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ANGULAR MOMENTUM

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Contents

1 Orbital angular momentum and central potentials

Classically the angular momentum vector $\vec{L}$ is defined as the cross-product of the position vector $\vec{r}$ and the momentum vector $\vec{p}$:

$$\vec{L} \;=\; \vec{r} \times \vec{p}. \tag{1.1}$$

In cartesian components, this equation reads

$$
\begin{aligned}
L_x &= yp_z - zp_y\,, \\
L_y &= zp_x - xp_z\,, \\
L_z &= xp_y - yp_x\,.
\end{aligned}
\tag{1.2}
$$

In quantum mechanics the classical vectors $\vec{r}$, $\vec{p}$ and $\vec{L}$ become operators. More precisely, they give us triplets of operators:

$$\begin{aligned}
\vec{r} &\to (\hat{x}, \hat{y}, \hat{z}), \\
\vec{p} &\to (\hat{p}_x, \hat{p}_y, \hat{p}_z), \\
\vec{L} &\to (\hat{L}_x, \hat{L}_y, \hat{L}_z).
\end{aligned} \tag{1.3}$$

When we want more uniform notation, instead of x, y, and z labels we use $1, 2$ and 3 labels:

$$\begin{aligned}
(\hat{x}_1, \hat{x}_2, \hat{x}_3) &\equiv (\hat{x}, \hat{y}, \hat{z}), \\
(\hat{p}_1, \hat{p}_2, \hat{p}_3) &\equiv (\hat{p}_x, \hat{p}_y, \hat{p}_z), \\
(\hat{L}_1, \hat{L}_2, \hat{L}_3) &\equiv (\hat{L}_x, \hat{L}_y, \hat{L}_z).
\end{aligned} \tag{1.4}$$

The basic canonical commutation relations then are easily summarized as

$$\left[\hat{x}_i, \hat{p}_j\right] = i\hbar\,\delta_{ij}, \quad \left[\hat{x}_i, \hat{x}_j\right] = 0, \quad \left[\hat{p}_i, \hat{p}_j\right] = 0. \tag{1.5}$$

Thus, for example, $\hat{x}$ commutes with $\hat{y}, \hat{z}, \hat{p}_y$ and $\hat{p}_z$, but fails to commute with $\hat{p}_x$. In view of (1.2) and (1.3) it is natural to define the angular momentum *operators* by

$$\begin{aligned}
\hat{L}_x &\equiv \hat{y}\,\hat{p}_z - \hat{z}\,\hat{p}_y, \\
\hat{L}_y &\equiv \hat{z}\,\hat{p}_x - \hat{x}\,\hat{p}_z, \\
\hat{L}_z &\equiv \hat{x}\,\hat{p}_y - \hat{y}\,\hat{p}_x.
\end{aligned} \tag{1.6}$$

Note that these equations are free of ordering ambiguities: each product involves a coordinate and a momentum that commute! In terms of numbered operators

$$\begin{aligned}
\hat{L}_1 &\equiv \hat{x}_2\,\hat{p}_3 - \hat{x}_3\,\hat{p}_2, \\
\hat{L}_2 &\equiv \hat{x}_3\,\hat{p}_1 - \hat{x}_1\,\hat{p}_3, \\
\hat{L}_3 &\equiv \hat{x}_1\,\hat{p}_2 - \hat{x}_2\,\hat{p}_1.
\end{aligned} \tag{1.7}$$

Note that the angular momentum operators are Hermitian, since $\hat{x}_i$ and $\hat{p}_i$ are and the products can be reordered without cost:

$$\hat{L}_i^{\dagger} = \hat{L}_i. \tag{1.8}$$

1.1 Quantum mechanical vector identities

We will write triplets of operators as boldfaced vectors, each element of the triplet multiplied by a unit basis vector, just like we do for ordinary vectors. Thus, for example, we have

$$\begin{aligned}
\mathbf{r} &\equiv \hat{x}_1\,\vec{e}_1 + \hat{x}_2\,\vec{e}_2 + \hat{x}_3\,\vec{e}_3, \\
\mathbf{p} &\equiv \hat{p}_1\,\vec{e}_1 + \hat{p}_2\,\vec{e}_2 + \hat{p}_3\,\vec{e}_3, \\
\mathbf{L} &\equiv \hat{L}_1\,\vec{e}_1 + \hat{L}_2\,\vec{e}_2 + \hat{L}_3\,\vec{e}_3.
\end{aligned} \tag{1.9}$$

These boldface objects are a bit unusual. They are vectors whose components happen to be operators! Moreover, the basis vectors $\vec{e}_i$ must be declared to commute with any of the operators. The boldface objects are useful whenever we want to use the dot products and cross products of three-dimensional space.

Let us, for generality consider vectors **a** and **b**

$$\begin{aligned} \mathbf{a} &\equiv a_1\,\vec{e}_1 + a_2\,\vec{e}_2 + a_3\,\vec{e}_3\,, \\ \mathbf{b} &\equiv b_1\,\vec{e}_1 + b_2\,\vec{e}_2 + b_3\,\vec{e}_3\,, \end{aligned} \tag{1.10}$$

and we will assume that the a_i's and b_j's are operators that do not commute. The following are then standard definitions:

$$\begin{aligned} \mathbf{a}\cdot\mathbf{b} &\equiv a_i\,b_i\,, \\ (\mathbf{a}\times\mathbf{b})_i &\equiv \epsilon_{ijk}\,a_j\,b_k\,. \end{aligned} \tag{1.11}$$

The order of the operators in the above right-hand sides cannot be changed; it was chosen conveniently, to be the same as the order of the operators on the left-hand sides. We also define,

$$\mathbf{a}^2 \equiv \mathbf{a}\cdot\mathbf{a}\,. \tag{1.12}$$

Since the operators do not commute, familiar properties of vector analysis do not hold. For example $\mathbf{a}\cdot\mathbf{b}$ is not equal to $\mathbf{b}\cdot\mathbf{a}$. Indeed,

$$\mathbf{a}\cdot\mathbf{b} = a_i\,b_i = [\,a_i\,,\,b_i\,] + b_i\,a_i\,, \tag{1.13}$$

so that

$$\boxed{\mathbf{a}\cdot\mathbf{b} = \mathbf{b}\cdot\mathbf{a} + [\,a_i\,,\,b_i\,]\,.} \tag{1.14}$$

As an application we have

$$\mathbf{r}\cdot\mathbf{p} = \mathbf{p}\cdot\mathbf{r} + [\,\hat{x}_i\,,\,\hat{p}_i\,]\,, \tag{1.15}$$

The right-most commutator gives $i\hbar\,\delta_{ii} = 3i\hbar$ so that we have the amusing three-dimensional identity

$$\boxed{\mathbf{r}\cdot\mathbf{p} = \mathbf{p}\cdot\mathbf{r} + 3\,i\hbar\,.} \tag{1.16}$$

For cross products we typically have $\mathbf{a}\times\mathbf{b} \neq -\mathbf{b}\times\mathbf{a}$. Indeed,

$$\begin{aligned} (\mathbf{a}\times\mathbf{b})_i &= \epsilon_{ijk}\,a_j\,b_k = \epsilon_{ijk}\left([\,a_j\,,\,b_k\,] + b_k\,a_j\right) \\ &= -\,\epsilon_{ikj}\,b_k\,a_j + \epsilon_{ijk}\,[\,a_j\,,\,b_k\,] \end{aligned} \tag{1.17}$$

where we flipped the k, j indices in one of the epsilon tensors in order to identify a cross product. Indeed, we have now

$$\boxed{(\mathbf{a}\times\mathbf{b})_i = -(\mathbf{b}\times\mathbf{a})_i + \epsilon_{ijk}\,[\,a_j\,,\,b_k\,]\,.} \tag{1.18}$$

3

The simplest example of the use of this identity is one where we use $\mathbf{r}$ and $\mathbf{p}$. Certainly

$$\mathbf{r} \times \mathbf{r} = 0, \quad \text{and} \quad \mathbf{p} \times \mathbf{p} = 0, \tag{1.19}$$

and more nontrivially,

$$(\mathbf{r} \times \mathbf{p})_i = -(\mathbf{p} \times \mathbf{r})_i + \epsilon_{ijk}[\hat{x}_j, \hat{p}_k]. \tag{1.20}$$

The last term vanishes for it is equal to $i\hbar\,\epsilon_{ijk}\delta_{jk} = 0$ (the epsilon symbol is antisymmetric in j, k while the delta is symmetric in j, k, resulting in a zero result). We therefore have, quantum mechanically,

$$\boxed{\mathbf{r} \times \mathbf{p} = -\mathbf{p} \times \mathbf{r}.} \tag{1.21}$$

Thus $\mathbf{r}$ and $\mathbf{p}$ can be moved across in the cross product but not in the dot product.

Exercise 1. Prove the following identities for Hermitian conjugation

$$\begin{aligned}(\mathbf{a} \cdot \mathbf{b})^\dagger &= \mathbf{b}^\dagger \cdot \mathbf{a}^\dagger, \\ (\mathbf{a} \times \mathbf{b})^\dagger &= -\mathbf{b}^\dagger \times \mathbf{a}^\dagger.\end{aligned} \tag{1.22}$$

Our definition of the angular momentum operators in (1.7) and the notation developed above imply that we have

$$\boxed{\mathbf{L} = \mathbf{r} \times \mathbf{p} = -\mathbf{p} \times \mathbf{r}.} \tag{1.23}$$

Indeed, given the definition of the product, we have

$$\boxed{\hat{L}_i = \epsilon_{ijk}\,\hat{x}_j\,\hat{p}_k.} \tag{1.24}$$

If you write out what this means for $i = 1, 2, 3$ (do it!) you will recover the expressions in (1.7). The angular operator is Hermitian. Indeed, using (1.22) and recalling that $\mathbf{r}$ and $\mathbf{p}$ are Hermitian we have

$$\mathbf{L}^\dagger = (\mathbf{r} \times \mathbf{p})^\dagger = -\mathbf{p}^\dagger \times \mathbf{r}^\dagger = -\mathbf{p} \times \mathbf{r} = \mathbf{L}. \tag{1.25}$$

The use of vector notation implies that, for example,

$$\mathbf{L}^2 = \mathbf{L} \cdot \mathbf{L} = \hat{L}_1\hat{L}_1 + \hat{L}_2\hat{L}_2 + \hat{L}_3\hat{L}_3 = \hat{L}_i\hat{L}_i. \tag{1.26}$$

The classical angular momentum operator is orthogonal to both $\vec{r}$ and $\vec{p}$ as it is built from the cross product of these two vectors. Happily, these properties also hold for the quantum angular momentum. Take for example the dot product of $\mathbf{r}$ with $\mathbf{L}$ to get

$$\mathbf{r} \cdot \mathbf{L} = \hat{x}_i\,\hat{L}_i = \hat{x}_i\epsilon_{ijk}\,\hat{x}_j\,\hat{p}_k = \epsilon_{ijk}\,\hat{x}_i\,\hat{x}_j\,\hat{p}_k = 0. \tag{1.27}$$

The last expression is zero because the $\hat{x}$'s commute and thus form an object symmetric in i, j, while the epsilon symbol is antisymmetric in i, j. Similarly,

$$\mathbf{p} \cdot \mathbf{L} \;=\; \hat{p}_i \, \hat{L}_i \;=\; -\hat{p}_i (\mathbf{p} \times \mathbf{r})_i \;=\; -\hat{p}_i \epsilon_{ijk} \, \hat{p}_j \, \hat{x}_k \;=\; -\epsilon_{ijk} \, \hat{p}_i \, \hat{p}_j \, \hat{x}_k \;=\; 0 \,. \tag{1.28}$$

In summary:

$$\boxed{\mathbf{r} \cdot \mathbf{L} \;=\; \mathbf{p} \cdot \mathbf{L} \;=\; 0 \,.} \tag{1.29}$$

In manipulating vector products the following identity is quite useful

$$\epsilon_{ijk} \, \epsilon_{ipq} \;=\; \delta_{jp}\delta_{kq} \;-\; \delta_{jq}\delta_{kp} \,. \tag{1.30}$$

Its contraction is also needed sometimes:

$$\epsilon_{ijk} \, \epsilon_{ijq} \;=\; 2\delta_{kq} \,. \tag{1.31}$$

For triple products we find

$$\begin{aligned}
\left[\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) \right]_k \;&=\; \epsilon_{kji} \, a_j \, (\mathbf{b} \times \mathbf{c})_i \\
&=\; \epsilon_{kji} \, \epsilon_{ipq} \, a_j \, b_p \, c_q \\
&=\; -\,\epsilon_{ijk} \, \epsilon_{ipq} \, a_j \, b_p \, c_q \\
&=\; -\,\big(\delta_{jp}\delta_{kq} \;-\; \delta_{jq}\delta_{kp}\big) a_j \, b_p \, c_q \\
&=\; a_j \, b_k \, c_j \;-\; a_j \, b_j \, c_k \\
&=\; [\,a_j \,,\, b_k\,]\, c_j \;+\; b_k \, a_j \, c_j \;-\; a_j \, b_j \, c_k \\
&=\; [\,a_j \,,\, b_k\,]\, c_j \;+\; b_k \, (\mathbf{a} \cdot \mathbf{c}) \;-\; (\mathbf{a} \cdot \mathbf{b})\, c_k
\end{aligned} \tag{1.32}$$

We can write this as

$$\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) \;=\; \mathbf{b} \, (\mathbf{a} \cdot \mathbf{c}) \;-\; (\mathbf{a} \cdot \mathbf{b})\, \mathbf{c} \;+\; [\,a_j \,,\, \mathbf{b}\,]\, c_j \,. \tag{1.33}$$

The first two terms are familiar from vector analysis, the last term is quantum mechanical.

Another familiar relation from vector analysis is the classical

$$(\vec{a} \times \vec{b})^2 \;\equiv\; (\vec{a} \times \vec{b}) \cdot (\vec{a} \times \vec{b}) \;=\; \vec{a}^2 \, \vec{b}^2 \;-\; (\vec{a} \cdot \vec{b})^2 \,. \tag{1.34}$$

In deriving such an equation you assume that the vector components are commuting numbers, not operators. If we have vector operators additional terms arise.

Exercise 2. Show that

$$\begin{aligned}
(\mathbf{a} \times \mathbf{b})^2 \;=\;\; &\mathbf{a}^2 \, \mathbf{b}^2 - (\mathbf{a} \cdot \mathbf{b})^2 \\
&- a_j \,[a_j, b_k]\, b_k + a_j \,[a_k, b_k]\, b_j - a_j \,[a_k, b_j]\, b_k \;-\; a_j a_k \,[b_k, b_j] \,,
\end{aligned} \tag{1.35}$$

5

and verify that this yields

$$(\mathbf{a} \times \mathbf{b})^2 \;=\; \mathbf{a}^2\,\mathbf{b}^2 - (\mathbf{a} \cdot \mathbf{b})^2 + \gamma\,\mathbf{a} \cdot \mathbf{b}\,, \qquad \text{when} \quad [a_i, b_j] = \gamma\,\delta_{ij}\,, \quad \gamma \in \mathbb{C}\,, \quad [b_i, b_j] = 0\,. \quad (1.36)$$

As an application we calculate $\mathbf{L}^2$

$$\mathbf{L}^2 \;=\; (\mathbf{r} \times \mathbf{p})^2\,, \tag{1.37}$$

equation (1.36) can be applied with $\mathbf{a} = \mathbf{r}$ and $\mathbf{b} = \mathbf{p}$. Since $[a_i, b_j] = [\hat{x}_i, \hat{p}_j] = i\hbar\,\delta_{ij}$ we read that $\gamma = i\hbar$, so that

$$\boxed{\mathbf{L}^2 \;=\; \mathbf{r}^2\,\mathbf{p}^2 - (\mathbf{r} \cdot \mathbf{p})^2 + i\hbar\,\mathbf{r} \cdot \mathbf{p}\,.} \tag{1.38}$$

Another useful and simple identity is the following

$$\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) \;=\; (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}\,, \tag{1.39}$$

as you should confirm in a one-line computation. In commuting vector analysis this triple product is known to be cyclically symmetric. Note, that in the above no operator has been moved across each other –that's why it holds.

1.2   Properties of angular momentum

A key property of the angular momentum operators is their commutation relations with the $\hat{x}_i$ and $\hat{p}_i$ operators. You should verify that

$$\boxed{\begin{aligned} [\,\hat{L}_i\,,\,\hat{x}_j\,] \;&=\; i\hbar\,\epsilon_{ijk}\,\hat{x}_k\,, \\[4pt] [\,\hat{L}_i\,,\,\hat{p}_j\,] \;&=\; i\hbar\,\epsilon_{ijk}\,\hat{p}_k\,. \end{aligned}} \tag{1.40}$$

We say that these equations mean that $\mathbf{r}$ and $\mathbf{p}$ are vectors *under* rotations.

Exercise 3. Use the above relations and (1.18) to show that

$$\mathbf{p} \times \mathbf{L} \;=\; -\mathbf{L} \times \mathbf{p} \;+\; 2i\hbar\,\mathbf{p}\,. \tag{1.41}$$

Hermitization is the process by which we construct a Hermitian operator starting from a non-Hermitian one. Say Ω is not hermitian, its Hermitization Ω_h is defined to be

$$\Omega_h \;\equiv\; \frac{1}{2}(\Omega + \Omega^\dagger)\,. \tag{1.42}$$

Exercise 4. Show that the Hermitization of $\mathbf{p} \times \mathbf{L}$ is

$$(\mathbf{p} \times \mathbf{L})_h \;=\; \frac{1}{2}\big(\mathbf{p} \times \mathbf{L} \;-\; \mathbf{L} \times \mathbf{p}\big) \;=\; \mathbf{p} \times \mathbf{L} \;-\; i\hbar\,\mathbf{p}\,. \tag{1.43}$$

Inspired by the behavior of $\mathbf{r}$ and $\mathbf{p}$ under rotations, we declare that an operator $\mathbf{u}$ defined by the triplet $(\hat{u}_1, \hat{u}_2, \hat{u}_3)$ is a *vector under rotations* if

$$\left[\,\hat{L}_i\,,\,\hat{u}_j\,\right] \;=\; i\hbar\,\epsilon_{ijk}\,\hat{u}_k\,. \tag{1.44}$$

Exercise 5. Use the above commutator to show that with $\mathbf{n}$ a constant vector,

$$\left[\,\mathbf{n}\cdot\mathbf{L}\,,\,\mathbf{u}\,\right] \;=\; -i\hbar\,\mathbf{n}\times\mathbf{u}\,. \tag{1.45}$$

Given two operators $\mathbf{u}$ and $\mathbf{v}$ that are vectors under rotations you will show that their dot product is a scalar –it commutes with all $\hat{L}_i$– and their cross product is a vector:

$$
\begin{aligned}
\left[\,\hat{L}_i\,,\mathbf{u}\cdot\mathbf{v}\,\right] &\;=\; 0\,, \\[2mm]
\left[\,\hat{L}_i\,,(\mathbf{u}\times\mathbf{v})_j\,\right] &\;=\; i\hbar\,\epsilon_{ijk}\,(\mathbf{u}\times\mathbf{v})_k\,.
\end{aligned}
\tag{1.46}
$$

Exercise 6. Prove the above equations.

A number of useful commutator identities follow from (1.46). Most importantly, from the second one, taking $\mathbf{u} = \mathbf{r}$ and $\mathbf{v} = \mathbf{p}$ we get

$$\left[\,\hat{L}_i\,,(\mathbf{r}\times\mathbf{p})_j\,\right] \;=\; i\hbar\,\epsilon_{ijk}\,(\mathbf{r}\times\mathbf{p})_k\,, \tag{1.47}$$

which gives the celebrated Lie algebra of angular momentum[1]

$$\left[\,\hat{L}_i\,,\hat{L}_j\,\right] \;=\; i\hbar\,\epsilon_{ijk}\,\hat{L}_k\,. \tag{1.48}$$

More explicitly,

$$
\begin{aligned}
\left[\,\hat{L}_x\,,\,\hat{L}_y\,\right] &\;=\; i\hbar\,\hat{L}_z\,, \\
\left[\,\hat{L}_y\,,\,\hat{L}_z\,\right] &\;=\; i\hbar\,\hat{L}_x\,, \\
\left[\,\hat{L}_z\,,\,\hat{L}_x\,\right] &\;=\; i\hbar\,\hat{L}_y\,.
\end{aligned}
\tag{1.49}
$$

Note the cyclic nature of these equations: take the first and cycle indices $(x \to y \to z \to x)$ to obtain the other two. Another set of examples follows from the first identity in (1.46) using our list of vector operators. For example

$$\left[\,\hat{L}_i\,,\mathbf{r}^2\,\right] \;=\; \left[\,\hat{L}_i\,,\mathbf{p}^2\,\right] \;=\; \left[\,\hat{L}_i\,,\mathbf{r}\cdot\mathbf{p}\,\right] \;=\; 0\,, \tag{1.50}$$

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[1]We do not know who celebrated it because we were not invited.

and, very importantly,

$$[\hat{L}_i, \mathbf{L}^2] = 0. \tag{1.51}$$

This equation is the reason the operator $\mathbf{L}^2$ plays a very important role in the study of central potentials. $\mathbf{L}^2$ will feature as one of the operators in complete sets of commuting observables. An operator, such as $\mathbf{L}^2$, that commutes with all the angular momentum operators is called a "Casimir" of the algebra of angular momentum. Note that the validity of (1.51) just uses the algebra of the $\hat{L}_i$ operators not, for example, how they are built from $\mathbf{r}$ and $\mathbf{p}$.

Exercise 7. Use (1.18) and the algebra of $\hat{L}$ operators to show that

$$\mathbf{L} \times \mathbf{L} = i\hbar \mathbf{L}. \tag{1.52}$$

This is a very elegant way to express the algebra of angular momentum. In fact, we can show that it is totally equivalent to (1.48). Thus we write

$$\boxed{\mathbf{L} \times \mathbf{L} = i\hbar \mathbf{L} \quad \Longleftrightarrow \quad [\hat{L}_i, \hat{L}_j] = i\hbar \epsilon_{ijk} \hat{L}_k.} \tag{1.53}$$

Commutation relations of the form

$$[a_i, b_j] = \epsilon_{ijk} c_k, \tag{1.54}$$

admit a natural rewriting in terms of cross products. From (1.18)

$$(\mathbf{a} \times \mathbf{b})_i + (\mathbf{b} \times \mathbf{a})_i = \epsilon_{ijk}[a_j, b_k] = \epsilon_{ijk}\epsilon_{jkp}c_p = 2c_i. \tag{1.55}$$

This means that

$$\boxed{[a_i, b_j] = \epsilon_{ijk} c_k \quad \rightarrow \quad \mathbf{a} \times \mathbf{b} + \mathbf{b} \times \mathbf{a} = 2\mathbf{c}.} \tag{1.56}$$

The arrow does *not* work in the reverse direction. One finds $[a_i, b_j] = \epsilon_{ijk} c_k + s_{ij}$ where $s_{ij} = s_{ji}$ is arbitrary and is *not* determined. If the arrow could be reversed, $\mathbf{a} \times \mathbf{b} + \mathbf{b} \times \mathbf{a} = 0$ would imply that $\mathbf{a}$ and $\mathbf{b}$ commute. We have, however, a familiar example where this does not happen: while $\mathbf{r} \times \mathbf{p} + \mathbf{p} \times \mathbf{r} = 0$ (see (1.23)), the operators $\mathbf{r}$ and $\mathbf{p}$ don't commute.

For a vector $\mathbf{u}$ under rotations, equation (1.56) becomes

$$\mathbf{L} \times \mathbf{u} + \mathbf{u} \times \mathbf{L} = 2i\hbar \mathbf{u}. \tag{1.57}$$

1.3 The central potential Hamiltonian

Angular momentum plays a crucial role in the study of three-dimensional central potential problems. Those are problems where the Hamiltonian describes a particle moving in a potential $V(r)$ that depends just on r, the distance of the particle to the chosen origin. The Hamiltonian takes the form

$$H = \frac{\mathbf{p}^2}{2m} + V(r). \tag{1.58}$$

When writing the Schrödinger equation in position space we identify

$$\mathbf{p} = \frac{\hbar}{i} \nabla, \tag{1.59}$$

and therefore

$$\mathbf{p}^2 = -\hbar^2 \nabla^2, \tag{1.60}$$

where ∇^2 denotes the Laplacian operator –a second order differential operator. In spherical coordinates the Laplacian is well known and gives us

$$\mathbf{p}^2 = -\hbar^2 \left[\frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right) \right]. \tag{1.61}$$

Our goal is to relate the "angular" part of the above differential operator to angular momentum operators. This will be done by calculating $\mathbf{L}^2$ and relating it to $\mathbf{p}^2$. Since we had from (1.38)

$$\mathbf{L}^2 = \mathbf{r}^2 \mathbf{p}^2 - (\mathbf{r} \cdot \mathbf{p})^2 + i\hbar \mathbf{r} \cdot \mathbf{p}, \tag{1.62}$$

We solve for $\mathbf{p}^2$ to get

$$\mathbf{p}^2 = \frac{1}{\mathbf{r}^2} \left[(\mathbf{r} \cdot \mathbf{p})^2 - i\hbar \mathbf{r} \cdot \mathbf{p} + \mathbf{L}^2 \right]. \tag{1.63}$$

Let us now consider the above equation in coordinate space, where $\mathbf{p}$ is a gradient. We then have:

$$\mathbf{r} \cdot \mathbf{p} = \frac{\hbar}{i} r \frac{\partial}{\partial r}, \tag{1.64}$$

and thus

$$(\mathbf{r} \cdot \mathbf{p})^2 - i\hbar \mathbf{r} \cdot \mathbf{p} = -\hbar^2 \left(r \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + r \frac{\partial}{\partial r} \right) = -\hbar^2 \left(r^2 \frac{\partial^2}{\partial r^2} + 2r \frac{\partial}{\partial r} \right). \tag{1.65}$$

It then follows that

$$\frac{1}{\mathbf{r}^2} \left[(\mathbf{r} \cdot \mathbf{p})^2 - i\hbar \mathbf{r} \cdot \mathbf{p} \right] = -\hbar^2 \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) = -\hbar^2 \frac{1}{r} \frac{\partial^2}{\partial r^2} r, \tag{1.66}$$

where the last step is readily checked by explicit expansion. Back in (1.63) we get

$$\mathbf{p}^2 = -\hbar^2 \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \mathbf{L}^2. \tag{1.67}$$

9

Comparing with (1.61) we identify $\mathbf{L}^2$ as the operator

$$\mathbf{L}^2 = -\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right). \qquad (1.68)$$

Note that the units are fully carried by the $\hbar^2$ in front and that the differential operator is completely angular: it has no radial dependence. Given our expression (1.67) for $\mathbf{p}^2$ we can now rewrite the three-dimensional Hamiltonian as

$$H = \frac{\mathbf{p}^2}{2m} + V(r) = -\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{2mr^2} \mathbf{L}^2 + V(r). \qquad (1.69)$$

A key property of central potential problems is that the angular momentum operators commute with the Hamiltonian

$$\text{Central potential Hamiltonians:} \quad [\hat{L}_i, H] = 0. \qquad (1.70)$$

We have seen that $\hat{L}_i$ commutes with $\mathbf{p}^2$ so it is only needed to show that the $\hat{L}_i$ commute with $V(r)$. This is eminently reasonable, for $\hat{L}_i$ commutes with $\mathbf{r}^2 = r^2$, so one would expect it to commute with any function of $\sqrt{\mathbf{r}^2} = r$. In the problem set you will consider this question and develop a formal argument that confirms the expectation.

The above commutator implies that the $\hat{L}_i$ operators are conserved in central potentials. Indeed

$$i\hbar \frac{d}{dt} \langle \hat{L}_i \rangle = \langle [\hat{L}_i, H] \rangle = 0. \qquad (1.71)$$

We can now consider the issue of complete sets of commuting observables. The list of operators that we have is

$$H, \quad \hat{x}_1, \hat{x}_2, \hat{x}_3, \quad \hat{p}_1, \hat{p}_2, \hat{p}_3, \quad \hat{L}_1, \hat{L}_2, \hat{L}_3, \quad \mathbf{r}^2, \mathbf{p}^2, \mathbf{r}\cdot\mathbf{p}, \mathbf{L}^2, \dots \qquad (1.72)$$

where, for the time being, we included all operators up to squares of coordinates, momenta, and angular momenta. Since we want to understand the spectrum of the Hamiltonian, one of the labels of states will be the energy and thus H must be in the list of commuting observables. Because of the potential $V(r)$ none of the $\hat{p}_i$ operators commute the Hamiltonian. Because of the $\mathbf{p}^2$ term in the Hamiltonian none of the $\hat{x}_i$ commute with the Hamiltonian. Nor will $\mathbf{r}^2, \mathbf{p}^2$ and $\mathbf{r}\cdot\mathbf{p}$. The list is thus reduced to

$$H, \quad \hat{L}_1, \hat{L}_2, \hat{L}_3, \quad \mathbf{L}^2. \qquad (1.73)$$

where there are no dots anymore, since without $\hat{x}_i$ or $\hat{p}_i$ there are no other operators to build (recall also that $\mathbf{L} \times \mathbf{L} = i\hbar\mathbf{L}$ and thus it is not new). All the operators in the list commute

10

with H: the $\hat{L}_i$ as discussed in (1.70), and $\mathbf{L}^2$ because, after all, it is built from $\hat{L}_i$. But all the operators do not commute with each other. From the $\hat{L}_i$ we can only pick at most one, for then the other two necessarily do not commute with the chosen one. Happily we can also keep $\mathbf{L}^2$ because of its Casimir property (1.51). Conventionally, everybody chooses $\hat{L}_3 = \hat{L}_z$ as one element of the set of commuting observables. Thus we have

$$\boxed{\text{Commuting observables:} \quad H\,,\ \hat{L}_z\,,\ \mathbf{L}^2\,.} \tag{1.74}$$

We can wonder if this set is complete in the sense that all energy eigenstates are uniquely labelled by the eigenvalues of the above operators. The answer is yes, for the bound state spectrum of a particle that has no other degrees of freedom (say, no spin).

2 Algebraic theory of angular momentum

Hermitian operators $\hat{J}_x, \hat{J}_y, \hat{J}_z$ are said to satisfy the algebra of **angular momentum** if the following commutation relations:

$$[\hat{J}_i\,,\ \hat{J}_j] \ = \ i\hbar\,\epsilon_{ijk}\,\hat{J}_k\,. \tag{2.1}$$

More explicitly, in components

$$\begin{aligned}
[\hat{J}_x, \hat{J}_y] &= i\hbar\hat{J}_z \\
[\hat{J}_y, \hat{J}_z] &= i\hbar\hat{J}_x \\
[\hat{J}_z, \hat{J}_x] &= i\hbar\hat{J}_y\,.
\end{aligned} \tag{2.2}$$

The $\hat{J}_i$ operators could be $\hat{L}_i$, or $\hat{S}_i$ or something else! Will only use this algebra and the Hermiticity of the operators. From this algebra it also follows that

$$[\hat{J}_i\,, \mathbf{J}^2] \ = \ 0\,. \tag{2.3}$$

This can be checked explicitly, but our proof of the analogous result (1.51): $[\hat{L}_i, \mathbf{L}^2] = 0$ only used the algebra of the operators $\hat{L}_i$, so this also holds for the $\hat{J}_i$, which satisfy the same algebra. It is not convenient to define

$$\boxed{\begin{aligned}
\hat{J}_+ &\equiv\ \hat{J}_x + i\hat{J}_y\,, \\
\hat{J}_- &\equiv\ \hat{J}_x - i\hat{J}_y\,,
\end{aligned}} \tag{2.4}$$

such that the two operators are Hermitian conjugates of each other:

$$(\hat{J}_+)^\dagger \ = \ \hat{J}_-\,. \tag{2.5}$$

Note that both $\hat{J}_x$ and $\hat{J}_y$ can be solved for in terms of $\hat{J}_+$ and $\hat{J}_-$. It is useful to compute the algebra of the operators $\hat{J}_+, \hat{J}_-$, and $\hat{J}_z$. We begin by computing the product $\hat{J}_+\hat{J}_-$:

$$\hat{J}_+\hat{J}_- = \hat{J}_x^2 + \hat{J}_y^2 - i[\hat{J}_x\,,\,\hat{J}_y] = \hat{J}_x^2 + \hat{J}_y^2 + \hbar\hat{J}_z\,. \tag{2.6}$$

Together with the product in the opposite order we have

$$\begin{aligned} \hat{J}_+\hat{J}_- &= \hat{J}_x^2 + \hat{J}_y^2 + \hbar\hat{J}_z\,, \\ \hat{J}_-\hat{J}_+ &= \hat{J}_x^2 + \hat{J}_y^2 - \hbar\hat{J}_z\,. \end{aligned} \tag{2.7}$$

From these two we can quickly get the commutator:

$$[\hat{J}_+\,,\,\hat{J}_-] = 2\hbar\hat{J}_z\,. \tag{2.8}$$

Moreover, we obtain two expressions for $\hat{J}_x^2 + \hat{J}_y^2$

$$\hat{J}_x^2 + \hat{J}_y^2 = \hat{J}_+\hat{J}_- - \hbar\hat{J}_z = \hat{J}_-\hat{J}_+ + \hbar\hat{J}_z\,. \tag{2.9}$$

Adding $\hat{J}_z^2$ to both sides of the equation we find

$$\boxed{\mathbf{J}^2 = \hat{J}_+\hat{J}_- + \hat{J}_z^2 - \hbar\hat{J}_z = \hat{J}_-\hat{J}_+ + \hat{J}_z^2 + \hbar\hat{J}_z\,.} \tag{2.10}$$

Of course, since $\hat{J}_i$ and $\mathbf{J}^2$ commute, we also have

$$[\,\hat{J}_\pm\,,\,\mathbf{J}^2\,] = 0\,. \tag{2.11}$$

We finally have to compute the commutator of $\hat{J}_\pm$ with $\hat{J}_z$. This is quickly done:

$$[\hat{J}_z,\hat{J}_+] = [\hat{J}_z,\hat{J}_x] + i[\hat{J}_z\,,\,\hat{J}_y] = i\hbar\hat{J}_y + i(-i\hbar\hat{J}_x) = \hbar(\hat{J}_x + i\hat{J}_y) = \hbar\hat{J}_+\,. \tag{2.12}$$

Similarly, $[\hat{J}_z,\hat{J}_-] = -\hbar\hat{L}_-$ and therefore, all in all

$$\boxed{[\hat{J}_z,\hat{J}_\pm] = \pm\hbar\,\hat{J}_\pm\,.} \tag{2.13}$$

This is similar to our harmonic oscillator commutators $[\hat{N},\hat{a}^\dagger] = \hat{a}^\dagger$ and $[N,\hat{a}] = -\hat{a}$, if we identify $\hat{N}$ with $\hat{J}_z$, $\hat{a}^\dagger$ with $\hat{J}_+$ and $\hat{a}$ with $\hat{J}_-$. In the oscillator case we learned from these that, acting on states, $\hat{a}^\dagger$ raises the $\hat{N}$ eigenvalue by one unit while $\hat{a}$ decreases it by one unit. As we will see, $\hat{J}_+$ adds $\hbar$ to the $\hat{J}_z$ eigenvalue and $\hat{J}_-$ subtracts $\hbar$ to the $\hat{J}_z$ eigenvalue.

Since $\mathbf{J}^2$ and $\hat{J}_z$ are hermitian and commute, they can be simultaneously diagonalized. In fact, there are no more operators in the angular momentum algebra can be added to this list of simultaneously diagonalizable operators. The common eigenstates form an orthonormal basis

for the relevant vector space. We thus introduce eigenstates $|j, m\rangle$, with $j, m \in \mathbb{R}$, where the first label relates to the $\mathbf{J}^2$ eigenvalue and the second label to the $\hat{J}_z$ eigenvalue:

$$
\begin{aligned}
\mathbf{J}^2 |j, m\rangle &= \hbar^2\, j(j+1) |j, m\rangle\,, \\
\hat{J}_z |j, m\rangle &= \hbar m |j, m\rangle\,.
\end{aligned}
\tag{2.14}
$$

The orthonormality of states implies that

$$
\langle j', m'|j, m\rangle = \delta_{j',j}\delta_{m',m}\,,
\tag{2.15}
$$

where we assumed that we will not have to deal with continuous values of j, m that would require delta function normalization. This will be confirmed below. Since j and m are real, the eigenvalues of the hermitian operators are real, as they have to be. The first line shows that the eigenvalue of $\mathbf{J}^2$ is defined to be $\hbar^2 j(j+1)$. This can seem curious: why not $\hbar^2 j^2$? The answer is convenience, as we will see below. Alternatively, if we know $\hbar^2 j(j+1)$, how do we get j? For this first note that $\hbar^2 j(j+1)$ must be non-negative:

$$
\hbar^2\, j(j+1) = \langle j, m|\mathbf{J}^2|j, m\rangle = \sum_{i=1}^{3}\langle j, m|\hat{J}_i\hat{J}_i|j, m\rangle = \sum_{i=1}^{3}||\hat{J}_i|j, m\rangle||^2 \geq 0\,,
\tag{2.16}
$$

where in the first step we used the eigenvalue definition and orthonormality. Therefore the condition

$$
j(j+1) \geq 0
\tag{2.17}
$$

is the only a priori condition on the values of j. Since what matters is the eigenvalue of $\mathbf{J}^2$ we can use any of the two j's that give a particular value of $j(j+1)$. As shown in the figure below, the positivity of $j(j+1)$ requires $j \geq 0$ or $j \leq -1$. We can simply use $j \geq 0$.

$$
\text{States are labeled as } |j, m\rangle \text{ with } j \geq 0\,.
\tag{2.18}
$$

You should not think that there are two different states, with two different j's associated with the eigenvalue $\hbar j(j+1)$. It is just one state, that we are labeling in an unusual way. Of course, a theory may end up having more than one state with the same $\mathbf{J}^2$ eigenvalue. In that case we will have more than one state with the same $j > 0$.

Let us now investigate what the operators $\hat{J}_\pm$ do when acting on the above eigenstates. Since they commute with $\mathbf{J}^2$, the operators J_+ or J_- do not change the j value of a state:

$$
\mathbf{J}^2(\hat{J}_\pm|j, m\rangle) = \hat{J}_\pm\mathbf{J}^2|j, m\rangle = \hbar j(j+1)(\hat{J}_\pm|j, m\rangle)\,,
\tag{2.19}
$$

so that we must have

$$
J_\pm|j, m\rangle \propto |j, m'\rangle\,, \quad \text{for some } m'\,.
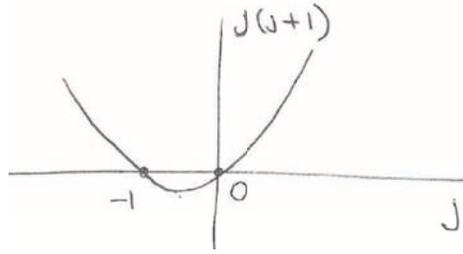\tag{2.20}
$$

13

Figure 1: Since $j(j+1) \geq 0$ for consistency, we can label the states $|j, m\rangle$ using $j \geq 0$.

On the other hand, as anticipated above, the $\hat{J}_\pm$ operators change the value of m:

$$\begin{aligned}
\hat{J}_z(\hat{J}_\pm|j, m\rangle) &= ([\hat{J}_z, J_\pm] + J_\pm\hat{J}_z)|j, m\rangle \\
&= (\pm\hbar J_\pm + \hbar m J_\pm)|j, m\rangle \\
&= \hbar(m \pm 1)(J_\pm|j, m\rangle),
\end{aligned} \tag{2.21}$$

from which we learn that

$$\hat{J}_\pm|j, m\rangle = C_\pm(j, m)|j, m \pm 1\rangle, \tag{2.22}$$

where $C_\pm(j, m)$ is a constant to be determined. Indeed, we see that $\hat{J}_+$ raised the m eigenvalue by one unit while $\hat{J}_-$ decreases the m eigenvalue by one unit. To determine $C_\pm(j, m)$ we first take the adjoint of the above equation

$$\langle j, m|\hat{J}_\mp = \langle j, m \pm 1|C_\pm(j, m)^*, \tag{2.23}$$

and then form the overlap

$$\langle j, m|J_\mp J_\pm|j, m\rangle = |C_\pm(j, m)|^2. \tag{2.24}$$

To evaluate the left-hand side use (2.10) in the form

$$\hat{J}_\mp \hat{J}_\pm = \mathbf{J}^2 - \hat{J}_z^2 \mp \hbar\hat{J}_z \tag{2.25}$$

as well as $\langle j, m|j, m\rangle = 1$:

$$|C_\pm(j, m)|^2 = \langle j, m|(\mathbf{J}^2 - \hat{J}_z^2 \mp \hbar\hat{J}_z)|j, m\rangle = \hbar^2 j(j+1) - \hbar^2 m^2 \mp \hbar^2 m. \tag{2.26}$$

We have thus found that

$$\boxed{|C_\pm(j, m)|^2 = \hbar^2 \left(j(j+1) - m(m \pm 1)\right) = ||\hat{J}_\pm|j, m\rangle||^2.} \tag{2.27}$$

Here we learn a few things. If we start with a consistent state $|j, m\rangle$ of norm one (as assumed above), the states $\hat{J}_\pm|j, m\rangle \sim |j, m \pm 1\rangle$ created by the action of $\hat{J}_\pm$ on $|j, m\rangle$ are inconsistent if

14

the middle expression in the above relation is negative. This is because that middle expression is in fact the norm-squared of $\hat{J}_{\pm}|j, m\rangle$. Assuming that middle expression is positive (or zero) we can take $C_{\pm}(j, m)$ real and equal to the positive square root

$$C_{\pm}(j, m) = \hbar\sqrt{j(j+1) - m(m \pm 1)}. \tag{2.28}$$

We have thus obtained

$$\boxed{J_{\pm}|j, m\rangle = \hbar\sqrt{j(j+1) - m(m \pm 1)}\,|j, m \pm 1\rangle.} \tag{2.29}$$

Given a consistent state $|j, m\rangle$, how far can we raise or lower the value of m? Our classical intuition is that $|\hat{J}_z| \leq |\mathbf{J}|$. So we should get something like $|m| \lesssim \sqrt{j(j+1)}$.

Consider this in two steps:

1. For the raised state to be consistent we must have $||J_+|j, m\rangle||^2 \geq 0$ and therefore

$$j(j+1) - m(m+1) \geq 0 \quad \rightarrow \quad m(m+1) \leq j(j+1) \tag{2.30}$$

The solution to the inequality is given in figure 2:

$$-j-1 \leq m \leq j. \tag{2.31}$$

Had we not chosen $\hbar^2 j(j+1)$ to be the eigenvalue of $\mathbf{J}^2$ this inequality would not have had a simple solution.
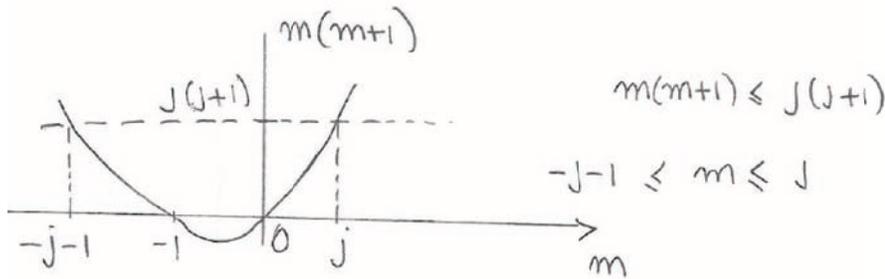

Figure 2: Solving the inequality $m(m+1) \leq j(j+1)$.

Since we are raising m we can focus on the troubles that raising can give given that $m \leq j$. Assume $m = j - \beta$ with $0 < \beta < 1$ so that the inequality (2.31) is satisfied and m is less than one unit below j. Then the raising once gives us a state with $m' = m + 1 > j$ and since the inequality is now violated raising one more time would then give an inconsistent

15

state. To prevent such inconsistency the process of raising must terminate: there must be a state that raising gives no state (the zero state). That indeed happens only if $m = j$ since then $C_+(j, j) = 0$

$$\hat{J}_+|j, j\rangle \;=\; 0 \,. \tag{2.32}$$

2. For the lowered state to be consistent we must have $||\hat{J}_-|j, m\rangle||^2 \geq 0$ and therefore

$$j(j + 1) - m(m - 1) \geq 0 \quad \rightarrow \quad m(m - 1) \leq j(j + 1) \tag{2.33}$$

The solution to this inequality is obtained using figure 3 and gives

$$-j \;\leq m \;\leq j + 1 \,. \tag{2.34}$$
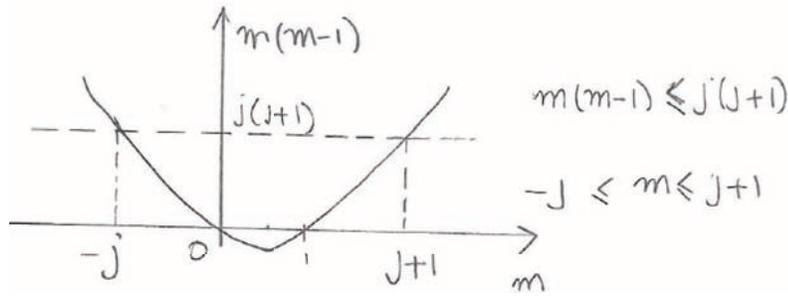
Figure 3: Solving the inequality $m(m - 1) \leq j(j - 1)$.

This time we can focus here on $m \geq -j$ and the complications due to lowering. Assume $m = -j + \beta$ with $0 < \beta < 1$ so that the constraint (2.34) is satisfied and m is less than one unit above $-j$. Then lowing once gives us a state with $m' = m - 1 < -j$ and since the inequality is now violated lowering one more time would then give an inconsistent state. To prevent such inconsistency we need that lowering terminates on some state for which lowering gives no state (the zero state). That indeed happens only if $m = -j$ since then $C_-(j, -j) = 0$

$$\hat{J}_-|j, -j\rangle \;=\; 0 \,. \tag{2.35}$$

The above analysis shows that for consistency a multiplet of states with some given fixed j must be such that the m values must include $-j$ and $+j$. Since m is increased or decreased by integer steps via the $\hat{J}_\pm$ operators, the distance $2j$ between j and $-j$ must be an integer:

$$\boxed{2j \in \mathbb{Z} \quad \rightarrow \quad j \in \mathbb{Z}/2 \,, \quad \rightarrow \quad j = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, 2, \dots \,.} \tag{2.36}$$

16

This is the fundamental quantization of angular momentum. Angular momentum can be integral or half-integral. For any allowed value of j the m values will be $j, j-1, \ldots, -j$. Thus the multiplet with angular momentum j has the following $2j+1$ states

$$
\begin{aligned}
&|j, j\rangle, \\
&|j, j-1\rangle, \\
&\quad\vdots \\
&|j, -j\rangle.
\end{aligned}
\tag{2.37}
$$

For $j = 0$ there is just one state, the **singlet** with $m = 0$: $|0, 0\rangle$.
For $j = \frac{1}{2}$ we have two states:

$$
\begin{aligned}
&\left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle, \\
&\left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle.
\end{aligned}
\tag{2.38}
$$

These are the states of a spin-1/2 particle, when we identify the angular momentum $\mathbf{J}$ with the spin angular momentum operator $\mathbf{S}$. The top state has $\hat{S}_z = \hbar/2$ and the lower state has $\hat{S}_z = -\hbar/2$. These are our conventional $|+\rangle$ and $|-\rangle$ states, respectively.
For $j = 1$ we have three states :

$$
\begin{aligned}
&|1, 1\rangle, \\
&|1, 0\rangle, \\
&|1, -1\rangle.
\end{aligned}
\tag{2.39}
$$

For $j = 3/2$ we have four states:

$$
\begin{aligned}
&\left|\tfrac{3}{2}, \tfrac{3}{2}\right\rangle \\
&\left|\tfrac{3}{2}, \tfrac{1}{2}\right\rangle \\
&\left|\tfrac{3}{2}, -\tfrac{1}{2}\right\rangle \\
&\left|\tfrac{3}{2}, -\tfrac{3}{2}\right\rangle
\end{aligned}
\tag{2.40}
$$

One last one! For $j = 2$ we have five states:

$$
\begin{aligned}
&|2, 2\rangle, \\
&|2, 1\rangle, \\
&|2, 0\rangle, \\
&|2, -1\rangle, \\
&|2, -2\rangle.
\end{aligned}
\tag{2.41}
$$

On any state of a multiplet with angular momentum j the eigenvalue J^2 of $\mathbf{J}^2$ is

$$
J^2 = \hbar^2 j(j+1) \quad \rightarrow \quad \frac{1}{\hbar} J = \sqrt{j(j+1)}
\tag{2.42}
$$

In the limit as j is large

$$\frac{1}{\hbar} J = j\sqrt{1 + \frac{1}{j}} \simeq j + \frac{1}{2} + \mathcal{O}(1/j) . \tag{2.43}$$

So for large j the angular momentum is roughly $J \simeq j$.

3 Comments on spherical harmonics

We have constructed the $\mathbf{L}^2$ operator as a differential operator in position space, with coordinates r, θ, ϕ. The operator happens to depend only on θ and ϕ and takes the form (1.68)

$$\mathcal{L}^2 = -\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right) . \tag{3.1}$$

where we denoted it with a calligraphic symbol to make it clear we are talking about a differential operator. We also have, with the same notation

$$\hat{\mathcal{L}}_z = \frac{\hbar}{i} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) . \tag{3.2}$$

A short calculation, passing to spherical coordinates (do it!) shows that

$$\hat{\mathcal{L}}_z = \frac{\hbar}{i} \frac{\partial}{\partial\phi} . \tag{3.3}$$

Finally, a longer calculation shows that

$$\mathcal{L}_\pm = \hbar e^{\pm i\phi} \left(i \cot\theta \frac{\partial}{\partial\phi} \pm \frac{\partial}{\partial\theta} \right) . \tag{3.4}$$

Recall now how things work for coordinate representations. For a single coordinate x we had that the operator $\hat{p}$ can be taken out of the matrix element as the differential operator $\mathfrak{p}$:

$$\langle x | \hat{p} | \psi \rangle = \mathfrak{p} \langle x | \psi \rangle , \quad \text{where} \quad \mathfrak{p} = \frac{\hbar}{i} \frac{\partial}{\partial x} \tag{3.5}$$

We will let $\langle \theta\phi |$ denote position states on the unit sphere and the spherical harmonic $Y_{\ell m}$ will be viewed as the wavefunction for the state $|\ell m\rangle$ so that

$$Y_{\ell m}(\theta, \phi) \equiv \langle \theta\phi | \ell, m \rangle . \tag{3.6}$$

Consider now (2.14) in the form

$$\begin{aligned} \mathbf{L}^2 |\ell, m\rangle &= \hbar^2 \ell(\ell+1) |\ell, m\rangle , \\ \hat{L}_z |\ell, m\rangle &= \hbar m |\ell, m\rangle . \end{aligned} \tag{3.7}$$

18

Letting the bra $\langle\theta\phi|$ act on them we have

$$
\begin{aligned}
\langle\theta\phi|\mathbf{L}^2|\ell,m\rangle &= \hbar^2\,\ell(\ell+1)\,\langle\theta\phi|\ell,m\rangle\,, \\
\langle\theta\phi|\hat{L}_z\,|\ell,m\rangle &= \hbar m\,\langle\theta\phi|\ell,m\rangle\,.
\end{aligned}
\tag{3.8}
$$

Using the analog of (3.5) for our operators we have

$$
\begin{aligned}
\mathcal{L}^2\langle\theta\phi|\ell,m\rangle &= \hbar^2\,\ell(\ell+1)\,\langle\theta\phi|\ell,m\rangle\,, \\
\hat{\mathcal{L}}_z\langle\theta\phi|\ell,m\rangle &= \hbar m\,\langle\theta\phi|\ell,m\rangle\,.
\end{aligned}
\tag{3.9}
$$

These are equivalent to

$$
\boxed{
\begin{aligned}
\mathcal{L}^2\,Y_{\ell m}(\theta,\phi) &= \hbar^2\,\ell(\ell+1)\,Y_{\ell m}(\theta,\phi)\,, \\
\hat{\mathcal{L}}_z\,Y_{\ell m}(\theta,\phi) &= \hbar m\,Y_{\ell m}(\theta,\phi)\,.
\end{aligned}
}
\tag{3.10}
$$

where $\mathcal{L}^2$ and $\hat{\mathcal{L}}_z$ are the coordinate representation operators for $\mathbf{L}^2$ and $\hat{L}_z$ respectively.

On the unit sphere the measure of integration is $\sin\theta d\theta d\phi$ so we postulate that the completeness relation for the $|\theta\phi\rangle$ position states reads

$$
\int_0^\pi d\theta\sin\theta\int_0^{2\pi}d\phi\,|\theta\phi\rangle\langle\theta\phi| = \mathbf{1}\,.
\tag{3.11}
$$

The integral will be written more briefly as

$$
\int d\Omega\,|\theta\phi\rangle\langle\theta\phi| = \mathbf{1}
\tag{3.12}
$$

where

$$
\int d\Omega = \int_0^\pi d\theta\sin\theta\int_0^{2\pi}d\phi = -\int_1^{-1}d(\cos\theta)\int_0^{2\pi}d\phi = \int_{-1}^1 d(\cos\theta)\int_0^{2\pi}d\phi\,.
\tag{3.13}
$$

Our orthogonality relation

$$
\langle\ell',m'|\ell,m\rangle = \delta_{\ell',l}\delta_{m',m}\,,
\tag{3.14}
$$

gives, by including a complete set of position states

$$
\int d\Omega\,\langle\ell',m'|\theta\phi\rangle\langle\theta\phi|\ell,m\rangle = \delta_{\ell',l}\delta_{m',m}\,.
\tag{3.15}
$$

This gives the familiar orthogonality property of the spherical harmonics:

$$
\int d\Omega\,Y_{\ell'm'}^*(\theta,\phi)\,Y_{\ell m}(\theta,\phi) = \delta_{\ell',l}\delta_{m',m}\,.
\tag{3.16}
$$

Note that the equation

$$
\hat{\mathcal{L}}_z Y_{\ell m} = \hbar m\,Y_{\ell m}
\tag{3.17}
$$

19

together with (3.3) implies that

$$Y_{\ell m}(\theta, \phi) = P_{\ell m}(\theta) \, e^{im\phi} \,. \tag{3.18}$$

The ϕ dependence of the spherical harmonics is very simple indeed!

One can show that for spherical harmonics, which are related to **orbital** angular momentum, one can only have integer ℓ. While j can be half-integral, any attempt to define spherical harmonics for half-integral ℓ fails. You will indeed show in the homework that this is necessarily the case.

4   The radial equation

Recall that from (1.69) we have

$$H = \frac{\mathbf{p}^2}{2m} + V(r) = -\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{2mr^2} \mathcal{L}^2 + V(r) \tag{4.1}$$

where we used the differential operator realization $\mathcal{L}^2$ of the operator $\mathbf{L}^2$. The Schrödinger equation will be solved using the following ansatz for energy eigenstates

$$\Psi_{E\ell m}(\mathbf{x}) = f_{E\ell m}(r) \, Y_{\ell m}(\theta, \phi) \tag{4.2}$$

We have the product of a radial function $f_{E\ell m}(r)$ times an angular function $Y_{\ell m}$ which is an eigenstate of $\mathbf{L}^2$ and of $\hat{L}_z$:

$$\mathcal{L}^2 Y_{\ell m} = \hbar^2 \ell(\ell+1) Y_{\ell m} \,, \qquad \hat{L}_z Y_{\ell m} = \hbar m \, Y_{\ell m} \tag{4.3}$$

Plugging this into the Schrödinger equation $H\Psi = E\Psi$, the $Y_{\ell m}$ dependence can be cancelled out and we get

$$-\frac{\hbar^2}{2m} \frac{1}{r} \frac{d^2}{dr^2} (r f_{E\ell m}) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} f_{E\ell m} + V(r) f_{E\ell m} = E f_{E\ell m} \tag{4.4}$$

We note that this equation does not depend on the quantum number m (do not confuse this with the mass m!) Therefore the label m is not needed in the radial function and we let $f_{E\ell m} \to f_{E\ell}$ so that we have

$$\Psi_{E\ell m}(\mathbf{x}) = f_{E\ell}(r) \, Y_{\ell m}(\theta, \phi) \tag{4.5}$$

and the differential equation, multiplying by r becomes

$$-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} (r f_{E\ell}) + \left(V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} \right) (r f_{E\ell}) = E \, (r f_{E\ell}) \tag{4.6}$$

This suggests writing introducing a modified radial function $u_{E\ell}(r)$ by

$$f_{E\ell}(r) = \frac{u_{E\ell}(r)}{r} \tag{4.7}$$

20

so that we have

$$\Psi_{E\ell m}(\mathbf{x}) = \frac{u_{E\ell}(r)}{r} Y_{\ell m}(\theta, \phi),$$

(4.8)

with radial equation

$$-\frac{\hbar^2}{2m} \frac{d^2 u_{E\ell}}{dr^2} + V_{\text{eff}}(r) u_{E\ell} = E u_{E\ell},$$

(4.9)

where the effective potential V_{eff} constructed by adding to the potential $V(r)$ the centrifugal barrier term proportional to $\mathbf{L}^2$:

$$V_{\text{eff}}(r) \equiv V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}$$

(4.10)

This is like a one-dimensional Schrödinger equation in the variable r, but as opposed to our usual problems with $x \in (-\infty, \infty)$, the radius $r \in [0, \infty]$ and we will need some special care for $r = 0$.

The normalization of our wavefunctions proceeds as follows

$$\int d^3\mathbf{x}\, |\Psi_{E\ell m}(\mathbf{x})|^2 = 1$$

(4.11)

This gives

$$\int r^2 dr\, d\Omega\, \frac{|u_{E\ell}(r)|^2}{r^2}\, Y^*_{\ell m}(\Omega) Y_{\ell m}(\Omega) = 1$$

(4.12)

the angular integral gives one and we get

$$\int_0^\infty dr\, |u_{E\ell}(r)|^2 = 1$$

(4.13)

a rather natural result for the function $u_{E\ell}$ that plays the role of radial wavefunction.

Behavior of solutions as $r \to 0$. We claim that

$$\lim_{r \to 0} u_{E\ell}(r) = 0.$$

(4.14)

This requirement does not arise from normalization: as you can see in (4.13) a finite $u_{E\ell}$ at $r = 0$ would cause no trouble. Imagine taking a solution u_{E0} with $\ell = 0$ that approaches a constant as $r \to 0$:

$$\lim_{r \to 0} u_{E0}(r) = c \neq 0.$$

(4.15)

The full solution Ψ near the origin would then take the form

$$\Psi(\mathbf{x}) \simeq \frac{c}{r} Y_{00} = \frac{c'}{r},$$

(4.16)

21

since Y_{00} is simply a constant. The problem with this wavefunction is that it simply *does not solve* the Schrödinger equation! You may remember from electromagnetism that the Laplacian of the $1/r$ function has a delta function at the origin, so that as a result

$$\nabla^2 \Psi(\mathbf{x}) = -4\pi c' \delta(\mathbf{x}). \tag{4.17}$$

Since the Laplacian is part of the Hamiltonian, this delta function must be cancelled by some other contribution, but there is none, since the potential $V(r)$ does not have delta functions[2].

We can learn more about the behavior of the radial solution under the reasonable assumption that the *centrifugal barrier dominates the potential as* $r \to 0$. In this case the most singular terms of the radial differential equation must cancel each other out, leaving less singular terms that we can ignore in this leading term calculation. So we set:

$$-\frac{\hbar^2}{2m}\frac{d^2 u_{E\ell}}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}u_{E\ell} = 0, \quad \text{as } r \to 0. \tag{4.18}$$

or equivalently

$$\frac{d^2 u_{E\ell}}{dr^2} = \frac{\ell(\ell+1)}{r^2}u_{E\ell}, \tag{4.19}$$

The solutions of this can be taken to be $u_{E\ell} = r^s$ with s a constant to be determined. We then find

$$s(s-1) = \ell(\ell+1) \quad \to \quad s = \ell+1, \ s = -\ell \tag{4.20}$$

thus leading to two possible behaviors near $r = 0$:

$$u_{E\ell} \sim r^{\ell+1}, \quad u_{E\ell} \sim \frac{1}{r^\ell}. \tag{4.21}$$

For $\ell = 0$ the second behavior was shown to be inconsistent with the Schrödinger equation at $r = 0$ (because of a delta function). For $\ell > 0$ the second behavior is not consistent with normalization. Therefore we have established that

$$\boxed{u_{E\ell} \sim c\,r^{\ell+1}, \quad \text{as } r \to 0.} \tag{4.22}$$

Note that the full radial dependence is obtained by dividing by r, so that

$$f_{E\ell} \sim c\,r^\ell, \tag{4.23}$$

This allows for a constant non-zero wavefunction at the origin only for $\ell = 0$. Only for $\ell = 0$ a particle can be at the origin. For $\ell \neq 0$ the angular momentum "barrier" prevents the particle from reaching the origin.

---

[2] Delta function potentials in more than one dimension are very singular and require regulation.

<u>Behavior of solutions as $r \to \infty$.</u> Again, we can make some definite statements once we assume some properties of the potential. Let us consider the case when the potential $V(r)$ vanishes beyond some radius or at least decays fast enough as the radius grows without bound

$$V(r) \ = \ 0 \, , \ \text{for } r > r_0 \, , \quad \text{or} \quad \lim_{r \to \infty} rV(r) \ = \ 0 \, . \tag{4.24}$$

Curiously, the above assumptions are violated for the $1/r$ potential of the Hydrogen atom (an extended discussion of related issues can be found in Shankar around page 344). Under these assumptions we ignore the effective potential completely (including the centrifugal barrier) and the equation becomes

$$-\frac{\hbar^2}{2m} \frac{d^2 u_{E\ell}}{dr^2} \ = \ E u_{E\ell}(r) \, . \tag{4.25}$$

The equation is the familiar

$$\frac{d^2 u_{E\ell}}{dr^2} \ = \ -\frac{2mE}{\hbar^2} u_{E\ell} \, . \tag{4.26}$$

The resulting $r \to \infty$ behavior follows immediately

$$\begin{aligned} E < 0 \, , \quad & u_{E\ell} \ \sim \ \exp\left(-\sqrt{\frac{2m|E|}{\hbar^2}} \, r\right) , \\ E > 0 \, , \quad & u_{E\ell} \ \sim \ \exp(\pm ikr) \, , \quad k = \sqrt{\frac{2mE}{\hbar^2}} \, . \end{aligned} \tag{4.27}$$

The first behavior, for $E < 0$ is typical of bound states. For $E > 0$ we have a continuous spectrum with degenerate solutions (hence the $\pm$). Having understood the behavior of solutions near $r = 0$ and for $r \to \infty$ this allows for qualitative plots of radial solutions.

The discrete spectrum is organized as follows. We have energy eigenstates for all values of ℓ. In fact for each value of ℓ the potential V_{eff} in the radial equation is different. So this equation must be solved for $\ell = 0, 1, \ldots$. For each fixed ℓ we have a one-dimensional problem, so we have no degeneracies in the bound state spectrum. We have a set of allowed values of energies that depend on ℓ and are numbered using an integer $n = 1, 2 \ldots$. For each allowed energy $E_{n\ell}$ we have a single radial solution $u_{n\ell}$.

$$\text{Fixed } \ell, \ \text{Energies:} \ \ E_{n\ell} \, , \quad \text{Radial function:} \ u_{n\ell} \, , \quad n = 1, 2, \ldots \tag{4.28}$$

Of course each solution $u_{n\ell}$ for the radial equation represents $2\ell + 1$ degenerate solutions to the Schrödinger equation corresponding to the possible values of $\hat{L}_z$ in the range $(-\ell\hbar, \ell\hbar)$. Note that n has replaced the label E in the radial solution, and the energies have now been labeled. This is illustrated in the diagram of Figure 4, where each solution of the radial equation is shown as a short line atop an ℓ label on the horizontal axis. This is the spectral diagram for the central-potential Hamiltonian. Each line of a given ℓ represents the $(2\ell + 1)$ degenerate states obtained with $m = -\ell, \ldots, \ell$. Because the bound state spectrum of a one-dimensional potential

is non-degenerate, our radial equation can't have any degeneracies for any fixed ℓ. Thus the lines on the diagram are single lines! Of course, other types of degeneracies of the spectrum can exist: some states having different values of ℓ may have the same energy. In other words, the states may match across columns on the figure. Finally, note that since the potential becomes more positive as ℓ is increased, the lowest energy state occurs for $\ell = 0$ and the energy $E_{1,\ell}$ of the lowest state for a given ℓ increases as we increase ℓ.
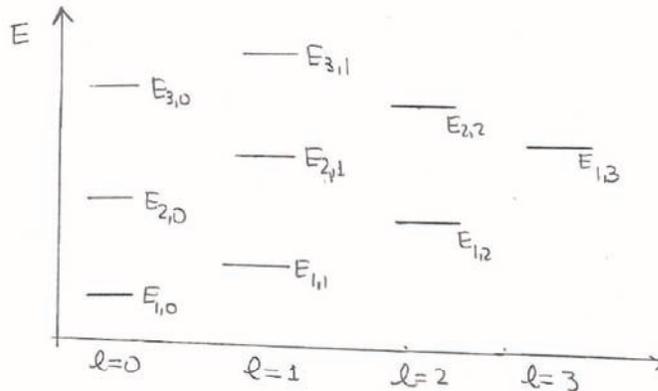
Figure 4: The generic discrete spectrum of a central-potential Hamiltonian, showing the angular momentum ℓ multiplets and their energies.

5   The free particle and the infinite spherical well

5.1   Free particle

It may sound funny at first, but it is interesting to find the radial solutions that correspond to a free particle! A particle that moves in $V(r) = 0$. This amounts to a very different description of the energy eigenstates. In cartesian coordinates we would write solutions as momentum eigenstates, for all values of the momentum. To label such solutions we could use three labels: the components of the momentum. Alternatively, we can use the energy and the direction defined by the momentum, which uses two labels. Here the solutions will be labeled by the energy and (ℓ, m), the usual two integers that describe the angular dependence (of course, ℓ affects the radial dependence too). The radial equation is

$$-\frac{\hbar^2}{2m}\frac{d^2 u_{E\ell}}{dr^2} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}u_{E\ell} \;=\; E u_{E\ell} \tag{5.29}$$

which is, equivalently

$$-\frac{d^2 u_{E\ell}}{dr^2} + \frac{\ell(\ell+1)}{r^2}u_{E\ell} \;=\; k^2 u_{E\ell}, \qquad k \equiv \sqrt{\frac{2mE}{\hbar^2}} \tag{5.30}$$

In this equation there is no quantization of the energy. Indeed we can redefine the radial coordinate in a way that the energy does not appear, namely, k does not appear. Letting $\rho = kr$ the equation becomes

$$-\frac{d^2 u_{E\ell}}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2} u_{E\ell} = u_{E\ell}, \qquad (5.31)$$

The solution of this differential equation with regular behavior at the origin is $u_{E\ell} = c\rho j_\ell(\rho)$, where c is an arbitrary constant. This means that we can take

$$u_{E\ell} = r j_\ell(kr). \qquad (5.32)$$

Here the $j_\ell(x)$ are the spherical Bessel functions. All in all we have

$$\text{Free particle:} \qquad \Psi_{E\ell m}(\mathbf{x}) = j_\ell(kr) Y_{lm}(\theta, \phi). \qquad (5.33)$$

The spherical Bessel functions have the following behavior

$$x j_\ell(x) \sim \frac{x^{\ell+1}}{(2\ell+1)!!}, \quad \text{as } x \to 0, \qquad \text{and} \qquad x j_\ell(x) \sim \sin\left(x - \frac{\ell\pi}{2}\right) \text{ as } x \to \infty. \qquad (5.34)$$

which implies the correct behavior for $u_{E\ell}$ as $r \to 0$ and $r \to \infty$. Indeed, for $r \to \infty$ we have

$$\text{Free particle :} \qquad u_{E\ell} \sim \sin\left(kr - \frac{\ell\pi}{2}\right), \quad \text{as } r \to \infty. \qquad (5.35)$$

Whenever the potential is not zero, but vanishes beyond some radius, the solutions, for $r \to \infty$ take the form

$$u_{E\ell} \sim \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell(E)\right), \quad \text{as } r \to \infty. \qquad (5.36)$$

Here $\delta_\ell(E)$ is called the **phase shift** and by definition vanishes if there is no potential. The form of the solution above is consistent with our general behavior, as this is a superposition of the two solutions available in (4.27) for $E > 0$. The phase shift contains all the information about a potential $V(r)$ available to someone probing the potential from far away by scattering particles off of it.

5.2 The infinite spherical well

An infinite spherical well of radius a is a potential that forces the particle to be within the sphere $r = a$. The potential is zero for $r \le a$ and it is infinite for $r > a$.

$$V(r) = \begin{cases} 0, & \text{if } r \le a \\ \infty, & \text{if } r > a \end{cases} \qquad (5.37)$$

The Schrödinger radial equation is the same as the one for the free particle

$$-\frac{d^2 u_{E\ell}}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2} u_{E\ell} = u_{E\ell}, \qquad \rho = kr \qquad (5.38)$$

25

where k again encodes the energy E, which is greater than zero. It follows that the solutions are the ones we had before, with spherical Bessel functions, but this time quantization of the energy arises because the wavefunctions must vanish for $r = a$.

Let us do the case $\ell = 0$ without resorting to the Bessel functions. The above equation becomes

$$-\frac{d^2 u_{E,0}}{d\rho^2} = u_{E,0} \quad \rightarrow \quad u_{E,0} = A\sin\rho + B\cos\rho. \tag{5.39}$$

Since the solution must vanish at $r = 0$ we must choose the sin function:

$$u_{E,0}(r) = \sin kr. \tag{5.40}$$

Since this must vanish for $r = a$ we have that k must take values k_n with

$$k_n a = n\pi, \quad \text{for} \quad n = 1, 2, \ldots \infty. \tag{5.41}$$

Those values of k_n correspond to energies $E_{n,0}$ where the n indexes the solutions and the 0 represents $\ell = 0$:

$$E_{n,0} = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2ma^2}(k_n a)^2 = \frac{\hbar^2}{2ma^2} n^2 \pi^2. \tag{5.42}$$

Note that $\frac{\hbar^2}{2ma^2}$ is the natural energy scale for this problem and therefore it is convenient to define the unit-free scaled energies $\mathcal{E}_{n,\ell}$ by dividing $E_{n,\ell}$ by the natural energy by

$$\mathcal{E}_{n,\ell} \equiv \frac{2ma^2}{\hbar^2} E_{n,\ell}. \tag{5.43}$$

It follows that the 'energies' for $\ell = 0$ are

$$\mathcal{E}_{n,0} = n^2 \pi^2, \quad u_{n,0} = \sin\left(\frac{n\pi r}{a}\right). \tag{5.44}$$

We have

$$\mathcal{E}_{1,0} \simeq 9.8696, \quad \mathcal{E}_{2,0} \simeq 39.478, \quad \mathcal{E}_{3,0} \simeq 88.826, \tag{5.45}$$

Let us now do $\ell = 1$. Here the solutions are $u_{E,1} = r\, j_1(kr)$. This Bessel function is

$$j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho} \tag{5.46}$$

The zeroes of $j_1(\rho)$ occur for $\tan\rho = \rho$. Of course, we are not interested in the zero at $\rho = 0$. You can check that the first three zeroes occur for $4.4934, 7.7252, 10.904$. For higher values of ℓ it becomes a bit more complicated but there are tables of zeroes on the web.

There is notation in which the nontrivial zeroes are denoted by $z_{n,\ell}$ where

$$z_{n,\ell} \text{ is the } n\text{-th zero of } j_\ell : \ j_\ell(z_{n,\ell}) = 0. \tag{5.47}$$

26

The vanishing condition at $r = a$ quantizes k so that

$$k_{n,\ell}\, a \;=\; z_{n,\ell} \tag{5.48}$$

and the energies

$$E_{n,\ell} \;=\; \frac{\hbar^2}{2ma^2}\,(k_{n,\ell}a)^2 \quad\to\quad \mathcal{E}_{n,\ell} \;=\; z_{n,\ell}^2 \tag{5.49}$$

We have

$$
\begin{aligned}
z_{1,1} &= 4.4934\,, \quad & z_{2,1} &= 7.7252\,, \quad & z_{3,1} &= 10.904 \\
z_{1,2} &= 5.7634\,, \quad & z_{2,2} &= 9.095\,, \\
z_{1,3} &= 6.9879\,, \quad & z_{2,3} &= 10.417\,.
\end{aligned} \tag{5.50}
$$

which give us

$$
\begin{aligned}
\mathcal{E}_{1,1} &= 20.191\,, \quad & \mathcal{E}_{2,1} &= 59.679\,, \quad & \mathcal{E}_{3,1} &= 118.89 \\
\mathcal{E}_{1,2} &= 33.217\,, \quad & \mathcal{E}_{2,2} &= 82.719\,, \\
\mathcal{E}_{1,3} &= 48.83\,, \quad & \mathcal{E}_{2,3} &= 108.51\,.
\end{aligned} \tag{5.51}
$$

The main point to be made is that there are no accidental degeneracies: the energies for different values of ℓ never coincide. More explicitly, with $\ell \neq \ell'$ we have that $\mathcal{E}_{n,\ell} \neq \mathcal{E}_{n',\ell'}$ for any choices of n and n'. This is illustrated in figure 5.
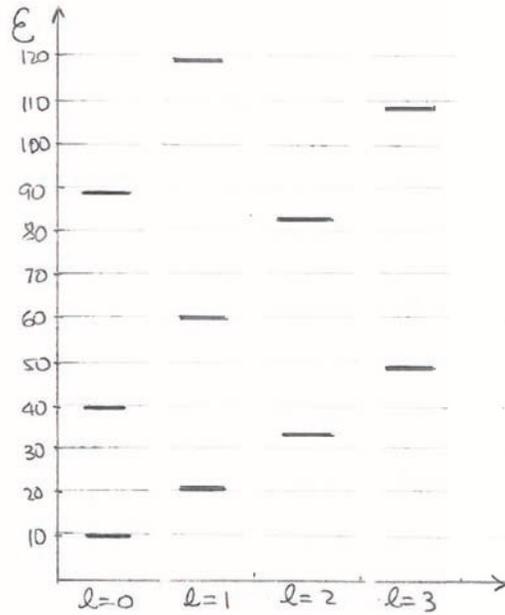

Figure 5: The spectrum of the infinite spherical square well. There are no accidental degeneracies.

6 The three-dimensional isotropic oscillator

The potential of the 3D isotropic harmonic oscillator is as follows:

$$V = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2) = \frac{1}{2}m\omega^2 r^2 \,. \tag{6.52}$$

As we will see, the spectrum for this quantum mechanical system has degeneracies, that are explained by the existence of some **hidden symmetry**, a symmetry that is not obvious from the start. Thus in some ways this quantum 3D oscillator is a lot more symmetric than the infinite spherical well.

As you know, for the 3D oscillator we can use creation and annihilation operators $\hat{a}_x^\dagger, \hat{a}_y^\dagger, \hat{a}_z^\dagger$ and $\hat{a}_x, \hat{a}_y, \hat{a}_z$ associated with 1D oscillators in the $x, y,$ and z directions. The Hamiltonian then takes the form:

$$H = \hbar\omega\big(\hat{N}_1 + \hat{N}_2 + \hat{N}_3 + \tfrac{3}{2}\big) \;=\; \hbar\omega\big(\hat{N} + \tfrac{3}{2}\big) \,. \tag{6.53}$$

where we defined $\hat{N} \equiv \hat{N}_1 + \hat{N}_2 + \hat{N}_3$.

We now want to explain how tensor products are relevant to the 3D oscillator. We have discussed tensor products before to describe two particles, each associated with a vector space and the combined system associated with the tensor product of vector spaces. But tensor products are also relevant to single particles, if they have degrees of freedom that live in different spaces, or more than one set of attributes, each of which described by states in some vector space. For example, if a spin 1/2 particle can move, the relevant states live in the tensor product of momentum space and the 2-dimensional complex vector space of spin. States are obtained by superposition of basic states of the form $|p\rangle \otimes (\alpha|+\rangle + \beta|-\rangle)$

For the 3D oscillator, the Hamiltonian is the sum of commuting Hamiltonians of 1D oscillators for the x, y, and z directions. Thus the general states are obtained by tensoring the state spaces $\mathcal{H}_x, \mathcal{H}_y,$ and $\mathcal{H}_z$ of the three independent oscillators. It is a single particle oscillating, but the description of what it is doing entails saying what is doing in each of the independent directions. Thus we write

$$\mathcal{H}_{3D} \;=\; \mathcal{H}_x \otimes \mathcal{H}_y \otimes \mathcal{H}_z \,. \tag{6.54}$$

Instead of this tensor product reflecting the behavior of three different particles, this tensor product allows us to describe the behavior of one particle in three different directions. The vacuum state $|0\rangle$ of the 3D oscillator can be viewed as

$$|0\rangle \;\equiv\; |0\rangle_x \otimes |0\rangle_y \otimes |0\rangle_z \,. \tag{6.55}$$

The associated wavefunction is

$$\Psi(x, y, z) \;=\; \langle x| \otimes \langle y| \otimes \langle z| \, |0\rangle \;=\; \langle x|0\rangle_x \langle y|0\rangle_y \langle z|0\rangle_z \;=\; \psi_0(x)\psi_0(y)\psi_0(z) \,. \tag{6.56}$$

where ψ_0 is the ground state wavefunction of the 1D oscillator. This is the expected answer. Recalling the form of (non-normalized) basis states for $\mathcal{H}_x, \mathcal{H}_y,$ and $\mathcal{H}_z$:

$$\text{basis states for } \mathcal{H}_x : \ (\hat{a}_x^\dagger)^{n_x}|0\rangle_x, \ n_x = 0, 1, \ldots$$
$$\text{basis states for } \mathcal{H}_y : \ (\hat{a}_y^\dagger)^{n_y}|0\rangle_y, \ n_y = 0, 1, \ldots \qquad (6.57)$$
$$\text{basis states for } \mathcal{H}_z : \ (\hat{a}_z^\dagger)^{n_z}|0\rangle_z, \ n_z = 0, 1, \ldots$$

We then have that the basis states for the 3D state space are

$$\text{basis states of } \mathcal{H}_{3D} : \ (\hat{a}_x^\dagger)^{n_x}|0\rangle_x \otimes (\hat{a}_y^\dagger)^{n_y}|0\rangle_y \otimes (\hat{a}_z^\dagger)^{n_z}|0\rangle_z, \ n_x, n_y, n_z \in \{0, 1, \ldots\} \quad (6.58)$$

This is what we would expect intuitively, we simply pile arbitrary numbers of $\hat{a}_x^\dagger, \hat{a}_y^\dagger,$ and $\hat{a}_z^\dagger$ on the vacuum. It is this multiplicative structure that is the signature of tensor products. Having understood the above, for brevity we write such basis states simply as

$$(\hat{a}_x^\dagger)^{n_x}(\hat{a}_y^\dagger)^{n_y}(\hat{a}_z^\dagger)^{n_z}|0\rangle. \qquad (6.59)$$

Each of the states in (6.58) has a wavefunction that is the product of $x, y,$ and z-dependent wavefunctions. Once we form superpositions of such states, the total wavefunction cannot any longer be factorized into $x, y,$ and z-dependent wavefunctions. The $x, y,$ and z-dependences become 'entangled'. These are precisely the analogs of entangled states of three particles.

We are ready to begin constructing the individual states of the 3D isotropic harmonic oscillator system. The key property is that the states must organize themselves into representations of angular momentum. Since angular momentum commutes with the Hamiltonian, angular momentum multiplets represent degenerate states.

We already built the ground state, which is a single state with $\hat{N}$ eigenvalue $N = 0$. All other states have higher energies, so this state must be, by itself a representation of angular momentum. It can only be the singlet $\ell = 0$. Thus we have

$$N = 0, \ E = \tfrac{3}{2}\hbar\omega, \ |0\rangle \ \leftrightarrow \ \ell = 0. \qquad (6.60)$$

The states with $N = 1$ have $E = (5/2)\hbar\omega$ and are

$$\hat{a}_x^\dagger|0\rangle, \ \hat{a}_y^\dagger|0\rangle, \hat{a}_z^\dagger|0\rangle \qquad (6.61)$$

These three states fit precisely into an $\ell = 1$ multiplet (a triplet). There is no other possibility, in fact: any higher ℓ multiplet has too many states and we only have 3 degenerate ones. Moreover, we cannot have three singlets, this is a degeneracy inconsistent with the lack of degeneracy for 1D bound states (as discussed earlier). The $\ell = 0$ ground state and the $\ell = 1$ triplet at the first excited level are indicated in Figure 7.

Let us proceed now with the states at $N = 2$ or $E = (7/2)\hbar\omega$. These are, the following six states:

$$(\hat{a}_x^\dagger)^2|0\rangle \,, \ (\hat{a}_y^\dagger)^2|0\rangle \,, \ (\hat{a}_z^\dagger)^2|0\rangle \,, \ \hat{a}_x^\dagger\hat{a}_y^\dagger|0\rangle \,, \ \hat{a}_x^\dagger\hat{a}_z^\dagger|0\rangle \,, \ \hat{a}_y^\dagger\hat{a}_z^\dagger|0\rangle \,. \tag{6.62}$$

To help ourselves in trying to find the angular momentum multiplets recall that that the number of states # for a given ℓ are

ℓ	#
0	1
1	3
2	5
3	7
4	9
5	11
6	13
7	15

Since we cannot use the triplet twice, the only way to get six states is having five from $\ell = 2$ and one from $\ell = 0$. Thus

$$\text{Six } N = 2 \text{ states}: \quad (\ell = 2) \oplus (\ell = 0) \,. \tag{6.63}$$

Note that here we use the direct sum (not the tensor product!) the six states define a six dimensional vector space spanned by five vectors in $\ell = 0$ and one vector in $\ell = 0$. Had we used a tensor product we would just have 5 vectors.

Let us continue to figure out the pattern. At $N = 3$ with $E = (9/2)\hbar\omega$ we actually have 10 states (count them!) It would seem now that there are two possibilities for multiplets

$$(\ell = 3) \oplus (\ell = 1) \quad \text{or} \quad (\ell = 4) \oplus (\ell = 0) \tag{6.64}$$

We can argue that the second possibility cannot be. The problem with it is that the $\ell = 3$ multiplet, which has not appeared yet, would not arise at this level. If it would arise later, it would do so at a higher energy, and we would have the lowest $\ell = 3$ multiplet above the lowest $\ell = 4$ multiplet, which is not possible. You may think that perhaps $\ell = 3$ multiplets never appear and the inconsistency is avoided, but this is not true. At any rate we will give below a more rigorous argument. The conclusion, however is that

$$\text{Ten } N = 3 \text{ states}: \quad (\ell = 3) \oplus (\ell = 1) \,. \tag{6.65}$$

Let us do the next level! At $N = 4$ we find 15 states. Instead of writing them out let us count them without listing them. In fact, we can easily do the general case of arbitrary integer $N \geq 1$. The states we are looking for are of the form

$$(\hat{a}_x^\dagger)^{n_x}(\hat{a}_y^\dagger)^{n_y}(\hat{a}_z^\dagger)^{n_z}|0\rangle \,, \quad \text{with} \ \ n_x + n_y + n_z = N \,. \tag{6.66}$$

We need to count how many different solutions there are to $n_x + n_y + n_z = N$, with $n_x, n_y, n_z \geq 0$. This is the number of states $\#(N)$ at level N. To visualize this think of $n_x + n_y + n_z = N$ as the equation for a plane in three-dimensional space with axes n_x, n_y, n_z. Since no integer can be negative, we are looking for points with integer coordinates in the region of the plane that lies on the positive octant, as shown in Figure 6. Starting at one of the three corners, say $(n_x, n_y, n_z) = (N, 0, 0)$ we have one point, then moving towards the origin we encounter two points, then three, and so on until we find $N+1$ points on the (n_y, n_z) plane. Thus, the number of states $\#(N)$ for number N is

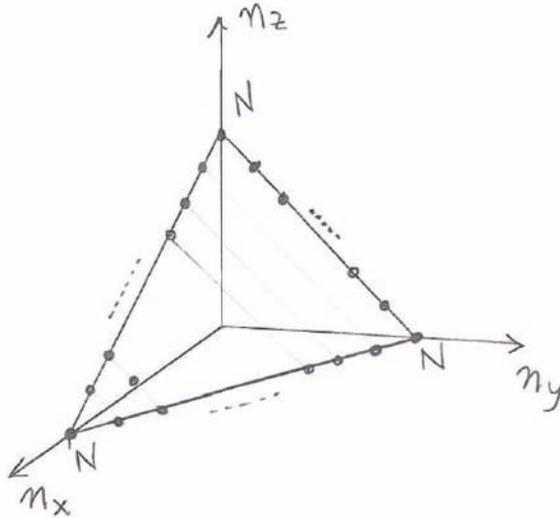$$\#(N) = 1 + 2 + \ldots + (N + 1) = \frac{(N + 1)(N + 2)}{2} \tag{6.67}$$

Figure 6: Counting the number of degenerate states with number N in the 3D simple harmonic oscillator.

Back to the $N = 4$ level, $\#(4)=15$. We rule out a single $\ell = 7$ multiplet since states with $\ell = 4, 5, 6$ have not appeared yet. By this logic the highest ℓ multiplet for $N = 4$ must be the lowest that has not appeared yet, thus $\ell = 4$, with 9 states. The remaining six must appear as $\ell = 2$ plus $\ell = 0$. Thus, we have

$$15 \ N = 4 \text{ states}: \quad (\ell = 4) \oplus (\ell = 2) \oplus (\ell = 0). \tag{6.68}$$

Thus we see that ℓ jumps by steps of two, starting from the maximal ℓ. This is in fact the rule. It is quickly confirmed for the $\#(5)=21$ states with $N = 5$ would arise from $(\ell = 5) \oplus (\ell = 3) \oplus (\ell = 1)$. All this is shown in Figure 7.
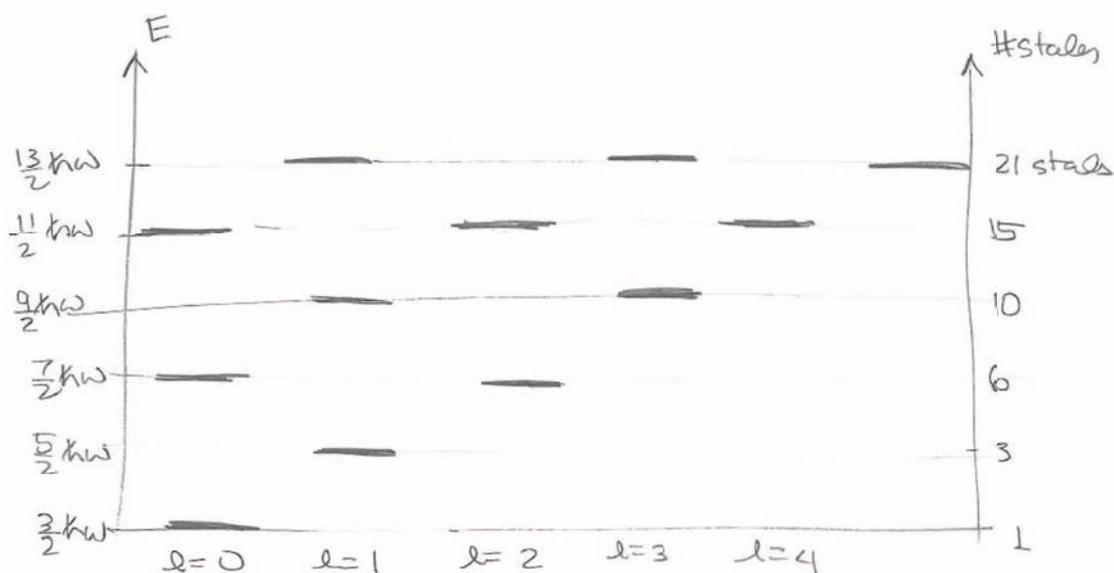
Figure 7: Spectral diagram for angular momentum multiplets in the 3D isotropic harmonic oscillator.

Some of the structure of angular momentum multiplets can be seen more explicitly using the $\hat{a}_L$ and $\hat{a}_R$ operators introduced for the 2D harmonic oscillator:

$$\hat{a}_L = \frac{1}{\sqrt{2}}(\hat{a}_x + i\hat{a}_y), \quad \hat{a}_R = \frac{1}{\sqrt{2}}(\hat{a}_x - i\hat{a}_y). \tag{6.69}$$

L and R objects commute with each other and we have $[\hat{a}_L, \hat{a}_L^\dagger] = [\hat{a}_R, \hat{a}_R^\dagger] = 1$. With number operators $\hat{N}_R = \hat{a}_R^\dagger \hat{a}_R$ and $\hat{N}_L = \hat{a}_L^\dagger \hat{a}_L$ we then have $H = \hbar\omega(\hat{N}_R + \hat{N}_L + \hat{N}_z + \frac{3}{2})$ and, more importantly, the z component $\hat{L}_z$ of angular momentum takes the simple form

$$\hat{L}_z = \hbar(\hat{N}_R - \hat{N}_L). \tag{6.70}$$

Note that $\hat{a}_z$ carries no z-component of angular momentum. States are now build acting with arbitrary numbers of $\hat{a}_L^\dagger, \hat{a}_R^\dagger$ and $\hat{a}_z^\dagger$ operators on the vacuum. The $N = 1$ states are then presented as

$$\hat{a}_R^\dagger|0\rangle, \ \hat{a}_z^\dagger|0\rangle, \ \hat{a}_L^\dagger|0\rangle. \tag{6.71}$$

We see that the first state has $L_z = \hbar$, the second $L_z = 0$ and the third $\hat{L}_z = -\hbar$, exactly the three expected values of the $\ell = 1$ multiplet identified before. For number $N = 2$ the state with highest L_z is $(\hat{a}_R^\dagger)^2|0\rangle$ and it has $L_z = 2\hbar$. This shows that the highest ℓ multiplet is $\ell = 2$. For arbitrary positive integer number N, the state with highest L_z is $(\hat{a}_R^\dagger)^N|0\rangle$ and it has $L_z = \hbar N$. This shows we must have an $\ell = N$ multiplet. This is in fact what we got before! We can also understand the reason for the jump of two units from the top state of the multiplet. Consider

32

the above state with maximal $\hat{L}_z/\hbar$ equal to N and then the states with one and two units less of $\hat{L}_z/\hbar$:

$$
\begin{aligned}
\hat{L}_z/\hbar = N &\quad : \quad (\hat{a}_R^\dagger)^N |0\rangle \\
\hat{L}_z/\hbar = N-1 &\quad : \quad (\hat{a}_R^\dagger)^{N-1} \hat{a}_z^\dagger |0\rangle \\
\hat{L}_z/\hbar = N-2 &\quad : \quad (\hat{a}_R^\dagger)^{N-2}(\hat{a}_z^\dagger)^2 |0\rangle, \quad (\hat{a}_R^\dagger)^{N-1}\, \hat{a}_L^\dagger |0\rangle
\end{aligned}
\tag{6.72}
$$

While there is only one state with one unit less of $\hat{L}_z/\hbar$ there are two states with two units less. One linear combination of these two states must belong to the $\ell = N$ multiplet, but the other linear combination must be the top state of an $\ell = N - 2$ multiplet! This is the reason for the jump of two units.

For arbitrary N we can see why $\#(N)$ can be reproduced by ℓ multiplets skipping by two

$$
\begin{aligned}
N \text{ odd}: \quad \#(N) &= \underbrace{1+2}_{\ell=1} + \underbrace{3+4}_{\ell=3} + \underbrace{5+6}_{\ell=5} + \underbrace{7+8}_{\ell=7} + \ldots + \underbrace{N+(N+1)}_{\ell=N} \\
N \text{ even}: \quad \#(N) &= \underbrace{1}_{\ell=0} + \underbrace{2+3}_{\ell=2} + \underbrace{4+5}_{\ell=4} + \underbrace{6+7}_{\ell=6} + \ldots + \underbrace{N+(N+1)}_{\ell=N}
\end{aligned}
\tag{6.73}
$$

The accidental degeneracy is "explained" if we identify an operator that commutes with the Hamiltonian (a symmetry) and connects the various ℓ multiplets that appear for a fixed number N. One such operator is

$$
K \equiv \hat{a}_R^\dagger \hat{a}_L .
\tag{6.74}
$$

You can check it commutes with the Hamiltonian, and with a bit more work, that acting on the top state of the $\ell = N - 2$ multiplet it gives the top state of the $\ell = N$ multiplet.

7 Hydrogen atom and Runge-Lenz vector

The hydrogen atom Hamiltonian is

$$
H = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{r} .
\tag{7.75}
$$

The natural length scale here is the Bohr radius a_0, which is the unique length that can be built using the constants in this Hamiltonian: $\hbar, m,$ and e^2. We determine a_0 by setting $p \sim \hbar/a_0$ and equating magnitudes of kinetic and potential terms, ignoring numerical factors:

$$
\frac{\hbar^2}{ma_0^2} = \frac{e^2}{a_0} \quad \rightarrow \quad a_0 = \frac{\hbar^2}{me^2} \simeq 0.529 \text{\AA} .
\tag{7.76}
$$

Note that if the charge of the electron e^2 is decreased, the attraction force decreases and, correctly, the Bohr radius increases. The Bohr radius is the length scale of the hydrogen atom.

A natural energy scale E_0 is

$$E_0 = \frac{e^2}{a_0} = \frac{e^4 m}{\hbar^2} = \left(\frac{e^2}{\hbar c}\right)^2 mc^2 = \alpha^2(mc^2) \tag{7.77}$$

where we see the appearance of the fine-structure constant α that, in cgs units, takes the form

$$\alpha \equiv \frac{e^2}{\hbar c} \simeq \frac{1}{137} . \tag{7.78}$$

We thus see that the natural energy scale of the hydrogen atom is about $\alpha^2 \simeq 1/18770$ smaller than the rest energy of the electron. This gives about $E_0 = 27.2\text{eV}$. In fact $-E_0/2 = -13.6\text{eV}$ is the bound state energy of the electron in the ground state of the hydrogen atom.

One curious way to approach the calculation of the ground state energy and ground state wavefunction is to factorize the Hamiltonian. One can show that

$$H = \gamma + \frac{1}{2m} \sum_{k=1}^{3} \left(\hat{p}_k + i\beta \frac{\hat{x}_k}{r}\right)\left(\hat{p}_k - i\beta \frac{\hat{x}_k}{r}\right) \tag{7.79}$$

for suitable constants β and γ that you can calculate. The ground state $|\Psi_0\rangle$ is then the state for which

$$\left(\hat{p}_k - i\beta \frac{\hat{x}_k}{r}\right)|\Psi_0\rangle = 0 . \tag{7.80}$$

The spectrum of the hydrogen atom is described in Figure 8. The energy levels are $E_{\nu\ell}$, where we used $\nu = 1, 2, \ldots$, instead of n to label the various solutions for a given ℓ. This is because the label n is reserved for what is called the "principal quantum number". The degeneracy of the system is such that multiplets with equal $n \equiv \nu + \ell$ have the same energy, as you can see in the figure. Thus, for example, $E_{2,0} = E_{1,1}$, which is to say that the first excited solution for $\ell = 0$ has the same energy as the lowest energy solution for $\ell = 1$. It is also important to note that for any fixed value of n the allowed values of ℓ are

$$\ell = 0, 1, \ldots, n - 1 \tag{7.81}$$

Finally, the energies are given by

$$E_{\nu\ell} = -\frac{e^2}{2a_0} \frac{1}{(\nu + \ell)^2} , \quad n \equiv \nu + \ell . \tag{7.82}$$

The large amount of degeneracy in this spectrum asks for an explanation. The hydrogen Hamiltonian has in fact some hidden symmetry. It has to do with the so-called Runge-Lenz vector. In the following we discuss the classical origin of this conserved vector quantity.

Imagine we have an energy functional
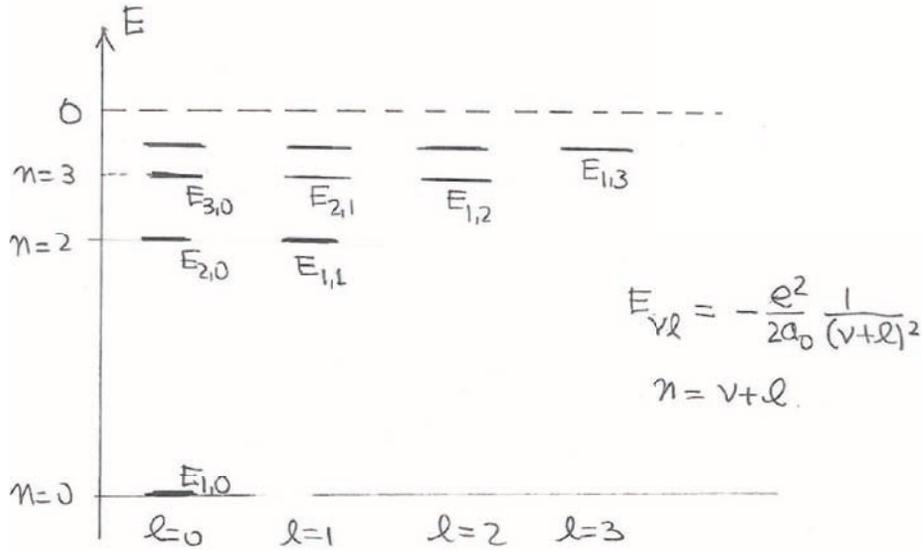
$$E = \frac{\mathbf{p}^2}{2m} + V(r) \tag{7.83}$$

34

Figure 8: Spectrum of angular momentum multiplets for the hydrogen atom. Here $E_{\nu\ell}$ with $\nu = 1, 2, \ldots$, denotes the energy of the ν-th solution for any fixed ℓ. States with equal values of $n \equiv \nu + \ell$ are degenerate. For any fixed n, the values of ℓ run from zero to $n - 1$. Correction: the $n = 0$ in the figure should be $n = 1$.

then the force on the particle moving in this potential is

$$\mathbf{F} = -\nabla V = -V'(r)\frac{\mathbf{r}}{r}, \tag{7.84}$$

where primes denote derivatives with respect to the argument. Newton's equation is

$$\frac{d\mathbf{p}}{dt} = -V'(r)\frac{\mathbf{r}}{r} \tag{7.85}$$

and it is simple to show (do it!) that in this central potential the angular momentum is conserved

$$\frac{d\mathbf{L}}{dt} = 0. \tag{7.86}$$

We now calculate (all classically) the time derivative of $\mathbf{p} \times \mathbf{L}$:

$$\frac{d}{dt}(\mathbf{p} \times \mathbf{L}) = \frac{d\mathbf{p}}{dt} \times \mathbf{L} = -\frac{V'(r)}{r}\mathbf{r} \times (\mathbf{r} \times \mathbf{p})$$

$$= -\frac{mV'(r)}{r}\mathbf{r} \times (\mathbf{r} \times \dot{\mathbf{r}}) \tag{7.87}$$

$$= -\frac{mV'(r)}{r}\left[\mathbf{r}(\mathbf{r} \cdot \dot{\mathbf{r}}) - \dot{\mathbf{r}}\, r^2\right].$$

We now note that

$$\mathbf{r} \cdot \dot{\mathbf{r}} = \frac{1}{2}\frac{d}{dt}(\mathbf{r} \cdot \mathbf{r}) = \frac{1}{2}\frac{d}{dt}r^2 = r\dot{r}. \tag{7.88}$$

35

Using this

$$\frac{d}{dt}(\mathbf{p} \times \mathbf{L}) = -\frac{mV'(r)}{r}\left[\mathbf{r}\, r\dot{r} - \dot{\mathbf{r}}\, r^2\right] = mV'(r)r^2\left[\frac{\dot{\mathbf{r}}}{r} - \frac{\mathbf{r}\,\dot{r}}{r^2}\right]$$
$$= mV'(r)r^2\,\frac{d}{dt}\left(\frac{\mathbf{r}}{r}\right) \tag{7.89}$$

Because of the factor $V'(r)r^2$, the right-hand side fails to be a total time derivative. But if we focus on potentials for which this factor is a constant we will get a conservation law. So, assume

$$V'(r)\,r^2 = \gamma, \tag{7.90}$$

for some constant γ. Then

$$\frac{d}{dt}(\mathbf{p} \times \mathbf{L}) = m\gamma\,\frac{d}{dt}\left(\frac{\mathbf{r}}{r}\right) \quad \rightarrow \quad \frac{d}{dt}\left(\mathbf{p} \times \mathbf{L} - m\gamma\,\frac{\mathbf{r}}{r}\right) = 0 \tag{7.91}$$

We got a conservation law: that complicated vector inside the parenthesis is constant in time! Back to (7.90) we have

$$\frac{dV}{dr} = \frac{\gamma}{r^2} \quad \rightarrow \quad V(r) = -\frac{\gamma}{r} + c_0. \tag{7.92}$$

This is the most general potential for which we get a conservation law. For $c_0 = 0$ and $\gamma = e^2$ we have the hydrogen atom potential

$$V(r) = -\frac{e^2}{r}, \tag{7.93}$$

so we have

$$\frac{d}{dt}\left(\mathbf{p} \times \mathbf{L} - me^2\,\frac{\mathbf{r}}{r}\right) = 0. \tag{7.94}$$

Factoring a constant we obtain the unit-free conserved **Runge-Lenz** vector $\mathbf{R}$:

$$\boxed{\mathbf{R} \equiv \frac{1}{me^2}\mathbf{p} \times \mathbf{L} - \frac{\mathbf{r}}{r}, \qquad \frac{d\mathbf{R}}{dt} = 0.} \tag{7.95}$$

The conservation of the Runge-Lenz vector is a property of inverse squared central forces. The second vector in $\mathbf{R}$ is simply minus the unit radial vector.

To understand the Runge-Lenz vector, we first examine its value for a circular orbit, as shown in figure 9. The vector $\mathbf{L}$ is out of the page and $\mathbf{p} \times \mathbf{L}$ points radially outward. The vector $\mathbf{R}$ is thus a competition between the outward radial first term and the inner radial second term. If these two terms would not cancel, the result would be a radial vector (outwards or inwards) but in any case, not conserved, as it rotates with the particle. Happily, the two terms cancel. Indeed for a circular orbit

$$m\frac{v^2}{r} = \frac{e^2}{r^2} \quad \rightarrow \quad \frac{m^2v^2r}{me^2} = 1 \quad \rightarrow \quad \frac{(mv)(mvr)}{me^2} = 1 \quad \rightarrow \quad \frac{pL}{me^2} = 1, \tag{7.96}$$
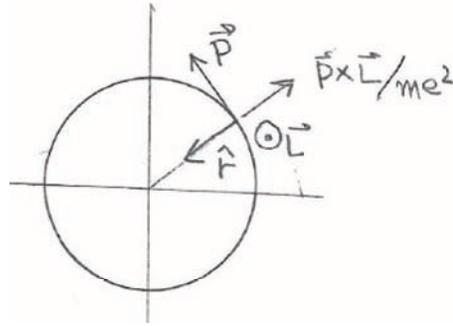
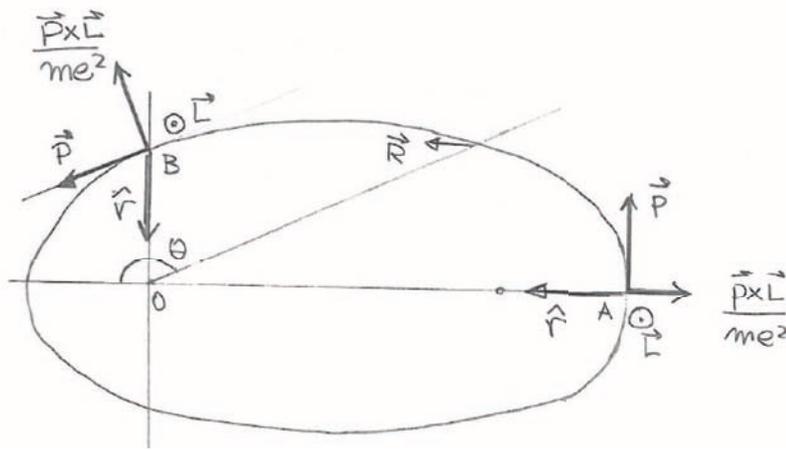Figure 9: The Runge-Lenz vector vanishes for a circular orbit.

Figure 10: In an elliptic orbit the Runge-Lenz vector is a vector along the major axis of the ellipse and points in the direction from the aphelion to the focus.

which is the statement that the first vector in $\mathbf{R}$, for a circular orbit, is of unit length and being outward directed cancels with the second term. The Runge-Lenz vector indeed vanishes for a circular orbit.

We now argue that for an elliptical orbit the Runge-Lenz vector is not zero. Consider figure 10. At the aphelion (point furthest away from the focal center), denoted as point A we have the first term in $\mathbf{R}$ point outwards and the second term point inwards. Thus, if $\mathbf{R}$ does not vanish it must be a vector along the line joining the focus and the aphelion, a horizontal vector on the figure. Now consider point B right above the focal center of the orbit. At this point $\mathbf{p}$ is no longer perpendicular to the radial vector and therefore $\mathbf{p} \times \mathbf{L}$ is no longer radial. As you can see, it points slightly to the left. It follows that $\mathbf{R}$ points to the left side of the figure. $\mathbf{R}$ is a vector along the major axis of the ellipse and points in the direction from the aphelion to the focus.

To see more quantitatively the role of $\mathbf{R}$ we dot its definition with the radial vector $\mathbf{r}$:

$$\mathbf{r} \cdot \mathbf{R} \;=\; \frac{1}{me^2}\, \mathbf{r} \cdot (\mathbf{p} \times \mathbf{L}) - r \tag{7.97}$$

referring to the figure, with the angle θ as defined there and $R \equiv |\mathbf{R}|$, we get

$$rR\cos\theta \;=\; \frac{1}{me^2}\, \mathbf{L} \cdot (\mathbf{r} \times \mathbf{p}) - r \;=\; \frac{1}{me^2}L^2 - r\,. \tag{7.98}$$

Collecting terms proportional to r:

$$r(1 + R\cos\theta) \;=\; \frac{L^2}{me^2} \quad \rightarrow \quad \boxed{\frac{1}{r} \;=\; \frac{me^2}{L^2}(1 + R\cos\theta)\,,} \tag{7.99}$$

We identify the magnitude R of the Runge-Lenz vector with the eccentricity of the orbit! Indeed if $R = 0$ the orbit if circular: r does not depend on θ.

This whole analysis has been classical. Quantum mechanically we will need to change some things a bit. The definition of $\mathbf{R}$ only has to be changed to guarantee that $\mathbf{R}$ is a hermitian (vector) operator. As you will verify the hermitization gives

$$\mathbf{R} \;\equiv\; \frac{1}{2me^2}\,(\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}) - \frac{\mathbf{r}}{r} \tag{7.100}$$

The quantum mechanical conservation of $\mathbf{R}$ is the statement that it commutes with the hydrogen Hamiltonian

$$[\,\mathbf{R}\,,H\,] \;=\; 0\,. \tag{7.101}$$

You will verify this; it is the analog of our classical calculation that showed that the time-derivative of $\mathbf{R}$ is zero. Moreover, the length-squared of the vector is also of interest. You will show that

$$\mathbf{R}^2 \;=\; 1 + \frac{2}{me^4}\, H(\mathbf{L}^2 + \hbar^2)\,. \tag{7.102}$$

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8.05 Quantum Physics II

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