Symmetric Functions and the Symmetric Group 10
B. G. Wybourne

> *Oh, he seems like an okay person, except for being a little strange in some ways. All day he sits at his desk and scribbles, scribbles. scribbles. Then at the end of the day, he takes the sheets of paper he's scribbled on, scrunges them all up, and throws them in the trash can*
>
> — J von Neumann's housekeeper

■ 10.1 A Hamiltonian for Quantum Dots

Experimentally the electrons of a quantum dot are contained in a parabolic potential and hence we expect a close relationship with a many-electron system subject to a harmonic oscillator potential. The interaction potential $V(r_i, r_j)$ between particles i and j moving in a two-dimensional confining potential in the $x-y$ plane is taken to saturate at small particle separations and to decrease quadratically with increasing separation. In free space we would expect the interaction between two electrons to vary as $|r_i - r_j|^{-1}$. In a quantum dot the form of $V(r_i, r_j)$ is modified by the presence of image charges. The wavefunctions of the electrons confined in the quantum dots have a small but finite extent in the $z-$direction perpendicular to the $x-y$ plane. This results in a smearing of the electron charges along the $z-$direction. As a result the interparticle repulsion tends to saturate at small distances. This suggests choosing the interaction as

$$V(r_i, r_j) = 2V_0 - \frac{1}{2}m^*\Omega^2|r_i - r_j|^2 \tag{10.1}$$

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

$$H_{space} = \frac{1}{2m^*}\sum_i \left[p_i + \frac{eA_i}{c}\right]^2 + \frac{1}{2}m^*\omega_0^2\sum_i |r_i|^2 + \sum_{i<j} V(r_i, r_j) \tag{10.2}$$

and the spin part as

$$H_{spin} = -g^*\mu_B B\sum_i s_{z,i} \tag{10.3}$$

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

$$p_i = (p_{x,i}, p_{y,i}) \qquad A_i = (A_{x,i}, A_{y,i}) \tag{10.4}$$

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. (10.2) becomes

$$H_{space} = \frac{1}{2m^*}\sum_i p_i^2 + \frac{1}{2}m^*\omega_0^2(B)\sum_i |r_i|^2 + \sum_{i<j}\left[2V_0 - \frac{1}{2}m^*\Omega^2|r_i, r_j|^2\right] + \frac{\omega_c}{2}\sum_i L_{z,i} \tag{10.5}$$

where $\omega_0^2(B) = \omega_0^2 + \omega_c^2/4$ and $\omega_c = eB/m^*c$.

■ 10.2 Note on Commutators and Second-quantisation

In much that follows we will need to be able to manipulate bosonic annihilation (a_i) and creation operators $(a_i^\dagger)$. The basic bosonic commutation relations are

$$[a_i, a_j] = 0, \quad [a_i^\dagger, a_j^\dagger] = 0, \quad [a_i, a_j^\dagger] = \delta_{i,j} \tag{10.6}$$

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

$$[a_i^\dagger a_j + a_j a_i^\dagger, a_k] = [a_i^\dagger a_j, a_k] + [a_j a_i^\dagger, a_k] \tag{10.7}$$

Expanding out the first commutator we have

$$[a_i^\dagger a_j, a_k] = a_i^\dagger a_j a_k - a_k a_i^\dagger a_j \tag{10.8}$$

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. (10.6) we can rearrange the first term as

$$a_i^\dagger a_j a_k \to a_i^\dagger a_k a_j \tag{10.9}$$

and hence the right-hand-side of Eqn. (10.9) becomes

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

■ **Exercise**

Show that if

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

then

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

■ 10.3 The Degeneracy Group for Mesoscopic Systems

In this lecture we enlarge the concept of a *degeneracy* group to a *dynamical* group. The degeneracy group for the isotropic harmonic oscillator was found to be $SU(3)$. Each irreducible representation $\{n00\}$ is spanned by a set of $\frac{(n+1)(n+2)}{2}$ eigenstates of the Hamiltonian and associated with the *same* energy eigenvalue E_n of the harmonic oscillator. There is one weight vector for every eigenstate. The algebra of the degeneracy group contains a set of operators that allow us to start from any eigenstate and ladder through the entire set of degenerate eigenstates associated with a given degenerate eigenvalue. Thus the angular momentum ladder operators $L_\pm$ take us from one $|\alpha LM\rangle$ eigenstate to another $|\alpha LM \pm 1\rangle$ but leaving L fixed. The operators $L_z, L_\pm$ that generate the angular momentum group SO_3 but cannot take us from states belonging to one irreducible representation of SO_3 to another. To do that we must use the operators contained in the degeneracy algebra that lie outside of those of the angular momentum algebra. In addition the algebra of the degeneracy group contains operators that allow us to ladder between states of a given $SU(3)$ multiplet changing *both* L and M quantum numbers but *not* n. These additional operators reflect the fact that the isotropic harmonic oscillator has, like the $H-$atom, symmetry higher that just rotational symmetry.

■ 10.4 A Dynamical Group

We seek a *dynamical* group that contains the degeneracy group as a subgroup and has the energy eigenstates belonging to a single irreducible representation. Such a group contains among its generators operators that allow one to ladder between different irreducible representations of the degeneracy group. The degeneracy group contains an infinite set of finite dimensional unitary irreducible representations and hence the dynamical group must necessarily be a non-compact group with infinite dimensional unitary irreducible representations . We now construct the dynamical group for mesoscopic quantum systems.

■ 10.5 The Dynamical Group for Mesoscopic Quantum Systems

1. Assume the Hamiltonian of the $N-$particle system is a function of coordinate and momentum operators of the individual particles.

2. Designate the coordinates of the $r-$th particle by x_{ri} with $r = 1, \ldots, N$ and the momentum by p_{ri} with $i = 1, \ldots, d$.
3. The associated operators X_{ri} and P_{ri} obey the usual Heisenberg commutation relations (We choose units such that $\hbar = 1$)
$$[X_{ri}, X_{sj}] = 0, [X_{ri}, P_{sj}] = i\delta_{rs}\delta_{ij}, [P_{ri}, P_{sj}] = 0 \tag{10.10}$$
4. The $(2Nd)^2$ bilinear operators
$$\{X_{ri}X_{sj}, X_{ri}P_{sj}, P_{ri}X_{sj}, P_{ri}P_{sj}\} \tag{10.11}$$
close under commutation. However, only
$(2Nd + 1)Nd$ of these operators are independent since
$$P_{ri}X_{sj} = X_{sj}P_{ri} - i\delta_{rs}\delta_{ij} \tag{10.12}$$
5. Consider the $(2Nd + 1)Nd$ independent operators
$$\begin{aligned} Q_{risj} &= \frac{1}{2}\{X_{ri}, X_{sj}\}, \quad V_{risj} = \frac{1}{2}\{X_{ri}, P_{sj}\}, \\ K_{risj} &= \frac{1}{2}\{P_{ri}, P_{sj}\} \end{aligned} \tag{10.13}$$
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.

■ 10.6 Subalgebras of the Dynamical Algebra

1. We can construct subalgebras of $Sp(2Nd, R$ by forming subsets of the defining generators that close under commutation. Thus, for example, the V's close under commutation forming the elements of the $GL(Nd, R)$ algebra.
2. Contracting on particle or spatial indices can yield further Lie subalgebras. Thus the two sets of operators (summing on repeated indices)
$$\begin{aligned} Q_{ij} &= X_{ri}X_{rj}, \quad L_{ij} = X_{ri}P_{rj} - X_{rj}P_{ri}, \\ K_{ij} &= P_{ri}P_{rj} \\ T_{ij} &= \frac{1}{2}(X_{ri}P_{rj} + X_{rj}P_{ri} + P_{ri}X_{rj} + P_{rj}X_{ri}) \end{aligned} \tag{10.14}$$
and
$$\begin{aligned} Q_{rs} &= X_{ri}X_{si}, \quad L_{rs} = X_{ri}P_{si} - X_{si}P_{ri}, \\ K_{rs} &= P_{ri}P_{si} \\ T_{rs} &= \frac{1}{2}(X_{ri}P_{si} + X_{si}P_{ri} + P_{ri}X_{si} + P_{si}X_{ri}) \end{aligned} \tag{10.15}$$
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
$$\begin{aligned} [L_{ij}, L_{kl}] &= i(L_{ik}\delta_{jl} - L_{il}\delta_{jk} + L_{jk}\delta_{il} + L_{jk}\delta_{il} - L_{jl}\delta_{ik}) \\ [L_{rs}, L_{tu}] &= i(L_{rt}\delta_{su} - L_{ru}\delta_{st} + L_{st}\delta_{ru} - L_{su}\delta_{rt}) \end{aligned} \tag{10.16}$$
and form the generators of the subalgebras $O(d)$ and $O(N)$.
4. Continuing we are led to the following possible Lie subalgebras of $Sp(2Nd, R)$:-
$$\begin{aligned} Sp(2, R) \times O(Nd) &\supset Sp(2, R) \times O(N) \times O(d) \\ &\supset U(1) \times O(N) \times O(d) \end{aligned} \tag{10.17}$$
$$Sp(2N, R) \times O(d) \supset U(N) \times O(d) \supset U(1) \times O(N) \times O(d) \tag{10.18}$$
$$Sp(2d) \times O(N) \supset U(d) \times O(N) \supset U(1) \times O(d) \times O(N) \tag{10.19}$$

$$U(Nd) \supset U(N) \times U(d) \supset U(1) \times O(N) \times O(d) \tag{10.20}$$

Note the separation of the spatial and particle dependencies.

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

Let us introduce three operators defined by

$$Q = X_{ri}X_{ri}, \quad T = X_{ri}P_{ri} + P_{ri}X_{ri}, \quad K = P_{ri}P_{ri} \tag{10.21}$$

and having the non-zero commutation relations

$$[Q,K] = 2iT, \quad [Q,T] = 4iQ, \quad [K,T] = -4iK \tag{10.21}$$

These commutation relations are those of a three element Lie algebra. Let us first decide if the algebra is compact or non-compact. This we may do by calculating the metric tensor

$$g_{ij} = c^t_{ik}c^k_{jt} \tag{10.22}$$

where the c^t_{ik} are the structure constants of the Lie algebra. Noting Eqn. (10.21) we have

$$c^T_{QK} = 2i, \quad c^Q_{QT} = 4i, \quad c^K_{KT} = -4i \tag{10.23}$$

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

$$\begin{aligned} &g_{QQ} = g_{KK} = 0 \\ &g_{TT} = c^Q_{TQ}c^Q_{TQ} + c^K_{TK}c^K_{TK} = -4i \times -4i + 4i \times 4i = -32 \end{aligned} \tag{10.24}$$

In addition we have the off-diagonal elements

$$g_{QK} = g_{KQ} = c^Q_{QT}c^T_{KQ} + c^T_{QK}c^K_{KT} = 4i \times -2i + 2i \times -4i = 16 \tag{10.25}$$

and thus the complete metric tensor is represented by the matrix

$$[g_{ij}] = \begin{array}{c} \\ Q \\ K \\ T \end{array} \begin{array}{c} \begin{array}{ccc} Q & K & T \end{array} \\ \begin{pmatrix} 0 & 16 & 0 \\ 16 & 0 & 0 \\ 0 & 0 & -32 \end{pmatrix} \end{array} \tag{10.26}$$

We can produce a diagonal metric tensor by putting

$$A_{\pm} = \frac{1}{\sqrt{2}}(Q \pm K) \tag{10.27}$$

to give the Lie algebra as

$$[A_{\pm}, T] = 4iA_{\mp}, \qquad [A_+, A_-] = 2iT \tag{10.28}$$

and the metric tensor as

$$[g_{ij}] = \begin{array}{c} \\ A_+ \\ A_- \\ T \end{array} \begin{array}{c} \begin{array}{ccc} A_+ & A_- & T \end{array} \\ \begin{pmatrix} -16 & 0 & 0 \\ 0 & +16 & 0 \\ 0 & 0 & -32 \end{pmatrix} \end{array} \tag{10.29}$$

We first note that the metric tensor has $\det|g_{ij}| \neq 0$ 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

$$SO(2,1) \sim Sp(2,R) \tag{10.30}$$

■ 10.8 Back to the Quantum Dot Hamiltonian

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

$$H_o = \frac{1}{2m}P_{ri}P_{ri} + \frac{m\omega^2}{2}X_{ri}X_{ri} \tag{10.31}$$

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

$$\frac{1}{2m}P_{ri}P_{ri} = \frac{1}{2m}K \tag{10.31}$$

and

$$\frac{m\omega^2}{2}X_{ri}X_{ri} = \frac{m\omega^2}{2}Q \tag{10.32}$$

to give

$$H_o = \frac{1}{2m}K + \frac{m\omega^2}{2}Q \tag{10.33}$$

Now consider our earlier Hamiltonian

$$H_{space} = \frac{1}{2m^*}\sum_i p_i^2 + \frac{1}{2}m^*\omega_0^2(B)\sum_i |r_i|^2 + \sum_{i<j}\left[2V_0 - \frac{1}{2}m^*\Omega^2|r_i,r_j|^2\right] + \frac{\omega_c}{2}\sum_i L_{z,i} \tag{10.5}$$

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

$$H_{space} = \frac{1}{2m}K + \frac{m\Omega_0^2}{2}Q - \frac{eB}{4mc}L_{12} + N(N-1)V_0 + \frac{m\Omega^2}{2}\sum_{rs}Q_{rs} \tag{10.34}$$

with

$$\Omega_0^2 = \omega^2 + (\frac{eB}{2mc})^2 - N\Omega^2 \tag{10.35}$$

The significance of these results is that the first three terms in Eqno. (10.34) have been expressed in terms of the generators of $Sp(2,R)$ (K,Q) and $O(d)$ (L_{12}) and the last term in terms of generators of the group $Sp(2N,R)$. A practical calculation then involves the evaluation of matrix elements of the group generators in a harmonic oscillator basis.