(4)$ symmetrised states to give

$$\begin{aligned}
|[11]^3_\pm P\rangle &= \frac{1}{\sqrt{2}}(|2p^{2\ 3}P> \pm |2s2p\ ^3P\rangle) \\
|[20]^1D\rangle &= |2p^{2\ 1}D\rangle \\
|[20]^1P\rangle &= -|2s2p\ ^1P\rangle \\
|[20]^1S\rangle &= \frac{\sqrt{3}}{2}|2s^{2\ 1}S\rangle - \frac{1}{2}|2p^{2\ 1}S\rangle \\
|[00]^1S\rangle &= \frac{1}{2}|2s^{2\ 1}S\rangle + \frac{\sqrt{3}}{2}|2p^{2\ 1}S\rangle
\end{aligned} \tag{47}$$

Note that the states $|[11]^3_\pm P\rangle$ involve linear combinations of *odd* and *even* parity states. States of the same parity can be formed from linear combinations

$$|[p|q|]SL\rangle^\pm = \frac{1}{\sqrt{2}}(|[pq]SL\rangle \pm |[p,-q]SL\rangle) \tag{48}$$

Continuous Symmetries VII.

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The sagacious reader who is capable of reading between these lines what does not stand written in them, but is nevertheless implied, will be able to form some conception.

— Goethe

The Dynamical Group of the Hydrogen Atom

Introduction

We have found the degeneracy group of the H-atom to be $SO(4) \sim SO(3) \times SO(3) \sim SU(2) \times SU(2)$ and now seek a dynamical group for the H-atom. We first give a description of $SO(4)$ in terms of bosonic creation and annihilation operators and then obtain a realisation of the dynamical group also in terms of bosonic operators.

Boson Operators and $SO(4)$

Let us introduce the two-component boson spin operators $a_i, a_i^\dagger \quad (i,j = 1,2)$ where

$$[a_i, a_j^\dagger] = \delta_{ij} \tag{1}$$

Using the Pauli spin matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2}$$

we can write the generators of $SU(2)$ as

$$J_i = \frac{1}{2}\mathbf{a}^\dagger \sigma_i \mathbf{a} \tag{3}$$

with

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \qquad \mathbf{a}^\dagger = \begin{pmatrix} a_1^\dagger & a_2^\dagger \end{pmatrix} \tag{4}$$

The creation operators $\mathbf{a}^\dagger$ acting on the vacuum state $|0\rangle$ can be used to create an arbitrary $SU(2)$ ket $|jm\rangle$,

$$|jm\rangle = \frac{(a_1^\dagger)^{j+m}(a_2^\dagger)^{j-m}}{[(j+m)!(j-m)!]^{\frac{1}{2}}}|0\rangle \tag{5}$$

Since the group $SO(4)$ is locally isomorphic to $SU(2) \times SU(2)$ we may obtain a realisation of the generators of $SO(4)$ by putting

$$J_i = \frac{1}{2}\mathbf{a}^\dagger \sigma_i \mathbf{a} \quad and J_i' = \frac{1}{2}\mathbf{b}^\dagger \sigma_i \mathbf{b} \tag{6}$$

where

$$[a_i, a_j^\dagger] = \delta_{ij} \qquad [b_i, b_j^\dagger] = \delta_{ij} \tag{7}$$

and the components of $\mathbf{a}^\dagger$ and $\mathbf{a}$ commute with those of $\mathbf{b}^\dagger$ and $\mathbf{b}$. The $SO(4)$ kets then become

$$|jm, j'm'\rangle = \frac{(a_1^\dagger)^{j+m}(a_2^\dagger)^{j-m}(b_1^\dagger)^{j'+m'}(b_2^\dagger)^{j'-m'}}{[(j+m)!(j-m)!(j'+m')!(j'-m')!]^{\frac{1}{2}}}|0\rangle \tag{8}$$

The ladder operators in this basis then become

$$J_+ = a_1^\dagger a_2 \qquad J'_+ = b_1^\dagger b_2$$
$$J_- = a_2^\dagger a_1 \qquad J'_- = b_2^\dagger b_1 \tag{9}$$

The operators **L** and **A** then become

$$L_i = J_i + J'_i = \frac{1}{2}\left(\mathbf{a}^\dagger \sigma_i \mathbf{a} + \mathbf{b}^\dagger \sigma_i \mathbf{b}\right) \tag{10}$$

$$A_i = J_i - J'_i = \frac{1}{2}\left(\mathbf{a}^\dagger \sigma_i \mathbf{a} - \mathbf{b}^\dagger \sigma_i \mathbf{b}\right) \tag{11}$$

It is convenient to introduce the antisymmetric tensors

$$L_{ij} = -L_{ji} \qquad (i \neq j) \tag{12}$$

where

$$L_k = L_{ij} = \frac{1}{2}\left(\mathbf{a}^\dagger \sigma_k \mathbf{a} - \mathbf{b}^\dagger \sigma_k \mathbf{b}\right)$$
$$(i,j,k = 1,2,3 \quad \textit{and cyclic permutations}) \tag{13}$$

and

$$-A_i = L_{i4} = -\frac{1}{2}\left(\mathbf{a}^\dagger \sigma_i \mathbf{a} - \mathbf{b}^\dagger \sigma_i \mathbf{b}\right) \tag{14}$$

Under commutation we then have

$$[L_{ij}, L_{kl}] = i\left(\delta_{ik} L_{jl} + \delta_{il} L_{kj} + \delta_{jk} L_{il} + \delta_{jl} L_{ik}\right) \tag{15}$$

The principal quantum number of the $H-$Atom

So far we have found the degeneracy group as $SO(4)$ and the energy spectrum generating group as $SO(2,1)$. The dynamical group must contain these two groups as subgroups of some larger non-compact group. Traditionally the states of an $H-$atom are labelled by the quantum numbers $|n\ell m\rangle$. In constructing the dynamical group we want to include operators that will ladder n and ℓ but first we construct an operator L_{56} whose eigenvalues are the principal quantum number n.

Consider the operator

$$\Gamma_0 = L_{56} = \frac{1}{2}\left(\mathbf{a}^\dagger \mathbf{a} - \mathbf{b}^\dagger \mathbf{b} + 2\right) \tag{16}$$

which commutes with all the generators of $SO(4)$ and has the form of a *number operator*. If we apply L_{56} to both sides of Eqn.(8), use the commutation properties of the annihilation and creation operators and remember that

$$a_i|0\rangle \tag{17}$$

and

$$\left[a_i, a_i^{\dagger x}\right] = x a_i^{\dagger x-1} \tag{18}$$

then

$$L_{56}|jm, j'm'\rangle = (j + j' + 1)|jm, j'm'\rangle \tag{19}$$

But for a hydrogen atom $j = j'$ and $2j + 1 = n$ and hence

$$L_{56}|n\ell m\rangle = n|n\ell m\rangle \tag{19}$$

and the eigenvalues of L_{56} are just the principal quantum number n.

The operator L_{56} taken with the generators of $SO(4)$ generate the compact direct product group $SO(2) \times SO(4)$ which should be a subgroup of our non-compact dynamical group.

The Dynamical Group Obtained

Let us consider two further scalar operators,

$$T = L_{45} = \frac{1}{2}\left(\mathbf{a}^\dagger \sigma_2 \mathbf{b}^\dagger - \mathbf{a}\sigma_2 \mathbf{b}\right) \tag{20}$$

and

$$S = L_{46} = \frac{1}{2}\left(\mathbf{a}^\dagger \sigma_2 \mathbf{b}^\dagger + \mathbf{a}\sigma_2 \mathbf{b}\right) \tag{21}$$

Under commutation,

$$[L_{45}, L_{46}] = iL_{56} \tag{22}$$

Now consider

$$N_\pm = L_{45} \mp iL_{46} \tag{23}$$

or

$$N_+ = \mathbf{a}^\dagger \sigma_2 \mathbf{b}^\dagger = -i(a_1^\dagger b_2^\dagger - a_2^\dagger b_1^\dagger) \tag{24a}$$

$$N_- = \mathbf{a}\sigma_2 \mathbf{b} = -i(a_1 b_2 - a_2 b_1) \tag{24b}$$

Since

$$[L_{56}, N_\pm] = \pm N_\pm \tag{25}$$

we anticipate that $N_\pm$ raises or lowers n by ± 1.

Consider the ket

$$|n\ell\ell\rangle \equiv |jj, jj\rangle \tag{26}$$

which has $n = 2j + 1$ and $\ell = n - 1$,

$$\begin{aligned} iN_+|n\ell\ell\rangle &= (a_1^\dagger b_2^\dagger - a_2^\dagger b_1^\dagger)|jj, jj\rangle \\ &= \frac{\left(a_1^{\dagger 2j+1} b_1^{\dagger 2j} b_2^\dagger - a_1^{\dagger 2j} a_2^\dagger b_1^{\dagger 2j+1}\right)}{2j!}|0\rangle \\ &= n\left\{|j + \frac{1}{2}\ j + \frac{1}{2}, j + \frac{1}{2}\ j - \frac{1}{2}\rangle - |j + \frac{1}{2}\ j - \frac{1}{2}, j + \frac{1}{2}\ j + \frac{1}{2}\rangle\right\} \\ &= (-1)^{n-1} n\left[1 - (-1)^{n+\ell'}\right](2\ell' + 1)^{\frac{1}{2}} \\ &\times \begin{pmatrix} \frac{n}{2} & \frac{n}{2} & \ell' \\ \frac{n}{2} & \frac{n}{2} - 1 & -n + 1 \end{pmatrix} |n + 1\ell'\ell\rangle \end{aligned} \tag{27}$$

where we have transformed to the $n\ell m$ basis. Inspection of the $3j-$symbol together with the phase factor $(-1)^{n+\ell'}$ shows that ℓ' is limited to $\ell' = n - 1 = \ell$. Explicit evaluation of the $3j-$symbol leads to

$$iN_+|n\ell\ell\rangle = (-1)^n 2n\sqrt{6(2n+1)}|n + 1\ell\ell\rangle \tag{28}$$

where $\ell = n - 1$.

Similarly,

$$-iN_-|n + 1\ell\ell\rangle = \frac{(-1)^n 2}{\sqrt{6(2n+1)}}|n\ell\ell\rangle \tag{29}$$

and

$$[N_+, N_-] = -2L_{56} \tag{30}$$

The operators L_{ij}, L_{i4}, L_{45} and L_{46} allow us to ladder from the vacuum state $|0\rangle$ to any ket $|n\ell m\rangle$. However, this set of operators, together with L_{56} do not close under commutation, to do that we need two additional vector operators $\mathbf{M}$ and $\mathbf{\Gamma}$ with components

$$M_i = L_{i5} = i[L_{i4}, L_{45}] = -\frac{1}{2}\left(\mathbf{a}^\dagger \sigma_i C \mathbf{b}^\dagger - \mathbf{a}\sigma_i C \mathbf{b}\right) \tag{31}$$

$$\Gamma_i = L_{i6} = -i[L_{i5}, L_{56}] = -\frac{i}{2}\left(\mathbf{a}^\dagger \sigma_i C \mathbf{b}^\dagger + \mathbf{a}\sigma_i C \mathbf{b}\right) \tag{32}$$

where

$$C = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{33}$$

We now have a set of 15 operators, $\{L_{ij}, L_{i4}, L_{i5}, L_{45}, L_{46}, L_{56}\}$ that close under commutation:

$$[L_{ab}, L_{cd}] = -i(g_{ac}L_{bd} + g_{ad}L_{cb} + g_{bc}L_{da} + g_{bd}L_{ac}) \tag{34}$$

where g_{ab} is associated with the metric $(- \; - \; - \; - \; + \; +)$. The corresponding Lie algebra formed by the 15 operators is that associated with the non-compact group $SO(4,2)$ which holds invariant the real form

$$-\sum g_{ab} x_a x_b \tag{35}$$

and is isomorphic to the group $SU(2,2)$ that holds invariant the complex form

$$z_1 z_1^* + z_2 z_2^* - z_3 z_3^* - z_4 z_4^* \tag{36}$$

Since the operators of $SO(4,2)$ allow us to pass from any ket $|n\ell m\rangle$ to any other ket $|n'\ell' m'\rangle$ we conclude that $SO(4,2)$ contains a single irreducible representation that covers all the states of a hydrogenic atom and is indeed the dynamical group of a hydrogenic atom.

Casimir Operators of $SO(4,2)$

The group $SO(4,2)$ is a group of rank 3 and hence has three independent Casimir operators which we may take as

$$C_2 = L_{ab} L^{ab} \quad C_3 = \varepsilon_{abcdef} L^{ab} L^{cd} L^{ef} \quad C_4 = L_{ab} L^{bc} L_{cd} L^{da} \tag{37}$$

where

$$L^{ab} = g_{ab} L_{ab} \tag{38}$$

Acting on an arbitrary ket $|n\ell m\rangle$ we find the eigenvalues

$$C_2 = 6 \qquad C_3 = 0 \qquad C_4 = 0 \tag{39}$$

Exercises

1. Show that the set of 15 operators

$$\begin{aligned}
\mathbf{L} &= \mathbf{r} \times \mathbf{p} \\
\mathbf{A} &= \frac{1}{2}\mathbf{r}\mathbf{p}^2 - \mathbf{p}(\mathbf{r}\cdot\mathbf{p}) - \frac{1}{2}\mathbf{r} \\
\mathbf{M} &= \frac{1}{2}\mathbf{r}\mathbf{p}^2 - \mathbf{p}(\mathbf{r}\cdot\mathbf{p}) + \frac{1}{2}\mathbf{r} \\
\mathbf{\Gamma} &= r\mathbf{p} \\
T &= \mathbf{r}\cdot\mathbf{p} - i \\
\Gamma_0 &= \frac{1}{2}(r\mathbf{p}^2 + r) \\
S &= \frac{1}{2}(r\mathbf{p}^2 - r)
\end{aligned} \tag{40}$$

   give an alternative realisation of the generators of $SO(4,2)$.

2. Show that in the above realisation the Casimir invariants and their eigenvalues are

$$\begin{aligned}
C_2 &= \mathbf{L}^2 + \mathbf{A}^2 - \mathbf{M}^2 - \mathbf{\Gamma}^2 + S^2 - T^2 - \Gamma_0^2 = -3 \\
C_3 &= 0 \\
C_4 &= 0
\end{aligned} \tag{41}$$

3. Use the commutation relations of the generators of $SO(4,2)$ to establish the following subgroups of $SO(4,2)$

$SO(2) \times SO(4)$	$(L_{56})(L_{ij}, L_{i4})$
$SO(4,1)$	$L_{ij}, L_{i4}, L_{i5}, L_{45}$
$SO(4,1)'$	$L_{ij}, L_{i4}, L_{i6}, L_{46}$
$SO(3,2)$	$L_{ij}, L_{i5}, L_{i6}, L_{56}$
$SO(3,1)$	L_{ij}, L_{i6}
$SO(3,1)'$	L_{ij}, L_{i5}
$SO(4)$	L_{ij}, L_{i4}
$SO(2,1) \times SO(3)$	$(L_4 5, L_{46}, L_{56})(L_{ij})$
$SO(2,1) \times SO(2,1)$	$(N_\pm^1, N_3^1)(N_\pm^2, N_3^2)$

(42)

where in the last case we define the generators as

$$N_1^1 = \frac{1}{2}(L_{46} + L_{35})$$
$$N_2^1 = \frac{1}{2}(L_{45} - L_{36})$$
$$N_3^1 = \frac{1}{2}(L_{56} + L_{34}) \tag{43}$$

and

$$N_1^2 = \frac{1}{2}(L_{46} - L_{35})$$
$$N_2^2 = \frac{1}{2}(L_{45} + L_{36})$$
$$N_3^2 = \frac{1}{2}(L_{56} - L_{34}) \tag{44}$$

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

Continuous Symmetries VIII.

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Some Aspects of Two-electron Systems

..his Majesty's mathematicians, having taken the height of my body by the help of a quadrant, and finding it to exceed theirs in the proportion of twelve to one, they concluded from the similarity of their bodies, that mine must contain at least 1724 of theirs, and consequently would require as much food as was necessary to support that number of Lilliputans.
—Johnathan Swift *Gulliver's travels (1726)*

Introduction

We saw in the previous lectures how one may construct $SO(4)-$symmetrised states involving two electrons in orbitals having a given principal quantum number n. This resulted in forming linear combinations of states involving various two-electron configurations but only those that are degenerate in the $SO(4)$ scheme. We also found that it was possible to describe the complete set of states of a hydrogenic-like atom in terms of a single irreducible representation of the dynamical group $SO(4,2) \sim SU(2,2)$. Suppose we were to consider two-electrons. We might consider the states formed from the direct product of that irreducible representation with itself or better still resolving the direct product into its symmetric and antisymmetric parts which could be respectively associated with spin singlets and triplets. In this lecture I want to sketch how one might proceed to construct states symmetrised with respect to a group chain of the form

$$U(2,2) \supset U(2) \times U(2) \supset SU(2) \times SU(2) \sim SO(4) \supset SO(3) \supset SO(2) \tag{1}$$

The Hydrogenic Representation

The systematic labelling of the irreducible representations of the non-compact group $U(p,q)$ group has been developed by King and Wybourne[1] and is based upon its maximal compact subgroup $U(q) \times U(p)$. Furthermore they give an algorithm to evaluate the $U(p,q) \rightarrow U(q) \times U(p)$ branching rules. For the hydrogen atom we are interested in the case with $p = q = 2$ and in particular the irreducible representation they label as

$$H_0 = \{1(\bar{0};0)\} \tag{2}$$

and under $U(2,2) \rightarrow U(2) \times U(2)$

$$H_0 \rightarrow \sum_{m=0}^{\infty} \{\bar{m}\} \times \{m\} \tag{3}$$

Under $U(2) \times U(2) \rightarrow SU(2) \times SU(2) \sim SO(4)$

$$\{\bar{m}\} \times \{m\} \rightarrow \{m\} \times \{m\} \rightarrow [m,0] \tag{4}$$

Thus the irreducible representation H_0 does indeed contain *all* the discrete states of the $H-$atom.

More generally we have under $U(2) \rightarrow SU(2)$ the branching rules

$$\{\lambda_1\lambda_2\} \rightarrow \{\lambda_1 - \lambda_2\}$$

$$\{\overline{\lambda_1\lambda_2}\} \rightarrow \{\lambda_1 - \lambda_2\} \tag{5}$$

Thus, for example,

$$\{42\} \rightarrow \{2\}$$

$$\{\overline{42}\} \rightarrow \{2\}$$

$$\{m\} \rightarrow \{m\}$$

$$\{\overline{m}\} \rightarrow \{m\}$$

Finally, we note that an arbitrary irreducible representation $\{\bar{\mu}\} \times \{\nu\}$ of the direct product group $U(2) \times U(2)$ goes irreducibly into an irreducible representation of $SO(4)$ as

$$\{\bar{\mu}\} \times \{\nu\} \rightarrow [\frac{\mu_1 - \mu_2 + \nu_1 - \nu_2}{2}, \frac{\mu_1 - \mu_2 - \nu_1 + \nu_2}{2}] \tag{6}$$

Thus, for example

$$\{\overline{41}\} \times \{32\} \rightarrow [2,1]$$
$$\{\overline{32}\} \times \{41\} \rightarrow [2,-1]$$
$$\{\bar{m}\} \times \{m\} \rightarrow [m,0]$$

The Two-electron Basis States

The Kronecker product $H_0 \times H_0$ may be resolved into its symmetric and antisymmetric parts as[2]

$$H_0 \otimes \{2\} = \sum_{k=0}^{\infty} \{2(\overline{2k}; 2k)\} \tag{7a}$$

$$H_0 \otimes \{1^2\} = \sum_{k=0}^{\infty} \{2(\overline{2k+1}; 2k+1)\} \tag{7b}$$

The symmetric terms are associated with spin singlets, $S = 0$, and the antisymmetric terms with spin triplets, $S = 1$.

The next step is to identify the $U(2) \times U(2)$ content of each of the infinite dimensional irreducible representations appearing on the right-hand-side of (7a) and (7b). This requires use of the algorithms described in ref. (1). We now give a partial table:-

$\{2(\overline{0}; 0)\} \rightarrow$			
$\{\overline{0}\} \times \{0\}$	$+ \{\overline{1}\} \times \{1\}$	$+ \{\overline{1^2}\} \times \{1^2\}$	$+ \{\overline{2}\} \times \{2\}$
$+ \{\overline{21}\} \times \{21\}$	$+ \{\overline{2^2}\} \times \{2^2\}$	$+ \{\overline{3}\} \times \{3\}$	$+ \{\overline{31}\} \times \{31\}$
$+ \{\overline{32}\} \times \{32\}$	$+ \{\overline{3^2}\} \times \{3^2\}$	$+ \{\overline{4}\} \times \{4\}$	$+ \{\overline{41}\} \times \{41\}$
$\{2(\overline{1}; 1)\} \rightarrow$			
$\{\overline{1}\} \times \{1\}$	$+ \{\overline{1^2}\} \times \{2\}$	$+ \{\overline{2}\} \times \{1^2\}$	$+ \{\overline{2}\} \times \{2\}$
$+ \{\overline{21}\} \times \{21\}$	$+ \{\overline{21}\} \times \{3\}$	$+ \{\overline{2^2}\} \times \{31\}$	$+ \{\overline{3}\} \times \{21\}$
$+ \{\overline{3}\} \times \{3\}$	$+ \{\overline{31}\} \times \{2^2\}$	$+ \{\overline{31}\} \times \{31\}$	$+ \{\overline{31}\} \times \{4\}$
$+ \{\overline{32}\} \times \{32\}$	$+ \{\overline{32}\} \times \{41\}$	$+ \{\overline{3^2}\} \times \{42\}$	$+ \{\overline{4}\} \times \{31\}$
$\{2(\overline{2}; 2)\} \rightarrow$			
$\{\overline{2}\} \times \{2\}$	$+ \{\overline{21}\} \times \{3\}$	$+ \{\overline{2^2}\} \times \{4\}$	$+ \{\overline{3}\} \times \{21\}$
$+ \{\overline{3}\} \times \{3\}$	$+ \{\overline{31}\} \times \{31\}$	$+ \{\overline{31}\} \times \{4\}$	$+ \{\overline{32}\} \times \{41\}$
$\{2(\overline{3}; 3)\} \rightarrow$			
$\{\overline{3}\} \times \{3\}$	$+ \{\overline{31}\} \times \{4\}$	$+ \{\overline{32}\} \times \{5\}$	$+ \{\overline{3^2}\} \times \{6\}$
$\{2(\overline{4}; 4)\} \rightarrow$			
$\{\overline{4}\} \times \{4\}$	$+ \{\overline{41}\} \times \{5\}$	$+ \{\overline{42}\} \times \{6\}$	$+ \{\overline{43}\} \times \{7\}$

(8)

(A more extensive table can be found at my website.)

Recall that at the $U(2)\times U(2)$ level the infinite discrete states of an H-atom involve the representations

$$\{\bar{0}\}\{0\}+\{\bar{1}\}\{1\}+\{\bar{2}\}\{2\}+\{\bar{3}\}\{3\}+\{\bar{4}\}\{4\}+\ldots$$

Two-electron states may be formed by taking products of pairs of the above irreducible representations with each set of states being associated with a pair of principal quantum numbers (n_1,n_2). When $n_1\neq n_2$ the various orbital states have spins $S=0,1$. When $n_1=n_2$ care must be taken with antisymmetrisation, this amounts to taking symmetrised products of the pair of identical $U(2)\times U(2)$ irreducible representations . Technically this may be done using the theory of plethysm[3,4]. In particular we have for the symmetric part of $\{m\}\times\{m\}$

$$\{m\}\otimes\{2\}=\{2m\}+\{2m-2,2\}+\{2m-4,4\}+\ldots \tag{9a}$$

and for the antisymmetric part of the square

$$\{m\}\otimes\{1^2\}=\{2m-1,1\}+\{2m-3,3\}+\{2m-5,5\}+\ldots \tag{9b}$$

and for $\{\bar{m}\}\times\{\bar{m}\}$

$$\{\bar{m}\}\otimes\{2\}=\{\overline{2m}\}+\{\overline{2m-2,2}\}+\{\overline{2m-4,4}\}+\ldots \tag{10a}$$

and for the antisymmetric part of the square

$$\{\bar{m}\}\otimes\{1^2\}=\{\overline{2m-1,1}\}+\{\overline{2m-3,3}\}+\{\overline{2m-5,5}\}+\ldots \tag{10b}$$

leading to

$$(\{\bar{m}\}\{m\})\otimes\{2\}=\{\bar{m}\}\otimes\{2\}\cdot\{m\}\otimes\{2\}+\{\bar{m}\}\otimes\{1^2\}\cdot\{m\}\otimes\{1^2\} \tag{11a}$$

$$(\{\bar{m}\}\{m\})\otimes\{1^2\}=\{\bar{m}\}\otimes\{1^2\}\cdot\{m\}\otimes\{2\}+\{\bar{m}\}\otimes\{2\}\cdot\{m\}\otimes\{1^2\} \tag{11b}$$

Thus, for example,

$$\begin{aligned}(\{\bar{1}\}\{1\})\otimes\{2\}&=\{\bar{1}\}\otimes\{2\}\cdot\{1\}\otimes\{2\}+\{\bar{1}\}\otimes\{1^2\}\cdot\{1\}\otimes\{1^2\}\\&=\{\bar{2}\}\{2\}+\{\bar{1^2}\}\{1^2\}\end{aligned} \tag{12a}$$

$$\begin{aligned}(\{\bar{1}\}\{1\})\otimes\{1^2\}&=\{\bar{1}\}\otimes\{1^2\}\cdot\{1\}\otimes\{2\}+\{\bar{1}\}\otimes\{2\}\cdot\{1\}\otimes\{1^2\}\\&=\{\bar{1^2}\}\{2\}+\{\bar{2}\}\{1^2\}\end{aligned} \tag{12b}$$

Those in (12a) are symmetrical in the orbital space and hence will belong to spin singlets ($S=0$) while those in (12b) are antisymmetrical in the orbital space and will belong to spin triplets ($S=1$). These we could identify with the two-electron states

$$(S=0)\ |2s^2\ {}^1S\rangle,\ |2p^2\ {}^1S\rangle,\ |2p^2\ {}^1D\rangle,\ |2s2p^1P\rangle \tag{13a}$$

$$(S=1)\ |2s2p^3P\rangle,\ |2p^2\ {}^3P\rangle \tag{13b}$$

These are just the two-electron states we described in Lecture VI in Eqn. (47).

Description of the two-electron states

There is an infinite set of discrete two-electron states described by an infinite set of infinite-dimensional irreducible representations of $U(2,2)$. These states may be each described by a set of quantum numbers associated with the irreducible representation labels arising in the group chain

$$U(2,2)\supset U(2)\times U(2)\supset SO(4)\supset SO(3)\supset SO(2) \tag{14}$$

The decompositions occurring along every step in the chain are multiplicity free and hence the set of irreducible representation labels unambiguously defines every two-electron state. The $U(2,2)$ irreducible representations are all of the form $\{2(\bar{m};m)\}$ and hence a general two-electron basis state could be described as

$$\{2(\bar{m};m)\}\{\bar{\mu}\}\times\{\nu\}[pq]LM\rangle \tag{15}$$

with $[pq]$ being determined from Eqn.(6) and the values of the L quantum number from

$$[pq]\rightarrow[p]+[p-1]+\ldots+[|q|] \tag{16}$$

A ket symmetrised as in Eqn. (15) can be expanded as a sum of products of one-particle kets such that

$$
\begin{aligned}
&|\{2(\bar{m};m)\}\{\bar{\mu}\}\times\{\nu\}[pq]LM\rangle \\
&=\sum_{p_1,p_2,\ell_1,\ell_2}\langle\{1(\bar{0};0)\}\{\bar{p_1}\}\times\{p_1\}[p_10]\ell_1m_1;\{1(\bar{0};0)\}\{\bar{p_2}\}\times\{p_2\}[p_20]\ell_2m_2|\{2(\bar{m};m)\}\{\bar{\mu}\}\times\{\nu\}[pq]LM\rangle \\
&\times|\{1(\bar{0};0)\}\{\bar{p_1}\}\times\{p_1\}[p_10]\ell_1m_1\rangle|\{1(\bar{0};0)\}\{\bar{p_2}\}\times\{p_2\}[p_20]\ell_2m_2\rangle \qquad (17)
\end{aligned}
$$

The first term on the right-hand-side of (17) is a generalised coupling coefficient which may be factorised to a triple product of coupling coefficients as

$$
\begin{aligned}
&\langle\{1(\bar{0};0)\}\{\bar{p_1}\}\times\{p_1\}[p_10]\ell_1m_1;\{1(\bar{0};0)\}\{\bar{p_2}\}\times\{p_2\}[p_20]\ell_2m_2|\{2(\bar{m};m)\}\{\bar{\mu}\}\times\{\nu\}[pq]\rangle \\
&=\langle\{1(\bar{0};0)\}\{\bar{p_1}\}\times\{p_1\}[p_10];\{1(\bar{0};0)\}\{\bar{p_2}\}\times\{p_2\}[p_20]|\{2(\bar{m};m)\}\{\bar{\mu}\}\times\{\nu\}[pq]\rangle \\
&\times\langle[p_10]\ell_1;[p_20]\ell_2|[pq]L\rangle \\
&\times\langle\ell_1m_1;\ell_2m_2|LM\rangle \qquad (18)
\end{aligned}
$$

The third coupling coefficient we recognise as the standard CG-coefficient of angular momentum theory while the second is the $SO(4)\supset SO(3)$ coupling coefficient given as Eqn.(44) of Lecture VI. The first coupling coefficient could be further factorised as

$$
\begin{aligned}
&\langle\{1(\bar{0};0)\}\{\bar{p_1}\}\times\{p_1\}[p_10];\{1(\bar{0};0)\}\{\bar{p_2}\}\times\{p_2\}[p_20]|\{2(\bar{m};m)\}\{\bar{\mu}\}\times\{\nu\}[pq]\rangle \\
&=\langle\{1(\bar{0};0)\}\{\bar{p_1}\}\times\{p_1\};\{1(\bar{0};0)\}\{\bar{p_2}\}\times\{p_2\}|\{2(\bar{m};m)\}\{\bar{\mu}\}\times\{\nu\}\rangle \\
&\times\langle\{\bar{p_1}\}\times\{p_1\}[p_10];\{\bar{p_2}\}\times\{p_2\}[p_20]|\{\bar{\mu}\}\times\{\nu\}[pq]\rangle \qquad (19)
\end{aligned}
$$

Neither of these coupling coefficients appear in the literature. The orthognality conditions on isoscalar factors[5] are such that the second factor can be, at most, a phase which we shall take as $+1$ with the first factor absorbing the phase. This leaves the first factor

$$\langle\{1(\bar{0};0)\}\{\bar{p_1}\}\times\{p_1\};\{1(\bar{0};0)\}\{\bar{p_2}\}\times\{p_2\}|\{2(\bar{m};m)\}\{\bar{\mu}\}\times\{\nu\}\rangle \qquad (20)$$

to be determined.

Two-electron states and $U(2)\times U(2)$ irreducible representations

Any two-electron state transforming under $U(2)\times U(2)$ as $\{\overline{p_1q_1}\}\times\{p_2q_2\}$ may be associated with one or more pairs of principal quantum numbers (n_1,n_2). We may determine these pairs as follows:- Let

$$m_1=\min(q_1+1,q_2+1)\qquad and\qquad m_2=\max(p_1+1,p_2+1) \qquad (21)$$

then

$$(n_1,n_2)=\{(m_1,m_2),\ (m_1+1,m_2-1),\ \ldots,\ (m_1+x,m_2-x)\} \qquad (22)$$

where x is such that $(n_2\geq n_1)$. Thus, for example,

$$
\begin{aligned}
\{\bar{3}\}\times\{3\}&\in\{(1,4),\ (2,3)\} \\
\{\overline{53}\}\times\{62\}&\in\{(4,6),\ (5,5)\} \\
\{\overline{61}\}\times\{52\}&\in\{(3,6),\ (4,5)\}
\end{aligned}
$$

Note that under $U(2,2)\rightarrow U(2)\times U(2)$ the decomposition of the irreducible representation $\{2(\bar{m};m)\}$ always yields irreducible representations $\{\bar{\mu}\}\times\{\nu\}$ of $U(2)\times U(2)$ such that the weights of $\{\bar{\mu}\}$ and $\{\nu\}$ are the same. i.e.

$$\omega_\mu=\omega_\nu \qquad (23)$$

Assigning quantum numbers

A determination of the isoscalar factor in Eqn. (20) would immediately allow one to expand any symmetrised two-electron state as a linear combination of products of one-electron states. Inspection of the irreducible representations appearing in Eqn. (8) permits some straightforward assignments:-

$$
\begin{aligned}
\{2(\bar{0};0)\}\{\bar{0}\}\times\{0\}[00]&\sim\ |1s^2\,{}^1S\rangle \\
\{2(\bar{0};0)\}\{\bar{1}\}\times\{1\}[10]&\sim\ |1s2s\,{}^1S\rangle,\ |1s2p\,{}^1P\rangle \\
\{2(\bar{1};1)\}\{\bar{1}\}\times\{1\}[10]&\sim\ |1s2s\,{}^3S\rangle,\ |1s2p\,{}^3P\rangle
\end{aligned}
$$

$$\{2(\bar{0};0)\}\{\overline{1^2}\} \times \{1^2\}[00] \sim \frac{1}{2}|2s^{2\,1}S\rangle + \frac{\sqrt{3}}{2}|2p^{2\,1}S\rangle$$
$$\{2(\bar{1};1)\}\{\bar{2}\} \times \{2\}[20] \sim \{|1s3s^3S\rangle,\ |1s3p^3P\rangle,\ |1s3d^3D\rangle\} \quad (24)$$

A problem arises when one considers the states associated with the $\{\bar{2}\} \times \{2\}$ states of $U(2) \times U(2)$ as this irreducible representation occurs with three irreducible representations of $U(2,2)$, namely the irreducible representations $\{2(\bar{0};0)\}$, $\{2(\bar{1};1)\}$, $\{2(\bar{2};2)\}$. It follows from Eqn. (22) that these three sets of states are associated with the principal quantum number pairs $(1,3)$, $(2,2)$. The $S = 1$ arising from $(1,3)$ can only be assigned as in Eqn. (24). There remain two sets of 9 $S = 0$ states, one set coming from $(1,3)$ and the other from $(2,2)$. One cannot simply assign these to $\{2(\bar{0};0)\}$, $\{2(\bar{2};2)\}$ without additional information which must come either from the solution of Eqn. (8) or from explicit construction of the states by use of the ladder operators of the dynamical group $U(2,2)$.

Concluding remarks

We end with two open problems that I am content to leave to the future.

1. Find an explicit form for the isoscalar factors defined in Eqn. (8).
2. Use the ladder operators of $U(2,2)$ to give an explicit expansion of symmetrised two-electron states in two-electron configuration space.

Note that while for a single electron one has a dynamical group equipped with a complete set of ladder operators that allow one to move from any discrete state to any other discrete state such is not the case for a many-electron atom. One can only ladder within a given irreducible representation of $U(2,2)$.

I have no clear idea where this will lead to but without solving such problems one does not know what new problems may arise, possibly in entirely different fields such as in the theory of special functions.

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Continuous Symmetries IX.

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Maybe history repeats itself - but I must have the facts.
— *Alamut Ambush xii,* A. Price (1971)

$SO(4)$ Symmetry and Doubly Excited States

Introduction

In this lecture we extend lecture VI to an examination of some of the properties of doubly excited states of two-electron atoms starting with some historical remarks.

A little History

In 1959 Layzer[1] introduced the concept of an electron configuration *complex*. A complex consisted of all those $N-$electron configurations involving occupation of orbitals characterised by the same principal quantum number n. Thus a given complex can be specified by simply giving (N,n). Thus the complex $(2,2)$ consists of the configuration set

$$2s^2 + 2s2p + 2p^2 \tag{1}$$

while $(3,2)$ consists of

$$2s^2 2p + 2s2p^2 + 2p^3 \tag{2}$$

and $(2,3)$ consists of

$$3s^2 + 3s3p + 3s3d + 3p^2 + 3p3d + 3d^2 \tag{3}$$

etc.

Note that for the two-electron complexes $(2,n)$ there are $n(n+1)/2$ two-electron configurations and that there are configurations of both parities in a given complex. Layzer asserted that configuration interaction within a complex was a fundamental feature of atomic spectra. This feature he also associated with his $Z-$expansion model for the properties of complexes. It was found that if one diagonalised the Coulomb repulsion term in the complex $(2,2)$ one obtained for the two ^1S states

$$|^1S_a\rangle = -0.476|2s^{21}S\rangle + 0.880|2p^{21}S\rangle \tag{4a}$$

$$|^1S_b\rangle = -0.880|2s^{21}S\rangle - 0.476|2p^{21}S\rangle \tag{4b}$$

This strong configuration interaction between $2s^2$ and $2p^2$ had been noted by Condon and Shortley[2] who pointed out that the energy ratio

$$\frac{E(^1S) - E(^1D)}{E(^1S) - E(^3P)} = \frac{3}{5} \tag{5}$$

should, in the absence of configuration interaction, be independent of the choice of Slater radial integrals. The ratio showed strong departures from $\frac{3}{2}$.

Could one have predicted the coefficients appearing in (4a) and (4b)? To that end Wulfman[3] and Alper and Sinanoŏglu[4] introduced a calculation based upon the group $SO(4)$ much as outlined in lecture VI. Their results were surprisingly close to the values given in (4). Butler and Wybourne[5] asked "Is the Group R_4 an Approximate Symmetry for Many-Electron Theory ?" pointing out that both sets of authors had made a phase error which when corrected destroyed the agreement (see[6,7] for further details).

Approximate dynamical symmetry of two-electron atoms

Bendar[8] discussed some of the properties of hydrogenic electron repulsion integrals in terms of the $O(4,2)$ group while Butler *etal*[9] tabulated algebraic expressions for the integrals. Wulfman and Kumei[10] tried to approximate hydrogenic Coulomb integrals in terms of the generators of the $O(4,2)$

group. Wulfman[11] then realised that one could obtain an alternative realisation for two-electron systems by requiring that the *difference* in the Runge-Lenz vectors of the two electrons be minimised rather than their *sum*. At first this seems a trivial change as the $SO(4)$ group structure remains, the Kronecker products, $SO(4) \rightarrow SO(3)$ branching rules and the commutation relations are unchanged. However, the two-electron $SO(4)$ basis states are not quite the same as those where the generators are built from the the sum of the Runge-Lenz vectors of the two electrons. The recoupling analogue of Eq.(45) of Lecture VI can differ by at most a phase but in this case a critically important phase. Wulfman[11] obtained

$$\begin{aligned}
&|[n_1-1][n_2-1];[PQ]LM\rangle \\
&= \sum_{\ell_1,\ell_2} (-1)^{\ell_2-n_2+1}[(2\ell_1+1)(2\ell_2+1)(P+Q+1)(P-Q+1)]^{\frac{1}{2}} \left\{ \begin{array}{ccc} \frac{1}{2}(n_1-1) & \frac{1}{2}(n_1-1) & \ell_1 \\ \frac{1}{2}(n_2-1) & \frac{1}{2}(n_2-1) & \ell_2 \\ \frac{1}{2}(P+Q) & \frac{1}{2}(P-Q) & L \end{array} \right\} \\
&\times |[n_1-1]\ell_1[n_2-1]\ell_2;LM\rangle \qquad (6)
\end{aligned}$$

Explicit evaluation then yields

$$|[00]^1S\rangle = -\tfrac{1}{2}|2s^{2\,1}S\rangle + \tfrac{\sqrt{3}}{2}|2p^{2\,1}S\rangle \qquad (7a)$$

$$|[20]^1S\rangle = -\frac{\sqrt{3}}{2}|2s^{2\,1}S\rangle - \tfrac{1}{2}|2p^{2\,1}S\rangle \qquad (7b)$$

which is remarkably close to (4a) and (4b) respectively, and indeed was what was found in the original incorrect calculations[3,4].

History is just a collection of footnotes?
— *Natterjack* Niall Duthie (Faber&Faber 1996)

Why does it Work?

The agreement between (4) and (7) is rather remarkable and demands an explanation. Imagine you have two electrons in a doubly excited state. Classically you would have said the most likely arrangement of the two electrons would be on the opposite sides of the central nucleus, rather like a XYX molecule. Recall the generators of $SO(4)_{12}$ have been chosen to involve the *difference* in the Runge-Lenz operators for the pair of electrons. As Wulfman showed[10,11] this has the effect of giving a good approximation to the Coulomb repulsion contribution to the energy of the two-electron states. Note that the Wulfman and Kumei paper[10] plays the key role in the analysis. A point often missed in subsequent publications.

$U(4) \rightarrow SO(4)$ Models

There has been much emphasis in the literature on grouping the various $SO(4)$ irreducible representations into supermultiplets treating the atom very much like a XYX molecule[12-16]. To that end attempts have been made to embed the group $SO(4)$ into the higher group $U(4)$ very much as done in vibron models of molecules[17,18]. Basically the idea has been to embed the $O(4)$ states of the one-electron Coulomb problem into a $U(4)$ and then the states of the two-electron problem are embedded in a coupled $U(4)_1 \times U(4)_2$ group[14] with the two-electron states being classified in terms of the group chain

$$U(4)_1 \times U(4)_2 \supset U(4)_{12} \supset O(4)_{12} \supset O(3)_{12} \qquad (8)$$

The problem with such a model is that it inevitably leads to spurious states and their interpretation is by no means obvious. Let us sketch an alternative possibility based upon the group $SO(5)$.

Sketch of a $SO(5)$ model for doubly excited states

We first note that under $SO(5) \rightarrow SO(4)$ we have

$$[n-1] \rightarrow [n-1] + [n-2] + \ldots + [0] \qquad (9)$$

and hence we can cover the complete set of orbital states of a hydrogen atom, up to principal quantum number n, in a single irreducible representation $[n-1]$ of $SO(5)$. This irreducible representation is of

degree

$$Dim[n-1] = \frac{n(n+1)(2n+1)}{2} \tag{10}$$

For two-electrons, the complete set of $S = 0$ states involving principal quantum numbers up to n span the $SO(5)$ irreps that arise in the $SO(5)$ plethysm $[n-1] \otimes \{2\}$ of degree

$$Dim[n-1] \otimes \{2\} = \frac{n(n+1)(n+2)(2n+1)(2n^2-n+3)}{72} \tag{11a}$$

while the $S = 1$ states come from the plethysm $[n-1,0] \otimes \{1^2\}$ of degree

$$\frac{(n-1)n(n+1)(2n+1)(2n^2+5n+6)}{72} \tag{11b}$$

One notes that under $SO(5) \rightarrow SO(4)$ the branching rule[19,20] is

$$[\lambda] \rightarrow [\lambda/M] \tag{12}$$

with the understanding that for two-part partitions on the right-hand-side of (12) we have the equivalence

$$[\lambda_1\lambda_2] \equiv [\lambda_1\lambda_2]_+ + [\lambda_1\lambda_2]_- \tag{13}$$

where the subscript $\pm$ signifies that the second part of the partition is $\pm$. Thus $[21]_- = [2,-1]$ while $[21]_+ = [2,1]$.

Now consider the case of $n = 3$. The one-electron states span the [2] irreducible representation of $SO(5)$ and

$$[2] \otimes \{2\} = [4] + [2^2] + [2] + [0] \quad S = 0 \tag{14a}$$

$$[2] \otimes \{1^2\} = [31] + [1^2] \quad S = 1 \tag{14b}$$

Note that for $SO(5)$ in general the terms in the plethysm $[n] \otimes \{2\}$ comprise all irreducible representations of $SO(5)$ involving at most two *even* parts with with the sum of the two parts $\leq 2n$ while the terms in the plethysm $[n] \otimes \{1^2\}$ comprise all irreducible representations of $SO(5)$ involving two *odd* parts with with the sum of the two parts $\leq 2n$. Thus, for example,

$$[3] \otimes \{2\} = [6] + [42] + [4] + [2^2] + [2] + [0]$$
$$[3] \otimes \{1^2\} = [51] + [3^2] + [31] + [1^2]$$

Under $SO(5) \rightarrow SO(4)$ one has, for example,

$$\begin{aligned}
[4] &\rightarrow [4] + [3] + [2] + [1] + [0] \\
[2^2] &\rightarrow [22]_+ + [22]_- + [21]_+ + [21]_- + [2] \\
[2] &\rightarrow [2] + [1] + [0] \\
[0] &\rightarrow [0] \\
[31] &\rightarrow [31]_+ + [31]_- + [3] + [21]_+ + [21]_- + [2] + [11]_+ + [11]_- + [1] \\
[1^2] &\rightarrow [11]_+ + [11]_- + [1]
\end{aligned} \tag{15}$$

These are precisely the $SO(4)$ irreducible representations that one expects for the various two-electron configurations that arise for orbitals involving principal quantum numbers $n \leq 3$. These, of course, are also the $SO(4)$ irreducible representations that arise in the $SO(4)$ plethysms

$$([2] + [1] + [0]) \otimes \{2\} = [4] + [3] + [2^2] - + [2^2] + + [21] - + [21] + + 3[2] + 2[1] + 3[0] \tag{16a}$$

$$([2] + [1] + [0]) \otimes \{1^2\} = [31] - + [31] + + [3] + [21] - + [21] + + [2] + 2[1^2] - + 2[1^2] + + 2[1] \tag{16b}$$

Note that for two electrons the plethysms in $SO(5)$ are multiplicity free and the quantum numbers associated with the canonical embedding

$$SO(5) \supset SO(4) \supset SO(3) \supset SO(2) \tag{17}$$

are complete. This should have the consequence of permitting a complete algebraic construction of the symmetrised two-electron states up to a chosen principal quantum number n with all the recoupling

coefficients algebraic in the same sense as for the $SO(4) \rightarrow SO(3)$ recoupling coefficients. This problem I leave to others to complete. An now for a little more history.

History, it is said, repeats itself... Few are but reminded
almost everyday... of something that has gone before.
— *Marian Rooke III* H Sedley (1865)

Effective Hamiltonians

The use of effective Hamiltonians is well-known in nuclear physics where the knowledge of the Hamiltonian is more incomplete than in atomic physics. Nevertheless there has been interest in constructing effective Hamiltonians for complex atomic spectra[21–24] that has allowed one to correlate experimental data with theoretical calculations in terms of parameterised effective operators. Initially calculations simply treated the Slater radial Coulomb integrals and the spin-orbit radial integral as parameters. Trees[25] observed that the addition of an effective operator $L(L+1)$ led to a considerable reduction in the least-squares error between experimental and theoretical atomic levels in the $3d-$shell. This became known as the "Trees correction". Runciman and Wybourne[26] showed that the inclusion of such a correction was significant in the $4f-$shell. At that time the origin of the Trees correction was unknown. In 1963 Rajnak and Wybourne[21] showed that the Trees correction, and indeed other corrections, were miming configuration interaction effects. This led to a whole industry of effective operators which continues to this day not only in atomic physics but also in extensions of the Judd-Ofelt theory of transitions[27,28] in lanthanide and actinide bearing crystals and solutions.

In constructing effective operators one is really trying to set up a minimal basis of invariants, or technically an *integrity basis*[29]. All other invariants are then polynomials in those of the integrity basis set of invariants. Thus in the f^n-shell the three invariants arising from second-order perturbation theory can be taken in parameterised form as

$$\alpha L(L+1) + \beta C_2(G_2) + \gamma C_2(SO_7) \tag{18}$$

where the three operators are just the second-order Casimir invariants of the groups SO_3, G_2 and SO_7 respectively. Add to those the four Slater Coulomb integrals F_0, $F_2(f,f)$, $F_4(f,f)$ and $F_6(f,f)$ as parameters and one has seven parameters which is precisely the number of SL terms in the two-electron configuration f^2.

Effective operators have been, largely, the success of the interacting boson model (IBM) of nuclei(see ref.[30] and references contained therein). In that case one has a chain of groups to describe the basis states and constructs effective Hamiltonians in terms of invariant operators and endeavours to fit the observed nuclear level spectra.

Clearly effective operators are our way of hiding our ignorance and lack of success with *ab initio* methods.

Back to Electron Complexes

Kellman[16] has recently discussed the construction of effective Hamiltonians for two-electron $n=2$ complexes starting with the Casimir operators $P(P+2)+Q^2$ for his group $O(4)_{12}$ and $L(L+1)$ for the $O(3)_{12}$ subgroup. It is somewhat surprising that he does not include the second $SO(4)$ Casimir operator, $Q(P+1)$, which has the effect of lifting the degeneracy of the $SO(4)$ states $[PQ]_{\pm}$ for $Q \neq 0$. He gives detailed examples with fits to actual spectra in the case of doubly excited states. As he notes one of the difficulties is that the group $O(4)_{12}$ has been constructed in terms of the difference in the Runge-Lenz vector of the two electrons and hence his effective Hamiltonian cannot be consistently extended to more than two electrons. In addition there is the problem of interpreting spurious states if $U(4)_{12}$ is introduced. An alternative might be to use the $SO(5)$ model suggested above. In that case one has, in addition to the usual $O(4)_{12}$ effective operators, the possibility of using the two independent Casimir invariants for $SO(5)$. Again I leave that task to someone else. The methods outlined in ref. [30] are probably relevant.

Fini ...

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> *For a man to commit his thoughts to writing when he can neither arrange them nor bring any new light to bear upon them and, indeed, when he has no attraction whatsoever to offer his reader, is a senseless waste of time, and of paper, too.*
>
> — *Tuscalanae Disputationes, Book 1* Cicero