Quantum Mechanics and Atomic Physics

Lecture 18: Angular Momentum Raising and Lowering

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Prof. Eva Halkiadakis
Hydrogen Atom Summary

- $\Psi$ is a product of
  - $\Phi$ which is oscillatory
  - $\Theta$ which is a polynomial in $\cos \theta$
  - $R$ which is a product of a decaying exponential and a polynomial in $r$

- $\Psi$ depends on 3 quantum numbers
  - **Principal quantum number** $n = 1, 2, 3, \ldots$
  - **Orbital angular momentum quantum number** $\ell = 0, 1, 2, \ldots (n-1)$
    - Today we will concentrate on this
  - **Magnetic quantum number** $m_\ell = 0, \pm 1, \ldots \pm \ell$ or $m_\ell = -\ell, -\ell+1, \ldots \ell-1, \ell$
    - Next time we will focus on this

Coulomb Potential:

$$V(r) = \frac{1}{4\pi \varepsilon_0} \frac{Q_1 Q_2}{r} = -\frac{e^2}{4\pi \varepsilon_0 r}$$
First, a few words on
The Effective Potential

- Recall the radial equation with the Coulomb Potential:

\[
\frac{d^2}{dr^2} (\psi(r)) + \frac{2\mu}{\hbar^2} \left[ E + \frac{e^2}{4\pi \epsilon_0 r} - \frac{\ell (\ell + 1) \hbar^2}{2\mu r^2} \right] \psi(r) = 0
\]

\[
- \frac{d^2}{dr^2} (\psi(r)) + \frac{\ell (\ell + 1)}{r^2} \psi(r) - \frac{2\mu}{\hbar^2} \frac{e^2}{4\pi \epsilon_0 r} \psi(r) = \frac{2\mu}{\hbar^2} E \psi(r)
\]

\[
V_{\text{eff}} = -\frac{2\mu}{\hbar^2} \frac{e^2}{4\pi \epsilon_0 r} + \frac{\ell (\ell + 1)}{r^2}
\]

\[
\Rightarrow - \frac{d^2}{dr^2} \psi(r) + V_{\text{eff}} \psi(r) = \frac{2\mu}{\hbar^2} E \psi(r)
\]

- This looks like the 1D S.E.!
$V_{\text{eff}}$

- $V_{\text{eff}}$ vs. $\rho$, where $\rho = r/a_0$
- Striking difference between $\ell=0$ and $\ell \neq 0$
  - When $\ell \neq 0$ the combination of the two terms in the effective potential leads to potential wells with infinite walls as $r \to 0$ (see radial nodes in Fig. 7.10 in textbook)
- $V_{\text{eff}}=0$ as $r \to \infty$
- Bohr energy levels get closer together as $n \to \infty$

Reed Chapter 7
The $\ell(\ell+1)/r^2$ term is known as the “centrifugal” term.

- Contributes a repulsive potential - drives the electron away from the nucleus.
- Stronger repulsion as $\ell$ increases and we expect to find the electron further from the nucleus.
Review of Orbital Angular Momentum

Recall that the orbital angular momentum in spherical coordinates is:

\[ \mathbf{L} = \mathbf{r} \times \mathbf{p} \quad \mathbf{\hat{\beta}} = -i\hbar \mathbf{\hat{\Sigma}} \]

\[ L_x = i\hbar (\sin \varphi \frac{\partial}{\partial \theta} + \cot \theta \cos \varphi \frac{\partial}{\partial \varphi}) \]

\[ L_y = i\hbar (-\cos \varphi \frac{\partial}{\partial \theta} + \cot \theta \sin \varphi \frac{\partial}{\partial \varphi}) \]

\[ L_z = -i\hbar \frac{\partial}{\partial \varphi} \]
Is the H atom an eigenstate of $L_x$, $L_y$, $L_z$?

- You should already be able to tell me the answer to this question!
- Let’s start with $L_z$:

Eigenstate means $Q_{0r} \Psi = (\text{const}) \Psi$

$L_z \Psi_{\text{me}} = -i \hbar \frac{\partial}{\partial \varphi} \Phi = -i \hbar \Theta \frac{\partial}{\partial \varphi} \Phi$

$\Phi = e^{i m \varphi}$

$\frac{\partial}{\partial \varphi} \Phi = i m e^{i m \varphi} = i m \Phi$

$\Rightarrow L_z \Psi = -i \hbar \Theta \Phi (\text{const}) = m \hbar \Psi$

- Yes, it is an eigenstate of $L_z$ with eigenvalue $m \hbar \Psi$!
Now let’s try $L_x$ and $L_y$

$L_x \Psi = i\hbar (R \sin \phi \frac{d\phi}{d\theta} + R \theta \cot \phi \cos \phi \frac{d\phi}{d\phi})$

$\neq (\text{const}) \Psi$

Similarly,

$\Psi = (\text{const}) \Psi$

- So, no, the H atom is not an eigenstate of either $L_x$ or $L_y$.
- But we can always evaluate the expectation values…
What about the expectation values of $L_x$ and $L_y$?

For example, as an exercise you can show that this is true for the (2,1,1) state. See problem 7-21 in your book.
What does this mean?

- So, the vector $L$ is continuously precessing about the $z$-axis.
- The plane of electron’s orbit is perpendicular to $L$ and precesses with it.
- There is a fixed value of $L_z$ but $L_x$ and $L_y$ are not fixed and average to zero.
More things to note...

- **Uncertainty principle:**
  - If $L_x$, $L_y$, and $L_z$ were all fixed, the electron would be moving in a definite fixed plane.
  - But then its momentum component perpendicular to the plane would be infinitely uncertain
    - So not bound in the H atom

- Also, H atom Coulomb potential is spherically symmetric but if atom is placed in an external magnetic field $\mathbf{B}$, symmetry is destroyed and the direction of $\mathbf{B}$ is chosen to be the z-axis.
  - We will see this next week!
Is H atom an eigenstate of $L^2$?

* Again you should know the answer to this!

\[ L_{op}^2 = l_x^2 + l_y^2 + l_z^2 = l_x l_x + l_y l_y + l_z l_z \]
\[ = -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \]

\[ L_{op} \Psi = -\hbar^2 \left[ \frac{R \Phi}{\sin \theta} \frac{d}{d \theta} \left( \sin \theta \frac{d \Phi}{d \theta} \right) + \frac{R \Phi}{\sin^2 \theta} \frac{d^2 \Phi}{d \phi^2} \right] \]

But $\Phi = e^{i m \phi}$ \implies $\frac{d^2 \Phi}{d \phi^2} = -m^2 \Phi$

\[ L_{op} \Psi = -\hbar^2 R \Phi \left[ \frac{1}{\sin \theta} \frac{d}{d \theta} \left( \sin \theta \frac{d \Phi}{d \theta} \right) - \frac{m^2}{\sin^2 \theta} \Phi \right] \]
Recall when we did the separation of variables in an earlier lecture (chapter 6):

\[
\frac{1}{\sin \theta} \frac{d}{d \theta} (\sin \theta \frac{d \Theta}{d \theta}) + \left[ l(l+1) - \frac{m^2}{\sin^2 \theta} \right] \Theta = \lambda
\]

\[
\Rightarrow L^2 \Psi = -\hbar^2 R \Phi' [-l(l+1) \Theta] = + l(l+1) \hbar^2 R \Phi \Phi
\]

\[
\Rightarrow L^2 \Psi = l(l+1) \hbar^2 \Psi
\]

So, yes, H atom is eigenstate of \( L^2 \) with eigenvalue \( l(l+1) \hbar^2 \)

We derived this already in chapter 6 but we did this by using S.E. directly
Recall Angular Momentum Commutation Relations

The components of L do not commute with each other!

No simultaneous eigenstates!

If you measure \( L_x \) \( \Rightarrow \) get a certain value

Next, measure \( L_y \) \( \Rightarrow \) get a certain value

Measure \( L_x \) again \( \Rightarrow \) in general, you won’t get the same value as before!

So, once a measurement has been made, knowledge of the other two components is irretrievably lost.
Let’s evaluate commutator

$$[L^2, L_x]$$

\[
[L^2, L_x] = L^2 (L_x \psi) - L_x (L^2 \psi) \\
= (L_x^2 + L_y^2 + L_z^2)(L_x \psi) - L_x (L_x^2 + L_y^2 + L_z^2) \psi \\
= (L_y^2 + L_z^2)L_x \psi - L_x (L_y^2 + L_z^2) \psi \\
= (L_y L_x - L_x L_y) \psi + (L_z^2 L_x - L_x L_z^2) \psi \\
= [L_y, L_x] \psi + [L_z^2, L_x] \psi \\
[L^2, L_x] = [L_y, L_x] + [L_z^2, L_x]
\]
Above comes from Chapter 4:

\[
[Ly^2, L_x] = Ly[Ny, L_x] + [Ly, L_x] Ly
\]

\[
[L_y^2, L_x] = L_y[N_y, L_x] + [L_y, L_x] L_y
\]

\[
[L_y^2, L_x] = L_y(-ith L_y) + (-ith) L_y L_y
\]

\[
= -ith L_y L_y + ith L_y L_y
\]

\[
[L_y^2, L_x] = L_y(iith L_y) + (ith L_y) L_y
\]

\[
= ith L_y L_y + ith L_y L_y
\]

- Put it all together ....
We can show similarly that:

\[
[\hat{L}^2, \hat{L}_x] = -i\hbar \hat{L}_y \hat{L}_z - i\hbar \hat{L}_z \hat{L}_y + i\hbar \hat{L}_z \hat{L}_y + i\hbar \hat{L}_y \hat{L}_z = 0
\]

\[
[\hat{L}^2, \hat{L}_y] = 0
\]

\[
[\hat{L}^2, \hat{L}_z] = 0
\]

\[
\Rightarrow [\hat{L}^2, \hat{L}] = \emptyset
\]

- So, \( \hat{L}^2 \) commutes with each of \( \hat{L}_x \), \( \hat{L}_y \) and \( \hat{L}_z \)
- But none of these commute with each other!
- We can measure \( \hat{L}^2 \) and any one of \( \hat{L}_y \), \( \hat{L}_y \) and \( \hat{L}_z \) and get sharp eigenvalues and simultaneous eigenstates
Raising and lowering angular momentum operators

Let’s introduce:

\[ L_+ = L_x + i L_y \]
\[ L_- = L_x - i L_y \]
\[ L_z = L_x + i L_y \]

Like raising and lowering operators of Harmonic Oscillator (H.O.) from chapter 4:

Raised/lowered energy eigenvalue by \((\hbar \omega)\)
What do these operators raise and lower?

Let’s find out ...

\[
[L_3, l_\pm] = L_3 l_\pm - l_\pm L_3
\]

\[
= L_3 (l_x i l_y) - (l_x i l_y) L_3
\]

\[
= L_3 l_x i l_y l_3 - l_x L_3 i l_y l_3
\]

\[
[ L_3, l_x ] \rightarrow \pm i [ L_3, l_y ]
\]
\[
\begin{align*}
\left[ L_3, L_t \right] &= \frac{\left[ L_3, L_x \right] + i \left[ L_3, L_y \right]}{i \hbar L_y} \\
&= i \hbar L_y + i(\hbar) L_x \\
&= i \hbar L_y + \hbar L_x \\
\Rightarrow \quad \left[ L_3, L_t \right] &= \pm \hbar L_t \\
\Rightarrow \quad (L_3 L_t - L_t L_3) &= \pm \hbar L_t \\
\Rightarrow \quad L_3 L_t &= L_t (L_3 \pm \hbar)
\end{align*}
\]

Let’s operate on wavefunction ...
Operate this on wavefunction

\[ L_3(L \pm \Psi) = \Psi \frac{1}{\sqrt{2}} (L_3 \pm \hbar) \Psi \]

\[ \Psi = \psi_{\ell, m_\ell} \]

\[ L_3(L \pm \psi_{\ell, m_\ell}) = \psi \frac{1}{\sqrt{2}} (L_3 \pm \hbar) \psi_{\ell, m_\ell} \]

Recall: \[ L_3 \psi_{\ell, m_\ell} = m_\ell \hbar \psi_{\ell, m_\ell} \]

\[ \Rightarrow L_3(L \pm \psi_{\ell, m_\ell}) = \psi \frac{1}{\sqrt{2}} (m_\ell \hbar \psi_{\ell, m_\ell} \pm \hbar \psi_{\ell, m_\ell}) \]

\[ = \psi \left( \hbar (m_\ell \pm 1) \frac{1}{\sqrt{2}} \right) \frac{1}{\sqrt{2}} \psi_{\ell, m_\ell} \]
What does this mean?

- $L_\pm$ operates on wavefunction and yields new function ($L_\pm Y_{\ell m}$), whose z component of angular momentum is exactly $\hbar$ more/less than that possessed by $Y_{\ell m}$.

- $L_+ \text{ and } L_- \text{ raise or lower the state of the z component of angular momentum of } Y_{\ell m} \text{ by one unit in terms of } \hbar$.

- Similar to case of H.O.
What effect does $L_{\pm}$ operators have on the $\ell$ eigenvalue?

\[
\left[ L^2, L_{\pm} \right] = L^2 L_{\pm} - L_{\pm} L^2
\]
\[
= L^2 (L_x \pm i L_y) \mp (L_x \pm i L_y) L^2
\]
\[
= L^2 L_{\pm} \mp i L^2 L_y \pm i L_y L^2
\]
\[
= L_{\pm} L^2 \mp i L^2 L_y \pm i L_y L^2
\]

\[
[L^2, L_x] = 0 \quad \text{and} \quad i[L^2, L_y] = 0
\]

\[
\Rightarrow \left[ L^2, L_{\pm} \right] = 0
\]

\[
L^2 (L_{\pm} Y_{\ell,m_{\lambda}}) = L_{\pm} (L^2 Y_{\ell,m_{\lambda}})
\]

\[
L^2 \Psi = \ell (\ell + 1) \hbar^2 \Psi
\]

\[
\Rightarrow \quad L^2 (L_{\pm} Y_{\ell,m_{\lambda}}) = \ell (\ell + 1) \hbar^2 \left( L_{\pm} Y_{\ell,m_{\lambda}} \right)
\]

- When $L^2$ operates on wavefunction $(L_{\pm} Y_{\ell,m_{\lambda}})$ the result is the same (same eigenvalue) as when it operates on wavefunction $(Y_{\ell,m_{\lambda}})$ alone!

- It has no effect on $\ell$ eigenvalue of $Y_{\ell,m_{\lambda}}$
What wavefunction does $L_\pm$ return?

- Recall H.O.:

\[
\begin{align*}
A^+ \Psi_n &= i \sqrt{n+1} \Psi_{n+1} \\
A^- \Psi_n &= -i \sqrt{n} \Psi_{n-1} \\
A^+ \Psi_n &\neq \Psi_{n+1}
\end{align*}
\]

- Similarly,

\[
\begin{align*}
L^+ \gamma_{\ell m_\ell} &= \gamma_{\ell, m_{\ell+1}} \\
L^+ \gamma_{\ell m_\ell} &= K^\pm_{\ell m_\ell} \gamma_{\ell, m_{\ell+1}} \\
K^\pm_{\ell m_\ell} &= \hbar \sqrt{\ell (\ell+1) - m_\ell (m_\ell \pm 1)} = \hbar \sqrt{\ell + m_\ell (\ell \pm m_\ell + 1)}
\end{align*}
\]

There is a very nice proof in your book!
Summary/Announcements

- **Next time:**
  - The Stern-Gerlach Experiment
    - evidence for quantized angular momentum

- **Next homework due on Monday Nov 12.**

- **Reminder:** Quiz on next Wed Nov 14 on Chapter 6/7.