#### 6 Addition of Angular Momentum

Back in section 2.3.1, we understood how to describe composite systems using the tensor product of the Hilbert spaces of the individual subsystems. However, in many circumstances, the basis of the tensor product formed by taking all possible pairs of basis elements from the individual subspaces is not the most convenient. A key case is when the subspaces transform under the action of a group G. We'd like to understand the effect of a G-transformation on the combined space, and the 'obvious' tensor product basis usually obscures this.

In this chapter, we'll see how this works for the case of the rotation group G = SO(3). Specifically, suppose two subsystems are each in states of definite total angular momentum – meaning mathematically that they transform in irreducible representations of SO(3) – with total angular momentum quantum numbers  $j_1$  and  $j_2$ , respectively. We'd like to express the tensor product of the subsystems in terms of a sum of Hilbert spaces,

$$\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2} = \bigoplus_j \mathcal{H}_j \,, \tag{6.1}$$

where each  $\mathcal{H}_j$  describes a state of the whole system with definite total angular momentum quantum number  $j^{56}$ . Physically, to understand this decomposition is to understand how to add the angular momentum of the two subsystems so as to find the possible values of the combined angular momentum of the whole system. For example, in a Hydrogen atom, both the proton and electron carry angular momentum  $\hbar/2$  by virtue of their spins, and further angular momentum may be present depending on the electron's orbit around the proton. If we wish to treat the atom as a whole, then we'll be concerned with the angular momentum of the combined system rather than that of the electron and proton individually. An even more familiar example is your bike: the total angular momentum comes from a combination of the back and front wheels which can be independent (at least in principle, though I don't recommend trying this while you're riding along!).

Our second task in this chapter is to fill in a gap left in our knowledge: While we know how to use the raising and lowering operators  $J_{\pm}$  to realign a given amount of angular momentum along or away from some axis, we've not yet learnt how to perform a mathematical operation that changes the total angular momentum of our state. In section 6.2.1, we'll understand that, as well as states, operators themselves can carry angular momentum. Applying such an operator to a state yields a new state whose total angular momentum can differ from that of the original state. We'll illustrate this using various physical examples, including radiative transitions induced by an electric dipole moment, and the special 'dynamical' symmetries present in the Coulomb and harmonic oscillator potentials.

<sup>&</sup>lt;sup>56</sup>In quantum mechanics we're concerned with Hilbert space, but in fact the inner product plays very little role in this story. The whole of this section carries over more generally to the case of representations of a general Lie group G, where we decompose the tensor product  $R_{j_1} \otimes R_{j_2}$  of two irreducible representations (vector spaces)  $R_{j_1}$  and  $R_{j_2}$  in terms of a sum  $\bigoplus_j R_j$  of further irreducible representations. You can learn more by taking the Part II Representation Theory course next term (and more still in the Part III courses).



**Figure 12**: Two gyroscopes, of individual angular momenta  $j_1$  and  $j_2$ , may be aligned relative to one another so that their total angular momentum ranges between  $j_1 + j_2$  and  $|j_1 - j_2|$ . For fixed relative alignment, the total angular momentum may be chosen to be aligned along any axis.

### 6.1 Combining the Angular Momenta of Two States

Suppose we have two subsystems ('gyros') enclosed in a box, where the first system has total angular momentum quantum number  $j_1$  and the second has total angular momentum quantum number  $j_2$ . As we saw in section 5.1, a basis of states of the first system is

$$\{|j_1, m_1\rangle\}$$
 where  $m_1 \in \{-j_1, -j_1 + 1, \dots, j_1\}$  (6.2)

while the second system may be described in terms of the basis

$$\{|j_2, m_2\rangle\}$$
 where  $m_2 \in \{-j_2, -j_2+1, \dots, j_2\}.$  (6.3)

From the general discussion of section 2.3.1, the state of the combined system can be expressed as

$$|\psi\rangle = \sum_{m_1 = -j_1}^{j_1} \sum_{m_2 = -j_2}^{j_2} c_{m_1 m_2} |j_1, m_1\rangle \otimes |j_2, m_2\rangle$$
(6.4)

with some coefficients  $c_{m_1m_2}$ . We can choose  $m_1$  and  $m_2$  independently, so there are a total of  $(2j_1 + 1)(2j_2 + 1)$  states here – this is the dimension of the tensor product  $\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2}$ . We want to understand how the states (6.4) behave under rotations; that is, we'd like to understand which linear combinations in (6.4) correspond to a definite amount of angular momentum for the system as a whole.

Let's first consider the corresponding classical situation, where we may wish to know the combined angular momentum of two gryroscopes. Although the total angular momentum of the individual components is fixed, that of the whole system is variable because it depends on the relative orientation of the two gyros: if they are aligned with eachother, the whole system might be expected to have total angular momentum labelled by  $j_1 + j_2$ , while if the two subsystems are aligned exactly against eachother, then you may expect the system as a whole to have total angular momentum  $|j_1 - j_2|$ . (See figure 12.) It's important to realise that we're *not* saying anything at all about how the individual subsystems may or may not be coupled to one another dynamically – that is, we're not assuming any form of interaction between them in the Hamiltonian. Rather, we're just considering the different relative alignments of their angular momenta *that are possible in principle*.

Quantum mechanically, the angular momentum operator for the combined system is

$$\mathbf{J} = (\mathbf{J}_1 \otimes \mathbf{1}_{\mathcal{H}_{j_2}}) + (\mathbf{1}_{\mathcal{H}_{j_1}} \otimes \mathbf{J}_2) \tag{6.5}$$

where  $\mathbf{J}_1$  and  $\mathbf{J}_2$  are the angular momentum operators for the two subsystems. It follows that

$$\mathbf{J}^2 = (\mathbf{J}_1^2 \otimes \mathbf{1}_{\mathcal{H}_{j_2}}) + (\mathbf{1}_{\mathcal{H}_{j_1}} \otimes \mathbf{J}_2^2) + 2(\mathbf{J}_1 \otimes \mathbf{J}_2)$$
(6.6)

where in the final term we take the scalar product of the two spin operators over their spatial vector indices. We'll often abuse notation by writing

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 \quad \text{and} \quad \mathbf{J}^2 = \mathbf{J}_1^2 + \mathbf{J}_2^2 + 2\mathbf{J}_1 \cdot \mathbf{J}_2, \quad (6.7)$$

with the tensor product and identity operators being understood.

We can rewrite the operator (6.6) in a way that allows us to understand its action on states  $|j_1, m_1\rangle |j_2, m_2\rangle$ , which form our basis in (6.4) (we've again dropped the  $\otimes$  symbol). Using the fact that

$$J_x = \frac{J_+ + J_-}{2}$$
 and  $J_y = \frac{J_+ - J_-}{2i}$ 

we have

$$2\mathbf{J}_{1} \cdot \mathbf{J}_{2} = 2(J_{1x}J_{2x} + J_{1y}J_{2y} + J_{1z}J_{2z})$$
  
=  $2\left(\frac{J_{1+} + J_{1-}}{2}\frac{J_{2+} + J_{2-}}{2} + \frac{J_{1+} - J_{1-}}{2\mathbf{i}}\frac{J_{2+} - J_{2-}}{2\mathbf{i}} + J_{1z}J_{2z}\right)$  (6.8)  
=  $J_{1+}J_{2-} + J_{1-}J_{2+} + 2J_{1z}J_{2z}$ .

Using this to eliminate  $\mathbf{J}_1 \cdot \mathbf{J}_2$  from (6.6) allows us to write the total angular momentum operator as

$$\mathbf{J}^{2} = \mathbf{J}_{1}^{2} + \mathbf{J}_{2}^{2} + J_{1+}J_{2-} + J_{1-}J_{2+} + 2J_{1z}J_{2z}, \qquad (6.9)$$

where we now understand how each of the terms on the *rhs* act on any state of the form  $|j_1, m_1\rangle |j_2, m_2\rangle$ .

Let's consider the action of this operator on states of the whole system. We'll start by examining the state  $|j_1, j_1\rangle |j_2, j_2\rangle$  in which both gyros are maximally aligned with the  $\hat{z}$ -axis. Since  $J_z = J_{1z} + J_{2z}$  we have

$$J_{z}|j_{1},j_{1}\rangle|j_{2},j_{2}\rangle = (j_{1}+j_{2})\hbar|j_{1},j_{1}\rangle|j_{2},j_{2}\rangle$$
(6.10)

so indeed this state is an eigenstate of  $J_z$  with the expected eigenvalue. Also, using (6.9) we have

$$\mathbf{J}^{2}|j_{1},j_{1}\rangle|j_{2},j_{2}\rangle = \left(\mathbf{J}_{1}^{2} + \mathbf{J}_{2}^{2} + J_{1+}J_{2-} + J_{1-}J_{2+} + 2J_{1z}J_{2z}\right)|j_{1},j_{1}\rangle|j_{2},j_{2}\rangle 
= \left(j_{1}(j_{1}+1) + j_{2}(j_{2}+1) + 2j_{1}j_{2}\right)\hbar^{2}|j_{1},j_{1}\rangle|j_{2},j_{2}\rangle$$

$$(6.11)$$

$$= \left(j_{1}+j_{2}\right)\left(j_{1}+j_{2}+1\right)\hbar^{2}|j_{1},j_{1}\rangle|j_{2},j_{2}\rangle$$

where we've used the fact that  $|j_1, j_1\rangle |j_2, j_2\rangle$  is annihilated by both  $J_{1+}$  and  $J_{2+}$ . Thus, setting  $j = j_1 + j_2$ , we may write

$$|j,j\rangle = |j_1,j_1\rangle|j_2,j_2\rangle \tag{6.12}$$

since  $|j_1, j_1\rangle |j_2, j_2\rangle$  satisfies both the defining equations for a state of total angular momentum labelled by  $j_1 + j_2$ , with it all aligned along  $\hat{\mathbf{z}}$ . (This is a highest weight state for  $j = j_1 + j_2$ .)

Now that we've found one mutual eigenstate of the combined  $\mathbf{J}^2$  and  $J_z$ , we may easily construct others by applying the lowering operator  $J_- = J_{1-} + J_{2-}$ . Acting on the left and using equation (5.16) we have

$$J_{-}|j,j\rangle = \hbar\sqrt{j(j+1) - j(j-1)}|j,j-1\rangle = \hbar\sqrt{2j}|j,j-1\rangle.$$
(6.13)

On the other hand, applying  $J_{-} = J_{1-} + J_{2-}$  to the *rhs* of (6.12) gives

$$\begin{aligned} (J_{1-} + J_{2-})|j_1, j_1\rangle|j_2, j_2\rangle \\ &= \hbar \left[ \sqrt{j_1(j_1+1) - j_1(j_1-1)} |j_1, j_1-1\rangle|j_2, j_2\rangle + \sqrt{j_2(j_2+1) - j_2(j_2-1)} |j_1, j_1\rangle|j_2, j_2-1\rangle \right] \\ &= \hbar \sqrt{2j_1} |j_1, j_1-1\rangle|j_2, j_2\rangle + \hbar \sqrt{2j_2} |j_1, j_1\rangle|j_2, j_2-1\rangle \,. \end{aligned}$$

$$(6.14)$$

Comparing the two sides we learn that

$$|j, j-1\rangle = \sqrt{\frac{j_1}{j}} |j_1, j_1-1\rangle |j_2, j_2\rangle + \sqrt{\frac{j_2}{j}} |j_1, j_1\rangle |j_2, j_2-1\rangle.$$
(6.15)

Note that the *lhs* is an eigenstate of  $J_z$  with eigenvalue  $(j-1)\hbar$ , and indeed the *rhs* is an eigenstate of  $J_{1z} + J_{2z}$  with eigenvalue  $(j_1 + j_2 - 1)\hbar$ . A further application of  $J_-$  to the *lhs* and  $J_{1-} + J_{2-}$  to the *rhs* would produce an expression for  $|j, j-2\rangle$  and so on.

Since  $[J^2, J_-] = 0$ , all the states we produce by acting on  $|j, j\rangle$  with  $J_-$  have total angular momentum quantum number  $j = j_1 + j_2$ . This corresponds to the individual angular momenta of the subsystems always being aligned with eachother, with the different  $|j, m\rangle$  telling us about how closely there mutual direction of alignment coincides with the z-axis.

It's perfectly possible for the individual subsystems to not line up with eachother. In such a configuration the net total angular momentum of the combined system will be less than the maximum value  $j_1 + j_2$ . Let's seek an expression for the state  $|j - 1, j - 1\rangle$ in which the total angular momentum of the whole system is just less than the maximum possible, but where this angular momentum still points along the  $\hat{z}$ -axis. It's trivial to verify that any simple state  $|j_1, m_1\rangle|j_2, m_2\rangle$  is an eigenstate of  $J_z = J_{1z} + J_{2z}$ , with eigenvalue  $(m_1 + m_2)\hbar$ . We require  $m_1 + m_2 = j - 1 = j_1 + j_2 - 1$ , so either  $(m_1, m_2) = (j_1 - 1, j_2)$ or  $(m_1, m_2) = (j_1, j_2 - 1)$ . Also, the state  $|j - 1, j - 1\rangle$  must be orthogonal to the state  $|j, j - 1\rangle$  we found in (6.15) since they are each eigenstates of the Hermitian operator  $\mathbf{J}^2$ with distinct eigenvalues. Therefore we must have

$$|j-1,j-1\rangle = \sqrt{\frac{j_2}{j}}|j_1,j_1-1\rangle|j_2,j_2\rangle - \sqrt{\frac{j_1}{j}}|j_1,j_1\rangle|j_2,j_2-1\rangle.$$
(6.16)



**Figure 13**: Decomposing the tensor product of two irreducible representations into a sum of irreducible representations, drawn as semicircles. The picture on the left shows states obtained by adding a system with  $j_1 = 2$  to one with  $j_2 = 1$ , while that on the right is for  $j_1 = 1$  and  $j_2 = 1/2$ .

with a relative sign between the two terms. Again, this is a highest weight state, now with  $j = j_1 + j_2 - 1$ . Given this state, we may now proceed to construct all the states  $|j - 1, m\rangle$  with  $-j + 1 \le m \le j - 1$  by applying the lowering operator  $J_{-}$ .

Figure 13 helps us to organise our results. States of the combined system with welldefined angular momentum are marked by dots. The radius of each semicircle is proportional to  $\sqrt{j'}$ , where  $j'(j'+1)\hbar^2$  is the state's eigenvalue  $\mathbf{J}^2$ . The height of a state above the centre of the semicircles is proportional to m. The outer semicircle thus contains all states with  $j' = j_1 + j_2$ ; going inwards we meet the states with  $j' = j_1 + j_2 - 1$ , then those with  $j' = j_1 + j_2 - 2$  and so on. To construct  $|j - 2, j - 2\rangle$  we note that it must be in the span of  $\{|j_1, j_1 - 2\rangle|j_2, j_2\rangle, |j_1, j_1 - 1\rangle|j_2, j_2 - 1\rangle, |j_1, j_1\rangle|j_2, j_2 - 2\rangle\}$ , and that  $|j, j - 2\rangle$  and  $|j - 1, j - 2\rangle$ , the state  $|j - 2, j - 2\rangle$  must be the unique orthogonal combination.

From our classical considerations, it's reasonable to conjecture that the smallest possible total angular momentum quantum number of the whole system is  $|j_1 - j_2|$ , coming when the two gyros are aligned against one another. Let's check this by working out the total number of states the conjecture leads to. Without loss, we can assume  $j_1 \ge j_2$ . If the combined system has j values running from  $j_1 + j_2$  to  $j_1 - j_2$ , then we count a total of

$$\sum_{j=j_1-j_2}^{j_1+j_2} (2j+1) = 2 \left( \sum_{j=j_1-j_2}^{j_1+j_2} j \right) + (2j_2+1) = (2j_1)(2j_2+1) + (2j_2+1)$$

$$= (2j_1+1)(2j_2+1),$$
(6.17)

in agreement with the dimension of the tensor product space we found earlier using the 'obvious' tensor product basis in (6.4). We've thus accounted for all the possible states of the system.

The numbers

$$C_{j,m}(j_1, m_1; j_2, m_2) = \langle j, m | (|j_1, m_1\rangle \otimes |j_2, m_2\rangle)$$
(6.18)

are known as Clebsch–Gordan coefficients. Physically, they represent the amplitude that, when the total system is in state  $|j,m\rangle$ , we will find the subsystems to be in states  $|j_1,m_1\rangle$ and  $|j_2,m_2\rangle$  when we peer inside the box. For example, from equation (6.15) we see that  $C_{3,2}(2,1;1,1) = \sqrt{2/3}$ , so if we know our box contains a gyro of spin 2 and a gyro of spin 1, if the box is in state  $|3,2\rangle$  then there's a 2/3 chance that the second gyro has its spin maximally aligned with the z-axis with the first significantly inclined, but only a 1/3 chance that it is the first gyro that is maximally aligned with the  $\hat{z}$ -axis.

Let's take a look at a few examples to familiarise ourselves with the above general formalism.

#### **6.1.1** $j \otimes 0 = j$

First, the trivial case: if one of the subsystems (say the second) has  $j_2 = 0$ , then it always lies in  $|j_2, m_2\rangle = |0, 0\rangle$ . Hence the tensor product is trivial

$$\mathcal{H} = \mathcal{H}_{j_1} \otimes \mathcal{H}_0 = \mathcal{H}_{j_1} \otimes \mathbb{C} \cong \mathcal{H}_{j_1}$$

because we have no choice about the state of the second subsystem. The states

$$\{|j,m\rangle = |j_1,m_1\rangle|0,0\rangle\}$$

therefore form a basis of the full system, and are immediately a single irreducible representation with  $j = j_1$ .

# **6.1.2** $\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0$

The first non-trivial case is when  $j_1 = j_2 = 1/2$ . Physically this is relevant, *e.g.* to the case of the ground state of the Hydrogen atom where to understand the spin of the whole atom we must combine the spins of both the proton and the electron. From above, we have

$$|1,1\rangle_{\rm H} = |\uparrow\rangle_{\rm e} |\uparrow\rangle_{\rm p} \tag{6.19}$$

where the subscripts refer to Hydrogen, the electron and the proton, respectively. In this state, the spins of the electron and proton are aligned with eachother, and they each have maximal possible spin along the  $\hat{\mathbf{z}}$ -axis. Applying  $J_{-H} = J_{-e} + J_{-p}$  we obtain

$$|1,0\rangle_{\rm H} = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_{\rm e} |\downarrow\rangle_{\rm p} + |\downarrow\rangle_{\rm e} |\uparrow\rangle_{\rm p}\right) , \qquad (6.20)$$

while applying  $J_{-H}$  a second time gives

$$|1, -1\rangle_{\mathrm{H}} = |\downarrow\rangle_{\mathrm{e}} |\downarrow\rangle_{\mathrm{p}} \,. \tag{6.21}$$

Since both the electron and proton are in the  $|\downarrow\rangle$  state here, any further applications of either lowering operator will annihilate the *rhs*, in agreement with the action of the total lowering operator  $J_{-H}$  on the state  $|1, -1\rangle_{\rm H}$  of the whole atom.

Let me point out a perhaps surprising feature of this multiplet. In state (6.20), we are certain to find that the z-component of the spins of the electron and proton are 'antiparallel'. This may seem surprising given that the atom is still in a spin-1 state, corresponding to the spins of the subsystems being aligned. The resolution of the paradox is that while the *z*-components are indeed antiparallel, the components in the *xy*-plane are aligned, although their precise direction is unknown to us. Similarly, in both the  $|1,1\rangle$  and  $|1,-1\rangle$  states, while the *z*-components of the electron and proton spins were aligned, their components in the *xy*-plane were in fact antiparallel. The poor alignment in the *xy*-plane accounts for the fact that  $\sqrt{\langle \mathbf{J}^2 \rangle} = \sqrt{2}\hbar$  for the atom, which is less than the sum of  $\sqrt{\langle \mathbf{J}^2 \rangle} = \sqrt{3/4}\hbar$  for the electron and proton individually.

The remaining state of the atom is  $|0,0\rangle$ , in which the atom has no angular momentum. This should be orthogonal to (6.20), so we find

$$|0,0\rangle_{\rm H} = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_{\rm e} |\downarrow\rangle_{\rm p} - |\downarrow\rangle_{\rm e} |\uparrow\rangle_{\rm p}\right) \,. \tag{6.22}$$

The change in sign on the rhs of this equation ensures that the electron and proton spins are antiparallel in the xy-plane as well as in the z-direction. In fact, one can check that this state may also be written as

$$|0,0\rangle_{\rm H} = -\frac{1}{\sqrt{2}} \left(|\uparrow_x\rangle_{\rm e} |\downarrow_x\rangle_{\rm p} - |\downarrow_x\rangle_{\rm e} |\uparrow_x\rangle_{\rm p}\right) \tag{6.23}$$

where  $|\uparrow_x\rangle$  and  $|\downarrow_x\rangle$  are eigenstates of  $J_x$ . Similarly,

$$|1,0\rangle_{\rm H} = \frac{1}{\sqrt{2}} \left(|\uparrow_x\rangle_{\rm e} |\uparrow_x\rangle_{\rm p} - |\downarrow_x\rangle_{\rm e} |\downarrow_x\rangle_{\rm p}\right) \tag{6.24}$$

as one can check straightforwardly.

Altogether, combining two states each with angular momentum 1/2, we've found a triplet of states with total angular momentum j = 1:

$$|1,1\rangle = |\uparrow\rangle |\uparrow\rangle, \qquad |1,0\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle |\downarrow\rangle + |\downarrow\rangle |\uparrow\rangle\right), \qquad |1,-1\rangle = |\downarrow\rangle |\downarrow\rangle \qquad (6.25)$$

and a singlet with total angular momentum j = 0:

$$|0,0\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\right) . \tag{6.26}$$

Note that each state in the triplet is symmetric under exchange of the angular momenta of the two subsystems, while the singlet state is antisymmetric under this exchange.

**6.1.3**  $1 \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2}$ 

If our subsystems have  $j_1 = 1$  and  $j_2 = \frac{1}{2}$ , then the total system can have  $j = \frac{3}{2}$  or  $j = \frac{1}{2}$ . Let's start as always with the highest state

$$\left|\frac{3}{2}, \frac{3}{2}\right\rangle = \left|1, 1\right\rangle \left|\uparrow\right\rangle. \tag{6.27}$$

Applying the lowering operator, we find successively the states

$$\left| \frac{3}{2}, \frac{1}{2} \right\rangle = \sqrt{\frac{2}{3}} \left| 1, 0 \right\rangle \left| \uparrow \right\rangle + \sqrt{\frac{1}{3}} \left| 1, 1 \right\rangle \left| \downarrow \right\rangle,$$

$$\left| \frac{3}{2}, -\frac{1}{2} \right\rangle = \sqrt{\frac{1}{3}} \left| 1, -1 \right\rangle \left| \uparrow \right\rangle + \sqrt{\frac{2}{3}} \left| 1, 0 \right\rangle \left| \downarrow \right\rangle,$$

$$\left| \frac{3}{2}, -\frac{3}{2} \right\rangle = \left| 1, -1 \right\rangle \left| \downarrow \right\rangle$$

$$(6.28)$$



**Figure 14**: Classically, the sum of two vectors lies on a sphere centred on the end of one of these vectors, at a location determined by their relative orientation.

which complete the  $j = \frac{3}{2}$  multiplet. The remaining states are

$$\left|\frac{1}{2},\frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left|1,0\right\rangle\left|\uparrow\right\rangle - \sqrt{\frac{2}{3}}\left|1,1\right\rangle\left|\downarrow\right\rangle \quad \text{and} \quad \left|\frac{1}{2},-\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|1,-1\right\rangle\left|\uparrow\right\rangle - \sqrt{\frac{1}{3}}\left|1,0\right\rangle\left|\downarrow\right\rangle. \tag{6.29}$$

The first of these is obtained by requiring it to be orthogonal to  $|\frac{3}{2}, \frac{1}{2}\rangle$ , and the second follows by applying the lowering operator to the first.

#### 6.1.4 The Classical Limit

We should expect to recover a classical picture when we combine two systems each with large amounts of total angular momentum. Let's see how this occurs. Classically, if we add two angular momentum vectors  $\mathbf{j}_1$  and  $\mathbf{j}_2$  then the resultant vector has magnitude

$$\mathbf{j}^2 = (\mathbf{j}_1 + \mathbf{j}_2)^2 = \mathbf{j}_1^2 + \mathbf{j}_2^2 + 2\mathbf{j}_1 \cdot \mathbf{j}_2.$$
 (6.30)

If we know nothing about the relative orientation of  $\mathbf{j}_1$  and  $\mathbf{j}_2$ , then all points on a sphere of radius  $|\mathbf{j}_2|$  centred on the end of  $\mathbf{j}_1$  are equally likely. Consequently, the probability dPthat  $\mathbf{j}_1$  and  $\mathbf{j}_2$  have relative alignment in the range  $(\theta, \theta + d\theta)$  is proportional to the area of the band shown in figure 14. The magnitudes of  $\mathbf{j}_1$  and  $\mathbf{j}_2$  are fixed, so  $d\mathbf{j}^2 = 2|\mathbf{j}_1||\mathbf{j}_2| d\cos\theta$ . Hence the probability of this alignment is

$$dP = \frac{2\pi \sin \theta \, d\theta}{4\pi} = \frac{|\mathbf{j}| \, d|\mathbf{j}|}{2|\mathbf{j}_1||\mathbf{j}_2|} \tag{6.31}$$

and hence  $dP/d|\mathbf{j}| = |\mathbf{j}|/2|\mathbf{j}_1||\mathbf{j}_2|$ .

In the quantum case, suppose  $j_1, j_2 \gg 1$ . Then the fraction of states in the combined system with some amount j of angular momentum is

$$\frac{2j+1}{(2j_1+1)(2j_2+1)} \approx \frac{j}{2j_1j_2} \tag{6.32}$$

provided  $|j_1 - j_2| \leq j \leq j_1 + j_2$ . Thus, if we know nothing about the original state of the subsystems, the probability that the combined system has total angular momentum j agrees with the classical probability computed above.

### 6.2 Angular Momentum of Operators

Suppose that V is a vector operator, so that in particular  $U^{-1}(\alpha)VU(\alpha) = \mathbf{R}(\alpha)V$  under rotations, or

$$[J_i, V_j] = i\hbar \sum_k \epsilon_{ijk} V_k \tag{6.33}$$

infinitesimally. We define the *spherical components* of  $\mathbf{V}$  by

$$V^{+1} = -\frac{1}{\sqrt{2}}(V_x + iV_y), \qquad V^{-1} = \frac{1}{\sqrt{2i}}(V_x - iV_y), \qquad V^0 = V_z$$
(6.34)

Then the commutation relations (6.33) are equivalent to

$$= m\hbar V^{m}$$

$$[J_{\pm}, V^{m}] = \hbar \sqrt{2 - m(m \pm 1)} V^{m \pm 1}.$$
(6.35)

## 6.2.1 The Wigner–Eckart Theorem

#### 6.2.2 Dipole Moment Transitions

## 6.2.3 The Runge–Lenz Vector in Hydrogen

For a spinless particle of mass<sup>57</sup> M in a generic central potential, the Hamiltonian takes the form

$$H = \frac{\mathbf{P}^2}{2M} + V(|\mathbf{X}|) \,. \tag{6.36}$$

By definition, any such Hamiltonian is rotationally invariant, so it follows that

$$[\mathbf{L}, H] = 0$$
 and  $[\mathbf{L}^2, H] = 0.$  (6.37)

Since we also have  $[L_i, \mathbf{L}^2] = 0$  we can find a complete set of simultaneous eigenstates of  $H, \mathbf{L}^2$  and  $L_z$ , so we can label our states as  $|n, \ell, m\rangle$ . The Hamiltonian does not involve  $L_z$  except through  $\mathbf{L}^2$ , so the energy level  $E_{n,\ell,m}$  of such a state must certainly be independent of m. However, the Hamiltonian *does* involve  $\mathbf{L}^2$  through the kinetic operator, so we do not generically expect the energy levels to be independent of  $\ell$ . Physically, if we give our particle more or less angular momentum, it will whizz round faster or slower. Typically, we'd expect this to change the energy.

Nonetheless, it occasionally happens that a Hamiltonian is invariant under transformations beyond those inherited from the transformations of the space  $\mathbb{R}^3$  in which the quantum system lives. If the algebra of the corresponding generators closes, meaning that the commutator of any pair of generators is equal to another generator (perhaps including the Hamiltonian), then we say we have a *dynamical symmetry*. In such cases, it may be possible to change the total angular momentum of a state without changing its energy, so that states of different orbital angular momentum quantum number  $\ell$  can be degenerate.

Hamiltonians with dynamical symmetry are very rare: for single-particle quantum systems moving on  $\mathbb{R}^3$  with a central potential, the only cases are the harmonic oscillator

<sup>&</sup>lt;sup>57</sup>We denote the mass with a capital M so as to avoid any confusion with the z angular momentum quantum number m.

and motion in a Coulomb potential. However, these two cases are so important that it's worth considering them from this point of view.

The treatment below closely follows section 4.8 of Weinberg – I think I'll modify it when I write the Wigner-Eckart part

The first case we'll study is for the Coulomb potential, relevant *e.g.* to the hydrogen atom. Classically, conservation of angular momentum in any central potential implies that the motion is confined to a plane, but the Kepler problem has a further conserved quantity known as the *Runge-Lenz vector*  $\mathbf{r}$ , given by

$$\mathbf{r} = -e^2 \frac{\mathbf{x}}{|\mathbf{x}|} + \frac{1}{M} \mathbf{p} \times \mathbf{L}$$
(6.38)

for a particle of mass M. Conservation of this vector implies that classical bound states have closed orbits; the motion is not just in a plane, but follows a fixed ellipse. (The observation of a gradual shift in Mercury's orbit – the precession of its perihelion – was one of the early confirmations of General Relativity's modifications to Newton's Laws of Gravity.)

Now let's consider the quantum mechanical case. We construct the Runge–Lenz operator

$$\mathbf{R} = -\frac{e^2}{|\mathbf{X}|}\mathbf{X} + \frac{1}{2M}\left(\mathbf{P} \times \mathbf{L} - \mathbf{L} \times \mathbf{P}\right)$$
  
$$= -\frac{e^2}{|\mathbf{X}|}\mathbf{X} + \frac{1}{M}\mathbf{P} \times \mathbf{L} - \frac{\mathrm{i}\hbar}{M}\mathbf{P} .$$
 (6.39)

Classically, the two terms in brackets on the first line of (6.39) are equal; we've written it this way to ensure that  $\mathbf{R}^{\dagger} = \mathbf{R}$ .

Since  $\mathbf{R}$  is a vector operator built from  $\mathbf{X}$  and  $\mathbf{P}$ , it follows that its commutation relations with  $\mathbf{L}$  are

$$[L_i, R_j] = i\hbar \sum_k \epsilon_{ijk} R_k \,. \tag{6.40}$$

so that it transforms as a vector under rotations. Therefore, the Wigner-Eckart theorem says that

$$\langle n', \ell', m' | R_1^k | n, \ell, m \rangle = C_{\ell', m'}(1, k'; \ell, m) \langle n' || R || n \rangle$$
 (6.41)

Furthermore, a somewhat tedious calculation (which I'll spare you, and which I don't expect you to reproduce) shows that  $[H, \mathbf{R}] = 0$  so the Runge-Lenz vector is conserved. Thus the reduced matrix element  $\langle n' || R || n \rangle$  vanishes unless n' = n.

The orbital angular momentum  $\mathbf{L} = \mathbf{X} \times \mathbf{P}$  is orthogonal to each of the three terms in this expression, so  $\mathbf{R} \cdot \mathbf{L} = \mathbf{L} \cdot \mathbf{R} = 0$ . We also have

$$\mathbf{L}^{2} = (\mathbf{X} \times \mathbf{P}) \cdot \mathbf{L} = \mathbf{X} \cdot (\mathbf{P} \times \mathbf{L})$$
$$= (\mathbf{P} \times \mathbf{L}) \cdot \mathbf{X} + \sum_{i,j,k=1}^{3} \epsilon_{ijk} [X_{i}, P_{j}L_{k}]$$
$$= (\mathbf{P} \times \mathbf{L}) \cdot \mathbf{X} + 2i\hbar \mathbf{P} \cdot \mathbf{X},$$
 (6.42)

as well as

$$\mathbf{P} \cdot (\mathbf{P} \times \mathbf{L}) = 0, \qquad (\mathbf{P} \times \mathbf{L}) \cdot \mathbf{P} = 2i\hbar \mathbf{P}^2 \qquad \text{and} \qquad (\mathbf{P} \times \mathbf{L})^2 = \mathbf{P}^2 \mathbf{L}^2 \qquad (6.43)$$

where we've been careful to keep track of operator orders. Using these results, we find that the length-squared of the Runge–Lenz operator is given by

$$\mathbf{R}^{2} = Z^{2}e^{4} + \frac{2H}{\mu} \left( L^{2} + \hbar^{2} \right) \,. \tag{6.44}$$

The point of this expression is that it relates  $\mathbf{R}$  to H; since we know the spectrum of  $L^2$ , we can find the eigenvalues of H if we can find the eigenvalues of  $\mathbf{R}$ . A rather longwinded calculation (that I won't expect you to reproduce) shows that the components of the Runge-Lenz operator obey the commutation relations

$$[R_i, R_j] = -\frac{2i\hbar}{\mu} H \sum_k \epsilon_{ijk} L_k , \qquad (6.45)$$

where we note that H commutes with  $\mathbf{L}$ .

We now introduce the operators

$$\mathbf{A}_{\pm} = \frac{1}{2} \left( \mathbf{L} \pm \sqrt{\frac{\mu}{-2H}} \, \mathbf{R} \right) \tag{6.46}$$

built from the orbital angular momentum operator, the Runge-Lenz operator and the Hamiltonian, where we recall that functions (such as the square root) of an operator are defined as in (2.42). The point of introducing these strange-looking combinations is that commutation relations (6.40) & (6.45) show that the  $\mathbf{A}_{\pm}$  obey the algebra

$$[A_{\pm i}, A_{\pm j}] = i\hbar \sum_{k} \epsilon_{ijk} A_{\pm k} \quad \text{and} \quad [\mathbf{A}_{\pm}, \mathbf{A}_{\mp}] = 0, \quad (6.47)$$

which we recognise<sup>58</sup> as two independent copies of the angular momentum algebra  $\mathfrak{so}(3)$ . In particular, just as for the total angular momentum, the eigenvalues of  $\mathbf{A}_{\pm}^2$  take the form  $a_{\pm}(a_{\pm}+1)\hbar^2$  where  $a_{\pm} \in \{0, 1/2, 1, 3/2, \ldots\}$ , with the eigenvalues of any component of  $\mathbf{A}_{\pm}$  running from  $-\hbar a_{\pm}$  to  $+\hbar a_{\pm}$  in steps of  $\hbar$ .

Since  $[\mathbf{A}_{\pm}, H] = 0$  we can find simultaneous eigenstates of H,  $\mathbf{A}_{\pm}^2$  and, say,  $A_{\pm z}$  and  $A_{-z}$ . However, taking the square of (6.46) and using the fact that  $\mathbf{L} \cdot \mathbf{R} = \mathbf{R} \cdot \mathbf{L} = 0$ ,

$$\mathbf{A}_{+}^{2} = \mathbf{A}_{-}^{2} = \frac{1}{4} \left( L^{2} + \frac{\mu}{2H} \mathbf{R}^{2} \right) = -\frac{Z^{2} e^{4} \mu}{8H} - \frac{\hbar^{2}}{4} \,. \tag{6.48}$$

In particular, we cannot choose these eigenvalues of  $\mathbf{A}^2_+$  and  $\mathbf{A}^2_-$  independently, but must have  $a_+ = a_-$ . Calling the common eigenvalue a, an simultaneous eigenstate of H and  $\mathbf{A}^2_{\pm}$ obeys

$$-\frac{Z^2 e^4 \mu}{8E} = \left(a(a+1) + \frac{1}{4}\right)\hbar^2 = \frac{\hbar^2}{4}(2a+1)^2.$$
(6.49)

<sup>&</sup>lt;sup>58</sup>For bound states of the Coulomb potential, the spectrum of H is negative-definite, so the operators  $\mathbf{A}_{\pm}$  are indeed Hermitian when acting on such states. At energies above the ionisation threshold, the square root in (6.46) means that  $\mathbf{A}_{\pm}$  can no longer be treated as Hermitian, and this algebra is then better described as  $\mathfrak{sl}(2)$ .

For a any non-negative half integer,  $2a + 1 \in \{1, 2, 3, ...\}$ , so the energy levels can be written

$$E_n = -\frac{Z^2 e^4 \mu}{2\hbar^2 n^2} \qquad \text{where} \qquad n \in \mathbb{N} \,. \tag{6.50}$$

These are the energy levels of hydrogenic atoms that you obtained in IB QM. The eigenvalues of  $A_{+z}$  and  $A_{-z}$  can be chosen independently, and each run from  $-a\hbar$  to  $a\hbar$  in steps of  $\hbar$ . Thus the degeneracy of the state with energy  $E_n$  is  $(2a+1)^2 = n^2$ . Again, this is bigger than the degeneracy of a generic central potential, and the degenerate states transform in representations of the enhanced  $\mathfrak{so}(3) \times \mathfrak{so}(3)$  symmetry algebra. The diagonal part of this, generated by  $\mathbf{L} = \mathbf{A}_+ + \mathbf{A}_-$  corresponds to spatial rotations.

Incidentally, it's useful to note that the energy levels of a hydrogenic atom can be written as -2, 2

$$E_n = -\frac{Z^2 \alpha^2}{2n^2} mc^2$$
 (6.51)

where the dimensionless number

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \tag{6.52}$$

is known as the *fine structure constant*. Experimentally,  $\alpha \approx 1/137$ . The significance of this is that, at least for small atomic number Z,  $|E_n/mc^2| \ll 1$  providing a posteriori justification of our use of non-relativistic quantum mechanics to study the hydrogen atom.

## 6.2.4 Enhanced Symmetry of the 3d Isotropic Harmonic Oscillator

As a second example, consider an isotropic 3d harmonic oscillator, with Hamiltonian

$$H = \frac{\mathbf{P}^2}{2M} + \frac{1}{2}M\omega^2 \mathbf{X}^2 \tag{6.53}$$

as in section 3.3. The fact that H is quadratic in **X** as well as in **P** means it has an enhanced symmetry beyond the obvious SO(3) rotational invariance. We can see this from the form

$$H = \hbar\omega \left(\sum_{i} A_{i}^{\dagger}A_{i} + \frac{3}{2}\right) \tag{6.54}$$

in terms of raising and lowering operators. Written this way, H is clearly invariant under the transformations

$$A_i \mapsto A'_i \sum_{j=1}^3 u_{ij} A_j \qquad A^{\dagger}_i \mapsto (A'_i)^{\dagger} = \sum_{k=1}^3 A^{\dagger}_k (u^{\dagger})_{ki}$$
(6.55)

for any  $3 \times 3$  unitary matrix u. These matrices must be unitary if the new  $\mathbf{A}'^{\dagger}$  is indeed to be the Hermitian conjugate of the new  $\mathbf{A}'$ . It's important to realise that, although they are unitary, the matrices  $u_{ij}$  do not act on the Hilbert space of the harmonic oscillator, but just on the spatial indices of the vector operators  $\mathbf{A}$  and  $\mathbf{A}^{\dagger}$ . They thus mix  $\mathbf{X}$  and  $\mathbf{P}$  together<sup>59</sup>.

<sup>&</sup>lt;sup>59</sup>For those taking Integrable Systems: classically these are symmetries of phase space that do not come from symmetries of space itself, and reflect the fact that the harmonic oscillator is (super-)integrable.

Note also that the new raising and lowering operators obey the same commutation relations as the original ones.

A  $3 \times 3$  unitary matrix has 9 independent real components, whereas a rotation in three dimensions is completely specified by only 3 independent Euler angles, so the U(3) symmetry of this Hamiltonian is much bigger than the SO(3) rotational invariance of a generic central potential. The fact that the Hamiltonian is invariant under the U(3) transformations (6.55) implies that there should be a total of nine conserved quantities corresponding to the nine generators of this symmetry. It's easy to check that these generators form the tensor operator  $\mathbf{T}$  with components  $T_{ij} = A_i^{\dagger}A_j$ . We have  $[H, \mathbf{T}] = 0$  and hence each component  $T_{ij}$  is conserved. To understand these operators, we decompose  $\mathbf{T}$  into its irreducible parts as in section 6.2.1, obtaining

$$T_{ij} = \mathbf{A}^{\dagger} \cdot \mathbf{A} \, \frac{\delta_{ij}}{3} + \frac{A_i^{\dagger} A_j - A_j^{\dagger} A_i}{2} + \left[ \frac{A_i^{\dagger} A_j + A_j^{\dagger} A_i}{2} - \mathbf{A}^{\dagger} \cdot \mathbf{A} \, \frac{\delta_{ij}}{3} \right] \,. \tag{6.56}$$

The trace  $\mathbf{A}^{\dagger} \cdot \mathbf{A}$  is (up to a constant) just the Hamiltonian itself, which is certainly conserved. Recalling the definition (3.33) of the raising and lowering operators, the anti-symmetric part can be combined into a vector with components

$$\sum_{j,k} \epsilon_{ijk} A_j^{\dagger} A_k = \frac{1}{2M\hbar\omega} \sum_{j,k} \epsilon_{ijk} (M\omega X_j - iP_j) (M\omega X_k + iP_k)$$
  
$$= \frac{i}{2\hbar} \sum_{j,k} \epsilon_{ijk} (X_j P_k - P_j X_k) = \frac{i}{\hbar} \mathbf{L}_i,$$
 (6.57)

where in the last equality we used the fact  $\epsilon_{ijk}(X_jP_k - P_jX_k) = 2\epsilon_{ijk}X_jP_k$ , with the  $\epsilon$ -symbol ensuring that the components of **X** and **P** commute. Thus

$$\mathbf{L} = -\mathrm{i}\hbar \left(\mathbf{A}^{\dagger} \times \mathbf{A}\right),\tag{6.58}$$

so that the vector part of  $\mathbf{T}$  is nothing but the usual orbital angular momentum operator for the 3*d* oscillator. It is no surprise that this is conserved.

The remaining five conserved quantities — the symmetric, traceless part  $(T_{ij}+T_{ji})/2 - \sum_i T_{ii}/3$  of  $\mathbf{T}$  — generate transformations that mix  $\mathbf{X}$  and  $\mathbf{P}$ , appropriately rescaled. They're less familiar, as they're special to the simple harmonic oscillator. The five components of this traceless symmetric part correspond to the spin-2 part of the operator  $\mathbf{T}$ 

We can see this degeneracy by examining the excited states of the oscillator. Just as in 1*d*, these may be obtained by acting on  $|\mathbf{0}\rangle$  with any component of the raising operators  $\mathbf{A}^{\dagger}$ . Since the ground state has energy  $3\hbar\omega/2$  and each application of a raising operator increases the energy by one unit of  $\hbar\omega$ , each of the states

$$A_{i_N}^{\dagger} \cdots A_{i_2}^{\dagger} A_{i_1}^{\dagger} | \mathbf{0} \rangle \tag{6.59}$$

has the same energy  $(N+3/2)\hbar\omega$ , where we can choose any  $\{i_1, i_2, \ldots, i_N\} \in \{1, 2, 3\}$ . We often call the (correctly normalised) such state  $|n_x, n_y, n_z\rangle$ , where  $n_x$  is the total number

of times we've applied the x-component of  $\mathbf{A}^{\dagger}$ , and similarly for  $n_y$  and  $n_z$ . Of course,  $N = n_x + n_y + n_z$ .

Since the components of the raising operators all commute with one another, we can consider the indices  $i_1, \ldots, i_N$  in (6.59) to be symmetrized. Consequently, the degeneracy of the  $N^{\text{th}}$  energy level is the same as the number of independent components of a rank Ntensor in 3 dimensions, which is (N + 1)(N + 2)/2. (Think 'stars & bars', or the number of ways to partition N into three non-negative integers  $(n_x, n_y, n_x)$ .) This is the larger degeneracy that we promised. It's easy to derive this degeneracy in number of ways; our derivation here makes clear that the degenerate energy states transform in representations of the larger  $\mathfrak{su}(3)$  algebra.

#### 6.3 Angular Momentum of the Isotropic Oscillator

We can find the spectrum of  $H_{\ell}$  using raising and lowering operators in a similar fashion to our treatment of the full H above. We introduce

$$A_{\ell} = \frac{1}{\sqrt{2\mu\hbar\omega}} \left( iP_r - \frac{(\ell+1)\hbar}{R} + \mu\omega R \right)$$
(6.60)

and a short computation using  $[R, P_r] = i\hbar$  shows that

$$H_{\ell} = \hbar\omega \left( A_{\ell}^{\dagger} A_{\ell} + \left( \ell + \frac{3}{2} \right) \right) \,. \tag{6.61}$$

This is very similar to the expression (3.35) above, but now we find the commutation relations

$$[A_{\ell}, A_{\ell}^{\dagger}] = 1 + \frac{(\ell+1)\hbar}{\mu\omega R^2} = \frac{H_{\ell+1} - H_{\ell}}{\hbar\omega} + 1$$
(6.62)

in place of (3.34) for the raising and lowering operators in Cartesian coordinates. In consequence, the commutator of  $H_{\ell}$  with  $A_{\ell}$  is

$$[A_{\ell}, H_{\ell}] = \hbar\omega[A_{\ell}, A_{\ell}^{\dagger}A_{\ell}] = \hbar\omega[A_{\ell}, A_{\ell}^{\dagger}]A_{\ell} = (H_{\ell+1} - H_{\ell} + \hbar\omega)A_{\ell}, \qquad (6.63)$$

or equivalently

$$H_{\ell+1}A_{\ell} - A_{\ell}H_{\ell} = -\hbar\omega A_{\ell}.$$
(6.64)

This is very close to showing that  $A_{\ell}$  is a lowering operator, but the presence of  $H_{\ell+1}$  means that the algebra does not close unless we consider all values of  $\ell$ . To understand the implications of this, let  $|E(\ell)\rangle$  be an eigenstate of  $H_{\ell}$ , with  $H_{\ell}|E(\ell)\rangle = E|E(\ell)\rangle$  where we emphasise that the energies depend on the total orbital angular momentum quantum number  $\ell$ . Then

$$H_{\ell+1}(A_{\ell}|E(\ell)\rangle) = (E - \hbar\omega)A_{\ell}|E(\ell)\rangle, \qquad (6.65)$$

which implies that  $A_{\ell}|E(\ell)\rangle$  is an eigenstate of  $H_{\ell+1}$  with eigenvalue  $E - \hbar\omega$ . The Hamiltonian  $H_{\ell+1}$  is the one appropriate for the radial part of wavefunctions with total angular momentum labelled by  $\ell + 1$ , so applying  $A_{\ell}$  to  $|E(\ell)\rangle$  has created a state with lower energy, but with a radial wavefunction corresponding to a state of greater orbital angular momentum.



**Figure 15**: The action of the operators  $A_{\ell}$  and  $A_{\ell}^{\dagger}$  on the states of the isotropic three dimensional oscillator.

By a now familiar argument, in any  $H_{\ell}$  eigenstate we have

$$\frac{E_{\ell}}{\hbar\omega} - \ell - \frac{3}{2} = \left\langle E(\ell) \left| \frac{H_{\ell}}{\hbar\omega} - \frac{3}{2} \right| E(\ell) \right\rangle = \left\langle E(\ell) | A_{\ell}^{\dagger} A_{\ell} | E(\ell) \right\rangle = \|A_{\ell} | E(\ell) \rangle \|^2 \ge 0.$$
(6.66)

Thus, for a fixed given energy E the maximum orbital angular momentum our state can have is

$$\ell_{\max} = \frac{E}{\hbar\omega} - \frac{3}{2}.$$
(6.67)

As  $\ell_{\text{max}}$  is a non-negative integer (since it is a possible value for  $\ell$  at given E) we see that, in agreement with the previous subsection, the ground state energy is  $3\hbar\omega/2$  which occurs when  $\ell_{\text{max}} = 0$ , meaning that this ground state is necessarily spherically symmetric.

For any given energy, the state  $|E(\ell_{\max})\rangle$  which saturates the bound (6.66) obeys  $A_{\ell_{\max}}|E(\ell_{\max})\rangle = 0$  and has the maximum possible total angular momentum out of all the states with this energy. It is thus the quantum equivalent of a *circular orbit*. In the position representation we have

$$0 = \langle r | A_{\ell_{\max}} | E(\ell_{\max}) \rangle = \frac{1}{\sqrt{2\mu\hbar\omega}} \left( \frac{\partial}{\partial r} + \frac{1}{r} - \frac{(\ell_{\max} + 1)}{r} + \frac{m\omega r}{\hbar} \right) \langle r | E(\ell_{\max}) \rangle$$
(6.68)

where we use  $|r\rangle$  to denote a state that is definitely located at radius r. This equation is solved by

$$\langle r|E(\ell_{\rm max})\rangle = C r^{\ell_{\rm max}} e^{-r^2/4r_0^2}$$
 (6.69)

where  $r_0 = \sqrt{\hbar/2\mu\omega}$  and C is a constant. Note that the exponential here is just the product of the exponentials we'd expect for Cartesian oscillators. This wavefunction varies with r, so quantum mechanically even a 'circular' orbit has some radial kinetic energy. In the limit of large  $\ell_{\text{max}}$  in which classical mechanics applies, the radial kinetic energy is negligible compared to the tangential kinetic energy. The full wavefunction is  $\langle \mathbf{r} | (|E(\ell_{\text{max}})\rangle \otimes |\ell_{\text{max}}, m \rangle)$  and so also involves the spherical harmonic  $Y^m_{\ell_{\text{max}}}(\theta, \phi)$ . Bearing in mind that  $d^3x = r^2 \sin\theta \, d\phi \, d\theta \, dr$ , the radial probability density P(r) for this state is  $P(r) \sim r^{2\ell_{\text{max}}+2} e^{-r^2/2r_0^2}$ . For  $r/r_0 \ll \sqrt{2\ell_{\text{max}}+2}$  this rises as  $r^{2\ell_{\text{max}}+2}$  and it falls as the

Gaussian takes over when  $r/r_0 > \sqrt{2\ell_{\text{max}} + 2}$ . The rms deviation in the radial location is  $\sim r_0$ , which is a small fraction of the expected radial location  $\langle R \rangle$  when  $\ell_{\text{max}}$  is large.

We can obtain the radial wavefunctions of more eccentric orbits using  $A_{\ell}^{\dagger}$ . Taking the adjoint of (6.64) we obtain

$$H_{\ell}A_{\ell}^{\dagger} - A_{\ell}^{\dagger}H_{\ell+1} = \hbar\omega A_{\ell}^{\dagger}.$$
(6.70)

Acting with this on  $|E(\ell+1)\rangle$  we have

$$H_{\ell}(A_{\ell}^{\dagger}|E(\ell+1)\rangle) = (E+\hbar\omega)\left(A_{\ell}^{\dagger}|E(\ell+1)\rangle\right)$$
(6.71)

so that  $A_{\ell}^{\dagger}|E(\ell+1)\rangle$  is a state of increased energy, whose radial wavefunction is appropriate for orbital angular momentum  $\ell$ . Thus  $A_{\ell}^{\dagger}|E(\ell+1)\rangle = c|E(\ell) + \hbar\omega\rangle$  for some constant c. The radial wavefunctions of the eccentric orbits follow by writing this equation in the position representation, though we won't perform this calculation here. The way the energy raising / angular momentum lowering operators  $A_{\ell}^{\dagger}$  and the energy lowering / angular momentum raising operators  $A_{\ell}$  act on the states is summarised in figure 15.

In the previous section we found that there were (N+2)(N+1)/2 degenerate states in the N<sup>th</sup> excited level of the isotropic oscillator, each with energy  $E = (N+3/2)\hbar\omega$ . From the point of view of the present section, with energy  $E = (N+3/2)\hbar\omega$  we have  $\ell_{\text{max}} = N$ and this degeneracy arises as

$$\sum_{\ell=0}^{\ell_{\max}} \sum_{m=-\ell}^{\ell} 1 = \sum_{\ell=0}^{\ell_{\max}} (2\ell+1) = \ell_{\max}(\ell_{\max}+1) = \frac{(N+1)(N+2)}{2}$$
(6.72)

since there are  $2\ell + 1$  possible states with total orbital angular momentum  $\ell$ .

#### 6.4 The Radial Hamiltonian for the Coulomb Potential

For some purposes, it's useful to study hydrogen from a point of view that emphasises the fact that the potential is central, so energy eigenstates may also be chosen to have definite angular momentum. In the first problem set you showed that the kinetic part of the Hamiltonian could be written as

$$T = \frac{1}{2\mu} \left( P_r^2 + \frac{\mathbf{L}^2}{R^2} \right) \,, \tag{6.73}$$

where  $R^2 = \mathbf{X} \cdot \mathbf{X}$  and  $P_r = \frac{1}{2}(\hat{\mathbf{X}} \cdot \mathbf{P} + \mathbf{P} \cdot \hat{\mathbf{X}})$  is the radial momentum. Thus, when acting on an orbital angular momentum eigenstate  $|\ell, m\rangle$ , the Hamiltonian of a hydrogenic atom with atomic number<sup>60</sup> Z reduces to

$$H_{\ell} = \frac{P_r^2}{2\mu} + \frac{\ell(\ell+1)\hbar^2}{2\mu R^2} - \frac{Ze^2}{4\pi\epsilon_0 R}.$$
(6.74)

As in IA Dynamics & Relativity, this is just what we'd find for a particle moving in one dimension under the influence of the *effective potential* 

$$V_{\rm eff}(R) = \frac{\ell(\ell+1)\hbar^2}{2\mu R^2} - \frac{Ze^2}{4\pi\epsilon_0 R}.$$
 (6.75)

<sup>&</sup>lt;sup>60</sup>The atomic number is the number of protons in the atom's nucleus.

 $H_{\ell}$  governs the oscillations of the particle around the minima of this potential. Note that since  $H_{\ell}$  depends only on the radius R and radial momentum  $P_r$ , in position space its eigenstates will determine the radial dependence  $R_E(r) = \langle r | E(\ell) \rangle$  of the full wavefunction. A basis of eigenstates  $|E, \ell, m\rangle$  of the full Hamiltonian H can be chosen to be (tensor) products of the eigenstates  $|E(\ell)\rangle$  of  $H_{\ell}$  and the eigenstates  $|\ell, m\rangle$  of  $\mathbf{L}^2$  and  $L_z$ , whose position space wavefunction  $Y_{\ell}^m(\theta, \phi) = \langle \hat{\mathbf{r}} | \ell, m \rangle$  is a spherical harmonic, as in section 5.4.1.

All three terms in  $H_{\ell}$  must have the same dimensions, and in particular the ratio of the two terms in  $V_{\text{eff}}$  must be dimensionless. Thus

$$\frac{\hbar^2}{\mu R^2} \times \frac{4\pi\epsilon_0 R}{e^2} = \frac{4\pi\epsilon_0 \hbar^2}{\mu e^2} \times \frac{1}{R} \qquad \text{is dimensionless.} \tag{6.76}$$

It follows that the Bohr radius

$$a_0 \equiv \frac{4\pi\epsilon_0\hbar^2}{\mu e^2} \tag{6.77}$$

is the characteristic length scale of the hydrogen atom. We have

$$H_{\ell} = \frac{\hbar^2}{2\mu} \left( \frac{P_r^2}{\hbar^2} + \frac{\ell(\ell+1)}{R^2} - \frac{2Z}{a_0 R} \right)$$
(6.78)

in terms of  $a_0$ .

Let's define a new operator  $A_{\ell}$  by

$$A_{\ell} = \frac{a_0}{\sqrt{2}} \left( \frac{\mathrm{i}}{\hbar} P_r - \frac{\ell+1}{R} + \frac{Z}{(\ell+1)a_0} \right) \,. \tag{6.79}$$

Then one finds

$$A_{\ell}^{\dagger}A_{\ell} = \frac{a_0^2}{2} \left( -\frac{\mathrm{i}}{\hbar}P_r - \frac{\ell+1}{R} + \frac{Z}{(\ell+1)a_0} \right) \left( \frac{\mathrm{i}}{\hbar}P_r - \frac{\ell+1}{R} + \frac{Z}{(\ell+1)a_0} \right) = \frac{a_0^2}{2} \left\{ \frac{P_r^2}{\hbar^2} + \left( \frac{Z}{(\ell+1)a_0} - \frac{\ell+1}{R} \right)^2 + \mathrm{i}\frac{\ell+1}{\hbar} \left[ P_r, \frac{1}{R} \right] \right\}.$$
(6.80)

Using the commutator  $[P_r, R] = -i\hbar$  this gives

$$\begin{aligned} A_{\ell}^{\dagger}A_{\ell} &= \frac{a_0^2}{2} \left\{ \frac{P_r^2}{\hbar^2} + \frac{Z^2}{(\ell+1)^2 a_0^2} + \frac{(\ell+1)^2}{R^2} - \frac{2Z}{a_0 R} - \frac{\mathrm{i}}{\hbar} \frac{\ell+1}{R} \left[ P_r, R \right] \right\} \\ &= \frac{a_0^2}{2} \left\{ \frac{P_r^2}{\hbar^2} + \frac{Z^2}{(\ell+1)^2 a_0^2} + \frac{\ell(\ell+1)}{R^2} - \frac{2Z}{a_0 R} \right\} \\ &= \frac{a_0^2 \mu}{\hbar^2} H_{\ell} + \frac{Z^2}{2(\ell+1)^2} \,. \end{aligned}$$
(6.81)

Had we instead evaluated  $A_{\ell}A_{\ell}^{\dagger}$  the only difference would have been the sign in front of the commutator, so we would instead find

$$A_{\ell}A_{\ell}^{\dagger} = \frac{a_0^2 \mu}{\hbar^2} H_{\ell+1} + \frac{Z^2}{2(\ell+1)^2}$$
(6.82)

which now involves the Hamiltonian appropriate for states whose orbital angular momentum is given by  $\ell + 1$ . Rearranging (6.81) allows us to write the radial Hamiltonian as

$$H_{\ell} = \frac{\hbar^2}{\mu a_0^2} \left( A_{\ell}^{\dagger} A_{\ell} - \frac{Z^2}{2(\ell+1)^2} \right)$$
(6.83)

while taking the difference of (6.81) and (6.82) gives the commutation relations

$$\left[A_{\ell}, A_{\ell}^{\dagger}\right] = \frac{a_0^2 \mu}{\hbar^2} \left(H_{\ell+1} - H_{\ell}\right) \,. \tag{6.84}$$

The final result we need is the commutation relation

$$[A_{\ell}, H_{\ell}] = \frac{\hbar^2}{\mu a_0^2} \left[ A_{\ell}, A_{\ell}^{\dagger} A_{\ell} \right] = \frac{\hbar^2}{\mu a_0^2} \left[ A_{\ell}, A_{\ell}^{\dagger} \right] A_{\ell} = (H_{\ell+1} - H_{\ell}) A_{\ell} , \qquad (6.85)$$

where the final step uses (6.84). Cancelling the  $H_{\ell}A_{\ell}$  term on both sides, this simplifies to

$$A_{\ell}H_{\ell} = H_{\ell+1}A_{\ell} \,, \tag{6.86}$$

and we also have  $A_{\ell}^{\dagger}H_{\ell+1} = H_{\ell}A_{\ell}^{\dagger}$  by taking the Hermitian conjugate.

Now let's understand these operators. Let  $|E, \ell\rangle$  be an eigenstate of  $H_{\ell}$  and  $\mathbf{L}^2$  with  $H_{\ell}|E, \ell\rangle = E|E, \ell\rangle$  and  $\mathbf{L}^2|E, \ell\rangle = \ell(\ell+1)\hbar^2 |E, \ell\rangle$ . Then

$$H_{\ell+1}\left(A_{\ell}|E,\ell\right) = A_{\ell}H_{\ell}|E,\ell\rangle = E\left(A_{\ell}|E,\ell\rangle\right) \tag{6.87}$$

so that  $A_{\ell}|E, \ell\rangle$  is an eigenstate of  $H_{\ell+1}$  with the same energy E. Thus, acting on  $|E, \ell\rangle$ ,  $A_{\ell}$  creates a new state with the same energy, but where the effective potential corresponds to the angular momentum quantum number  $\ell+1$ . Acting on the new state  $A_{\ell}|E, \ell\rangle$  with  $A_{\ell+1}$  again creates a new state with the same energy, but even more orbital angular momentum labelled by  $\ell + 2$ , and so on. We already know that our energy levels are not infinitely degenerate, so this process must eventually terminate. That is, just as in the harmonic oscillator, there must be a maximum value  $\ell_{\text{max}}$  such that

$$A_{\ell_{\max}}|E,\ell_{\max}\rangle = 0 \tag{6.88}$$

and again, by analogy with the classical case where a circular orbit has the highest possible orbital angular momentum for fixed energy, we can view this state as the quantum analogue of a circular orbit. Taking the norm and using equation (6.81) we have

$$0 = \|A_{\ell_{\max}}|E, \ell_{\max}\rangle\|^2 = \langle E, \ell_{\max}|A_{\ell_{\max}}^{\dagger}A_{\ell_{\max}}|E, \ell_{\max}\rangle = \frac{a_0^2\mu}{\hbar^2}E + \frac{Z^2}{2(\ell_{\max}+1)^2}, \quad (6.89)$$

or equivalently

$$E = -\frac{Z^2 \hbar^2}{2\mu a_0^2} \frac{1}{n^2} \tag{6.90}$$

where  $n \equiv \ell_{\text{max}} + 1$  labels the energy level. This agrees with the spectrum of the Hamiltonian computed earlier using the Runge–Lenz vector (or indeed in IB QM). The virtue

of the Runge–Lenz derivation is that it makes transparent the role of the additional, dynamical symmetry of Hydrogen, explaining why the energy levels fall into multiplets of  $\mathfrak{so}(3) \times \mathfrak{so}(3)$ . The virtue of the present derivation is that it makes transparent how the degeneracy arises because, aside from simply rotating our system, we can trade radial kinetic energy and Coulomb potential for different orbital kinetic energy whilst keeping the total energy constant.