The Central Force Problem in Dirac Theory.

4) The above formulation of the 2nd order Dirac Eqtn is best suited for showing the nature of the Dirac add-on compared to the Klein-Gordon Eqtn, and for establishing Lorentz covariance of the Dirac Eqtn in an external field A_μ (to do this, one begins from Eq.(10)). For practical calculations, however, it is easier to return to the Hamiltonian form of the Dirac Eqtn. We do this now, for the central force problem, w/ (q,m) moves in a radial potential $V(r)$.

CENTRAL FORCE PROBLEM: $\mathbf{A}=0$, $q\phi = V(r)$ the central potential

and/ $\rightarrow i\hbar\frac{\partial\psi}{\partial t} = \mathcal{H}\psi$, w/ $\psi = \begin{pmatrix}\varphi\\ \chi\end{pmatrix}$ &/ $\mathcal{H} = c\boldsymbol{\alpha}\cdot\mathbf{p} + \beta mc^2 + V$. ¶ (17)

In nonrelativistic Schrödinger theory, the central force problem has the "nice" feature that the orbital ∡ moment $\mathbb{L} = \mathbf{r}\times\mathbf{p} = -i\hbar\,\mathbf{r}\times\nabla$ is a constant of

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¶ Why does V just add to $\mathcal{H}$ this way? Go back to Eq.(2), p. DE 39...

$\{\gamma_\mu[p_\mu - \frac{q}{c}A_\mu] - imc\}\psi = 0$ ∫ recall standard repⁿ [Eq.(22), p. DE8: $\gamma_k = -i\beta\alpha_k$, $\gamma_4 = \beta$.

Put in the γ_μ equivalents. Choose $A_\mu = (0, i\phi)$ for central force problem. Then:

$\rightarrow \{-i\beta\alpha_k p_k + \beta(p_4 - \frac{q}{c}i\phi) - imc\}\psi = 0.$

Multiply this eqtn on the left by ic, and put in $p_4 = -i\hbar\frac{\partial}{\partial x_4} = -\frac{\hbar}{c}\frac{\partial}{\partial t}$ ...

$\rightarrow \{\beta c\alpha_k p_k - ic\beta\left(\frac{\hbar}{c}\frac{\partial}{\partial t} + i\frac{q\phi}{c}\right) + mc^2\}\psi = 0.$

Multiply on the left by $\beta = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$, w/ $\beta^2 = 1$. Set $\alpha_k p_k = \boldsymbol{\alpha}\cdot\mathbf{p}$, define $q\phi = V(r)$, and put the term in $\partial\psi/\partial t$ on the RHS. Then...

$\{c\boldsymbol{\alpha}\cdot\mathbf{p} + V(r) + \beta mc^2\}\psi = i\hbar\,\partial\psi/\partial t$.

This is equivalent to Eq.(17). V enters w/o any associated Dirac matrices.

the motion -- in particular, $[\mathcal{H}(\text{Schröd.}), \mathbb{L}] = 0$, and $\mathbb{L}$ has associated eigenfcns $Y_\ell^m(\theta,\phi)$ such that: $\mathbb{L}^2 Y_\ell^m = [\ell(\ell+1)\hbar^2] Y_\ell^m$, $\ell = 0,1,2,\ldots$; $L_z Y_\ell^m = m\hbar Y_\ell^m$, with: $m = -\ell, -\ell+1, \ldots, +\ell$. This "nice" feature no longer holds in Dirac theory, because of the intrinsic appearance of spin. For the $\mathcal{H}$ in Eq. (17)...

$$\rightarrow [\mathcal{H}(\text{Dirac}), \mathbb{L}] = -i\hbar c\, \boldsymbol{\alpha} \times \mathbb{p}; \qquad (18)$$

so: $d\mathbb{L}/dt = c\,\boldsymbol{\alpha} \times \mathbb{p}$, and $\mathbb{L}$ cannot be a cnst-of-the-motion. But, we suspect that $\mathbb{J} = \mathbb{L} + \mathbb{S}$, where $\mathbb{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$ is the electron spin, will qualify -- because a central force cannot affect the system's total ∡ momentum (this is a Newtonian verity). So, look at the commutator for $\mathcal{H}$(Dirac) and the super-spin operator $\boldsymbol{\Sigma}$ (as defined in Eq. (17), p. DE 17)...

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}$$

$\boldsymbol{\sigma}$ = 2×2 Pauli spin ½ matrices [see Eq. (15) above], $\boldsymbol{\Sigma}$ is 4×4, and acts on the 4-spinor $\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$;

$$\xrightarrow{\text{w/}} [\mathcal{H}(\text{Dirac}), \boldsymbol{\Sigma}] = 2ic(\boldsymbol{\alpha} \times \mathbb{p}); \qquad (19)$$

so: $d\boldsymbol{\Sigma}/dt = -\frac{2}{\hbar} c(\boldsymbol{\alpha} \times \mathbb{p})$, and $\boldsymbol{\Sigma}$ by itself is also not a cnst-of-motion. However, by adding Eqs. (18) & (19), we see: $[\mathcal{H}(\text{Dirac}), \mathbb{L} + \frac{\hbar}{2}\boldsymbol{\Sigma}] = 0$, so:

$$\boxed{\mathbb{J} = \mathbb{L} + \mathbb{S} \quad \text{w/ } \mathbb{S} = \frac{\hbar}{2}\boldsymbol{\Sigma}, \text{ is a cnst-of-the-motion;}} \qquad (20)$$

here $\mathbb{L} = \mathbb{r} \times \mathbb{p} \cdot$ (4×4 identity matrix), and $\mathbb{S} = \frac{\hbar}{2}\begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}$;

so/ $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\mathbb{L} + \frac{\hbar}{2}\boldsymbol{\sigma}$ acts on each of the bispinors φ & χ.

This means that for a Dirac central force problem, the entire 4-spinor $\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$ is an eigenfcn of $\mathbb{J}^2$ & J_z, w/ eigenvalues $j(j+1)\hbar^2$ & $m_j\hbar$, where $j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$, and $m_j = -j, -j+1, \ldots, +j$. In fact $j = \ell \oplus s$, and since $s = \frac{1}{2}$ only, the j-values are: $j = \ell \pm s$, for $\ell \neq 0$, and $j = \frac{1}{2}$, for $\ell = 0$.

The ∡ dependence of the Dirac central force problem can be incorporated into associated spherical harmonics $\mathcal{Y}_j^{m_j}(\theta,\phi)$ -- these are eigenfcns of $\mathbb{J}^2$ & J_z and are formed by "appropriate" linear combinations of products of the ordinary orbital ∡ momentum eigenfcns $Y_\ell^m(\theta,\phi)$, and the spin up & spin down bispinors $\underset{\sim}{u}=\begin{pmatrix}1\\0\end{pmatrix}$ & $\underset{\sim}{d}=\begin{pmatrix}0\\1\end{pmatrix}$. What combinations are "appropriate" here is prescribed by the Clebsch-Gordan transformation $|\ell,s,m,m_s\rangle \to |\ell,s,j,m_j\rangle$. For $\mathbb{J}=\mathbb{L}+\mathbb{S}$, and $\mathbb{S}=\frac{\hbar}{2}\sigma$ only, have $j=\ell\pm\frac{1}{2}$ (units of $\hbar$), and prescription is:

$$\left[\begin{array}{l} \mathcal{Y}_{j=\ell+\frac{1}{2}}^{m_j}(\theta,\phi)=\left[\frac{\ell+\frac{1}{2}+m_j}{2\ell+1}\right]^{\frac{1}{2}} Y_\ell^{m_j-\frac{1}{2}}(\theta,\phi)\,\underset{\sim}{u}+\left[\frac{\ell+\frac{1}{2}-m_j}{2\ell+1}\right]^{\frac{1}{2}} Y_\ell^{m_j+\frac{1}{2}}(\theta,\phi)\,\underset{\sim}{d}, \\ \mathcal{Y}_{j=\ell-\frac{1}{2}}^{m_j}(\theta,\phi)=\left[\frac{\ell+\frac{1}{2}-m_j}{2\ell+1}\right]^{\frac{1}{2}} Y_\ell^{m_j-\frac{1}{2}}(\theta,\phi)\,\underset{\sim}{u}-\left[\frac{\ell+\frac{1}{2}+m_j}{2\ell+1}\right]^{\frac{1}{2}} Y_\ell^{m_j+\frac{1}{2}}(\theta,\phi)\,\underset{\sim}{d}; \\ \text{w/}\ \mathbb{J}^2\mathcal{Y}_j^{m_j}=j(j+1)\mathcal{Y}_j^{m_j},\ J_z\mathcal{Y}_j^{m_j}=m_j\mathcal{Y}_j^{m_j};\ \langle\mathcal{Y}_j^{m_j}|\mathcal{Y}_{j'}^{m_j'}\rangle_{\text{all ∡s}}=\delta_{jj'}\delta_{m_jm_j'} \end{array}\right\} \quad (21)$$

Each $\mathcal{Y}_j^{m_j}$ is itself a bispinor, specifying the spatial ∡ dependence in the $\underset{\sim}{u}$ & $\underset{\sim}{d}$ spin states, with one $\mathcal{Y}_j^{m_j}$ for each of the values $j=\ell\pm\frac{1}{2}$. For the $\ell=0$ case (S states): $\mathcal{Y}_{j=\frac{1}{2}}^{m_j=+\frac{1}{2}}(\theta,\phi)=Y_0^0\,\underset{\sim}{u}$, $\mathcal{Y}_{j=\frac{1}{2}}^{m_j=-\frac{1}{2}}(\theta,\phi)=Y_0^0\,\underset{\sim}{d}$, with $Y_0^0=1/\sqrt{4\pi}$, so the $m_j=m_s=\pm\frac{1}{2}$ states are basically just $\underset{\sim}{u}$ or $\underset{\sim}{d}$.

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5) We can now reduce the Dirac central force problem in Eq.(17) to just a radial problem, by separating out the ∡ & spin dependence per Eqs.(21). For an eigenstate of energy E [i.e., $i\hbar\,\partial\psi/\partial t=E\psi$, $E=(\pm)$ve], we have:

$$\rightarrow [c\alpha\cdot\mathbb{p}+\beta mc^2+V(r)]\begin{pmatrix}\varphi\\ \chi\end{pmatrix}=E\begin{pmatrix}\varphi\\ \chi\end{pmatrix} \leftarrow \text{put in } \alpha=\begin{pmatrix}0&\sigma\\ \sigma&0\end{pmatrix} \text{ Eq.(11) p.DE5}$$

So//

$$\boxed{\begin{array}{l}(E-M-V)\varphi=c(\sigma\cdot\mathbb{p})\chi \\ (E+M-V)\chi=c(\sigma\cdot\mathbb{p})\varphi\end{array}} \quad \text{with: } M=mc^2. \qquad (22)$$

Each of the bispinors φ & χ must be eigenfcns of $\mathbb{J}^2$ & J_z, so write φ as...

$$\longrightarrow \underline{\varphi(\mathbb{r})=g(r)\,\mathcal{Y}_j^{m_j}(\theta,\phi)}, \quad g(r)=\text{scalar fcn of } r=|\mathbb{r}| \text{ only}. \qquad (23)$$

Elimination of the ∡ & spin-dependence of Dirac's central force Eqtn.

The radial fcn $g(r)$ must be a scalar, and thus the <u>same</u> for both the $\underset{\sim}{u}$ and $\underset{\sim}{d}$ components of $\varphi(\mathbf{r})$, otherwise we would be looking at some preferred spin direction in a central field -- which by definition has <u>no preferred axis</u>. Now the "small" bispinor $\chi(\mathbf{r})$ must also be an eigenfcn of $\mathbf{J}^2$ & J_z [recall remark below Eq.(20) on p. DE43] so it must be that $\chi(\mathbf{r}) \propto \mathcal{Y}_j^{m_j}(\theta,\phi)$ also. At the same time, however, <u>$\varphi(\mathbf{r})$ & $\chi(\mathbf{r})$ must have opposite parities</u> [recall Eq.(13), p. DE6; or Eq.(11), p. DE15]. The parity change cannot be accommodated by radial fcns like $g(r)$, since $r \to r$ under parity $P(x_k \to (-)x_k)$. So we contemplate a realization of P by the following operator...

$$\rightarrow \underline{\underline{P = (\sigma \cdot \hat{r})}}, \text{ w/ } \hat{r} = \mathbf{r}/r \quad \Big\lmoustache \begin{array}{l} P^2 = 1, \text{ eigenvalues of } P \text{ are } \pm 1; \text{ and:} \\ P \to (-)P \text{ on cd. reflection, also } [\mathbf{J}, P] = 0. \end{array} \tag{24}$$

So P does not affect the eigenfeatures of the $\mathcal{Y}_j^{m_j}$, and if we take...

$$\rightarrow \underline{\chi(\mathbf{r}) = -i f(r)\, P\, \mathcal{Y}_j^{m_j}(\theta,\phi)}, \quad f(r) = \text{scalar fcn of } r = |\mathbf{r}| \text{ only}, \tag{25}$$

then this χ is an eigenfcn of $\mathbf{J}^2$ & J_z just as φ of Eq.(23), but it has opposite intrinsic parity. NOTE: the factor $-i$ is inserted for convenience. If we plug φ of Eq.(23) and χ of Eq.(25) into Eqs(22), we get...

$$\boxed{\begin{array}{l} (E-M-V)\, g\, \mathcal{Y} = -ic(\sigma\cdot\mathbf{p})\, f P \mathcal{Y} \\ (E+M-V)\, f P \mathcal{Y} = +ic(\sigma\cdot\mathbf{p})\, g\, \mathcal{Y} \end{array}} \quad \Big\lmoustache \begin{array}{l} M = mc^2,\ V = V(r),\ P = \sigma\cdot\hat{r}, \\ \text{and/ } \mathcal{Y} = \mathcal{Y}_j^{m_j}(\theta,\phi). \end{array} \tag{26}$$

The idea now is to eliminate the ∡ dependence entirely by integrating over θ & ϕ.

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6) To do the ∡ integrations in Eqs.(26), first note, by use of Dirac identity...

$$\rightarrow \sigma\cdot\mathbf{p} = P^2(\sigma\cdot\mathbf{p}) = P\cdot\frac{1}{r}[(\sigma\cdot\mathbf{r})(\sigma\cdot\mathbf{p})] = P\cdot\frac{1}{r}\big[\underbrace{\mathbf{r}\cdot\mathbf{p}}_{= r p_r = -i\hbar r(\partial/\partial r)} + i\sigma\cdot(\overbrace{\mathbf{r}\times\mathbf{p}}^{\mathbf{L}})\big]$$

$$\underline{\underline{\sigma\cdot\mathbf{p} = i P\left[\frac{1}{r}(\sigma\cdot\mathbf{L}) - \hbar\frac{\partial}{\partial r}\right]}}. \tag{27}$$

Reduction of the Dirac central force problem to radial eqtns.

Use the identity in Eq. (27) on the quantities on the RHS of Eqs. (26), viz...

$$\left.\begin{aligned}&(\sigma\cdot\mathbb{p})\,f\,P\,\mathcal{Y} = i(f/r)\,P(\sigma\cdot\mathbb{L})\,P\,\mathcal{Y} - i\hbar(\partial f/\partial r)\,\mathcal{Y},\\ &(\sigma\cdot\mathbb{p})\,g\,\mathcal{Y} = i(g/r)\,P(\sigma\cdot\mathbb{L})\,\mathcal{Y} - i\hbar(\partial g/\partial r)\,P\,\mathcal{Y}.\end{aligned}\right\}\quad(28)$$

Now, put Eqs. (28) into Eqs. (26); and multiply the 2nd of the resulting eqtns on the left by P. With $P^2=1$ (and P commuting with fcns of r), we get...

$$\left.\begin{aligned}&①\ (E-M-V)\,g\,\mathcal{Y} = c(f/r)\,[P(\sigma\cdot\mathbb{L})P]\,\mathcal{Y} - \hbar c(\partial f/\partial r)\,\mathcal{Y},\\ &②\ (E+M-V)\,f\,\mathcal{Y} = -c(g/r)\,[\sigma\cdot\mathbb{L}]\,\mathcal{Y} + \hbar c(\partial g/\partial r)\,\mathcal{Y}.\end{aligned}\right\}\quad(29)$$

Multiply both of Eqs. (29) on the left by $\mathcal{Y}^\dagger$, and integrate over all $\measuredangle$s θ & φ. Since $\mathcal{Y}^\dagger$ commutes with fcns of r, and $\langle\mathcal{Y}|\mathcal{Y}\rangle=1$ [by Eq. (21)], we get...

$$\boxed{\begin{aligned}&①\ (E-M-V)\,g = -\hbar c(\partial f/\partial r) + c(f/r)\,\langle\mathcal{Y}|P(\sigma\cdot\mathbb{L})P|\mathcal{Y}\rangle_{\measuredangle s},\\ &②\ (E+M-V)\,f = +\hbar c(\partial g/\partial r) - c(g/r)\,\langle\mathcal{Y}|\sigma\cdot\mathbb{L}|\mathcal{Y}\rangle_{\measuredangle s}.\end{aligned}}\quad(30)$$

We finish the separation of variables (radial vs. $\measuredangle$ & spin) once we find the $\measuredangle$ integrals in Eq. (30). The integral in Eq. (30)② is easy, because $(\sigma\cdot\mathbb{L})$ is a cnst-of-the-motion. We have...

$\mathbb{J} = \mathbb{L} + \frac{1}{2}\hbar\sigma$, is a cnst-of-the-motion;

$$\xrightarrow{\text{so}} \mathbb{J}^2 = \underbrace{\mathbb{L}^2}_{l(l+1)\hbar^2} + \hbar(\sigma\cdot\mathbb{L}) + \frac{1}{4}\hbar^2\underbrace{\sigma^2}_{3} = j(j+1)\hbar^2 = \text{cnst} \int^{\text{w/}} j = l\pm\tfrac{1}{2}$$

[in rep$^{\text{n}}$ $|lsjm_j\rangle$]   [Pauli matrices: $\sigma_k^2=1$]

$$\underline{\underline{(\sigma\cdot\mathbb{L}) = [j(j+1) - l(l+1) - \tfrac{3}{4}]\,\hbar}} = \begin{cases}+l\hbar, & \text{for } j = l+\frac{1}{2};\\ -(l+1)\hbar, & \text{for } j = l-\frac{1}{2}.\end{cases}\quad(31)$$

For convenience, a new quantum # $\underline{\underline{\kappa = \mp(j+\frac{1}{2}),\ \text{for } j = l\pm\frac{1}{2}}}$, is introduced at this point. The two κ's are eigenvalues of yet another spin

Reduction to radial eqtns completed.

Spin operator: $K = \beta(\Sigma\cdot\mathbb{L} + \hbar) = \begin{pmatrix} \sigma\cdot\mathbb{L}+\hbar & 0 \\ 0 & -(\sigma\cdot\mathbb{L}+\hbar)\end{pmatrix}$. K commutes with $\mathcal{H}$(Dirac), and its eigenvalues κ determine whether the electron spin σ is parallel ($\kappa<0$) or anti-parallel ($\kappa>0$) to its orbital $\mathbb{L}$, in the nonrelativistic limit. Since: $\kappa = -(l+1)$ for $j = l+\frac{1}{2}$, and $\kappa = +l$ for $j = l-\frac{1}{2}$, Eq. (31) is succinctly written: $(\sigma\cdot\mathbb{L}) = -(\kappa+1)\hbar$, and so:

$$\rightarrow \underline{\langle \mathcal{Y}|\sigma\cdot\mathbb{L}|\mathcal{Y}\rangle = -(\kappa+1)\hbar}, \quad \text{w/ } \kappa = \mp(j+\tfrac{1}{2}) \text{ for } j = l\pm\tfrac{1}{2}.^{\bigstar} \tag{32}$$

This is to be used in Eq. (30)②. The ∡ integral in Eq. (30)① is trickier because of the parity operator $\mathbb{P} = \sigma\cdot\hat{r}$. One finds, however

$$\rightarrow \underline{\langle \mathcal{Y}|\mathbb{P}(\sigma\cdot\mathbb{L})\mathbb{P}|\mathcal{Y}\rangle = +(\kappa-1)\hbar}, \quad \kappa \text{ as in Eq. (32)}. \tag{33}$$

Using (32) & (33) in Eq. (30), we reduce the Dirac central force problem to the following radial problem... w/ $M = mc^2$, $\kappa = \mp(j+\frac{1}{2})$ for $j = l\pm\frac{1}{2}$...$^{\bigstar}$

$$\left.\begin{array}{l} \boxed{\begin{array}{l} ①\ \dfrac{\partial f}{\partial r} + (1-\kappa)\dfrac{f}{r} + \dfrac{1}{\hbar c}[E - M - V(r)]g = 0, \\ ②\ \dfrac{\partial g}{\partial r} + (1+\kappa)\dfrac{g}{r} - \dfrac{1}{\hbar c}[E + M - V(r)]f = 0; \end{array}} \\ \text{w/ Dirac 4-spinor: } \psi = \begin{pmatrix}\varphi \\ \chi\end{pmatrix} = \begin{pmatrix} g(r)\,\mathcal{Y}_j^{m_j}(\theta,\phi) \\ -i f(r)(\sigma\cdot\hat{r})\,\mathcal{Y}_j^{m_j}(\theta,\phi)\end{pmatrix}. \end{array}\right\} \tag{34}$$

This is for a spin $\frac{1}{2}$ particle (q, m) moving in the central potential $V = q\phi(r)$. The external magnetic field $\mathbb{B} \equiv 0$ (since we put $\mathbb{A} = 0$ at the outset).

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7) It is convenient to define new radial fcns $F(r)$ & $G(r)$ by:

$$\underline{F(r) = r f(r),\ G(r) = r g(r)}, \quad \text{so/ } \psi = \begin{pmatrix} \frac{1}{r} G\,\mathcal{Y} \\ -\frac{i}{r} F(\sigma\cdot\hat{r})\mathcal{Y}\end{pmatrix}. \tag{35}$$

$^{\bigstar}$ For S-states, $j = \frac{1}{2}$ only, the correct assignment for κ is: $\kappa = (-)1$.

Transmogrification of the Dirac radial eqtns. Dirac square well.

Eqs. (34) then take the form:

$$\frac{dF}{dr} - \frac{\kappa}{r}F + \frac{1}{\hbar c}(E-M-V)G = 0, \quad \frac{dG}{dr} + \frac{\kappa}{r}G - \frac{1}{\hbar c}(E+M-V)F = 0. \quad (36)$$

These two coupled 1st order differential eqtns can be separated into the system:

$$\boxed{\begin{aligned} &F = \frac{\hbar c}{(E+M-V)}\left(\frac{dG}{dr} + \frac{\kappa}{r}G\right), \text{ and with } \kappa = \mp(j+\tfrac{1}{2}) \text{ for } j = l \pm \tfrac{1}{2} \ldots \\ &\frac{d^2G}{dr^2} + \left[\frac{(E-V)^2 - M^2}{(\hbar c)^2} - \frac{\kappa(\kappa+1)}{r^2}\right]G + \frac{(dV/dr)}{E+M-V}\left[\frac{dG}{dr} + \frac{\kappa}{r}G\right] = 0. \end{aligned}} \quad (37)$$

For (+)ve energy solutions ($E>0$), G is the "large" and F is the "small" radial component of Dirac's ψ [per Eq. (35)]. Notice that $\kappa(\kappa+1) = l(l+1)$ for both $j = l \pm \frac{1}{2}$ values, so the term $\kappa(\kappa+1)/r^2$ plays the role of a centrifugal barrier. The first two terms LHS in the d^2G/dr^2 eqtn in (37) are similar in structure to the terms that appear in the radial eqtns for the Schrödinger & Klein-Gordon eqtns¶, but the 3rd term LHS in (37) is peculiar to the Dirac theory. In this term, the particle is coupled to the central force $\mathcal{F}(r) = -dV/dr$, in effect, as well as being coupled to the potential $V(r)$.

The G eqtn is simple in only one example, namely the radial potential well:

$V(r) = -V_0$, cnst, for $0 \leq r < a$;
$V(r) = 0$, for $r > a$.
Look at S-states, $\kappa = -1$.

So $\frac{d^2G}{dr^2} + \alpha^2 G = 0$ ∫ $\alpha = \frac{1}{\hbar c}\sqrt{(E+V_0)^2 - M^2}$, and: $0 \leq r < a$;

$\frac{d^2G}{dr^2} - \beta^2 G = 0$ ∫ $\beta = \frac{1}{\hbar c}\sqrt{M^2 - E^2}$, and: $r > a$.

Further details of Dirac's square-well problem are left as an exercise.

¶ Schrödinger radial eqtn: $\frac{d^2R}{dr^2} + \left[\frac{2m}{\hbar^2}(E-V-M) - \frac{l(l+1)}{r^2}\right]R = 0$ ∫ Eq. (3), p. II 2 of class notes

Klein-Gordon radial eqtn: $\frac{d^2R}{dr^2} + \left[\frac{(E-V)^2 - M^2}{(\hbar c)^2} - \frac{l(l+1)}{r^2}\right]R = 0$ ∫ Eq. (18), p. fs 18 of class notes

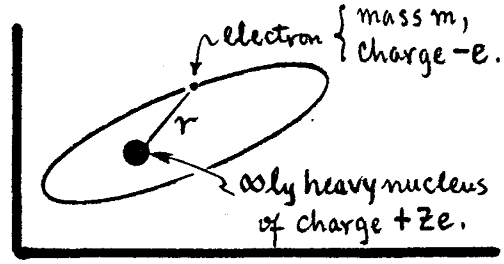
Dirac's radial problem for the Coulomb potential.

Dirac Equation: Solution for the Hydrogen Atom

We shall now solve Dirac's central force problem [pp. 42-48 preceding] for the Coulomb potential: $\underline{V(r) = -Ze^2/r}$. In particular, we want to find how the Bohr energies $\underline{E_n = -\frac{1}{2}(Z\alpha)^2 mc^2/n^2}$ turn out in the fully relativistic theory (recall $\underline{\alpha = e^2/\hbar c \simeq 1/137}$ is the fine-structure cnst). In principle, the energies E_n(Dirac) should be correct to all orders in $(Z\alpha)$, and should therefore include E_n(Bohr) + all the $\mathcal{O}(v/c)^2$ corrections we have previously added on [see pp. fs 5-13 for spin-orbit interaction, Pauli correction, etc].

1) Write the Coulomb potential as...

$$\rightarrow V(r) = -\hbar c Z\alpha/r, \qquad (1)$$



and, with $M = mc^2$ the electron rest energy, define...

$$\left[\begin{array}{ll} \underline{\underline{\lambda_1}} = (M+E)/\hbar c, \quad \underline{\underline{\lambda_2}} = (M-E)/\hbar c & \int \lambda_1 \,\&\, \lambda_2 \text{ have dimensions of (length)}^{-1}. \text{ For bound states } (E<M)\text{, both are +ve.} \\ \underline{\underline{\gamma}} = Z\alpha, \text{ and: } \underline{\underline{\rho}} = \sqrt{\lambda_1\lambda_2}\, r = \left[\sqrt{M^2-E^2}/\hbar c\right] r & \int \rho \text{ is dimensionless, and real for bound states.} \end{array}\right] \qquad (2)$$

In these terms, the radial equations for Dirac's central force problem become [ref. Eq. (36), p. DE 48], w/ $\kappa = \mp(j+\frac{1}{2})$ for $j = l \pm \frac{1}{2}$ (and $\kappa = -1$ for $l=0$): $\star$

$$\boxed{\left(\frac{d}{d\rho} - \frac{\kappa}{\rho}\right)F - \left(\sqrt{\frac{\lambda_2}{\lambda_1}} - \frac{\gamma}{\rho}\right)G = 0, \quad \left(\frac{d}{d\rho} + \frac{\kappa}{\rho}\right)G - \left(\sqrt{\frac{\lambda_1}{\lambda_2}} + \frac{\gamma}{\rho}\right)F = 0.} \qquad (3)$$

As boundary conditions, we want $\frac{1}{\rho}G$ & $\frac{1}{\rho}F$ finite as $\rho \to 0$, and zero as $\rho \to \infty$ (so that $\int d^3x\, \psi^\dagger\psi \propto \int_0^\infty (G^2+F^2)\,dr$ is bounded). For $\rho \to$ large, we note:

$$\left[\begin{array}{l} dF/d\rho - (\sqrt{\lambda_2/\lambda_1})\,G \simeq 0 \\ dG/d\rho - (\sqrt{\lambda_1/\lambda_2})\,F \simeq 0 \end{array}\right\} \quad \left[\frac{d^2}{d\rho^2} - 1\right](F \,\&\, G) \simeq 0, \ \text{w/}\ F \,\&\, G \propto e^{-\rho}, \text{ as } \rho\to\infty. \qquad (4)$$

$\star$ The full Dirac wavefcn is [from Eq. (35), p. DE 47]: $\psi(\mathbf{r}) = \frac{1}{r}\begin{pmatrix} G(r)\,\mathcal{Y}(\theta,\phi) \\ -iF(r)\,\boldsymbol{\sigma}\cdot\hat{\mathbf{r}}\,\mathcal{Y}(\theta,\phi)\end{pmatrix}$.

Power series solutions for the radial fcns. Comments on S-states.

That F & $G \propto e^{-\rho}$ as $\rho\to\infty$ is acceptable asymptotic behavior. For full solutions for $F(\rho)$ & $G(\rho)$, we try the power series [method of Frobenius]:

$$\underline{\underline{F(\rho) = e^{-\rho}\rho^s \sum_{\nu=0}^{\infty} a_\nu \rho^\nu}}, \quad \underline{\underline{G(\rho) = e^{-\rho}\rho^s \sum_{\nu=0}^{\infty} b_\nu \rho^\nu}}. \qquad (5)$$

Plug these expressions into Eqs. (3), and equate coefficients of $e^{-\rho}\rho^s\rho^{\nu-1}$ to zero to get (coupled) recursion relations for the a's & b's...

$$\left.\begin{array}{l}(s-\kappa+\nu)a_\nu - a_{\nu-1} + \gamma b_\nu - (\sqrt{\lambda_2/\lambda_1})\, b_{\nu-1} = 0,\\ (s+\kappa+\nu)b_\nu - b_{\nu-1} - \gamma a_\nu - (\sqrt{\lambda_1/\lambda_2})\, a_{\nu-1} = 0;\end{array}\right\rangle \text{for } \nu \geqslant 1. \qquad (6)$$

For $\nu=0$, $a_{\nu-1}$ & $b_{\nu-1}$ vanish, and Eqs. (6) yield...

$$\begin{pmatrix} s-\kappa & \gamma \\ -\gamma & s+\kappa\end{pmatrix}\begin{pmatrix} a_0 \\ b_0\end{pmatrix} = 0 \;\ldots\; \text{so, for } a_0 \,\&\, b_0 \neq 0,\; \det\begin{pmatrix} s-\kappa & \gamma \\ -\gamma & s+\kappa\end{pmatrix} = 0,$$

or// $\underline{\underline{s = \pm\sqrt{\kappa^2-\gamma^2}}}$ ← take (+) root only, if F & $G \propto \rho^s$ are to remain finite as $\rho\to 0$. (7)

ASIDE Behavior of S-state radial fcns as $\rho\to 0$.

For an S-state ($l=0$, $j=\frac{1}{2}$), have $\kappa=-1$, so in Eq. (7): $s=\sqrt{1-(Z\alpha)^2}<1$.

The radial dependence of ψ then goes as: $\frac{1}{\rho}(F \,\&\, G) \propto \rho^{-(1-s)}$, as $\rho\to 0$,

i.e.// $\underline{\frac{1}{\rho}(F \,\&\, G) \propto \rho^{-\epsilon/2}}$, where: $\underline{\epsilon = 2\left(1-\sqrt{1-(Z\alpha)^2}\right) \underset{Z\alpha \ll 1}{\simeq} (Z\alpha)^2}$. (8)

This shows that Dirac's S-state wavefcns ψ are formally singular at the origin. The singularity is "weak" so long as $Z\alpha \ll 1$, i.e. $Z \ll 137$, and one can argue that it will be removed at short distances by modifications of the Coulomb potential due to finite nuclear size. Anyway, the overall probability: $\int d^3x\, \psi^\dagger\psi \propto \int_0^\infty (G^2+F^2)\,d\rho$, with $G^2+F^2 \propto \rho^{2-\epsilon}$, does not show any divergence as $\rho\to 0$, so we are not in any dramatic trouble.

NOTE: For an atom with $Z>137$, radial fcns in (8) are $\frac{1}{\rho}(F \,\&\, G) \propto \rho e^{-i\zeta \ln\rho}$, where $\zeta = \sqrt{(Z\alpha)^2-1}$. Can such an atom exist, with an oscillatory radial fcn?

Solution for the Dirac eigen-energies in a Coulomb potential.

2) The power series for $F(\rho)$ & $G(\rho)$ in Eq.(5) diverge exponentially (as $e^{+\rho}$) when $\rho \to \infty$, and hence $F(\rho)$ & $G(\rho)$ will diverge as ρ^s, <u>unless</u> the series are truncated. We assume that both series terminate with the same power of ρ. So...

There must be some integer $n' \geqslant 0$ such that:

$$\underline{a_{n'+1} \;\&\; b_{n'+1} = 0, \;\; \text{but} \;\; a_{n'} \;\&\; b_{n'} \neq 0}, \;\; w/\; n' = 0, 1, 2, 3, \ldots \tag{9}$$

Set $\nu = n'+1$ in the recursion relations of Eq (6). Both yield the relation:

$$\underline{a_{n'} = -\sqrt{\lambda_2/\lambda_1}\, b_{n'}}, \text{ for highest power } \rho^{n'} \text{ appearing in series.} \tag{10}$$

Now, massage the recursion relations in Eq.(6) again. Multiply through the 1st eqtn by λ_1, and through the 2nd by $\sqrt{\lambda_1\lambda_2}$. Subtract the results to get...

$$[(s-\kappa+\nu)\lambda_1 + \gamma\sqrt{\lambda_1\lambda_2}\,]\,a_\nu - [(s+\kappa+\nu)\sqrt{\lambda_1\lambda_2} - \lambda_1\gamma\,]\,b_\nu = 0. \tag{11}$$

... set $\nu = n'$ here, and use $a_{n'} = -\sqrt{\lambda_2/\lambda_1}\, b_{n'}$ from (10)...

so/ $$\underline{[\,2(s+n')\sqrt{\lambda_1\lambda_2} - (\lambda_1-\lambda_2)\gamma\,]\, b_{n'} = 0}. \tag{12}$$

... but $b_{n'} \neq 0$ by hypothesis, so the [ ] = 0, and this yields...

$$[\;] = 0 \Rightarrow \underline{(s+n')\sqrt{\lambda_1\lambda_2} = \tfrac{1}{2}(\lambda_1-\lambda_2)\gamma}. \tag{13}$$

Eq.(13) gives the eigenvalue energies E for the Coulomb problem. Recall the notation from Eq.(2): $\lambda_{1,2} = \frac{1}{\hbar c}(M \pm E)$, $\gamma = Z\alpha$, so...

$$\rightarrow (s+n')\sqrt{M^2-E^2} = EZ\alpha, \;\; w/\; s = \sqrt{\kappa^2-(Z\alpha)^2}, \;\; \kappa = \mp(j+\tfrac{1}{2})$$

so/ $$E^2 = M^2\Big/\left[1+\frac{(Z\alpha)^2}{(n'+s)^2}\right], \;\; w/\; n' = 0,1,2,3,\ldots, \;\; M = mc^2,$$

or/ $$\boxed{E_{n'j} = \pm mc^2\Big/\left\{1+\left[Z\alpha\Big/\left(n'+\sqrt{(j+\tfrac{1}{2})^2-(Z\alpha)^2}\right)\right]^2\right\}^{1/2}}. \tag{14}$$

These are the bound state energies for a Dirac particle in the Coulomb potential of Eq (1). Note that now E depends on <u>two</u> quantum numbers, n' & $j = l \pm \frac{1}{2}$.

REMARKS On Dirac's Coulomb energies of Eq. (14).

1. The ± for $E_{n'j}$ are for the (±)ve energy states, of course. The ordinary H-atom energies are the +ve branch, with energies $0 < E_{n'j} \leq +mc^2$. The conventional eigenenergies are $\mathcal{E}_{n'j} = E_{n'j} - mc^2 \leq 0$.

2. Bohr's principal quantum # n is defined for the Dirac energies as...

$$\underline{n = n' + (j + \tfrac{1}{2})} = 1, 2, 3, \ldots \quad (n=1 \text{ is the ground state}) \tag{15}$$

so// $\mathcal{E}_{nj} = E_{nj} - mc^2$, are conventional eigenenergies...

or//

$$\mathcal{E}_{nj} = -mc^2 \left\{ 1 - \left[1 + \left(\frac{Z\alpha}{n - (j+\frac{1}{2}) + \sqrt{(j+\frac{1}{2})^2 - (Z\alpha)^2}} \right)^2 \right]^{-\frac{1}{2}} \right\} \tag{16}$$

This is the evolution of Bohr's energies $\mathcal{E}_n = -\frac{1}{2}(Z\alpha)^2 mc^2/n^2$ in the hands of Dirac. $\mathcal{E}_{nj}$ (Dirac) bears little resemblance to the <u>nonrelativistic</u> energies $\mathcal{E}_n$(Bohr), but has generic similarities to the <u>relativistic</u> energies $\mathcal{E}_{nl}$(KG) of the Klein-Gordon eqtn [see Eq. (21), p. fs (19) of class notes].

3. Eq (16) can be expanded in powers of the small parameter $(Z\alpha/n)$, with result

$$\boxed{\mathcal{E}_{nj} = \mathcal{E}_n \left\{ 1 + \left(\frac{Z\alpha}{n}\right)^2 \left[\frac{n}{j+\frac{1}{2}} - \frac{3}{4} \right] + \mathcal{O}\left(\frac{Z\alpha}{n}\right)^4 + \ldots \right\}}, \tag{17}$$

where: $\mathcal{E}_n = -\frac{1}{2} mc^2 (Z\alpha/n)^2$ = Bohr energies.

So $\mathcal{E}_{nj}$ (Dirac) <u>does</u> include $\mathcal{E}_n$(Bohr), as the lowest order approxn (good only when $c \to \infty$). The next term in the Dirac expansion, i.e. the 2nd term inside the { } in Eq. (17), is the <u>Dirac finestructure</u> -- it is a correction of $\mathcal{O}(v/c)^2$ w.r.t. $\mathcal{E}_n$ (Bohr), and agrees exactly with the patchwork version of the finestructure we achieved in Eq. (33), p. fs 13 of class notes.

REMARKS On Dirac's Coulomb energies in Eq. (14) [cont'd].

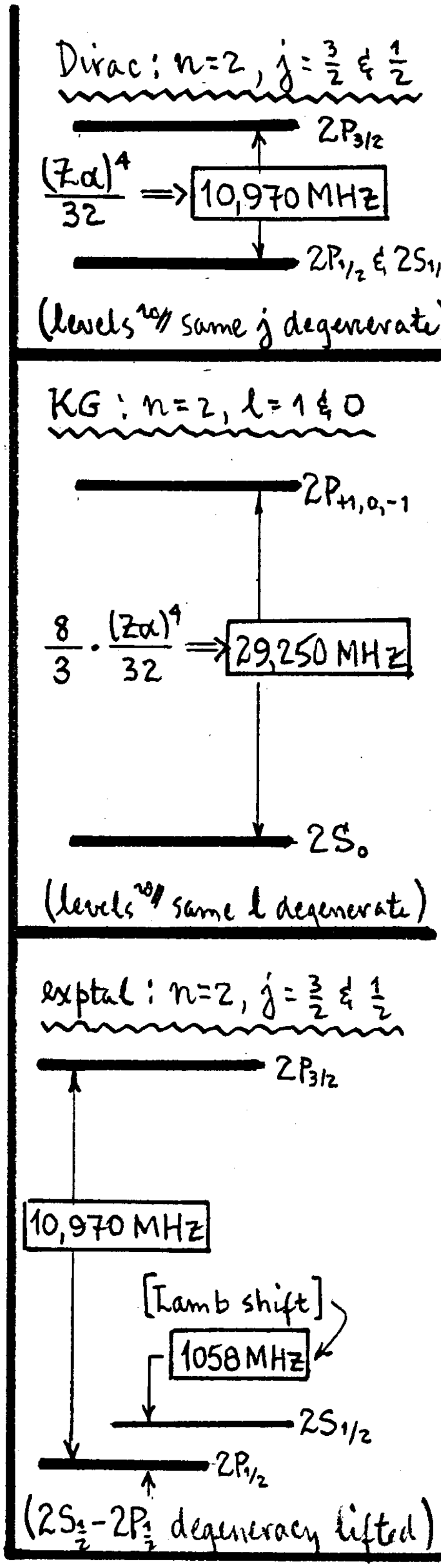
4. It is interesting to compare the Dirac fs (finestructure) with that calculated from Klein-Gordon theory [Eq. (32), p. fs 13, class notes]. Let the fs correction be $\Delta\mathcal{E}_{nj} = \mathcal{E}_{nj} - \mathcal{E}_n(\text{Bohr})$, so...

$$\left.\begin{matrix}\text{Dirac}\\ \text{fs}\end{matrix}\right\} \quad \frac{\Delta\mathcal{E}_{nj}}{mc^2} = -\left(\frac{Z\alpha}{n}\right)^4\left[\frac{n}{2j+1} - \frac{3}{8}\right], \; j = l \pm \tfrac{1}{2};$$

$$\Rightarrow \text{interval}: \frac{1}{mc^2}\Delta\mathcal{E}_{nj}\left(j = \tfrac{3}{2} \to \tfrac{1}{2}\right) = (Z\alpha)^4/4n^3. \quad (18)$$

$$\left.\begin{matrix}\text{KG}\\ \text{fs}\end{matrix}\right\} \quad \frac{\Delta\mathcal{E}_{nl}}{mc^2} = -\left(\frac{Z\alpha}{n}\right)^4\left[\frac{n}{2l+1} - \frac{3}{8}\right], \; l = 0, 1, 2, \ldots$$

$$\Rightarrow \text{interval}: \frac{1}{mc^2}\Delta\mathcal{E}_{nl}(l = 1 \to 0) = \frac{8}{3}(Z\alpha)^4/4n^3. \quad (19)$$



The resulting fs for the 2S & 2P levels in the $n=2$ state of the H-atom ($Z=1$) is shown in the sketch (more or less to scale). In comparing Eqs. (19) & (18), we see "all" that has happened in going from the KG solution to the Dirac solution is that we have replaced the orbital ∡ momentum quantum # l by the total ∡ momentum quantum # $j = l \pm \frac{1}{2}$, with the $\pm\frac{1}{2}$ present because of the electron spin. Although the Dirac & KG fs terms are formally similar under $j \to l$, they predict very different fs energy intervals, as shown; as well, they predict a different ordering of the levels.

The exptal results are shown at right, for H($n=2$). The Dirac fs correctly predicts the $2P_{3/2} - 2P_{1/2}$ splitting. BUT, the predicted $2P_{1/2} - 2S_{1/2}$ degeneracy is not there... it is lifted by the "Lamb shift" (of size ≃ 10% of the interval). This is the first crack in Dirac's monolith.

Terms contributing to the Dirac fs correction.

3) It is instructive to trace the terms that contribute to the Dirac fs correction in Eq. (18). Recall that when we did the $\mathcal{O}(1/c^2)$ reduction of the Dirac Eqtn [ref. pp. DE 22-23 above], we arrived at the expression [Eq. (10), p. DE 23]:

$$\rightarrow [\mathcal{H}_S + \mathcal{H}_{KE} + \mathcal{H}_{SO} + \mathcal{H}_D]\Phi = \mathcal{E}\Phi, \quad \text{w/ } \mathcal{E} = E - mc^2 = \text{conventional eigenenergy}, \tag{20}$$

where/

$$\left.\begin{array}{ll} & \mathcal{H}_S = (\mathbf{p}^2/2m) + q\phi \ \ldots \text{ Schrödinger Ham}^{\underline{n}} \text{ in external potential } \phi, \\ \boxed{1} & \mathcal{H}_{KE} = -\mathbf{p}^4/8m^3c^2 \ldots \ \mathcal{O}(v/c)^2 \text{ correction to kinetic energy}, \\ \boxed{2} & \mathcal{H}_{SO} = -(q\hbar/4m^2c^2)\,\boldsymbol{\sigma}\cdot(\mathbb{E}\times\mathbf{p}) \ldots \text{ spin-orbit interaction}, \\ \boxed{3} & \mathcal{H}_D = -\frac{1}{8}q(\hbar/mc)^2\,\nabla\cdot\mathbb{E} \ldots \text{ Darwin term (ZitterBewegung).} \end{array}\right\} \tag{21}$$

Here: $q = -e$ for an electron, $\mathbb{E} = -\nabla\phi$ is the external electric field, and the external magnetic field has been taken to be $\mathbb{B} \equiv 0$. NOTE: $\mathcal{H}_{KE}$, $\mathcal{H}_{SO}$, & $\mathcal{H}_D$ are all $\mathcal{O}(v/c)^2$ [i.e. $\mathcal{O}(\alpha^2)$] relative to $\mathcal{H}_S$, and can be considered as perturbations on the Schrödinger problem. To find their sizes, calculate in the Schrödinger basis, i.e. with two component spinor wavefcns $\Phi \times |u\rangle$ or $|d\rangle$ such that:

$$\mathcal{H}_S\Phi = \mathcal{E}_n\Phi \Rightarrow \text{Schrodinger solution} \begin{cases} \Phi = \Phi(nlm), \text{ nonrel. H-atom wavefcns;} \\ \underline{\underline{\mathcal{E}_n = -\frac{1}{2}mc^2(Z\alpha/n)^2}}, \text{ Bohr energies.} \end{cases} \tag{22}$$

The Dirac fs correction -- to $\mathcal{O}(\alpha^2)$ as in Eq. (18) -- is then composed of the perturbations on the Bohr energies $\mathcal{E}_n$ due to $\mathcal{H}_{KE}$, $\mathcal{H}_{SO}$, & $\mathcal{H}_D$. They are, in turn:

$\boxed{1}$ KE CORRECTION

see previous work in Eq. (27)-(32), pp. fs 12-13.

$$\Delta\mathcal{E}_{KE} = \langle\Phi|\mathcal{H}_{KE}|\Phi\rangle = -\frac{1}{8}mc^2\int\Phi^\dagger(\mathbf{p}/mc)^4\,\Phi\, d^3x$$

or/

$$\underline{\underline{\Delta\mathcal{E}_{KE} = \mathcal{E}_n\left(\frac{Z\alpha}{n}\right)^2\left[\frac{n}{l+\frac{1}{2}} - \frac{3}{4}\right]}}, \text{ all } l = 0, 1, 2, \ldots \tag{23}$$

This is identical to the Klein-Gordon fs to relative $\mathcal{O}(1/c^2)$ [Eq. (22), p. fs 19]. And there are no more $\mathcal{O}(v/c)^2$ corrections in the KG eqtn.

Terms contributing to Dirac fs correction (cont'd).

2 SPIN-ORBIT CORRECTION

For a central potential $V(r)$: $q\mathbb{E} = -\nabla V = -\hat{r}\,\frac{\partial V}{\partial r}$, w/ $\hat{r} = \frac{\mathbf{r}}{r}$.

so/ $\longrightarrow \mathcal{H}_{SO} = \frac{+\hbar}{4m^2c^2}\left(\frac{1}{r}\frac{\partial V}{\partial r}\right)\boldsymbol{\sigma}\cdot(\mathbf{r}\times\mathbf{p})$ ∫ set $(\mathbf{r}\times\mathbf{p}) = \hbar\mathbb{L}$, $\mathbb{L}$ = dimensionless orbital ∡ momentum operator; $\mathbb{S} = \frac{1}{2}\boldsymbol{\sigma}$, $\mathbb{S}$ = dimensionless spin ∡ mom. operator;

or/

$$\mathcal{H}_{SO} = 2\mu_0^2\left(\frac{1}{e^2}\frac{1}{r}\frac{\partial V}{\partial r}\right)\underbrace{\mathbb{S}\cdot\mathbb{L}}_{\text{spin-orbit}},\quad \text{w/ } \mu_0 = e\hbar/2mc = \text{Bohr magneton}. \tag{24}$$

For Coulomb potential $V = -\frac{Ze^2}{r}$: $(1/e^2)\frac{1}{r}(\partial V/\partial r) = +Z/r^3$ }

$$\mathcal{H}_{SO} = 2\left(\frac{Z\mu_0^2}{r^3}\right)\mathbb{S}\cdot\mathbb{L}. \tag{25}$$

In this form $\mathcal{H}_{SO}$ can be interpreted as a magnetic dipole energy--viz. a coupling between the electron spin magnetic moment $\boldsymbol{\mu}_e = 2\mu_0\mathbb{S}$ and the field $\mathbb{B}_L = (Z\mu_0/r^3)\mathbb{L}$ generated by the relative orbital motion of the nucleus. Note that $\mathbb{B}_L$ has its Thomas precession factor built-in [see p. fs10, Eq. (22)], and $\boldsymbol{\mu}_e$ shows the correct g-value: $g_s = 2$ [p. fs2, Eq. (6)].

$$\Delta\mathcal{E}_{SO} = \langle\Phi|\mathcal{H}_{SO}|\Phi\rangle = \frac{1}{2}(Z\alpha)^4 mc^2 \int \Phi^\dagger\left\{\left[\frac{a_0/Z}{r}\right]^3 \mathbb{S}\cdot\mathbb{L}\right\}\Phi\, d^3x,$$

or/

$$\Delta\mathcal{E}_{SO} = \frac{1}{2}mc^2\frac{(Z\alpha)^4}{n^3}\langle\mathbb{S}\cdot\mathbb{L}\rangle/\ell(\ell+1)(\ell+\tfrac{1}{2}),\quad \text{for } \ell\neq 0 \tag{26}$$

∫ see Davydov Eq. (38.17e)

$$\text{Here: } \langle\mathbb{S}\cdot\mathbb{L}\rangle = \frac{1}{2}\left[j(j+1)-\ell(\ell+1)-\frac{3}{4}\right] = \begin{cases} +\frac{1}{2}\ell, & \text{for } j=\ell+\frac{1}{2}, \\ -\frac{1}{2}(\ell+1), & \text{for } j=\ell-\frac{1}{2}. \end{cases} \tag{27}$$

Now combine the K.E. & S-O corrections, Eqs. (23) & (26), to form...

$$\boxed{(\Delta\mathcal{E}_{KE}+\Delta\mathcal{E}_{SO})\big|_{\ell\neq 0} = \mathcal{E}_n\left(\frac{Z\alpha}{n}\right)^2\left[\frac{n}{j+1/2}-\frac{3}{4}\right]\Big|_{j=\ell\pm\frac{1}{2}} = \Delta\mathcal{E}_{nj}(\text{Dirac})}. \tag{28}$$

This is exactly the Dirac fs correction [2nd term in { }, RHS of Eq. (17), p. DE52] for all but S-states ($\ell=0$). The $\ell\neq 0$ fs corrections evidently do not depend on the Darwin term $\mathcal{H}_D$ in Eq. (21); the S-state fs must depend on $\mathcal{H}_D$, otherwise they are moved only by $\mathcal{H}_{KE}$ (since $\langle\mathbb{S}\cdot\mathbb{L}\rangle \equiv 0$ for $\ell=0$ states).

The Darwin contribution to Dirac fs correction.

3 DARWIN CORRECTION

For a (strict) Coulomb potential: $V(r) = -\frac{Ze^2}{r}$, have: $\mathbb{E} = \frac{1}{e}\nabla V = \left(\frac{Ze}{r^3}\right)\mathbf{r}$, and $\nabla\cdot\mathbb{E} = 4\pi\rho(r)$, w/ $\rho(r) = Ze\,\delta(r)$. The charge density ρ is that of a point nucleus at the origin. For an electron ($q = -e$) the Darwin term in (21) is:

$$\underline{\mathcal{H}_D = +\frac{1}{8}e(\hbar/mc)^2\cdot 4\pi Ze\,\delta(r)}\,,\quad \delta(r) = \text{Dirac delta fcn.} \tag{29}$$

So/ $\Delta\mathcal{E}_D = \langle\Phi|\mathcal{H}_D|\Phi\rangle = 2\pi Z(e\hbar/2mc)^2\int\Phi^\dagger\delta(r)\Phi\,d^3x$

or/ $$\underline{\underline{\Delta\mathcal{E}_D = 2\pi Z\mu_0^2|\Phi(0)|^2}}\,,\quad \text{w/}\ \mu_0 = \frac{e\hbar}{2mc} = \text{Bohr magneton} \tag{30}$$

Here $\Phi(0)$ is the value of the Schrödinger wavefcn at the origin. All such wavefcns with $l\neq 0$ vanish at $r = 0$: $\Phi(0)|_{l\neq 0} \equiv 0$, so indeed the Darwin term does not contribute to the $l\neq 0$ Dirac fs calculated in Eq. (28). On the other hand, $\mathcal{H}_D$ does contribute to the fs of n S-states, since...

$$\left.\begin{array}{l}\text{for } n\text{S states, } l=0 \text{ only}\\ (\text{with: } a_0 = \hbar^2/me^2 = \text{Bohr radius})\end{array}\right\}\ |\Phi(0)|^2 = \frac{1}{\pi}(Z/na_0)^3 \tag{31}$$

$$\xrightarrow{\text{so}}\Delta\mathcal{E}_D = 2\left(\frac{Z\mu_0^2}{a_0^3}\right)[Z/n]^3 = \frac{1}{2}mc^2(Z\alpha/n)^4\frac{n}{j+1/2}\quad \sqrt{\ } j=\tfrac12 \text{ only for } n\text{S-states}\ \bigstar \tag{32}$$

The (μ_0^2/a_0^3) here implies $\Delta\mathcal{E}_D$ is a type of spin-orbit correction, but in fact for nS-states $\Delta\mathcal{E}_{so}$ in (26) vanishes (because $\mathbb{L} = 0$). So we combine...

$\mathcal{E}_n = \mathcal{E}_n(\text{Bohr}) = -\frac{1}{2}mc^2(Z\alpha/n)^2$

$$\boxed{(\Delta\mathcal{E}_{KE} + \Delta\mathcal{E}_D)\Big|_{l=0} = \mathcal{E}_n\left(\frac{Z\alpha}{n}\right)^2\left[\frac{n}{j+1/2} - \frac{3}{4}\right]\Big|_{j=1/2} = \Delta\mathcal{E}_{nj}(\text{Dirac})}\,. \tag{33}$$

We see that the Dirac form for the fs correction is the same for $l = 0$ states as for $l\neq 0$ [Eq. (28)], and that $\mathcal{H}$(Darwin) does for S-states what $\mathcal{H}$(Spin-orbit) does for non-S states. However, $\mathcal{H}_D$ has much different physics in it than $\mathcal{H}_{so}$ -- $\mathcal{H}_D$ results from an actual contact between the electron & nucleus, while $\mathcal{H}_{so}$ takes place at a distance.

$\bigstar = \mu_0^2/a_0^3 = \frac{1}{4}\alpha^4 mc^2$, w/ $\alpha = e^2/\hbar c$.

What Dirac has done to Schrödinger's ground state.

4) We close this section on Dirac's H-atom with a brief look at how the theory has changed in going from Schrödinger's account to Dirac's picture. As an exemplar, we choose the ground state w/ $n(\text{Bohr}) = 1$. So for $1^2S_{1/2}$ in H...

GROUND STATE (binding) ENERGY

Schrödinger : $\mathcal{E}^{(S)}_{gnd} = \mathcal{E}_n(\text{Bohr})\big|_{n=1} = -\frac{1}{2}mc^2(Z\alpha)^2$. (34A)

Dirac : $\mathcal{E}^{(D)}_{gnd} = \mathcal{E}_{nj}\,[\text{Eq.}(16)]\big|_{n=1,\,j=\frac{1}{2}} = -mc^2\left\{1 - \sqrt{1-(Z\alpha)^2}\right\}$. (34B)

... expanding : $\boxed{\mathcal{E}^{(D)}_{gnd} = \mathcal{E}^{(S)}_{gnd}\left[1 + \underbrace{\tfrac{1}{4}(Z\alpha)^2}_{13.3\times10^{-6}} + \underbrace{\tfrac{1}{8}(Z\alpha)^4}_{0.355\times10^{-9}} + \dots\right]}$ (for $Z=1$) (35)

The 2nd term RHS in (35), i.e. $\frac{1}{4}(Z\alpha)^2$, is just the Dirac fs correction calculated in Eq. (33) [for $n=1$ & $j=\frac{1}{2}$]. The term in $\frac{1}{8}(Z\alpha)^4$ is actually detectable, in the sense that the H-atom ionization energy $|\mathcal{E}_{gnd}|$ has been measured to $\sim 1\,\text{part}/10^{10}$.

GROUND STATE WAVEFUNCTION

Schrödinger : $\phi^{(S)}_{gnd}(r) = \frac{1}{\sqrt{\pi}}(Z/a_0)^{\frac{3}{2}}\exp\left(-\frac{Zr}{a_0}\right)$, $a_0 = \frac{\hbar^2}{me^2}$ = Bohr radius. (36A)

Dirac : $\psi^{(D)}_{gnd}(r) = \mathcal{N}\,\phi^{(S)}_{gnd}(r)\cdot\left(\frac{Zr}{a_0}\right)^{-(1-\delta)}\begin{bmatrix}\chi \\ \left(\frac{1-\delta}{Z\alpha}\right) i\sigma\cdot\hat{r}\,\chi\end{bmatrix}$,

w/ $\delta = \sqrt{1-(Z\alpha)^2}$, & $\mathcal{N} = \frac{1}{2^{1-\delta}}\left[(1+\delta)/\Gamma(1+2\delta)\right]^{1/2}$. (36B)

χ is a Pauli 2-component spinor : $\chi = \binom{1}{0}$ or $\binom{0}{1}$, depending on whether $m_j = +\frac{1}{2}$ or $-\frac{1}{2}$ for the electron. In the nonrelativistic limit $c\to\infty$, have $\alpha\to0$ & $\delta\to1$; then $\mathcal{N}\to1$, $(Zr/a_0)^{-(1-\delta)}\to1$, and $\underline{\underline{\psi^{(D)}_{gnd}\to\phi^{(S)}_{gnd}\,\chi}}$ ... i.e. the Dirac wavefcn is just the (Schrodinger wavefcn)×(Pauli spinor). The new factor $(Zr/a_0)^{\delta-1} = \exp\left[(1-\delta)\ln\left(\frac{a_0/Z}{r}\right)\right]$ is unity except at *very* small distances... $(1-\delta)\ln\left(\frac{a_0/Z}{r}\right)\sim1 \Rightarrow r\sim(a_0/Z)\cdot e^{-(1/(1-\delta))} = (a_0/Z)\cdot10^{-16224/Z^2}$.