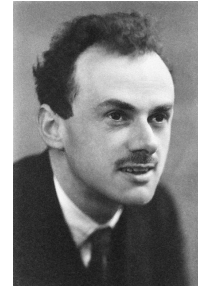


The Dirac Equation

Lit: Harald Friedrich
 "Theoretical Atomic Physics"
 Sec. 2.1.3. (Springer 2006)



Paul Adrien Maurice Dirac
 (* 8. August 1902 in Bristol;
 † 20. Oktober 1984 in Tallahassee)

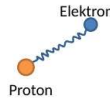
Nobel prize 1933

Aus
https://de.wikipedia.org/wiki/Paul_Dirac

Schrödinger's Hydrogen

Schrödinger Equation (SE)

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi \quad (1.1)$$



The Hamiltonian operator \hat{H} or simply "Hamiltonian" is very often also written without the "hat": $\hat{H} = H$

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(r) \quad (1.2)$$

m = electron mass. Proton shall be infinitely heavy for now

The Laplacian is, in cartesian coordinates

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (1.3)$$

time & space not on equal footing
 ↳ relativity

Dirac Hamiltonian

$$\hat{H} = c \vec{\alpha} \vec{p} + \beta m c^2$$

↑ ↑
 vector coefficient
 of } dimensionless
 coefficients

momentum \vec{p} : components $p_x = \frac{i}{\hbar} \frac{\partial}{\partial x}$

relativistic energy - momentum relation

$$E^2 = p^2 c^2 + m^2 c^4 \quad \hat{H} = c \vec{\alpha} \vec{p} + \beta m c^2$$

\hat{H} should obey this

$$\hat{H}^2 = c^2 \sum_{i,k=1}^3 \frac{1}{2} (\alpha_i \alpha_k + \alpha_k \alpha_i) \hat{p}_i \hat{p}_k + \dots$$

$$+ mc^3 \sum_{i=1}^3 (d_i \beta + \beta d_i) p_i = 0$$

$$+ \beta^2 m^2 c^4$$

$$\Rightarrow (d_i d_k + d_k d_i) = 2 \delta_{ik}$$

$$d_i \beta + \beta d_i = 0$$

$$\beta^2 = 1$$

cannot be fulfilled by simple numbers
must be at least 4×4 matrices

$$\Rightarrow \text{Dirac Equ. } (c \vec{\alpha} \vec{p} + \beta m c^2) \psi = i \hbar \frac{\partial}{\partial t} \psi$$

is for 4-component spinors

$$\psi = \begin{pmatrix} \psi_1(\vec{r}, t) \\ \psi_2(\vec{r}, t) \\ \psi_3(\vec{r}, t) \\ \psi_4(\vec{r}, t) \end{pmatrix}$$

\Rightarrow 4 coupled differential equations

Ansatz stationary solution

$$\psi(\vec{r}, t) = \psi(\vec{r}, t=0) e^{-\frac{i}{\hbar} E t}$$

\Rightarrow time-independent DE

$$(c \vec{\alpha} \vec{p} + \beta m c^2) \psi = E \psi$$

Standard representation

$$\beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Standard representation

$$\rightarrow d_i = \begin{pmatrix} 0 & \hat{\sigma}_i \\ \hat{\sigma}_i & 0 \end{pmatrix} \quad i = x, y, z$$

$$\beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \quad \mathbb{1} = 2 \times 2 \text{ identity matrix}$$

$$\beta = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Pauli matrices

$$\rightarrow \hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\Rightarrow d_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \text{ etc.} \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

4-component spinors $\psi =$

pairs of 2-component spinors

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \quad \text{with} \quad \psi_A = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad \psi_B = \begin{pmatrix} \psi_3 \\ \psi_4 \end{pmatrix}$$

$$\Rightarrow \begin{cases} \hat{\sigma} \cdot \vec{p} \psi_B = \frac{1}{c} (E - mc^2) \psi_A \\ \hat{\sigma} \cdot \vec{p} \psi_A = \frac{1}{c} (E + mc^2) \psi_B \end{cases}$$

$$\hookrightarrow (i\hbar \frac{\partial}{\partial t} + mc^2) \psi_1 - i\hbar \left(\frac{\partial \psi_4}{\partial x} - i \frac{\partial \psi_4}{\partial y} + \frac{\partial \psi_3}{\partial z} \right) = 0$$

and 3 more (cyclic)

e.g. particle at rest $(\vec{p} \psi_A = 0 \quad ; \quad \vec{p} \psi_B = 0)$

gives 2 decoupled equations

↳ 2 solutions with positive energy $E_0 = mc^2$

and $\psi_A = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

up down

⇒ spin states of particles

plus 2 solutions w/ negative energy $E_0 = -mc^2$

again $\psi_B = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

→ spin states of the antiparticle

if particle is not at rest then

pos. energy solutions get contributions from ψ_B

these are small if $E \ll mc^2$

⇒ ψ_B are called "small components"

ψ_A large

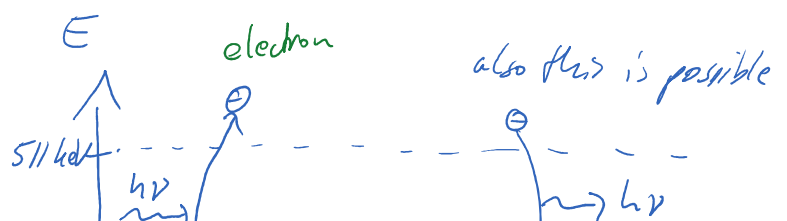
1928 Dirac

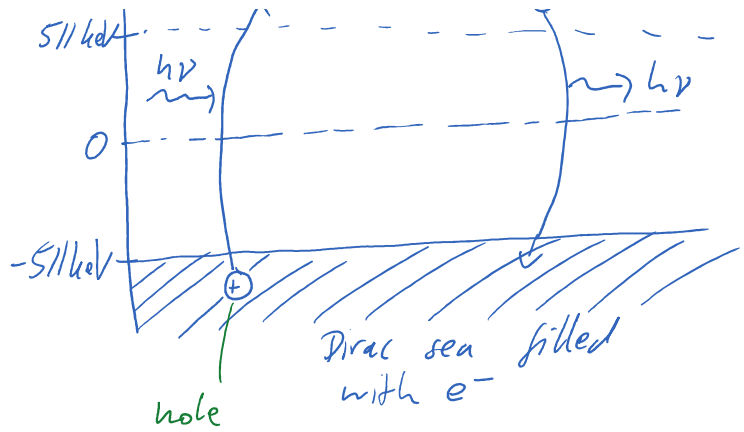
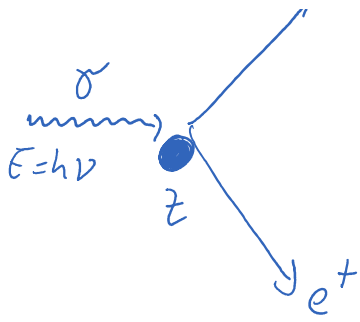
pos. energy solutions = well-known e^-

⊕ spin pops → explains Zeeman effect

neg. energy solutions as if it had a pos. charge: e^+

Dirac sea

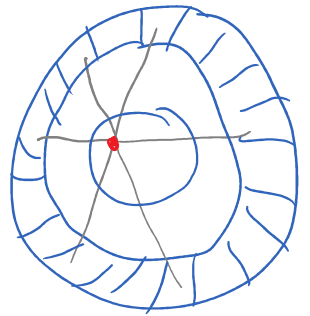




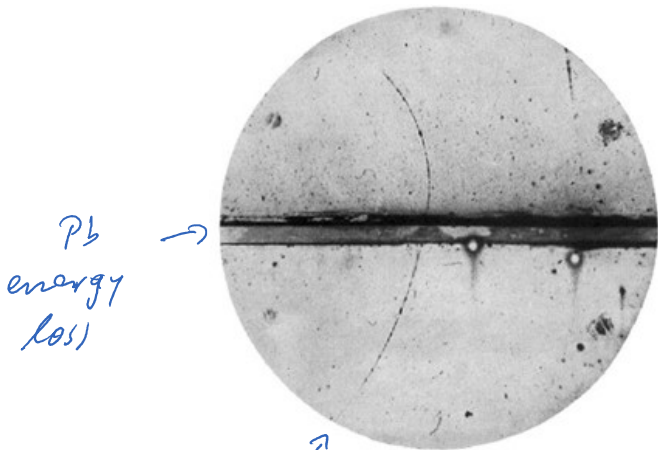
PET scanner

Positron
Emission
Tomography

Tumor
radioactive sugar
↳ β^+ emitter
 $e^+ + e^-$ from tissue
↳ $2 \times 511 \text{ keV}$



1933 ; Discovery of the positron



particle in
curvature from \vec{B}
 $\hat{=} e^+$

cloud chamber:

saturated H_2O vapor
charged particles ionize
→ form droplets

→ tracks particle id
from thickness

+ \vec{B} -field → curvature
→ sign of charge

The Positive Electron

CARL D. ANDERSON, *California Institute of Technology, Pasadena, California*
 (Received February 28, 1933)

Out of a group of 1300 photographs of cosmic-ray tracks in a vertical Wilson chamber 15 tracks were of positive particles which could not have a mass as great as that of the proton. From an examination of the energy-loss and ionization produced it is concluded that the charge is less than twice, and is probably exactly equal to, that of the proton. If these particles carry unit positive charge the

curvatures and ionizations produced require the mass to be less than twenty times the electron mass. These particles will be called positrons. Because they occur in groups associated with other tracks it is concluded that they must be secondary particles ejected from atomic nuclei.

Editor

Back to hydrogen:

potential energy $e \cdot V(r)$

$$V(r) = \frac{-ze}{4\pi\epsilon_0 r}$$

into \hat{H}

$z=1$ for H

$$\hat{O} \vec{p} \psi_B = \frac{1}{c} (E - eV(r) - mc^2) \psi_A$$

$$\psi_A = \dots + \dots \psi_B$$

solution: • separate (this) into radial
angular
spin

degrees of freedom

leads to coupling of spin & orbital angular momentum

$$\Rightarrow \text{total angular momentum } j = l \pm \frac{1}{2}$$

$$(SE) : l = 0, 1, 2, \dots, n-1$$

$$\Rightarrow j = \frac{1}{2}, \frac{3}{2}, \dots, n - \frac{1}{2}$$

• radial part:

energies
$$E_{n,j} = mc^2 \left[1 + \frac{(z\alpha_{fs})^2}{(n - \delta_j)^2} \right]^{-\frac{1}{2}}$$

$$\alpha_{fs} = \frac{1}{137} \dots \neq \alpha$$

$$n_{j,d} = \dots \left[(n - \delta_j)^2 \right] \quad \alpha_{fs} = 1/137.036 \dots$$

$$\delta_j = j + \frac{1}{2} - \sqrt{\left(j + \frac{1}{2}\right)^2 - (Z\alpha_{fs})^2}$$

with fine structure constant $\alpha_{fs} = \frac{e^2}{4\pi\epsilon_0 \hbar c} \approx \frac{1}{137.036 \dots}$

Zd-expansion $(Z\alpha_{fs})$

$$E_{n,j} = mc^2 \left[1 - \frac{(Z\alpha_{fs})^2}{2n^2} - \frac{(Z\alpha_{fs})^4}{2n^3} \left(\frac{1}{j + \frac{1}{2}} - \frac{3}{4n} \right) + \dots \right]$$

1st term : rest energy

2nd term : SE solution $-\frac{1}{(4\pi\epsilon_0)^2} \frac{Z^2 e^4 m}{2\hbar^2 n^2}$

3rd term : corrections

$-\frac{(Z\alpha_{fs})^2}{n}$ smaller than Schrödinger energy

- lowers energy levels

for a given n $j = \frac{1}{2}$ largest effect

$j = n - \frac{1}{2}$ smallest effect

- still degeneracy in l

Dirac energies depend on n, j, not on l

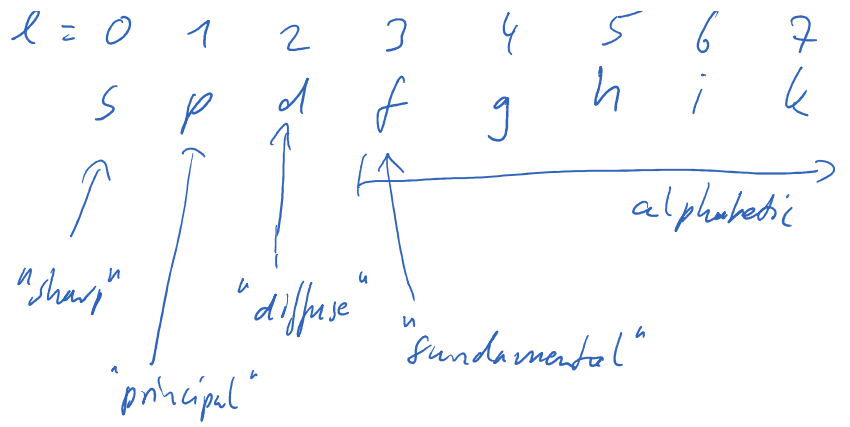
Spectroscopic notation for H-like electron systems

$$\boxed{n l_j}$$

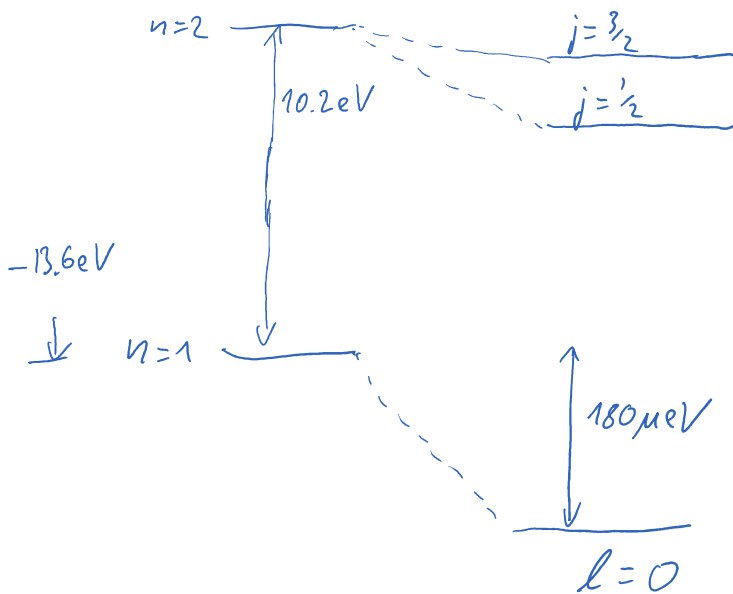
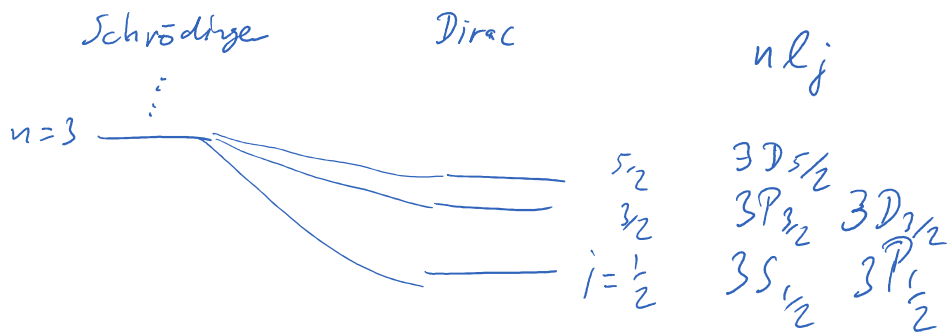
n = principal quantum number

$$n = 1, 2, 3, \dots$$

l = orbital angular momentum
written as a Letter

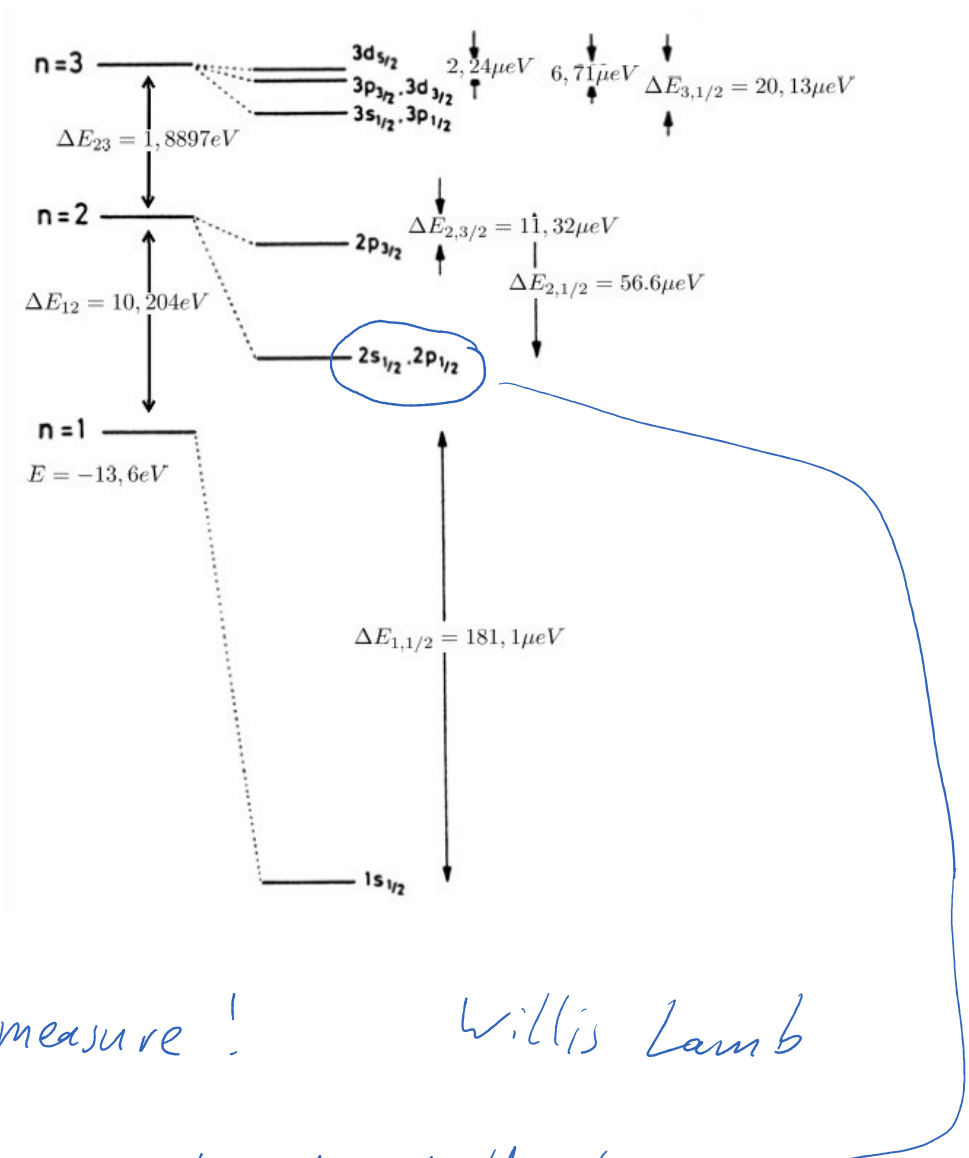


$l = 0, 1, 2, \dots, n-1$
 $j = \text{total angular momentum}$



$2P_{3/2} \leftarrow l=0$
 $2S_{1/2} \leftarrow j=l+1/2$
 $2P_{1/2} \leftarrow l=1$
 $2P_{1/2} \leftarrow j=l-1/2$

$1S_{1/2}$



measure ! Willis Lamb

→ Lamb shift ←

QED lifts degeneracy in j