E. Spin-orbit Interaction

- Physics: Electron's motion (hence related to $\vec{L}$) leads to an internal magnetic field acting on the electron's own spin magnetic moment (hence related to $\vec{S}$)

  [Important to note: No externally applied magnetic field is needed!]

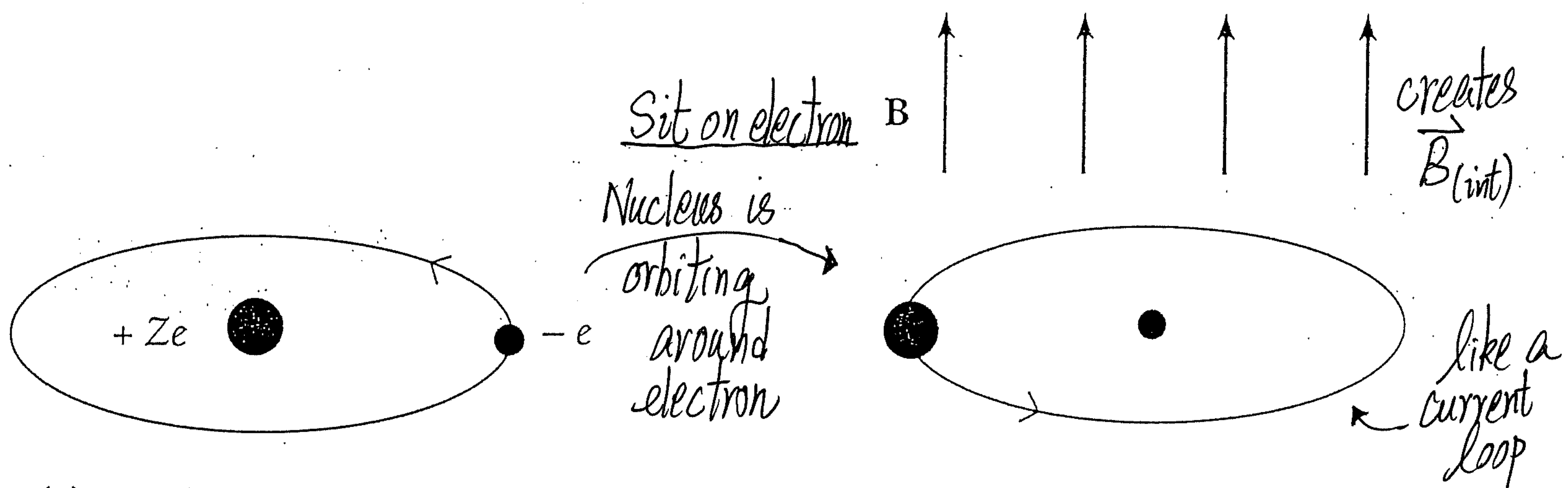
- Consequences:
  - an interaction energy $\sim -\vec{\mu}_s \cdot \vec{B}_{int} \sim \underbrace{\vec{S} \cdot \vec{L}}_{\text{"spin-orbit interaction"}}$

  - Help understand

    2p states ($\ell = 1$) Not — — — But $j = 3/2$, $j = 1/2$ $\boxed{\text{Fine structure}}$

    (No applied field)

Rough Picture of an Orbiting electron creating a $\vec{B}_{int}$ acting on itself



(*a*) An electron circles an atomic nucleus, as viewed from the frame of reference of the nucleus. (*b*) From the electron's frame of reference, the nucleus is circling it. The magnetic field the electron experiences as a result is directed upward from the plane of the orbit. The interaction between the electron's spin magnetic moment and this magnetic field leads to the phenomenon of spin-orbit coupling.

$$\vec{B} \propto \vec{L}$$

What we have been calling $\vec{B}_{int}$

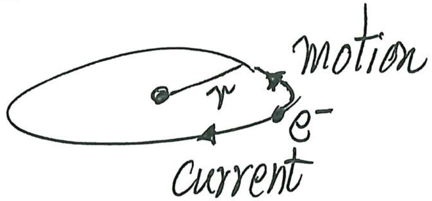
- But electron has $\vec{\mu}_s = \frac{-e}{m_e}\vec{S}$
- $\vec{\mu}_s$ and $\vec{B}$ interact to give an interaction energy $\propto \vec{S}\cdot\vec{L}$

Key Points up to here (Big Picture)

- No external applied B-field
- It is electron's $\vec{L}$ interacting with electron's $\vec{S}$
- $\vec{L}$ gives a $\vec{B}_{int}$; $\vec{S}$ gives $\vec{\mu}_s$
- Interacting energy $\sim -\vec{\mu}_s \cdot \vec{B}_{int} \propto \underbrace{\vec{S}\cdot\vec{L}}_{\text{spin-orbit interaction}}$
- This $\vec{S}\cdot\vec{L}$ term should be added to $\hat{H}_{atom}$ for accurate treatment of an atom, i.e. $\hat{H} = \hat{H}_{atom} + \underbrace{\hat{H}'_{SO}}_{\propto \vec{S}\cdot\vec{L}}$

The (internal) $\vec{B}$-field is NOT small

An estimation: (atom with 1 electron)



Field at center of current loop $|B| = \dfrac{\mu_0 i}{2r}$ (Biot-Savart Law) [EM Theory]

But $i = \dfrac{(-e)\,v}{2\pi r}$ [current is charge passing through a point per unit time]

$$= \frac{-e\,(\overbrace{r\, m_e v}^{|\vec{L}|})}{2\pi r^2 m_e} = \frac{-e}{2\pi m_e r^2}\,|\vec{L}|$$

[c.f. $|B|$ on Earth: $\sim 2.5\times10^{-5}$ Tesla]

$$\therefore\ |B| = \frac{\mu_0 e}{4\pi m_e}\,\frac{1}{r^3}\,|\vec{L}|$$

internal field is NOT small! $\underbrace{\text{(and it is free!)}}$

E.g. H-atom 2p $(n=2,\ l=1)$ thus $\underbrace{R_{21}(r)}\,Y_{1m_l}(\theta,\phi)$ (m_l: 1, 0, −1)

calculate[†] $\left\langle \dfrac{1}{r^3}\right\rangle$ and $|\vec{L}| = \sqrt{1(1+1)}\,\hbar = \sqrt{2}\,\hbar \Rightarrow |B| \sim 0.74$ Tesla

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† For H-atom, $\left\langle \frac{1}{r}\right\rangle$, $\left\langle \frac{1}{r^2}\right\rangle$, $\left\langle \frac{1}{r^3}\right\rangle$ can be evaluated analytically. Results are listed in books.

Hydrogen atom $(Z=1)$ and Hydrogen-like ions (Optional)

Values of $\langle r^k \rangle_{n\,l\,m_l} = \langle n\,l\,m_l \mid r^k \mid n\,l\,m_l \rangle$ for a Hydrogen-like Atom or Ion with Nuclear Charge Z for $k = 2, 1, -1, -2,$ and -3

$$\langle r^2 \rangle_{n\,l\,m_l} = \langle n\,l\,m_l \mid r^2 \mid n\,l\,m_l \rangle = \frac{a_0^2 n^4}{Z^2}\left\{1 + \frac{3}{2}\left[1 - \frac{l(l+1) - \frac{1}{3}}{n^2}\right]\right\}$$

$$\langle r \rangle_{n\,l\,m_l} = \langle n\,l\,m_l \mid r \mid n\,l\,m_l \rangle = \frac{a_0 n^2}{Z}\left\{1 + \frac{1}{2}\left[1 - \frac{l(l+1)}{n^2}\right]\right\}$$

$$\left\langle \frac{1}{r} \right\rangle_{n\,l\,m_l} = \left\langle n\,l\,m_l \left| \frac{1}{r} \right| n\,l\,m_l \right\rangle = \frac{Z}{a_0 n^2}$$

$$\left\langle \frac{1}{r^2} \right\rangle_{n\,l\,m_l} = \left\langle n\,l\,m_l \left| \frac{1}{r^2} \right| n\,l\,m_l \right\rangle = \frac{Z^2}{a_0^2 n^3 (l + \frac{1}{2})}$$

$$\left\langle \frac{1}{r^3} \right\rangle_{n\,l\,m_l} = \left\langle n\,l\,m_l \left| \frac{1}{r^3} \right| n\,l\,m_l \right\rangle = \frac{Z^3}{a_0^3 n^3 l (l + \frac{1}{2})(l+1)}$$

Source: Pauling, L., Wilson, E. B. *Introduction to Quantum Chemistry*. McGraw-Hill: New York, 1935.

e.g. $$\left\langle \frac{1}{r} \right\rangle_{n l m_l} = \int_0^\infty dr\, r^2 \left(\frac{1}{r}\right) \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi\, \psi^*_{n l m_l}(r,\theta,\phi)\, \psi_{n l m_l}(r,\theta,\phi)$$

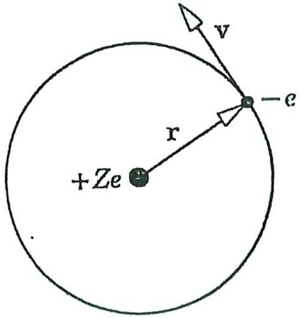
[Table taken from "Quantum Chemistry" by D. McQuarrie]

General Expression for Spin-Orbit Interaction: A partial derivation

- Why bother? Spin-orbit interaction is a hot topic in recent years in condensed matter physics (e.g. topological insulators) and in atomic physics (e.g. cold atoms)
- Why only a partial derivation?

  Formal derivation should start with relativistic QM (Dirac Equation) for which spin is part of the theory
- To get a sense on the physics behind the spin-orbit interaction energy term that should be included into the Hamiltonian

Consider one-electron atom for simplicity



- Electron is in motion $\left(\underbrace{m\vec{v} = \vec{p} = \text{momentum}}_{\vec{r}\times\vec{p} = \vec{L}}\right)$

- Electron is under the influence of the nucleus through an electric field

$$\vec{E} = \frac{Ze}{4\pi\varepsilon_0 r^2}\,\hat{r} \quad \text{(radially outward from +ve nucleus)}$$

potential energy

$$\vec{F} = \text{force on electron} = -e\vec{E} = -\vec{\nabla} V(\vec{r}) \quad \text{(true for conservative forces)}$$

$$= -\frac{dV(r)}{dr}\,\hat{r}$$

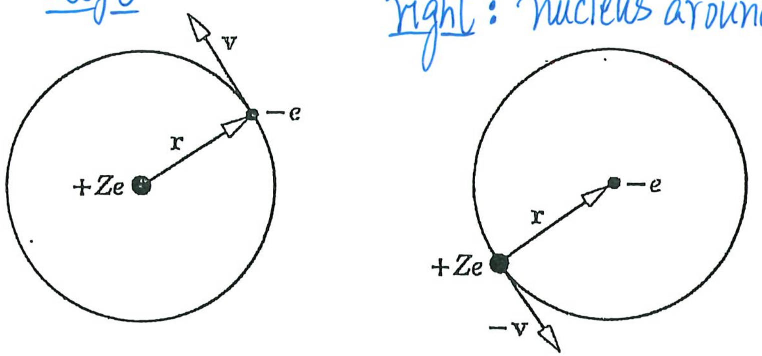
(true for central forces $\vec{E} \propto \hat{r}$, as $V(\vec{r}) = V(r)$ spherically symmetric)

$$= -\frac{dV(r)}{dr}\,\frac{\vec{r}}{r}$$

Questions: How do all these give $\vec{B}_{int}$ at the position of the electron?

How does $\vec{B}_{int}$ relate to $\vec{p}, \vec{L}, \vec{E}, -\vec{\nabla}V$?

left — right: nucleus around electron



Left: An electron moves in a circular Bohr orbit, the motion as seen by the nucleus. *Right:* The same motion, but as seen by the electron. From the point of view of the electron, the nucleus moves around it. The magnetic field **B** experienced by the electron is in the direction out of the page at the electron's location.

Note vectors in figures

$\vec{v}$ (left) thus $-\vec{v}$ (see right side)

$\vec{r}$ (left) $\vec{r}$ (right) (same magnitude, same direction)

Viewpoint of nucleus around electron: $\vec{J}$ = current density $= (+Ze)(-\vec{v}) = -Ze\vec{v}$

$$\vec{B} = \text{magnetic field at position of electron} = \frac{\mu_0}{4\pi}\frac{\vec{J}\times\vec{r}}{r^3} = -\frac{\mu_0}{4\pi}Ze\frac{\vec{v}\times\vec{r}}{r^3} = \frac{\mu_0}{4\pi}\frac{Ze}{r^3}\underbrace{\vec{r}\times\vec{v}}_{\vec{r}\times\frac{\vec{p}}{m} = \frac{1}{m}\vec{L} \;\propto \vec{L}}$$

this is $\vec{B}_{int}$

Biot-Savart Law [ignoring retardation] (Griffiths Ch.5)

$$\vec{B} = \frac{\mu_0}{4\pi}\frac{Ze}{r^3}\vec{r}\times\vec{V} = \mu_0\varepsilon_0 \frac{Ze}{4\pi\varepsilon_0}\frac{\vec{r}}{r^3}\times\vec{V} = \frac{1}{c^2}\vec{E}\times\vec{V} \qquad (14)$$

now back to what electron feels due to nucleus

Read/Recap Physics from Equation

$$\underbrace{\vec{B}}_{③} = \frac{1}{c^2}\underbrace{\vec{E}}_{②}\times\underbrace{\vec{V}}_{①} \qquad (14)$$

③ a magnetic field acting on the electron itself

① electron's motion in...

② electric field $\vec{E}$ due to the nucleus gives...

Read ①, ②, ③

Further explicit forms

$$(14)\quad \vec{B} = \frac{1}{c^2}\frac{(-e\vec{E})}{(-e)} \times \vec{v} = \frac{1}{emc^2}\,\overbrace{\vec{\nabla}V}^{\text{gradient of potential energy (due to nucleus' field)}} \times \underbrace{(m\vec{v})}_{\text{electron's linear momentum } \vec{p}}$$

$$= \frac{1}{emc^2}\vec{\nabla}V \times \vec{p} \qquad \text{(important in solid state physics)}$$

$$= \frac{1}{emc^2}\frac{dV(r)}{dr}\frac{\vec{r}}{r} \times \vec{p} \qquad (\vec{r} \times \vec{p} = \vec{L})$$

$$= \underbrace{\frac{1}{emc^2}\frac{1}{r}\frac{dV(r)}{dr}}_{\text{determines strength}}\vec{L} \qquad \text{(important in atomic physics)}$$

- The electron has $\vec{\mu}_s = \frac{-e}{m}\vec{S}$ due to its spin AM
  - $\vec{\mu}_s$ interacts with $\vec{B}$ as $-\vec{\mu}_s \cdot \vec{B}$ (interaction energy)
  - $$H' = -\vec{\mu}_s \cdot \vec{B} = \underbrace{\frac{1}{m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}}_{\text{strength } \underbrace{f(r)}_{\text{function of } r}} \underbrace{\vec{S}\cdot\vec{L}}_{\text{spin-orbit interaction}}$$

- Final expression:

$$\boxed{H'_{SO} = \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\,\vec{S}\cdot\vec{L}} \qquad (15) \qquad \text{[Key Result]}$$

(Done! Almost!)

for spin-orbit interaction

- a factor of ½ is not accounted for in our discussion
- it is related to the fact that we are transforming between accelerating frames
- Optional: See Eisberg and Resnick "Quantum Physics" (an appendix on Thomas Precession) for details

Alternative Forms

$$H'_{SO} = \frac{1}{2m^2c^2}\,\vec{S}\cdot(\vec{\nabla}V \times \vec{p})$$ [only needs[+] $V(\vec{r})$ and $\vec{\nabla}V$]

$$= \frac{\hbar}{4m^2c^2}\,\vec{\sigma}\cdot(\vec{\nabla}V \times \vec{p})$$ [used $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$] Pauli matrices as components

$$= \frac{\hbar}{4m^2c^2}\,(\vec{\sigma} \times \vec{\nabla}V)\cdot\vec{p} \qquad (16)$$

Forms often used in solid state physics

- Emphasizing that it is $\vec{\nabla}V(\vec{r})$ (gradient of potential energy function that leads to a force on the electron but its source is not crucial) and $\vec{p}$ (electron's motion) and their cross product $(\vec{\nabla}V \times \vec{p})$ that are important!

+ Does not need $V(\vec{r})$ to be spherical symmetrical

Let the formula talk...

$$H'_{so} = \underbrace{\frac{\hbar}{4m^2c^2}\vec{\sigma}\cdot\left(\vec{\nabla}V \times \vec{p}\right)}_{} \qquad (16)$$

① when an electron moves...

②... perpendicularly to a gradient of a potential energy landscape,

③ there is a (an effective) magnetic field that interacts with the electron's spin

$\vec{p}$: electron's momentum (so "moves")

$\vec{\sigma}$: Pauli spin matrix $\vec{\sigma} = \sigma_x \hat{x} + \sigma_y \hat{y} + \sigma_z \hat{z}$ (electron's spin)

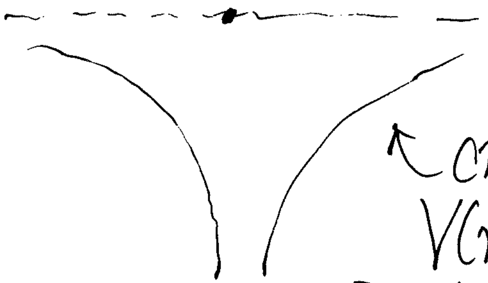
Pauli matrices

$$H'_{SO} = \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\,\vec{S}\cdot\vec{L} \quad (15) \quad \text{OR} \quad H'_{SO} = \frac{\hbar}{4m^2c^2}\,\vec{\sigma}\cdot(\vec{\nabla}V \times \vec{p}) \quad (16)$$

- Indicates a "cheap way" of getting a $\vec{B}$-field <u>without buying a magnet</u>
- Some sources
  - atom : Nucleus
  - Solid : array of atoms/nuclei

  $\Big\}$ creates $V(\vec{r})$ landscape for an electron to move on

<u>Atom</u>

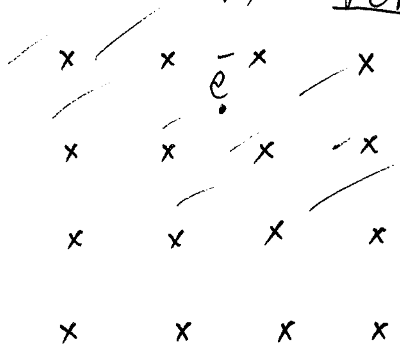


creates $V(r)$ [central force]

$V(r)$ is spherically symmetric (approximately)

<u>Solid</u>

$V(\vec{r})$ is <u>Periodic</u>



array of nuclei (creates $V(\vec{r})$)

$$\boxed{\sim (\vec{\nabla}V \times \vec{p}) \text{ is a field and acts on } \vec{\sigma}}$$

- In general, heavy atoms[+] give stronger spin-orbit interaction
- Recent years see new solid state systems in which the field so generated could lead to quantum effects (Hall effects) previously observed under a strong external magnetic field (look up "topological insulators").
- Besides electron, protons and neutrons are spin-half particles and carry intrinsic magnetic moments. Thus, for proton/neutron in a nucleus (other neutrons/protons create $V(\vec{r})$ via nuclear force so as to confine them), spin-orbit interaction also applies to determine the "magic numbers" observed in stable nuclei. (Nuclear Physics)

[+] Meaning: Hydrogen atom is not the perfect system to illustrate the effects!