# Hydrogen Dynamical Symmetry and Spectrum Generating Groups

Evan Frangipane
6 June 2019

# Hydrogen Symmetry and Degeneracy

-Spherically symmetric potential

$$V(r) = -\frac{e^2}{r} \tag{1}$$

-Implies 3D rotationally invariant hamiltonian making symmetry group SO(3) with familiar degeneracy 2l+1

$$\sum_{l=0}^{n-1} (2l+1) = n^2 \tag{2}$$

-Energy has larger degeneracy than explained by conservation of angular momentum. There must be a larger symmetry group

-Let classical Kepler problem guide us with LRL vector which points from the origin of an ellipse to the periapsis (closest point) and is a constant of motion

# Laplace Runge Lenz and Dynamical Symmetry

-Introduce Hermitian version of classically conserved LRL vector. I follow the treatment in Sakurai Chapter 5

$$\vec{M} = \frac{\vec{p}\times\vec{L} - \vec{L}\times\vec{p}}{2m} - \frac{e^2\vec{r}}{r} \tag{3}$$

-Conserved quantity ⇔ Commutes with H

-Useful relations:

$$\vec{L}\cdot\vec{M} = \vec{M}\cdot\vec{L} = 0 \tag{4}$$

$$\vec{M}^2 = \frac{2}{m}\mathcal{H}(\vec{L}^2 + \hbar^2) + e^4 \tag{5}$$

# Commutation Relations and Rescaling

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k \tag{6}$$

$$[M_i, L_j] = i\hbar\epsilon_{ijk}M_k \tag{7}$$

$$[M_i, M_j] = -i\hbar\epsilon_{ijk}\frac{2\mathcal{H}L_k}{m} \tag{8}$$

-Replace H with eigenvalue E.
-We can restrict to the Hilbert space to this eigenvalue E due to the fact that H commutes with L, M and is independent of time

$$\vec{N} = \sqrt{\frac{m}{2|E|}}\vec{M} \tag{9}$$

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k \tag{10}$$

$$[N_i, L_j] = i\hbar\epsilon_{ijk}N_k \tag{11}$$

$$[N_i, N_j] = \pm i\hbar\epsilon_{ijk}L_k \tag{12}$$

-Restriction and redefinition make the algebra closed by replacing H with E and rescaling to remove E
-Note the sign of Equation 12
This comes from E<0 or E>0 depending on being bound or scattering states, respectively

# Which Lie Group?

-Another redefinition of operators will make the answer more clear.

$$\vec{I} = \frac{\vec{L} + \vec{N}}{2} \tag{13}$$

$$\vec{K} = \frac{\vec{L} - \vec{N}}{2} \tag{14}$$

$$[I_i, I_j] = i\hbar\epsilon_{ijk} I_k \tag{15}$$

$$[I_i, K_j] = 0 \tag{16}$$

$$[K_i, K_j] = i\hbar\epsilon_{ijk} K_k \tag{17}$$

-These operators are analogous to angular momentum operators and the Lie Algebra for an angular momentum operator is:

$$\mathfrak{so}(3) \cong \mathfrak{su}(2)$$

-Another clue comes from the number of operators which is 6
4(4-1)/2 = 6 → Looks like SO(4)

# Which Lie Group?

-From previous slide, the full Lie algebra is the sum of the two subalgebras

$$\mathfrak{so}(4) = \mathfrak{su}(2) \oplus \mathfrak{su}(2)$$

-Thus, the Lie Group must be locally (near identity) isomorphic to SO(4) and I will call it SO(4)

-This accounts for the positive sign in equation 12, but the scattering (E>0) states have a slightly different algebra

-The algebra coincides with the algebra of the Lorentz Group with generators boost and rotation. Thus the group for scattering states is SO(3,1)

# SO(4) and SO(3,1) as Dynamical Symmetry Groups

-SO(4) is the four dimensional rotation group but does not represent a physical rotation for Hydrogen → this is called a dynamical symmetry

-Clearly SO(4) contains the geometrical symmetry group of 3D rotations SO(3)

-Similarly, SO(3,1) does not represent physical rotations for Hydrogen

-For the case of E=0, the dynamical symmetry group is E(4) which adds translations and reflections to SO(4) while conserving distance between points.

# Let’s Calculate E from the Operators

$$\vec{I}^2 + \vec{K}^2 = \frac{1}{2}(\vec{L}^2 + \frac{m}{2|E|}\vec{M}^2) \tag{18}$$

$$\vec{I}^2 - \vec{K}^2 = \vec{L} \cdot \vec{M} = 0 \tag{19}$$

$$\vec{I}^2, \vec{K}^2 = p(p+1)\hbar^2 \tag{20}$$

$$E = \frac{-e^4}{2\hbar^2}\frac{1}{(2p+1)^2} \tag{21}$$

$$2p+1 \leftrightarrow n \Rightarrow E \propto n^{-2} \tag{22}$$

-Some more useful relations derived using equations 4 and 5 and the fact that the commutation relations of I, K hint that they are angular momenta
-Eq. 19 and positive p implies that p is same for I and K.

-Use 18 and 20 together to derive 21

-Identify 2p+1 as the principal quantum number

-Degeneracy is (2p+1)*(2p+1) = n^2 as expected from equation 2 and we recover bound state energy

# Spectrum Generating Groups

-One example of a spectrum generating group is SO(2,1) which conserves the angular momentum quantum number and changes the principal quantum number and thus the energy. Here I follow the treatment in *Shattered Symmetries*

$$\mathcal{H}_r = \frac{p_r^2}{2m} + \frac{l(l+1)\hbar^2}{2mr^2} - \frac{e^2}{r} \tag{23}$$

-To investigate this claim, start with the radial part of the Hamiltonian and three new angular-momentum-like operators Q1,Q2,Q3

# Generators of so(2,1)

$$Q_1 = \frac{1}{2}(\frac{rp_r^2}{a} - ar + \frac{b}{r}) \tag{24}$$

$$Q_2 = rp_r \tag{25}$$

$$Q_3 = \frac{1}{2}(\frac{rp_r^2}{a} + ar + \frac{b}{r}) \tag{26}$$

$$[Q_1, Q_2] = -i\hbar Q_3 \tag{27}$$

$$[Q_2, Q_3] = i\hbar Q_1 \tag{28}$$

$$[Q_3, Q_1] = i\hbar Q_2 \tag{29}$$

$$(Q_3 - \frac{me^2}{a})\left|\Psi\right\rangle = 0 \tag{30}$$

$$\vec{Q}^2 = ab = l(l+1)\hbar^2 \tag{31}$$

-Constants a and b are introduced so we can rewrite eigenvalue equation in terms of Q Generators.

-Eigenstates of radial hamiltonian are also eignestates of Q3
-Q^2 eigenvalue found to be exactly the L^2 eigenvalue
-Many parallels with the generic angular momentum operator of SO(3)

-Eigenstates of Q are given by: $\left|jm_j\right\rangle$

-2j+1 options for m as usual

# Ladder Operators of so(2,1)

-Equation 31 tells us that l will be conserved by acting with Q’s analogous to l being conserved by acting with L’s on radial hamiltonian eigenstate.

-31 also tells us that j(j+1) = l(l+1)
-30 tells us that Q3 acting on ground state mj=m0 is a positive eigenvalue!

$$j(j+1) = l(l+1), m_0 = -j \Rightarrow j = -l-1 \qquad (32)$$

$$Q_\pm = Q_1 \pm iQ_2 \qquad (33)$$

-Introduce ladder operators that increment mj while conserving l

$$Q_\pm \left| j m_j \right\rangle = c_\pm \left| j m_j \pm 1 \right\rangle \qquad (34)$$

$$m_j = m_0 + n_r = l + 1 + n_r, n_r = 0, 1, 2, ... \qquad (35)$$

# Ladder Operators Change Bound State Energy

-From Q3 eigenvalue equation 30

$$\hbar(1+l+n_r)=\frac{me^2}{a},a=\sqrt{-2mE}\Rightarrow E=-\frac{me^4}{(1+l+n_r)^2} \tag{36}$$

$$1+l+n_r\leftrightarrow n\Rightarrow E\propto n^{-2} \tag{37}$$

-Ladder operators increment n_r which increments the principal quantum number and thus the energy while keeping angular momentum fixed.

# Concluding Remarks

-SO(3) can increment m by +/- 1

-SO(4) can increment l by +/- 1 ( Analogous to SO(3) and SO(2,1) )

-SO(2,1) can increment n by +/- 1

-Which group contains all of these as subgroups and thus is the complete spectrum generating group?

-SO(4,2)!

# The three different types of spectrum generators listed. Courtesy of *Shattered Symmetry*

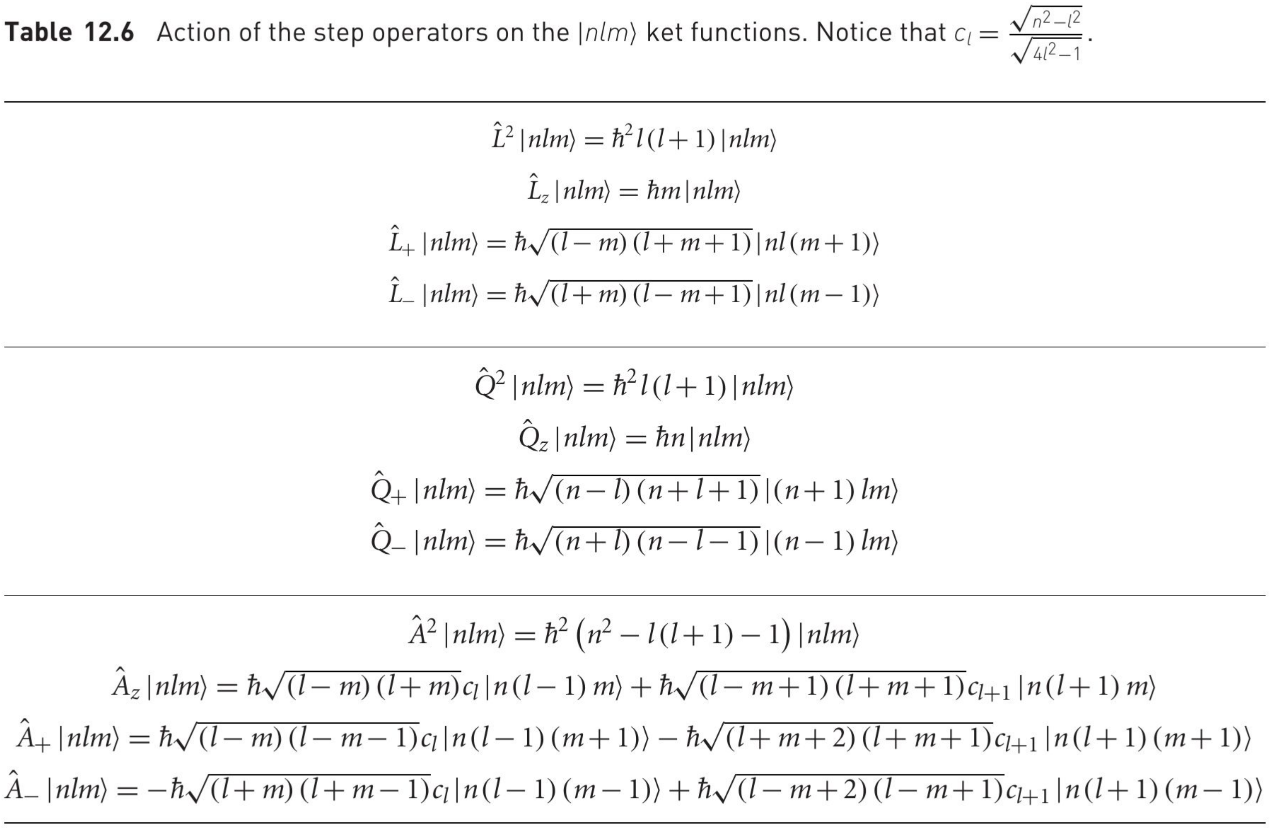

**Table 12.6** Action of the step operators on the $|nlm\rangle$ ket functions. Notice that $c_l = \frac{\sqrt{n^2-l^2}}{\sqrt{4l^2-1}}$.

$$\hat{L}^2\,|nlm\rangle = \hbar^2 l\,(l+1)\,|nlm\rangle$$

$$\hat{L}_z\,|nlm\rangle = \hbar m\,|nlm\rangle$$

$$\hat{L}_+\,|nlm\rangle = \hbar\sqrt{(l-m)\,(l+m+1)}\,|nl\,(m+1)\rangle$$

$$\hat{L}_-\,|nlm\rangle = \hbar\sqrt{(l+m)\,(l-m+1)}\,|nl\,(m-1)\rangle$$

$$\hat{Q}^2\,|nlm\rangle = \hbar^2 l\,(l+1)\,|nlm\rangle$$

$$\hat{Q}_z\,|nlm\rangle = \hbar n\,|nlm\rangle$$

$$\hat{Q}_+\,|nlm\rangle = \hbar\sqrt{(n-l)\,(n+l+1)}\,|(n+1)\,lm\rangle$$

$$\hat{Q}_-\,|nlm\rangle = \hbar\sqrt{(n+l)\,(n-l-1)}\,|(n-1)\,lm\rangle$$

$$\hat{A}^2\,|nlm\rangle = \hbar^2\left(n^2 - l\,(l+1) - 1\right)|nlm\rangle$$

$$\hat{A}_z\,|nlm\rangle = \hbar\sqrt{(l-m)\,(l+m)}\,c_l\,|n\,(l-1)\,m\rangle + \hbar\sqrt{(l-m+1)\,(l+m+1)}\,c_{l+1}\,|n\,(l+1)\,m\rangle$$

$$\hat{A}_+\,|nlm\rangle = \hbar\sqrt{(l-m)\,(l-m-1)}\,c_l\,|n\,(l-1)\,(m+1)\rangle - \hbar\sqrt{(l+m+2)\,(l+m+1)}\,c_{l+1}\,|n\,(l+1)\,(m+1)\rangle$$

$$\hat{A}_-\,|nlm\rangle = -\hbar\sqrt{(l+m)\,(l+m-1)}\,c_l\,|n\,(l-1)\,(m-1)\rangle + \hbar\sqrt{(l-m+2)\,(l-m+1)}\,c_{l+1}\,|n\,(l+1)\,(m-1)\rangle$$

The fifteen generators of the so(4,2) algebra. A is equivalent to the definition of N, the scaled LRL operator. Courtesy of *Shattered Symmetry*

$$\mathbb{L} \Longleftrightarrow \begin{pmatrix} 0 & \hat{L}_3 & -\hat{L}_2 & \hat{A}_1 & \hat{B}_1 & \hat{\Gamma}_1 \\ & 0 & \hat{L}_1 & \hat{A}_2 & \hat{B}_2 & \hat{\Gamma}_2 \\ & & 0 & \hat{A}_3 & \hat{B}_3 & \hat{\Gamma}_3 \\ & & & 0 & \hat{Q}_2 & \hat{Q}_1 \\ & & & & 0 & \hat{Q}_3 \\ & & & & & 0 \end{pmatrix}.$$

# Works Cited

Gilmore, Robert. *Lie Groups, Physics, and Geometry an Introduction for Physicists, Engineers and Chemists*. Cambridge Univ. Press, 2011.

Sakurai, J. J., and Jim J. Napolitano. *Modern Quantum Mechanics*. Pearson India Education Services, 2014.

Thyssen, Pieter, and Arnout Ceulemans. *Shattered Symmetry: Group Theory from the Eightfold Way to the Periodic Table*. Oxford University Press, 2017.

Tung, Wu-Ki. *Group Theory*. World Scientific, 1985.