# PHY2005
# Atomic Physics

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# (5) Single-electron atoms: spin, total angular momentum and spectroscopic notation

*Learning goals*

1. To formally introduce the spin part of the wavefunction.
2. To appreciate that spin has many similarities to orbital angular momentum, and has analogous compatible observables.
3. To introduce the total angular momentum **J**.
4. To introduce spectroscopic notation as used in atomic physics.
5. To conclude discussion of one-electron atoms with relativistic results.

# Electron spin

Spin is a fundamental (observed) property of the electron

- E.g. the Stern Gerlach experiment

Not accounted for in the Schrödinger equation: needs to be considered as a separate part of the wavefunction:

$$\text{complete eigenfunction} = \psi(\mathbf{r}) \times \sigma(\mathbf{S})$$

**Space part**

**Spin part**

# Electron spin

"Coordinates" for electron spin are discreet:

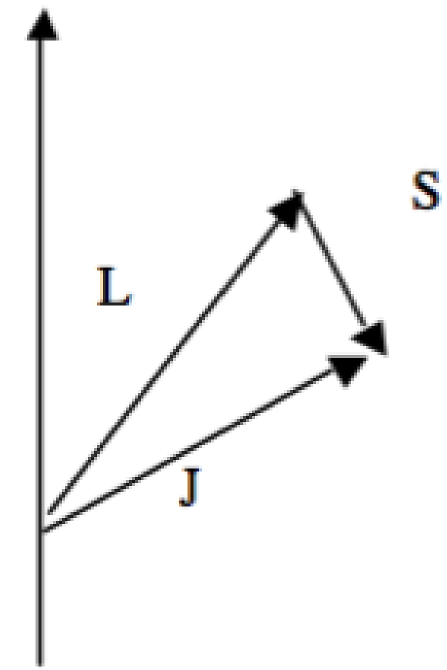
- Spin is an angular momentum vector
- For 1 electron, specified by two quantum numbers (magnitude and z-component):

| Physical quantity | Eigenvalue | Quantum number | Quantization |
|---|---|---|---|
| $\lvert \mathbf{S} \rvert$ | $\sqrt{s(s+1)}\hbar$ | $s$ | $s = \frac{1}{2}$ |
| $s_z$ | $m_s\hbar$ | $m_s$ | $m_s = -\frac{1}{2}$ or $\frac{1}{2}$ |

# Total angular momentum

Can sum orbital and spin parts

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$$




noting that this is a vector sum.

Result, ***J***, also an angular momentum: also described by two quantum numbers *j*, $m_j$

$$|\mathbf{J}| = \sqrt{j(j+1)}\hbar;$$

$$J_z = m_j\hbar$$

# Total angular momentum: allowed quantum numbers

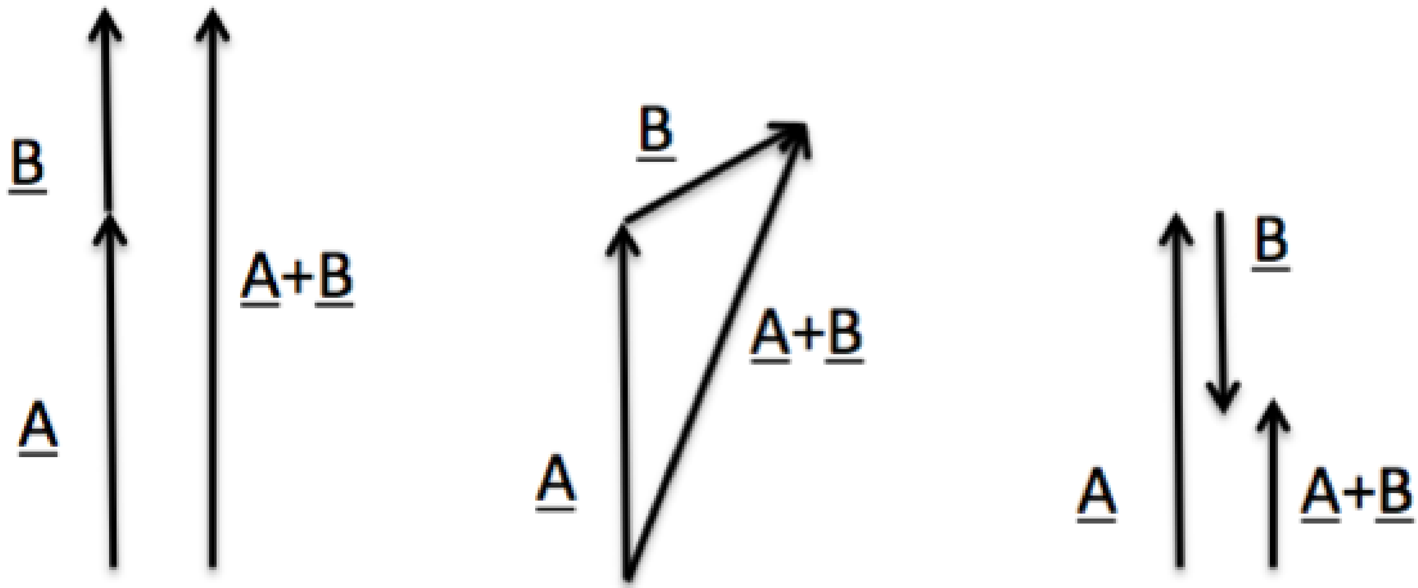
For single electron atom, allowed values are

$$\boxed{j = l + 1/2,\ l - 1/2}$$

and then

$$\boxed{m_j = -j, -j+1, ..., j-1, j}$$

# Reminder: vector addition



# Specifying states using J

For single electron atom, state fully specified by the quantum numbers in Table:

| Physical quantity | Eigenvalue | Quantum number | Quantization |
|---|---|---|---|
| $E$ | $-\frac{\mu Z^2 e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n^2}$ | $n$ | $n > 0$ |
| $\|\mathbf{L}\|$ | $\sqrt{l(l+1)}\hbar$ | $l$ | $0 \leq l < n$ |
| $\|\mathbf{S}\|$ | $\sqrt{s(s+1)}\hbar$ | $s$ | $s = \frac{1}{2}$ |
| $\|\mathbf{J}\|$ | $\sqrt{j(j+1)}\hbar$ | $j$ | $j = l \pm 1/2$ or $j = 1/2$ for $l = 0$ |
| $J_z$ | $m_j\hbar$ | $m_j$ | $-j, -j+1, ..., j-1, j$ |

# Spectroscopic notation: terms

Conventional to use standard notation to specify the angular momentum quantum numbers:

Single-electron: $\boxed{{}^{2s+1}l_j}$

*l* identified by "spectroscopic" letter:

| | | |
|---|---|---|
| 0 | S | sharp |
| 1 | P | principal |
| 2 | D | diffuse |
| 3 | F | fundamental |
| 4 | G | alphabetical |
| 5 | H | |

# Spectroscopic notation: terms

For single-electron atom, only additional information needed is *n*

Often written before term as an integer…e.g.:

$$1\,{}^{2}\mathrm{S}_{1/2}$$

Identifies the ground state of hydrogen atom

$$2\,{}^{2}\mathrm{S}_{1/2}\;,\;\; 2\,{}^{2}\mathrm{P}_{1/2}\;\text{ and }\; 2\,{}^{2}\mathrm{P}_{3/2}$$

are the sub-states of first excited energy level.

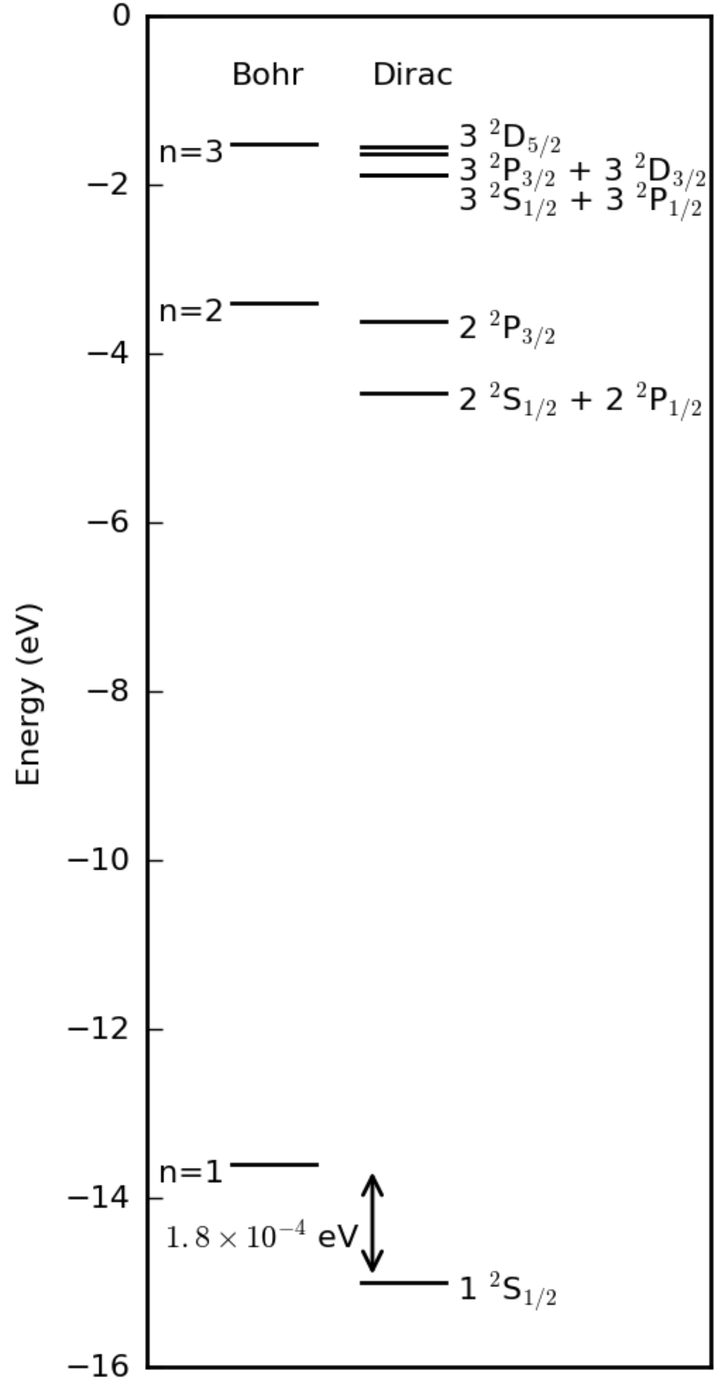
# Hydrogen atom: Dirac theory

Dirac’s theory of relativistic quantum mechanics predicts energy levels of the hydrogen atom:

$$E = -\frac{\mu e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n^2}\left[1 + \frac{\alpha^2}{n}\left(\frac{1}{j+1/2} - \frac{3}{4n}\right)\right]$$

where

$$\alpha = e^2/4\pi\epsilon_0\hbar c \approx 1/137$$



Energy (eV)
0
−2
−4
−6
−8
−10
−12
−14
−16
Bohr
Dirac
n=3
n=2
n=1
$3\ ^2D_{5/2}$
$3\ ^2P_{3/2} + 3\ ^2D_{3/2}$
$3\ ^2S_{1/2} + 3\ ^2P_{1/2}$
$2\ ^2P_{3/2}$
$2\ ^2S_{1/2} + 2\ ^2P_{1/2}$
$1.8 \times 10^{-4}$ eV
$1\ ^2S_{1/2}$

# Summary/Revision

- Spin ($\mathbf{S}$) must be included in the theory atomic physics. It behaves just like an angular momentum vector in quantum mechanics.
- The spin properties of a single electron are specified by two quantum numbers: $s$ and $m_s$ .
- $s$ specifies the magnitude of the spin: $|\mathbf{S}| = \sqrt{s(s+1)}\hbar$; for a single electron $s = 1/2$.
- $m_s$ gives the $z$-component of the spin: $S_z = m_s\hbar$. For a single electron, $m_s = -1/2$ or $+1/2$.
- The total angular momentum, $\mathbf{J} = \mathbf{L} + \mathbf{S}$ is widely used in identifying states.
- $\mathbf{J}$ is also defined by two quantum numbers, $j$ and $m_j$. These specify the magnitude $|\mathbf{J}| = \sqrt{j(j+1)}\hbar$ and $z$-component $J_z = m_j\hbar$.
- For a single-electron atom, the allowed values of $j$ are $l - 1/2$ and $l + 1/2$.
- For given $j$, allowed values of $m_j$ form a sequence:

$$m_j = -j, -j+1, ..., j-1, j$$

- For the simple one-electron Hamiltonian we considered in Section 4, the energy of a state is independent of $l$, $s$, $j$ and $m_j$. However, in Dirac theory, the energy levels are shifted and split by their $j$ values. These effects are small ($\sim 10^{-4}$eV) but accurately match observed fine structure in hydrogen lines.
- In spectroscopic notation, the quantum numbers for orbital, spin and total angular momenta of a complete atom are indicated by the *term*.