Lecture 3

Relativistic Hamiltonian of a particle moving in EM field:

$$\hat{H} = \frac{1}{2m_e}\left(\vec{p} - \frac{e}{c}\vec{A}(\vec{x},t)\right)^2 - \underbrace{\frac{e\hbar}{2m_e c}\,\vec{\sigma}\cdot\vec{\nabla}\times\vec{A} + e\varphi}_{\text{Interaction with the field}}$$

$$\underbrace{-\frac{\vec{p}^{\,4}}{8m_e^3c^2}}_{\text{Relativistic mass correction}} \underbrace{+\frac{e\hbar^2}{8m_e^2c^2}\vec{\nabla}^2\varphi}_{\text{Darwin term}} \underbrace{-\frac{e\hbar}{4m_e^2c^2}\,\vec{\sigma}\cdot\vec{\nabla}\varphi\times\vec{p}}_{\text{Spin-orbit interaction.}}$$

Zeeman effect: splitting of lines in a uniform magnetic field.

$\vec{B} = \vec{\nabla}\times\vec{A}$ If $\vec{B}(\vec{x},t) = \text{const}$, than $\vec{A}(\vec{x}) = -\frac{1}{2}\vec{B}\times\vec{r}$

(Because of Stoke's theorem: circulation of vector field $\vec{A}$ in closed surface is equivalent to the flux of its curl through this surface).

$$\int_l d\vec{l}\cdot\vec{A}(\vec{x}) = \iint_S d\vec{S}\cdot(\vec{\nabla}\times A) \quad \left(= \iint_S d\vec{S}\cdot\vec{B}\right)$$

if $\vec{B} \neq \phi(\vec{x}) \Rightarrow \iint_S d\vec{S}\cdot\vec{B} = B\cdot\iint_S d\vec{S} =$

$$= B\cdot\int_l \frac{1}{2}d\vec{l}\times\vec{r} = \frac{1}{2}\int_l d\vec{l}\cdot(\vec{r}\times\vec{B}),$$

so $\vec{A} = \frac{1}{2}\vec{r}\times\vec{B}$

Let us choose $\vec{B} = B\vec{z}$, than

$$\vec{A} = -\frac{1}{2}\left(|B|y\,\vec{x} - |B|x\,\vec{y}\right). \quad (1)$$

The Hamiltonian $H = \frac{1}{2m_e}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 \underbrace{- \frac{e\hbar}{2m_e c}\vec{\sigma}\cdot\vec{\nabla}\times\vec{A} + e\varphi}$ =

$$= \frac{\vec{p}^{\,2}}{2m_e} - \frac{e}{2m_e c}\left(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right) + \frac{e^2}{c^2 2m_e}\vec{A}^{\,2} + \text{—''—}$$

$\vec{p}\cdot\vec{A} = \vec{\nabla}\cdot\vec{A} = 0$ for vector field (1), and

$$\vec{A}\cdot p = |B|\left(-\frac{1}{2}yp_x + \frac{1}{2}xp_y\right) = \frac{1}{2}|B|\hat{L}_z$$

and $\vec A^2 = \frac{1}{4}|B|^2(x^2+y^2)$,

we finally obtain

$\frac{\vec\sigma}{2} = \vec S$, and $\vec\nabla\times\vec A = \vec B$, so $\frac{1}{2}\vec S\cdot\vec B = \frac{1}{2}S_z|B|$ for (1)

$$\hat H_{Zeeman} = \frac{\vec p^{\,2}}{2m_e} - \frac{e}{2m_e c}|B|\hat L_z + \frac{e\hbar}{2m_e c}\vec\sigma\,\vec\nabla\times\vec A + \frac{e^2}{8m_e c^2}|B|^2(x^2+y^2) + e\Phi =$$

$$\boxed{= \frac{\vec p^{\,2}}{2m_e} - \underbrace{\frac{e}{2m_e c}|B|(\hat L_z + 2S_z)}_{\substack{\text{most interesting term,}\\ \text{levels will move depending}\\ \text{on } \hat L_z \text{ and } \hat S_z.}} + \underbrace{\frac{e^2}{8m_e c^2}|B|^2(x^2+y^2)}_{\substack{\text{shift of all levels}\\ \text{with constant factor}}} + \underbrace{e\Phi}_{\substack{\text{coulomb}\\ \text{potential}}}}$$

The $\hat H_{Zeeman}$ contains $\hat L_z$ and $\hat S_z$ operator, which do not commute with $\hat H_{Spin\text{-}Orbit}$, so we should consider these two effects together.

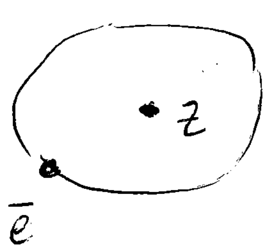
Depending on ratio between $\hat H_z$ and $\hat H_{SO}$ we can distinguish weak ZE and strong ZE.

if $B_{SO} \gg B$ – weak ZE

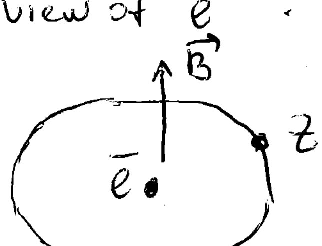
$B_{SO} \ll B$ – strong ZE,

$B_{SO} \approx B$ – intermediate case, no analytic solution.

Another point of view on SO-interaction:



, But from the point of view of $\bar e$: the nuclei orbiting the electron creates magnetic field,



so H_{SO} has some internal magnetic field $\vec B_{SO}$

1) Weak Zeeman effect

$$\hat{H} = \underbrace{\hat{H}_{S} + \hat{H}_{\substack{fine\\struct}}}_{H_0} + \hat{H}_{Zeeman}$$

We know the solutions of $H_0 |n l j m_j\rangle = E^0(n,j)\, |n l j m_j\rangle$

We are interested to find $\langle n l j m_j | \hat{H}_{Zeeman} | n l' j m_j' \rangle$.

$\hat{H}_z \sim L_z + 2S_z$, we know that $[\hat{L}^2, \hat{H}_z] = 0$, so for $l \neq l'$ matrix elements vanishes

and $[\hat{J}_z, \hat{H}_z] = 0$ and thus for $m_j \neq m_j'$ we also have zero matrix el.

We need to consider only the case when $l = l'$, and $m_j = m_j'$, the diagonal.

$$E^{(1)}(n,l,j,m_j) = \frac{eB}{2mc} \langle n l j m_j | \hat{L}_z + 2\hat{S}_z | n l j m_j \rangle$$

$$\hat{L}_z + 2\hat{S}_z = \hat{J}_z + S_z, \text{ so}$$

$$E^{(1)}(n,l,j,m_j) \sim \hbar m_j + \langle n l j m_j | \hat{S}_z | n l j m_j \rangle$$

$|n l j m_j\rangle$ can be understood as a linear combination of $|l,m\rangle \otimes |s,m_s\rangle$, so we can compute $\hat{S}_z |l,m\rangle \otimes |s,m_s\rangle$ explicitly. The coefficients in the sum are CG coefficients. Doing the required simplification we get

$$\langle S \rangle = \hbar m_j \frac{j(j+1) - l(l+1) + \frac{3}{4}}{2j(j+1)},$$ and finally

$$\langle \hat{L}_z + 2\hat{S}_z \rangle = \hbar m_j \left(1 + \frac{j(j+1) - l(l+1) + \frac{3}{4}}{2j(j+1)}\right) \sim \text{Lande g-factor.}$$

Strong field Zeeman effect.

$$\hat{H} = \underbrace{\hat{H}_{\mathcal{S}} + \hat{H}_{Zeeman}}_{H_0} + \hat{H}_{fs} ,$$ so we first solve

$$H_0 |n l m_\ell m_s\rangle = E^{(0)} |n l m_\ell m_s\rangle$$

because $[\hat{H}_{Zeeman}, \hat{H}_{\mathcal{S}}] = 0$

$$E^{(0)}(n, \ell, m_\ell, m_s) = E_{\mathcal{S}} + \frac{e\hbar}{2m_e c} B (m_\ell + 2m_s)$$

$\hat{H}_{fs} \sim \vec{L}\cdot\vec{S}$, then we get for both $\hat{H}_z$ and $\hat{H}_{fs}$:
(perturbation theory):

$$E_{z+fs} = E_z + \frac{m_e c^2 \alpha^4}{2n^3}\left\{\frac{3}{4n} - \left[\frac{\ell(\ell+1) - m_\ell m_s}{\ell(\ell+\frac{1}{2})(\ell+1)}\right]\right\}$$ Paschen-Back formula

---

Stark effect:

The electro-magnetic field

$$\vec{\mathcal{E}} = -\nabla\varphi - \frac{\partial}{\partial t}\vec{A}$$
$$\vec{B} = \vec{\nabla}\times A$$

The most general form of $\vec{A}(\vec{x},t) = \sum_{\omega,\vec{k}} A_0^{\omega,\vec{k}}(t)\, e^{\omega,\vec{k}} \exp\left[i(\vec{k}\cdot\vec{x} - \omega t + \varphi^{\omega,\vec{k}})\right]$
(plane wave expansion)

$e^{\omega,\vec{k}}$ – polarization vector

Using the expansion of $\exp(i\vec{k}\cdot\vec{x}) = \exp(i\vec{k}\cdot x_0)\exp(i\vec{k}\cdot(\vec{x}-\vec{x}_0)) =$

$$= \exp(i\vec{k}\cdot x_0)(1 + i\vec{k}\cdot\vec{x} + \dots)$$

We can write

$$\vec{A}(\vec{x},t) = A^{DA}(t) = \underbrace{\sum_{\omega,k} A_0^{\omega,k}(t)\, \vec{e}^{\,\omega,k} \exp(i(\vec{k}\cdot\vec{x}_0 - \omega t + \varphi))}_{\text{not a function of coordinates, so}}$$

not a function of coordinates, so $\vec{\nabla}\times A = 0$, no magnetic field.

Starting ~~with~~ from the Coulomb gauge:

$\nabla\cdot A' = 0$, $\varphi' = 0$,

we can use the gauge $\Lambda = -\vec{x}\cdot A^{DA}(t)$

$$\nabla\Lambda = -A^{DA}(t)$$

$$\boxed{\frac{\partial\Lambda}{\partial t} = -\vec{x}\cdot\frac{\partial A^{DA}}{\partial t}}$$, we can obtain $\varphi' = -x\cdot E(t)$ – dipole approx. for EM field.

Lamb shift:

Fluctuations at QED vacuum causes the fluctuations ~~of~~ the position of the electron.

The difference of PES is given by:

$$\Delta V = V(\vec{x} + \delta\vec{x}) - V(\vec{x}) = \delta\vec{x}\cdot\nabla V(\vec{x}) + \frac{1}{2}(\delta\vec{x}\cdot\nabla)^2 V(\vec{x}) + \dots$$

$\langle \delta\vec{x} \rangle_{vac} = 0$, so the fluctuations of vacuum ~~are~~ are isotropic.

but $\langle (\delta\vec{x}\cdot\vec{\nabla})^2 \rangle_{vac} = \frac{1}{3}\langle (\delta\vec{x})^2 \rangle_{vac} \nabla^2$

from QED we can obtain

$$\langle (\delta\vec{x})^2 \rangle_{vac} \cong \frac{1}{2\varepsilon_0 \pi^2}\left(\frac{e^2}{\hbar c}\right)\left(\frac{\hbar}{mc}\right)^2 \ln\frac{4\varepsilon_0 \hbar c}{e^2}$$

and $\langle \nabla^2 \underset{\substack{\uparrow \\ \text{coulomb pot.}}}{V(\vec{x})} \rangle = \frac{e^2}{\varepsilon_0}|\psi(0)|^2$

ε_0 – vacuum permittivity

So, combining $\frac{1}{3}\langle (\delta\vec{x})^2 \rangle_{vac} \langle \nabla^2 V(\vec{x}) \rangle = \alpha^5 mc^2 \frac{1}{6\pi} \ln\frac{1}{\pi\alpha}$

(for 2S orbital of hydrogen).