(3d) Dirac Equation

I. Recall: non-relativistic Sch. Eqn, ok only for $\beta = v/c << 1$, since use $E = \frac{p^2}{2m}$

OK e.g. for H-atom analysis where in g.s.

$\beta = \alpha \Leftrightarrow \frac{v}{c} = \frac{1}{137}$ ✓

... still measurable fine structure $\left(\left(\frac{p}{c}\right)^4\right)$ corrections.

- p^4 corrections.
- spin-orbit interactions
- spin (e.g., Zeeman effect) ?
- $g = 2$

$$H_{\text{nonrel.}} = \frac{p^2}{2m} + V \underset{\text{for } V=0}{\Leftrightarrow} E = \frac{p^2}{2m}$$

generalize to encode $E = \underbrace{\sqrt{p^2c^2 + m^2c^4}}$

how?
$$\underset{\beta<<1}{\simeq} mc^2 + \frac{p^2}{2m} - \left(\frac{p^2}{m^2c^2}\right)^2 \frac{mc^2}{8} + \dots$$

$H = \sqrt{\hat{p}^2c^2 + m^2c^4}$ ← not a good treatment

e.g., not symm treatment of $\vec{x}$ & t.

A. $H^2 = \hat{p}^2c^2 + m^2c^4 \equiv H_{\text{Klein-Gordon}}$

$$\Rightarrow -\hbar^2\partial_t^2|\psi\rangle = (\hat{p}^2c^2 + m^2c^4)|\psi\rangle$$

$$\Rightarrow \left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \left(\frac{m\cancel{c^2}}{\hbar}\right)^2\right]|\psi\rangle = 0 \quad \text{K-G eqn.}$$

but $|\psi\rangle$ is a scalar, not spinor, since H_{KG} is a scalar in spin space (not matrix)

good for pions, kaons, etc spinless bosons.

B. Dirac, P.A.M.

... taking the sqr-root of H_{KG}.
i.e.,
require $H_{KG} = H_{Dirac}^2$

$$p^2c^2 + m^2c^4 = (c\alpha_x p_x + c\alpha_y p_y + c\alpha_z p_z + \beta mc^2)^2$$
$$= (c\vec{\alpha}\cdot\vec{p} + \beta mc^2)^2$$
$$= c^2(\alpha_x^2 p_x^2 + \alpha_y^2 p_y^2 + \alpha_z^2 p_z^2) + \beta^2 m^2 c^4$$
$$+ c^2 p_x p_y (\alpha_x\alpha_y + \alpha_y\alpha_x) + \text{cyclic perm}$$
$$+ mc^3 p_x (\alpha_x\beta + \beta\alpha_x) + x\to y\to z$$

$$\Rightarrow \left.\begin{array}{ll} \alpha_i^2 = \beta^2 = 1 & (i = x, y, z) \\ \{\alpha_i, \alpha_j\} = 0 & (i \neq j) \end{array}\right\} \Leftrightarrow \{\alpha_i, \alpha_j\} = 2\delta_{ij}$$

$$\{\alpha_i, \beta\} = 0$$

$\alpha_x\alpha_y = -\alpha_y\alpha_x$

$\alpha_x\alpha_y^2 = -\alpha_y\alpha_x\alpha_y$

$\underline{\mathrm{Tr}\,\alpha_x = 0} \Leftarrow \mathrm{Tr}\,\alpha_x = -\mathrm{Tr}\,\alpha_y\alpha_x\alpha_y = -\mathrm{Tr}\,\alpha_x$

$\Rightarrow \alpha_i, \beta$ are matrices (obeying Clifford Algebra
Hermitian & traceless, eigen's ± 1.

$\Rightarrow$ also <u>even</u> dimensional.

[recall in 2d $\sigma_x, \sigma_y, \sigma_z$ satisfy these
props since $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$, etc

... but we need 4 matrices in 3d
3+1
space + time

covariant form:

$$i\hbar\,\partial_t \psi = (c\vec{\alpha}\cdot\vec{p} + \beta m c^2)\psi$$

$$\times\beta \quad \Big[\underbrace{i\hbar\beta\partial_t}_{\equiv\gamma^0} - c\underbrace{\beta\vec{\alpha}}_{\equiv\gamma^i}\cdot(-i\hbar\vec{\nabla}) - mc^2\Big]\psi = 0 \quad\Rightarrow\quad i\hbar\gamma^\mu\partial_\mu\psi - mc\psi = 0$$

$$c\frac{\partial}{\partial x_0}, \quad x_0 = ct$$

$$j^0 = \psi^\dagger\psi \equiv \overline{\psi}\gamma^0\psi, \quad \overline{\psi} = \psi^\dagger\gamma^0$$

$$j^i = c\psi^\dagger\alpha^i\psi = \overline{\psi}\gamma^i\psi$$

$$\Rightarrow \quad \partial_t n + \nabla\cdot j = 0 \iff \partial_\mu j^\mu = 0.$$

$$j^\mu = \overline{\psi}\gamma^\mu\psi$$

$$i\hbar\gamma^\mu\partial_\mu\psi - mc\psi = 0$$

$$\Rightarrow \quad i\hbar\gamma^\mu\left(\partial_\mu + i\frac{q}{\hbar c}A_\mu\right)\psi - mc\psi = 0$$

$$A_\mu = (\phi, \vec{A})$$

$\Rightarrow$ need (at least) 4×4 matrices.
not unique since $\vec{\alpha} \to S^{+}\vec{\alpha}S$, $\beta \to S^{+}\beta S$
preserve above props for unitary S.

common choice: $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$, $\beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}$

free Dirac Eqn:

$$\Rightarrow \boxed{i\hbar\,\partial_t|\psi\rangle = (c\,\vec{\alpha}\cdot\vec{p} + \beta mc^2)|\psi\rangle}$$

$\Rightarrow |\psi\rangle \to \vec{\psi}$ is a 4-component object.

Lorentz spinor

Why 4 (instead of 2) component?

Dirac discovered spin and antiparticles (e.g. positrons).

Conservation of particle #:

$$\int \psi^{+}\psi\, d^3r = \text{const} \quad \text{since } H_D^{+} = H_D$$

$\Rightarrow$ local conservation law (continuity eqn):

$$\partial_t P + \vec{\nabla}\cdot\vec{J} = 0$$

where $P = \psi^{+}\psi$, $\vec{J} = c\,\psi^{+}\vec{\alpha}\,\psi$

$\Leftrightarrow \partial_\mu j_\mu = 0$, w/ $j_\mu = [\psi^{+}(\mathbb{1}, \vec{\alpha}c)\psi]$

II. Dirac Eqn for $\underline{\text{photon}}$?

$\uparrow$ spin 1 particle

Maxwell's Eqns:

(1) $\vec{\nabla}\times\vec{E} = -\frac{1}{c}\partial_t\vec{B}$

(2) $\vec{\nabla}\times\vec{B} = \frac{1}{c}\partial_t\vec{E}$

$\Rightarrow \frac{1}{c}\partial_t^2\vec{E} - \nabla^2\vec{E} = 0$

(cf. Klein-Gordon Eqn w/ $m=0$)

same for $\vec{B}$

introduce $\vec{\Psi} = \vec{E} + i\vec{B}$

$\Rightarrow$ (1) $+ i$(2)

$$(i\epsilon_{ijk})(-i\hbar)\partial_i\Psi_j = +\frac{1}{c}i\hbar\partial_t\Psi_k$$

$$\Rightarrow \quad c(\vec{\alpha}\cdot\vec{p})_{ij}\Psi_j = i\hbar\partial_t\Psi_i$$

where $(\vec{\alpha}_{ij})^k = i\epsilon_{ijk} = \frac{i}{\hbar}S^k_{ij} \leftarrow$ 3 generators 3×3 of rotation for $S=1$ represent.

$E \Longleftrightarrow -E$ spectrum:

$$E\,\Psi_E = H_D\,\Psi_E$$

$$H_D = c\vec{\alpha}\cdot\vec{p} + \beta m c^2$$

consider $\gamma = \alpha_x \alpha_y \alpha_z \beta$

<u>Note that</u>: $\{\gamma, H_D\} = 0$

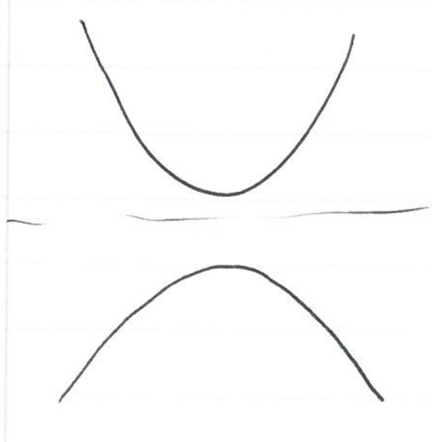
e.g. $\underbrace{\alpha_x \alpha_y \alpha_z}_{\gamma} \beta\, \alpha_x = (-1)\, \alpha_x \underbrace{\alpha_x \alpha_y \alpha_z}_{\gamma}$

etc.

$$\Rightarrow \quad E(\gamma \Psi_E) = \underbrace{\gamma H_D}_{-H_D \gamma} \Psi_E$$

$$\Rightarrow \quad (-E)(\gamma \Psi_E) = H_D(\gamma \Psi_E)$$

$$\Rightarrow \quad \underline{\Psi_{-E} \equiv \gamma \Psi_E}$$



Interactions / Potential

$$\underbrace{i\hbar\partial_t}\vec{\Psi} = (c\vec{\alpha}\cdot\vec{p} + \beta mc^2)\cdot\vec{\Psi}$$

$$E \to E + V$$

$V \leftarrow q\phi$

$$i\hbar\partial_{x_0} - \frac{q}{c}\phi$$

gauge invnce: $\begin{cases} i\hbar\partial_t \to i\hbar\partial_t - q\phi \sim i\partial_0 - \frac{q}{c}A_0 \\ -i\hbar\vec{\nabla} \to -i\hbar\vec{\nabla} - \frac{q}{c}\vec{A} \sim i\partial_i - A_i \end{cases}$

$(i\hbar\partial_\mu - \frac{q}{c}A_\mu)$

$$\Rightarrow \boxed{i\hbar\partial_t\vec{\Psi} = \left(c\vec{\alpha}\cdot(\vec{p} - \tfrac{q}{c}\vec{A}) + \beta mc^2 + q\phi\right)\cdot\vec{\Psi}}$$

III. Spin & $\vec{\mu}$ for electron.

take $\phi = 0$ & go to non-relativistic $\beta \ll 1$ limit.

$$\vec{\Psi}(t) = \vec{\Psi}\, e^{-iEt/\hbar}$$

$$\Rightarrow \left[c\vec{\alpha}\cdot\overbrace{(\vec{p} - \tfrac{q}{c}\vec{A})}^{\vec{\pi}} + \beta mc^2\right]\vec{\Psi} = E\vec{\Psi}$$

$$\vec{\Psi} = \begin{pmatrix} \chi \\ \varphi \end{pmatrix}$$ ← 2 component spinors.

$$\Rightarrow \begin{pmatrix} E - mc^2 & -c\vec{\sigma}\cdot\vec{\pi} \\ -c\vec{\sigma}\cdot\vec{\pi} & E + mc^2 \end{pmatrix}\begin{pmatrix} \chi \\ \varphi \end{pmatrix} = 0$$

$$\Rightarrow \underbrace{(E - mc^2)}_{E_{\text{schrodinger}}}\chi - c\vec{\sigma}\cdot\vec{\pi}\varphi = 0$$

$$(E + mc^2)\varphi - c\vec{\sigma}\cdot\vec{\pi}\chi = 0$$

$$\Rightarrow \varphi = \frac{c\vec{\sigma}\cdot\vec{\pi}}{E + mc^2}\chi \underset{\frac{v}{c}\ll 1}{\simeq} \frac{c}{2mc^2}\vec{\sigma}\cdot\vec{\pi}\chi$$

small components large

$$\Rightarrow E_s\chi = \frac{(\vec{\sigma}\cdot\vec{\pi})(\vec{\sigma}\cdot\vec{\pi})}{2m}\chi$$

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

& $\vec{\pi}\times\vec{\pi} = \frac{iq\hbar}{c}\vec{B}$

$\Rightarrow$ low $\frac{v}{c} \ll 1 \Rightarrow \left(\frac{(\vec{p} - \frac{q}{c}\vec{A})^2}{2m} - \frac{q\hbar}{2mc}\vec{\sigma}\cdot\vec{B}\right)\chi = E_s\chi$

$\Rightarrow$ spin ½ particle (χ w/ 2 comp., σ 2x2)

with $g = 2$ & $\vec{\mu} = g\frac{q\hbar}{2mc}\frac{\vec{\sigma}}{2} = g\mu_B\vec{S}$

$$\uparrow \quad 2 \quad \frac{q}{2mc} \quad \frac{\hbar\vec{\sigma}}{2}$$

IV. Spin-orbit interaction & H fine structure

$$\vec{A}=0, \quad V = e\phi = -\frac{e^2}{r}$$

$$\Rightarrow (E - V - mc^2)\chi - c\vec{\sigma}\cdot\vec{p}\varphi = 0$$

$$(E - V + mc^2)\varphi - c\vec{\sigma}\cdot\vec{p}\chi = 0$$

large comp.

$$\Rightarrow (E - V - mc^2)\chi = c\vec{\sigma}\cdot\vec{p}\Big(\underbrace{\frac{1}{E-V+mc^2}}_{\simeq 2mc^2}\Big)c\vec{\sigma}\cdot\vec{p}\chi$$

$$\frac{v}{c} \ll 1 \Rightarrow \quad E_s\chi = \underbrace{\frac{(\vec{\sigma}\cdot\vec{p})^2}{2m}}_{\frac{p^2}{2m}}\chi \quad \leftarrow \text{non-relativ. Sch. Eqn.}$$

need to go to higher v/c order, $\mathcal{O}\left(\left(\frac{v}{c}\right)^4\right)$

use $$\frac{1}{E-V+mc^2} \simeq \frac{1}{2mc^2} - \frac{E_s - V}{4m^2c^4} + \dots$$

$$\Rightarrow (E_s - V)\vec{\sigma}\cdot\vec{p}\,\chi = \vec{\sigma}\cdot\vec{p}(\underbrace{E_s - V}_{\simeq \frac{p^2}{2m}})\chi + \vec{\sigma}\cdot[E_s - V, \vec{p}]\chi$$

$$= (\vec{\sigma}\cdot\vec{p})\frac{p^2}{2m}\chi \quad + \quad \vec{\sigma}\cdot[\vec{p}, V]\chi$$

$$\Rightarrow E_s\chi = \left[\frac{p^2}{2m} + V - \frac{p^4}{8m^3c^2} - \frac{(\vec{\sigma}\cdot\vec{p})(\vec{\sigma}\cdot[\vec{p},V])}{4m^2c^2}\right]\chi$$

$$E_s\chi = \underbrace{\left[\frac{p^2}{2m} + V - \frac{p^4}{8m^3c^2} - \frac{i\vec{\sigma}\cdot(\vec{p}\times[\vec{p},V])}{4m^2c^2} - \frac{\vec{p}\cdot[\vec{p},V]}{4m^2c^2}\right]}_{H_{\text{sch w/ }\frac{p^4}{c^4}\text{ corrections.}}}\chi$$

$$-\frac{p^4}{8m^3c^2} = H_{p^4}$$ ✓

$$H_{so} = -\frac{i\vec{\sigma}\cdot(\vec{p}\times[\vec{p},V])}{4m^2c^2} = -\frac{i\vec{\sigma}\cdot(\vec{p}\times[-i\hbar\nabla,\frac{-e^2}{r}])}{4m^2c^2}$$

$$= \frac{e^2}{4m^2c^2r^3}\underbrace{(\hbar\vec{\sigma})}_{2\vec{S}}\cdot\underbrace{(\vec{r}\times\vec{p})}_{\vec{L}}$$ ✓

(Thomas $\frac{1}{2}$ factor is automatic)

$$\tilde{H}_{\text{Darwin}} = -\frac{\vec{p}\cdot[\vec{p},V]}{4m^2c^2} = -\frac{1}{4m^2c^2}\vec{p}\cdot(\vec{p}V - V\vec{p})$$

$$\left([\vec{p}\cdot(\vec{p}V - V\vec{p})]^+ = V\vec{p}\cdot\vec{p} - \vec{p}\cdot V\vec{p}\right)$$

non Hermitian

$\Rightarrow \int |\chi|^2 d^3r \neq$ non const in time.

since $\int |\chi|^2 + |\varphi|^2$ is conserved but not φ, χ indepen*d*.

but $|\varphi|^2 \simeq \left|\frac{\sigma\cdot p}{2mc}\chi\right|^2 = \chi^+\frac{p^2}{4m^2c^2}\chi$

$\Rightarrow$ expect $\int \chi^+\left(1+\frac{p^2}{4m^2c^2}\right)\chi\, d^3r \simeq \int\left[\left(1+\frac{p^2}{8m^2c^2}\right)\chi\right]^+\left[\left(1+\frac{p^2}{8m^2c^2}\right)\chi\right]$

$\simeq$ const.

$\Rightarrow$ use $\chi_s = \left(1+\frac{p^2}{8m^2c^2}\right)\chi$ as the sch. ψ.

$\Rightarrow E_s\left(1+\frac{p^2}{8m^2c^2}\right)^{-1}\chi_s = H\left(1+\frac{p^2}{8m^2c^2}\right)^{-1}\chi_s$

$\Rightarrow$

$$E_s \chi_s \simeq \left(1+\frac{p^2}{8m^2c^2}\right) H \left(1-\frac{p^2}{8m^2c^2}\right)\chi_s$$

$$= \underbrace{\left(H + \left[\frac{p^2}{8m^2c^2}, H\right]\right)}_{\equiv H_s .}\chi_s$$

$$\Rightarrow \quad H_{\text{Darwin}} = \frac{1}{8m^2c^2}\left(-2\vec{p}\cdot[\vec{p}, V] + [p\cdot p, V]\right)$$

$$= -\frac{1}{8m^2c^2}\left[\vec{p}\cdot[p, V]\right]$$

$$= +\frac{\hbar^2}{8m^2c^2}\nabla^2 V$$

$$\boxed{H_D = \frac{e^2\hbar^2\pi}{2m^2c^2}\,\delta^{(3)}(r)} \leftarrow \text{affects only S-states.}$$

e.g. $\langle 100 | H_D | 100 \rangle = \frac{e^2\hbar^2\pi}{2m^2c^2}\,\frac{1}{\pi a_0^3} = \underline{\frac{1}{2}mc^2\alpha^4}$

contributes to H's fine-structure.

$$\overline{V(r)} = V(r) + \frac{1}{2!}\sum_{ij}\frac{\partial^2 V}{\partial r_i \partial r_j}\overline{\delta r_i \delta r_j}$$

$$= V(r) + \frac{1}{6}\,\overline{\delta r^2}\,\nabla^2 V$$

$$\overline{\delta r^2} \simeq \frac{\hbar}{mc} \quad \text{Compton } \lambda_c .$$

relativistic particle cannot be localized to $< \lambda_c$.

for the record: exact soln for H: $E_{nj} = mc^2\left[1 + \left(\frac{\alpha}{\underbrace{n-(j+\frac{1}{2}) + [(j+\frac{1}{2})^2 - \alpha^2]^{1/2}}_{\ell\text{-degeneracy (only depends on } j)}}\right)^2\right]^{-1/2}$

... but split by quantum E&M: $\Rightarrow$ Lamb shift $< \begin{matrix} \overline{}\ 2P_{1/2} \\ \overline{}\ 2S_{1/2} \end{matrix}$

Inconsistency of Dirac Eqn

relativistic description $\Rightarrow$ E can be $> Nmc^2$
$\Rightarrow$ can produce many $p-\bar{p}$ pairs $\Rightarrow$

relativity & quantum mechanics inconsistent w/ single particle (fixed particle) description

$\Rightarrow$ quantum field theory of matter a/a qft of light

$\psi_\sigma(\vec{r})$ is a quantum field that annihilates electron at $\vec{r}$ & spin σ

$$\Rightarrow \quad H = \int_{\vec{r}} \psi^\dagger (c\vec{\alpha}\cdot\vec{p} + \beta mc^2)\psi$$

cf $$H_{\text{oscillators}} = \sum_i \hbar\omega_i a_i^\dagger a_i$$