VII.5 The relativistic Hydrogen problem

(A) Stationary solutions of Dirac Eq. in a central potential

(563) $$\left[c\vec{\alpha}\cdot\vec{p}+\beta m_0c^2+V(r)\right]\phi = E\phi$$

where

(564) $$eA_0(r) = V(r) = -\frac{Ze}{r}$$

is a central potential. In nonrelativistic quantum mechanics angular momentum and spin are conserved quantities. How is this here?

Orbital angular momentum

(565) $$\boxed{\hat{\vec{L}} = -\hbar i\left(\vec{r}\times\vec{\nabla}\right)}$$

Spin

(566) $$\boxed{\hat{\vec{S}} = \frac{\hbar}{2}\begin{pmatrix}\hat{\vec{\sigma}} & 0\\ 0 & \hat{\vec{\sigma}}\end{pmatrix} = \frac{\hbar}{2}\gamma^5\vec{\alpha}}$$

$$\vec{\alpha} = \begin{pmatrix}0 & \hat{\vec{\sigma}}\\ \hat{\vec{\sigma}} & 0\end{pmatrix}$$

$$\gamma^5 = \begin{pmatrix}0 & \mathbb{1}\\ \mathbb{1} & 0\end{pmatrix}$$

One finds that neither $\hat{\vec{L}}$ nor $\hat{\vec{S}}$ is a conserved quantity

$$[L^i, H] = \hbar\left[-i\,\varepsilon_{ijk}\, r^j \partial_k , -i\alpha_e \partial_e\right]$$

(567)
$$= \hbar\,\varepsilon_{ijk}\,\delta_{ej}\,\partial_k \alpha_e = \hbar\,\varepsilon_{iek}\,\alpha_e \partial_k \neq 0$$

and

$$[S^i, H] = \frac{\hbar}{2}\left[\gamma^5 \alpha_i , -i\alpha_j \partial_j\right] = -\frac{i\hbar}{2}\gamma^5 [\alpha_i, \alpha_j]\,\partial_j$$

(568)
$$= -\hbar\,\varepsilon_{iek}\,\alpha_e \partial_k \neq 0$$

However the ~~total~~ spin

(569)
$$\boxed{\hat{J}^i = \hat{L}^i + \hat{S}^i} \qquad \hat{\vec{J}} = \begin{pmatrix} \hat{\vec{L}} + \frac{\hbar}{2}\vec{\sigma} & 0 \\ 0 & \hat{\vec{L}} + \frac{\hbar}{2}\vec{\sigma} \end{pmatrix}$$

is <u>conserved</u>. Furthermore

$$\hat{\vec{S}}^2 = \hat{S}^j \cdot \hat{S}^j = \frac{\hbar^2}{4}\begin{pmatrix} \vec{\sigma}\cdot\vec{\sigma} & 0 \\ 0 & \vec{\sigma}\cdot\vec{\sigma} \end{pmatrix}$$

(570)
$$\boxed{\hat{\vec{S}}^2 = \frac{3}{4}\hbar^2\, \mathbb{1}} \qquad \hat{=} \text{ spin } 1/2 \text{ particle}$$

One could think that $\hat{\vec{L}}^2$ is conserved, however as you will show in the problem course

(571)
$$\left[\hat{\vec{L}}^2, H\right] \neq 0$$

The eigenstate of H will still have a fixed quantum number ℓ since H has another symmetry which is parity

(572) $$\boxed{\hat{P} = \gamma^0 P_0}$$

where P_0 is the spatial parity operator, i.e.

Def: $$P_0 f(\vec{r}) = f(-\vec{r})$$

γ^0 operator in the space of Dirac spinors

Since $$\gamma^0 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}$$

it flips sign of the lower spinor. One finds

$$[\hat{P}, H] = [\gamma^0 P_0, -i\alpha_j \partial_j]$$

(573) $$= -i\left(\gamma^0 \underbrace{P_0 \alpha_j \partial_j}_{=-\alpha_j \partial_j P_0} - \alpha_j \partial_j \gamma^0 P_0\right)$$

$$= -i\left(-\underbrace{\gamma^0 \alpha_j \partial_j - \alpha_j \gamma^0 \partial_j}_{=0}\right) P_0 = \underline{\underline{0}}$$

stationary solution

(574) $$\psi(\vec{r}, t) = \begin{pmatrix} \varphi(\vec{r}) \\ \chi(\vec{r}) \end{pmatrix} e^{-iEt/\hbar}$$

with

$$P\,\varphi(\vec{r}) = \varphi(-\vec{r}) \qquad (575)$$
$$P\,\chi(\vec{r}) = -\chi(-\vec{r})$$

stationary DE

$$\boxed{\begin{aligned} c(\hat{\vec{\sigma}}\cdot\hat{\vec{p}})\chi + m_0c^2\varphi + V\varphi &= E\varphi \\ c(\hat{\vec{\sigma}}\cdot\hat{\vec{p}})\varphi - m_0c^2\chi + V\chi &= E\chi \end{aligned}} \qquad (576)$$

spherical spinors

One can show tha common set of spinor eigenfunctions of $\hat{\vec{J}}^2$, $\hat{J}_z$, $\hat{\vec{S}}^2$ and P_0 (which fixes ℓ) are

$$\boxed{j = \ell + \frac{1}{2}}$$

$$\boxed{\Omega_{j=\ell+\frac{1}{2},\ell,m} = \begin{pmatrix} \sqrt{\frac{j+m}{2j}}\, Y_{\ell,m-\frac{1}{2}}(\vartheta,\varphi) \\ \sqrt{\frac{j-m}{2j}}\, Y_{\ell,m+\frac{1}{2}}(\vartheta,\varphi) \end{pmatrix}} \qquad (577)$$

only spinor, i.e. 2 components!

and for

$$\boxed{j = \ell - \frac{1}{2}}$$

(578) $$\Omega_{j=\ell-\frac{1}{2},\ell,m} = \begin{pmatrix} -\sqrt{\frac{j-m+1}{2j+2}}\, Y_{\ell,m-\frac{1}{2}}(\vartheta,\varphi) \\ \sqrt{\frac{j+m+1}{2j+2}}\, Y_{\ell,m+\frac{1}{2}}(\vartheta,\varphi) \end{pmatrix}$$

one finds

(579) $$\boxed{P_0\, \Omega_{j\ell m} = (-1)^{\ell}\, \Omega_{j\ell m}}$$

Now we make the ansatz for the upper and lower spinors

(580) $$\begin{aligned} \varphi_{j\ell m} &= i\, g(r)\, \Omega_{j\ell m}(\vartheta,\varphi) \\ \chi_{j\ell' m} &= -f(r)\, \Omega_{j\ell' m}(\vartheta,\varphi) \end{aligned}$$

where $\ell' = \ell \pm 1$ (± 1 to have opposite parity of χ as compared to φ see eq. (575))

and $\ell, \ell' = j \pm \frac{1}{2}$

(581) $$\ell' = \begin{cases} \ell + 1 & \text{for } j = \ell + \frac{1}{2} \\ \ell - 1 & \text{for } j = \ell - \frac{1}{2} \end{cases}$$

What is the action of $(\vec{\sigma} \cdot \vec{p})\, \Omega_{j\ell m} = ?$

For this we first note

$$\vec{\sigma}\cdot\frac{\vec{r}}{r}\,\Omega_{jem} = -\Omega_{je'm} \qquad \text{with } \ell' \text{ from (587)} \tag{582}$$

Such that

$$-(\vec{\sigma}\cdot\hat{\vec{p}})\,\Omega_{jem} = (\vec{\sigma}\cdot\hat{\vec{p}})\left(\vec{\sigma}\cdot\frac{\vec{r}}{r}\right)\Omega_{je'm} \tag{583}$$

Making use of the identity

$$(\vec{\sigma}\cdot\vec{A})(\vec{\sigma}\cdot\vec{B}) = \vec{A}\cdot\vec{B} + i\vec{\sigma}\cdot(\vec{A}\times\vec{B}) \tag{584}$$

we find

$$-(\vec{\sigma}\cdot\hat{\vec{p}})\,\Omega_{jem} = \left(\hat{\vec{p}}\cdot\frac{\vec{r}}{r} + i\vec{\sigma}\cdot\left(\hat{\vec{p}}\times\frac{\vec{r}}{r}\right)\right)\Omega_{je'm}$$

$$= \Big[-i\hbar(\vec{\nabla}\cdot\vec{r}) - i\hbar\,\underbrace{\vec{r}\cdot\vec{\nabla}}_{=\frac{\partial}{\partial r}} - i\vec{\sigma}\cdot(\vec{r}\times\hat{\vec{p}})\Big]\frac{1}{r}\,\Omega_{je'm} \tag{585}$$

$$= -i\left(\frac{2\hbar}{r} + \frac{1}{r}\vec{\sigma}\cdot\vec{L}\right)\Omega_{je'm}$$

To evaluate the last expression we make use of the fact that $\Omega_{je'm}$ is an eigenfunction of $\hat{\vec{J}}^2$

$$\hat{\vec{J}}^2 = \left(\vec{L} + \frac{\hbar}{2}\vec{\sigma}\right)^2 = \vec{L}^2 + \underbrace{\left(\frac{\hbar}{2}\vec{\sigma}\right)^2}_{=\frac{3}{4}\hbar^2} + \hbar\vec{\sigma}\cdot\vec{L}$$

i.e.

$$\hbar\,\hat{\vec{J}}\cdot\hat{\vec{L}}\,\Omega_{jl'm} = \left(\hat{J}^2 - \hat{L}^2 - \frac{3}{4}\hbar^2\right)\Omega_{jl'm}$$

(586) $$= \left(j(j+1) - l'(l'+1) - \frac{3}{4}\right)\hbar^2\,\Omega_{jl'm}$$

$$= -(1+\kappa)\hbar^2\,\Omega_{jl'm}$$

where

(587) $$\kappa = \begin{cases} -(l+1) = -(j+\frac{1}{2}) & \text{for } j = l+\frac{1}{2} \\ l = +(j+\frac{1}{2}) & \text{for } j = l-\frac{1}{2} \end{cases}$$

Inserting these expressions into the stationary DE, eq. (576) finally gives differential equations for the spatial functions

(588) $$\begin{aligned} &\hbar c\,\frac{dg(r)}{dr} + (1+\kappa)\hbar c\,\frac{g(r)}{r} - \left[E + m_0c^2 - V(r)\right] f(r) = 0 \\ &\hbar c\,\frac{df(r)}{dr} + (1-\kappa)\hbar c\,\frac{f(r)}{r} + \left[E - m_0c^2 - V(r)\right] g(r) = 0 \end{aligned}$$

Substituting

(589) $$g(r) = \frac{G(r)}{r} \qquad f(r) = \frac{F(r)}{r}$$

yields

(590) $$\boxed{\begin{aligned} &\hbar c\,\frac{dG(r)}{dr} + \hbar c\,\frac{\kappa}{r}\,G(r) - \left[E + m_0c^2 - V(r)\right] F(r) = 0 \\ &\hbar c\,\frac{dF(r)}{dr} - \hbar c\,\frac{\kappa}{r}\,F(r) + \left[E - m_0c^2 - V(r)\right] G(r) = 0 \end{aligned}}$$

Solution of radial equation

$$V(r) = -\frac{Ze}{r}$$

To solve the radial equation we again make use of the Sommerfeld method

(i) asymptotic behavior for $r \to 0$

(591) $\Rightarrow \cdots \Rightarrow \quad G(r) = a r^{\gamma} \qquad F = b r^{\gamma}$

where $\gamma = (\pm)\sqrt{\left(j+\frac{1}{2}\right)^2 - Z^2\alpha^2} \qquad \alpha = \frac{e^2}{\hbar c}$

fine-structure constant

As in the case of the Klein-Gordon equation there is

$$Z_{max} = \left(j+\frac{1}{2}\right)\frac{1}{\alpha}$$

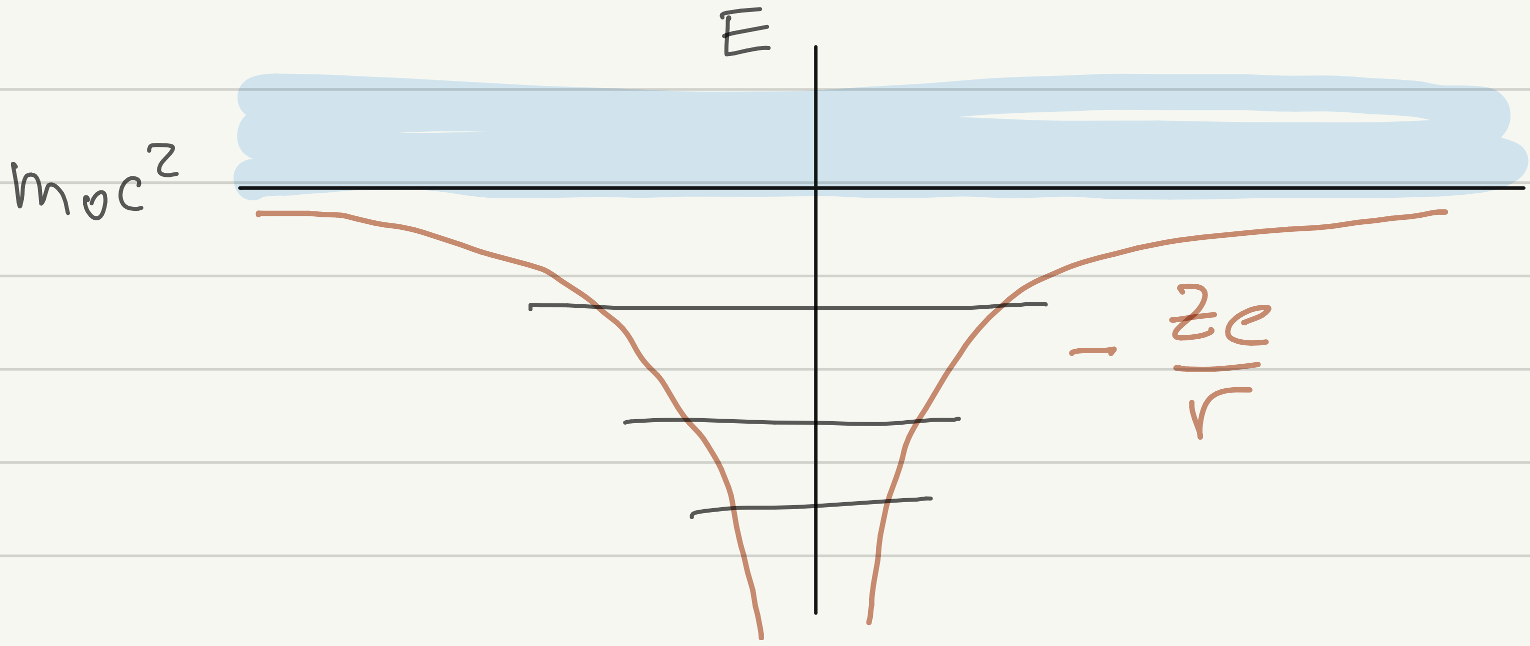
for which a state with total angular momentum $\hat{j}$ exists

(ii) asymptotic behaviour for $r \to \infty$

(592) $\Rightarrow \cdots \Rightarrow \quad G(r) \sim e^{-\rho/2} \qquad \rho = 2\lambda r$

$$\lambda = \frac{\left(m_0^2 c^4 - E^2\right)^{1/2}}{\hbar c}$$

Note that for a bound state $E < m_0 c^2$



(iii) general polynomial ansatz

$$G(\rho)=\sqrt{m_0c^2+E}\,e^{-\rho/2}\left(\phi_1(\rho)+\phi_2(\rho)\right)$$
$$F(\rho)=\sqrt{m_0c^2-E}\,e^{-\rho/2}\left(\phi_1(\rho)-\phi_2(\rho)\right) \tag{593}$$

and

$$\phi_1(\rho)=\rho^{\gamma}\sum_{m=0}^{\infty}\alpha_m\rho^m$$
$$\phi_2(\rho)=\rho^{\gamma}\sum_{m=0}^{\infty}\beta_m\rho^m \tag{594}$$

and we require that all coefficients α_m, β_m vanish identically above a certain index!

inserting (593) + (594) into (590) and sorting in terms of powers ρ^n gives a recursion relation for α_m, β_m

We require that the recursion stops at $m=n'$

Def: principle quantum number

(595) $$n = n' + |\kappa| = n' + j + \frac{1}{2} \qquad n = 1,2,3,\dots$$

$$j + \frac{1}{2} = 1,2,3 \quad \Rightarrow \text{eigenenergies}$$

$$\boxed{E_{nj} = m_0 c^2 \left[1 + \frac{(Z\alpha)^2}{\left(n - j - \frac{1}{2} + \left[(j+\frac{1}{2})^2 - (Z\alpha)^2\right]^{1/2}\right)^2} \right]^{-\frac{1}{2}}}$$

(596)

Sommerfeld finestructure equation

expanding E_{nj} into powers of $Z\alpha \mathrel{\hat{=}} \frac{Z}{?}$ yields

$$E_{nj} \simeq m_0 c^2 \left[1 - \frac{1}{2} \frac{Z^2 \alpha^2}{n^2} \left(1 + \frac{(Z\alpha)^2}{n^2} \left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4} \right) \right) + \dots \right]$$

(597)

↑ rest energy

↑ nonrelativist. hydrogen

ground state

(598) $$\boxed{E_{n=1, j=\frac{1}{2}} = m_0 c^2 \sqrt{1 - Z^2 \alpha^2}}$$

ground-state wavefunction

(599)
$$\phi_{n=1,j=\frac{1}{2},\uparrow}(r,\vartheta,\varphi) = A(r) \begin{bmatrix} 1 \\ 0 \\ \frac{i(1-\gamma)}{Z\alpha}\cos\vartheta \\ \frac{i(1-\gamma)}{Z\alpha}\sin\vartheta e^{i\varphi} \end{bmatrix}$$

(600)
$$\phi_{n=1,j=\frac{1}{2},\downarrow}(r,\vartheta,\varphi) = A(r) \begin{bmatrix} 0 \\ 1 \\ \frac{i(1-\gamma)}{Z\alpha}\sin\vartheta e^{-i\varphi} \\ -i\frac{(1-\gamma)}{Z\alpha}\cos\vartheta \end{bmatrix}$$

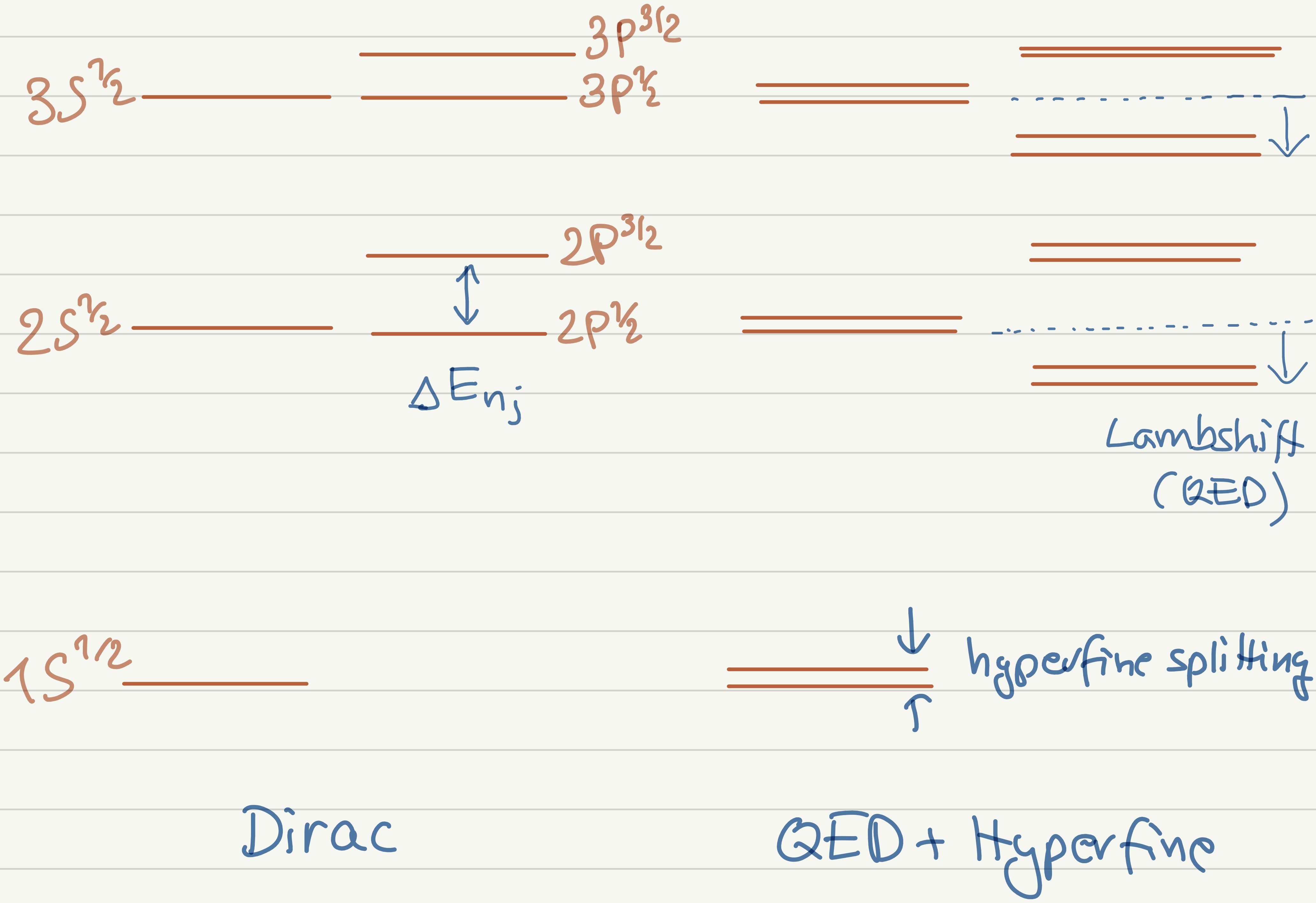
$\hbar = c = 1$

(601)
$$A(r) = \frac{(2m_0 Z\alpha)^{3/2}}{\sqrt{4\pi}}\left[\frac{1+\gamma}{2\Gamma(1+2\gamma)}\right]^{1/2}(2mZ\alpha r)^{\gamma-1} e^{-mZ\alpha r}$$

(602) with
$$\gamma = \sqrt{1 - Z^2\alpha^2}$$

fine structure splitting

$$\boxed{\Delta E_{nj} = -\frac{1}{2}\frac{(Z\alpha)^4 m_0 c^2}{n^4}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)} \tag{603}$$



(B) Approximation to the relativistic Hydrogen problem without mixing of positive and negative energies: Foldy-Wouthuysen transformation

- problem of the relativistic Hydrogen solution:

We recognize from eqs. (599) and (600) that the eigenbispinors of the Hydrogen problem have both positive and negative frequency components, where the contribution from negative frequencies scales as

$$\frac{1-\gamma}{Z\alpha} = \frac{1-\sqrt{1-Z^2\alpha^2}}{Z\alpha} \simeq \frac{1}{2} Z\alpha$$

This is because for highly charged nuclei the energies become comparable to m_0c^2; see eq. (598). This violates the single particle interpretation

$\Rightarrow$ Can we construct an approximate description that avoids the coupling of positive and negative frequencies?

$\Rightarrow$ Foldy-Wouthuysen approximation idea (sequence of) unitary transformations that (approximately) eliminates operators $\vec{\alpha}, \gamma_i, \gamma_5$ that couple upper and lower spinors!

ansatz

(604) $$\underline{\Phi} = \hat{U}\underline{\Psi} = e^{i\hat{S}}\underline{\Psi} \qquad \hat{S} = \hat{S}^{\dagger}$$

$$\hat{U}^{\dagger}\hat{U} = \underline{1}$$

equation of motion of $\underline{\Phi}$:

$$i\hbar\frac{\partial}{\partial t}\underline{\Phi} = -\hbar\frac{\partial\hat{S}}{\partial t}e^{i\hat{S}}\underline{\Psi} + e^{i\hat{S}}\hat{H}\underline{\Psi}$$

(605) $$= -\hbar\frac{\partial\hat{S}}{\partial t}\underline{\Phi} + e^{i\hat{S}}\hat{H}e^{-i\hat{S}}\underline{\Phi}$$

$$= \hat{H}_{\underline{\Phi}}\underline{\Phi}$$

$\Rightarrow$

(606) $$\boxed{H_{\underline{\Phi}} = e^{i\hat{S}}He^{-i\hat{S}} - \hbar\frac{\partial\hat{S}}{\partial t}}$$

- how to construct $\hat{S}$?

(i) free particle

we know $[\vec{p}, H] = 0 \rightarrow$ momentum representation
$\vec{p} \rightarrow \vec{p}$

$\Rightarrow$ ansatz

$$\hat{S} = -\frac{i}{2m_0c}\, \beta \vec{\alpha} \cdot \vec{p}\, f\left(\frac{p}{m_0c}\right) \tag{607}$$

f still needs to be found. Note that despite the i
$\hat{S}$ is hermitian as β and $\vec{\alpha}$ anti-commute.

The transformed Hamiltonian reads

$$H_\phi = e^{i\hat{S}} (c\vec{\alpha} \cdot \vec{p} + \beta m_0 c^2) e^{-i\hat{S}}$$

$$= e^{i\vec{S}} \beta \left(c\beta\vec{\alpha} \cdot \vec{p} + m_0c^2\right) e^{-i\vec{S}}$$

commute!

$$= \underbrace{e^{i\vec{S}} \beta e^{-i\hat{S}}}_{=\,?} \left(c\beta\vec{\alpha} \cdot \vec{p} + m_0c^2\right) \tag{608}$$

In the problem course you will show that

$$\beta e^{-i\hat{S}} = e^{i\hat{S}} \beta \tag{609}$$

i.e.

$$H_\phi = e^{2iS}\left(c\vec{\alpha} \cdot \vec{p} + \beta m_0 c^2\right) \tag{610}$$

Expanding e^{2iS} into a power series and using

$$(\beta\vec{\alpha}\cdot\vec{p})^2 = -\vec{p}^{\,2} \qquad y \equiv p/m_0c$$

yields: does not couple positive and negative frequencies

$$H\Phi = \beta\left[m_0c^2\cos(yf(y)) + cp\sin(yf(y))\right]$$

$$+\frac{\vec{\alpha}\cdot\vec{p}}{p}\underbrace{\left[pc\cos(yf(y)) - m_0c^2\sin(yf(y))\right]}_{\overset{!}{=}0 \quad \text{choose } f} \tag{611}$$

couples positive & negative frequencies

So choose

$$yf(y) \overset{!}{=} \arctan y \tag{612}$$

note in non-relativistic limit

$$f \approx 1 \tag{613}$$

then

$$H\Phi = \beta\left[m_0c^2\cos\left(\arctan\left(\frac{p}{m_0c}\right)\right) + cp\sin\left(\arctan\left(\frac{p}{m_0c}\right)\right)\right] \tag{614}$$

$$= \beta c\sqrt{p^2 + m_0c^2}$$

so

$$\boxed{H\Phi = \beta E_p \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}} \tag{615}$$

$E_p^2 = p^2 + m_0c^2$

decoupled!

(ii) electron/positron in external elm. field

Now there is no transformation that eliminates the coupling exactly

(6.16)
$$H = \beta m_0 c^2 + \underbrace{c\vec{\alpha}\cdot\left(\hat{\vec{p}} - \frac{e}{c}\vec{A}(\vec{r})\right)}_{\text{couples upper and lower spinors}} + eA_0(\vec{r})$$

ansatz

(6.17)
$$\hat{S} = -\frac{i}{2m_0 c}\,\beta\vec{\alpha}\cdot\left(\hat{\vec{p}} - \frac{e}{c}\vec{A}(\vec{r})\right) = -\frac{i}{2m_0c^2}\beta\hat{O}$$

i.e. $\hat{O} = c\vec{\alpha}\cdot\left(\hat{\vec{p}} - \frac{e}{c}\vec{A}(\vec{r})\right)$

remarks:
- Here $[\hat{\vec{p}}, H] \neq 0$ so no momentum representation
- Here no function $f\left(\frac{p}{m_0c}\right)$ as in case of free particle, but in non-relativistic limit $f=1$, so (6.17) will not remove the coupling but will do so in lowest order of relativistic corrections

$$\sim \frac{1}{m_0c^2}$$

so we define

$$H' = e^{i\hat{S}} H e^{-i\hat{S}} = H + i[S, H]$$

(618) $$-\frac{1}{2}[S,[S,H]] - \frac{i}{3!}[S,[S,[S,H]]] + \frac{1}{4!}[S,[S,[S,[S,H]]]] + \cdots$$

You will prove the last equation in the problem courses.

Up to terms $\left(\frac{1}{m_0c^2}\right)^3$ we find

$$H' = \beta\left(m_0c^2 + \frac{1}{m_0c^2}\hat{O}^2 - \frac{1}{8m_0^3c^6}\hat{O}^4\right) + eA_0$$

(619) $$- \frac{1}{8m_0^2c^4}[\hat{O},[\hat{O},eA_0]] + \frac{1}{2m_0c^2}\beta[\hat{O},eA_0] - \frac{1}{3m_0^2c^4}\hat{O}^3 - \frac{1}{48m_0^3c^6}\beta[\hat{O},[\hat{O},[\hat{O},eA_0]]]$$

- even powers of $\hat{O}$ do not couple upper and lower spinors ☺
- odd powers appear only $\sim \left(\frac{1}{m_0c^2}\right)^1$

One can now construct a succession of Foldy - Wouthuysen transformations to make the terms that couple upper and lower spinors (i.e. positive and negative frequencies) iteratively smaller!

2nd Foldy-Wouthuysen trafo

(620) $$\hat{S}' \equiv -\frac{i}{2m_0c^2}\beta\hat{O}' \qquad \hat{O}' = e^{i\hat{S}}\hat{O}e^{-i\hat{S}}$$

$\Rightarrow$ $\hat{H}''$ contains coupling terms $\sim \left(\frac{1}{m_0c^2}\right)^2$

3rd Foldy-Wouthuysen trafo

(621) $$\hat{S}'' \equiv -\frac{i}{2m_0c^2}\beta\hat{O}'' \qquad \hat{O}'' = e^{i\hat{S}'}\hat{O}'e^{-i\hat{S}''}$$

$\Rightarrow$ $\hat{H}'''$ contains coupling terms $\sim \left(\frac{1}{m_0c^2}\right)^3$

(622) $$\hat{H}''' = \beta\left(m_0c^2 + \frac{1}{2m_0c^2}\hat{O}^2 - \frac{1}{2m_0^3c^6}\hat{O}^4\right) + eA_0 - \frac{1}{8m_0^2c^4}\left[\hat{O},\left[\hat{O},eA_0\right]\right] + \mathcal{O}\left(\left(\frac{1}{m_0c^2}\right)^4\right)$$

explicit evaluation of $\hat{H}'''$ yields:

$$\boxed{\begin{aligned} H_{\Phi} = H''' = \beta\left[m_0c^2 + \frac{1}{2m_0}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 - \frac{1}{8m_0^3c^2}\vec{p}^{\,4}\right] \\ + eA_0 - \frac{1}{2m_0c}\beta e\hbar\,\vec{\Sigma}\cdot\vec{B} - \frac{ie\hbar^2c^2}{8m_0^2c^4}\vec{\Sigma}\cdot\mathrm{rot}\,\vec{E} \\ - \frac{e\hbar}{4m_0^2c^2}\vec{\Sigma}\cdot(\vec{E}\times\vec{p}) - \frac{e\hbar^2c^2}{8m_0^2c^4}\mathrm{div}\,\vec{E} \end{aligned}}$$

(623)

$$\beta = \begin{pmatrix} 1_2 & 0 \\ 0 & -1_2 \end{pmatrix} \qquad \vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$$

discussion of terms

- 1st term: series expansion of $\sqrt{m_0^2c^4 + c^2\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2}$
- 2nd term: electrostatic potential
- 3rd term: coupling of magnetic moment of spin to external magnetic field
- 4th term: for spherical symmetric electrostatic potentials $V(r) \curvearrowright \vec{E} = -\vec{e}_r\frac{\partial}{\partial r}V(r)$ and $\mathrm{rot}\,\vec{E} = 0$; so only relevant for non spherical problems

- 5th term: spin-orbit coupling

spherical potential $V(r)$

$$\vec{E} = -\vec{e}_r \frac{\partial}{\partial r} V(r)$$

$$\hat{\vec{\Sigma}} \cdot (\vec{E} \times \hat{\vec{p}}) = -\frac{1}{r}\frac{\partial V}{\partial r} \hat{\vec{\Sigma}} \cdot (\hat{\vec{r}} \times \hat{\vec{p}})$$

$$= -\frac{1}{r}\frac{\partial V}{\partial r} \hat{\vec{\Sigma}} \cdot \hat{\vec{L}}$$

(624) $$\boxed{H_{SO} = \frac{e\hbar}{4 m_0^2 c^2} \frac{1}{r}\frac{\partial V}{\partial r} \hat{\vec{\Sigma}} \cdot \hat{\vec{L}}}$$

- 6th term: Darwin term

contact interaction with the core

If the core is point-like $(Z=1)$

$$\operatorname{div} \vec{E} = -\Delta \phi = 4\pi e \delta(\vec{r})$$

(625) $$\boxed{H_{Darwin} = -\frac{4\pi e^2 \hbar^2}{8 m_0^2 c^2} \delta(\vec{r})}$$

(c) Hyperfinestructure

The Foldy-Wouthuysen Hamiltonian considers the atomic core (proton in case of Hydrogen) as a point particle with charge but without spin.

Simple extension: include spin of proton

proton spin has magnetic moment and creates a magnetic field at the position of the electron

$$\vec{B}_I(\vec{r}) = -\frac{g_p e}{2m_p} \int d^3r' \, \rho_p(r') \, \vec{\nabla} \times (\vec{\sigma}_I \times \vec{\nabla}) \frac{1}{4\pi|\vec{r}-\vec{r}'|} \tag{626}$$

$\vec{\sigma}_I$ – spin operator of proton

ρ_p – density of (magnetic moment of) proton

g_p – gyromagnetic factor of proton

m_p – mass of proton

$\Rightarrow \cdots \Rightarrow$

$$\vec{B}_I = -\frac{2}{3} g_p \frac{e}{2m_p} \hat{\vec{I}} \rho_p(\vec{r}) \tag{627}$$

where $\vec{\hat{I}} = \frac{\hbar}{2}\vec{\sigma}_I$ is the spin of the proton.

This gives the Hyperfine Hamiltonian

(628) $$\boxed{\hat{H}_{HF} = \frac{1}{6}\frac{g_p e^2}{m_0 m_p}\beta\left(\vec{\hat{\Sigma}}\cdot\vec{\sigma}_I\right)\delta_p(\vec{r})}$$

for the upper ~~ele~~ electron spinor we find

(629) $$\boxed{\hat{H}_{HF} = \frac{2}{3\hbar^2}\frac{g_p c^2}{m_0 m_p}\left(\vec{\hat{S}}\cdot\vec{\hat{I}}\right)\delta_p(\vec{r})}$$

total spin $\quad \vec{\hat{F}} = \vec{\hat{S}} + \vec{\hat{I}}$

(330) $\hat{F}^2 = \hat{I}^2 + \hat{S}^2 + 2\vec{\hat{S}}\cdot\vec{\hat{I}}$ conserved quantity!

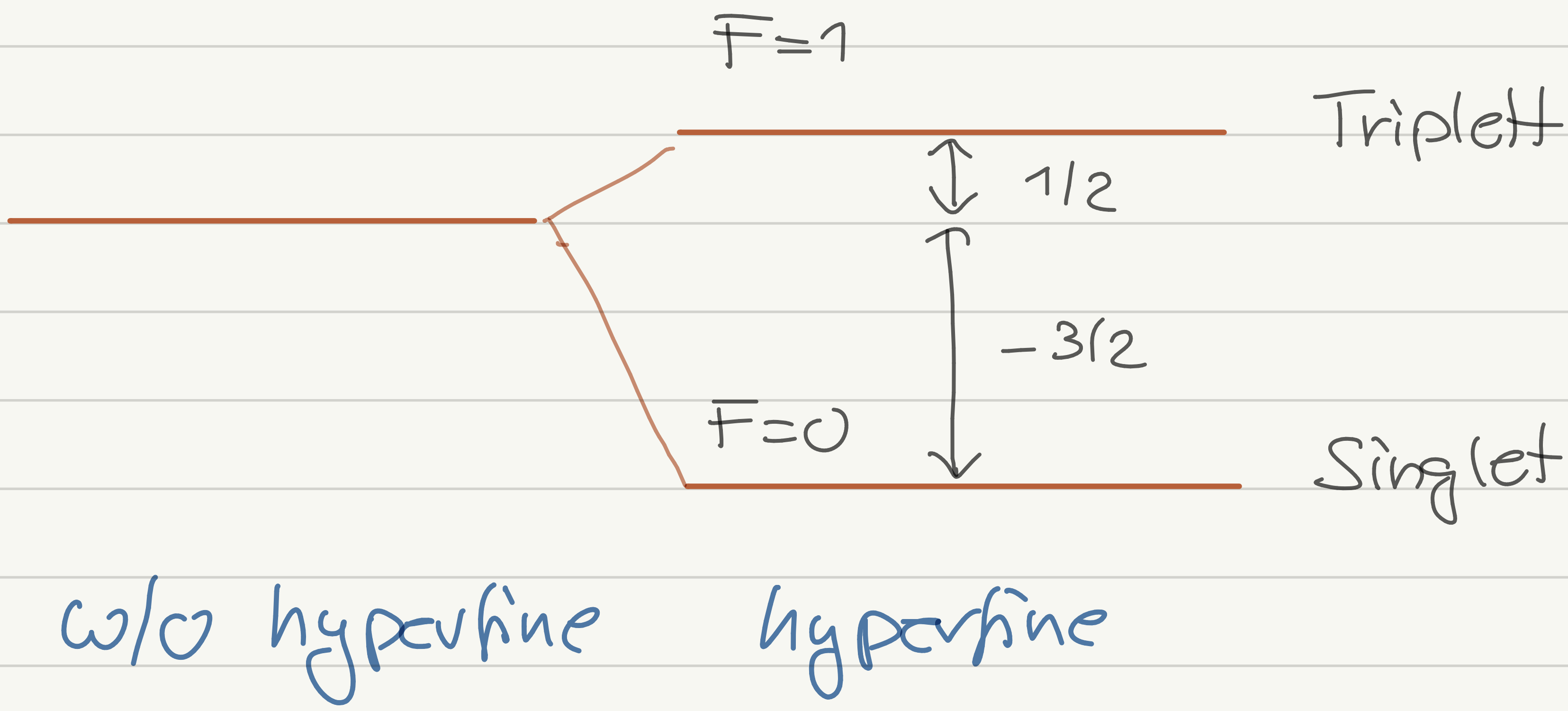
eigenvalues of $\hat{F}^2$: $\hbar^2 F(F+1)$

(331) $$F = \begin{cases} I + S = 1 & \text{Triplett} \\ I - S = 0 & \text{Singlett} \end{cases}$$

eigenvalues of

$$2\vec{S}\cdot\vec{I} = \begin{cases} 1(1+1) - \frac{1}{2}\left(\frac{1}{2}+1\right) - \frac{1}{2}\left(\frac{1}{2}+1\right) = \frac{1}{2} \\ 0 - \frac{1}{2}\left(\frac{1}{2}+1\right) - \frac{1}{2}\left(\frac{1}{2}+1\right) = -\frac{3}{2} \end{cases}$$

(332



VII.6 Dirac sea

The unboundedness from below of the energy spectrum of the Dirac equation creates a problem:

an electron can emitt elm. energy an continue to fall down in the spectrum