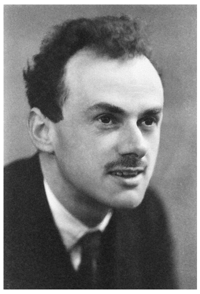
The Dirac Equation

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



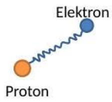
Paul Adrien Maurice Dirac
(* 8. August 1902 in Bristol;
† 20. Oktober 1984 in Tallahassee)

Nobel prize 1933

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

Schrödinger's Hydrogen

Schrödinger Equation (SE)



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

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

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

m = electron mass. Proton shall be infinitely heavy for now
The Laplacian is, in cartesian coordinates

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

time & space not on equal footing
↳ relativity

Dirac Hamiltonian

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

$\vec{\alpha}$: vector of coefficients; β: coefficient } dimensionless

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

relativistic energy - momentum relation

$$E^2 = p^2c^2 + m^2c^4$$

$\hat{H}$ should obey this ↺

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

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

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

$$\Rightarrow (\alpha_i \alpha_k + \alpha_k \alpha_i) = 2\delta_{ik}$$

$$\alpha_i \beta + \beta \alpha_i = 0$$

$$\beta^2 = 1$$

cannot be fulfilled by simple numbers

must be at least 4x4 matrices

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

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

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

$\Rightarrow$ time-independent DE

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

Standard representation

Standard representation

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

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

Pauli matrices

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

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

4-component spinors ψ =
pairs of 2-component spinors

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

$$\Rightarrow \boxed{\begin{aligned} \hat{\vec{\sigma}}\,\hat{\vec{p}}\;\psi_B &= \frac{1}{c}\left(E - mc^2\right)\psi_A \\ \hat{\vec{\sigma}}\,\hat{\vec{p}}\;\psi_A &= \frac{1}{c}\left(E + mc^2\right)\psi_B \end{aligned}}$$

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

and 3 more (cyclic)

---

e.g. particle at rest $\left(\hat{\vec{p}}\,\psi_A = 0 \;;\; \vec{p}\,\psi_B = 0\right)$

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

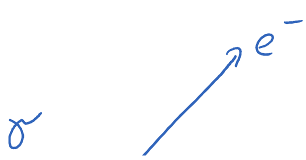
1928 Dirac

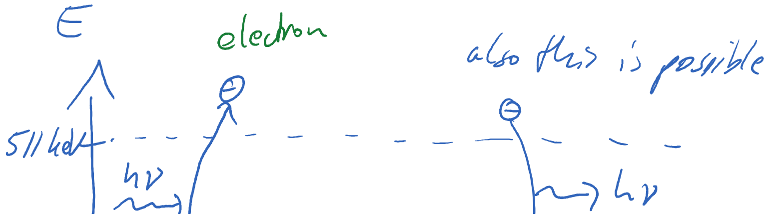
pos. energy solutions = well-known e^-

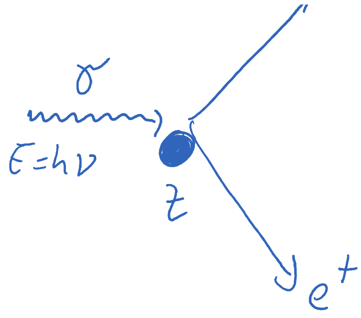
⊕ spin props → explains Zeeman effect

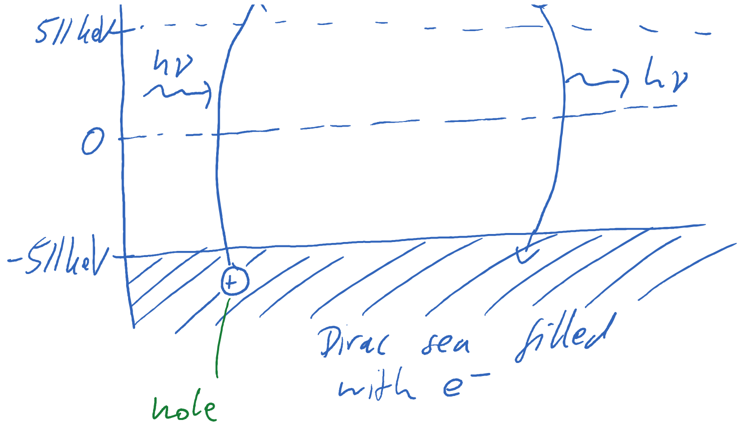
neg. energy solutions as if it had a pos. charge: e^+

Dirac sea



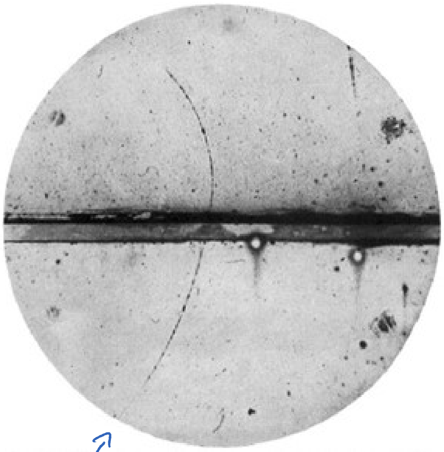






1933 : Discovery of the positron

Pb → energy loss



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

cloud chamber:

saturated H_2O vapor

charged particles ionize

→ form droplets

→ tracks   particle id from thickness

+ B-field → curvature

→ sign of charge

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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 $e \cdot V(r)$ $V(r) = \frac{-Ze}{4\pi\varepsilon_0 r}$

into $\hat{H}$ $\qquad Z = 1$ for H

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

$$\ldots\ \psi_A = \ldots\ldots + \ldots\ \psi_B$$

solution: • separate this into radial
angular
spin

degrees of freedom

leads to coupling of spin & orbital angular momentum

$\Rightarrow$ total angular momentum $\quad j = \ell \pm \frac{1}{2}$

$$(SE):\quad \ell = 0, 1, 2, \ldots\ n-1$$

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

• radial part:

energies
$$E_{n,j} = mc^2\left[1 + \frac{(Z\alpha_{fs})^2}{(n-\delta_j)^2}\right]^{-\frac{1}{2}} \qquad \alpha_{fs} = \frac{1}{137\ldots} \overset{!}{\neq} \vec{\alpha}$$

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

with
fine structure constant $\quad \alpha_{fs} = \dfrac{e^2}{4\pi\varepsilon_0 \hbar c} \approx \dfrac{1}{137.036\ldots}$

$Z\alpha$ - expansion $\qquad (Z\alpha_{fs})$

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

1st term: rest energy

$1 \qquad Z^2 e^4 m$

1st term : rest energy

2nd term : SE solution $\quad -\frac{1}{(4\pi\varepsilon_0)^2}\frac{Z^2 e^4 m}{2\hbar^2 n^2}$

3rd term : corrections

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

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

  $\quad j = n - \frac{1}{2}$ smallest effect
- still degeneracy in ℓ

Dirac energies depend on n, j, not on ℓ

Spectroscopic notation for H-like 1 electron systems

$\boxed{n\ell_j}$ $\quad n$ = principal quantum number

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

ℓ = orbital angular momentum written as a <u>Letter</u>

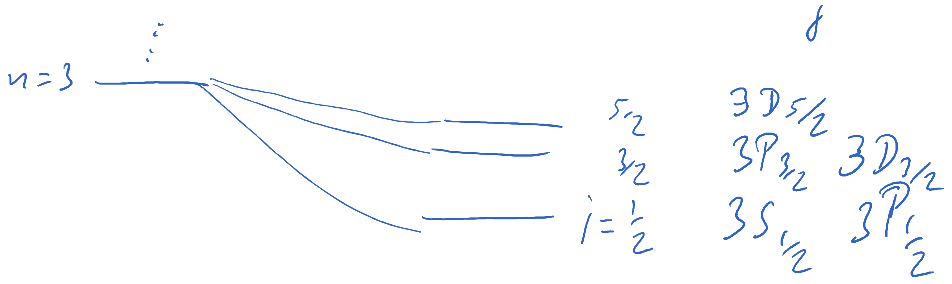
$\ell =$ 0	1	2	3	4	5	6	7
s	p	d	f	g	h	i	k

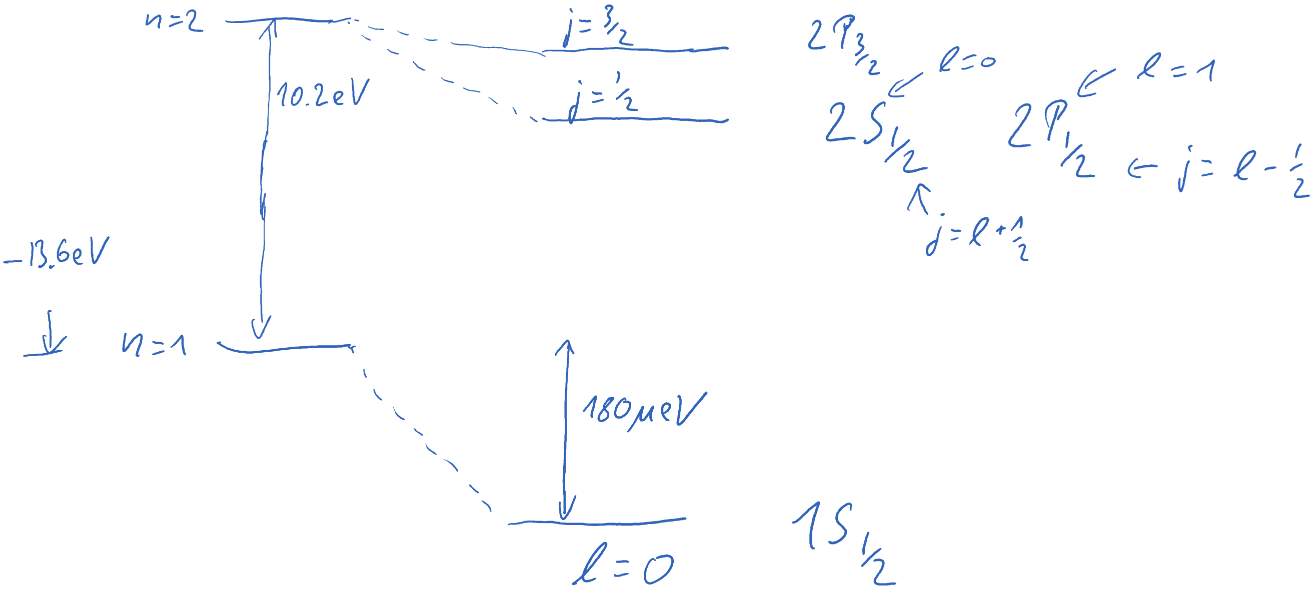
"sharp" "principal" "diffuse" "fundamental" alphabetic

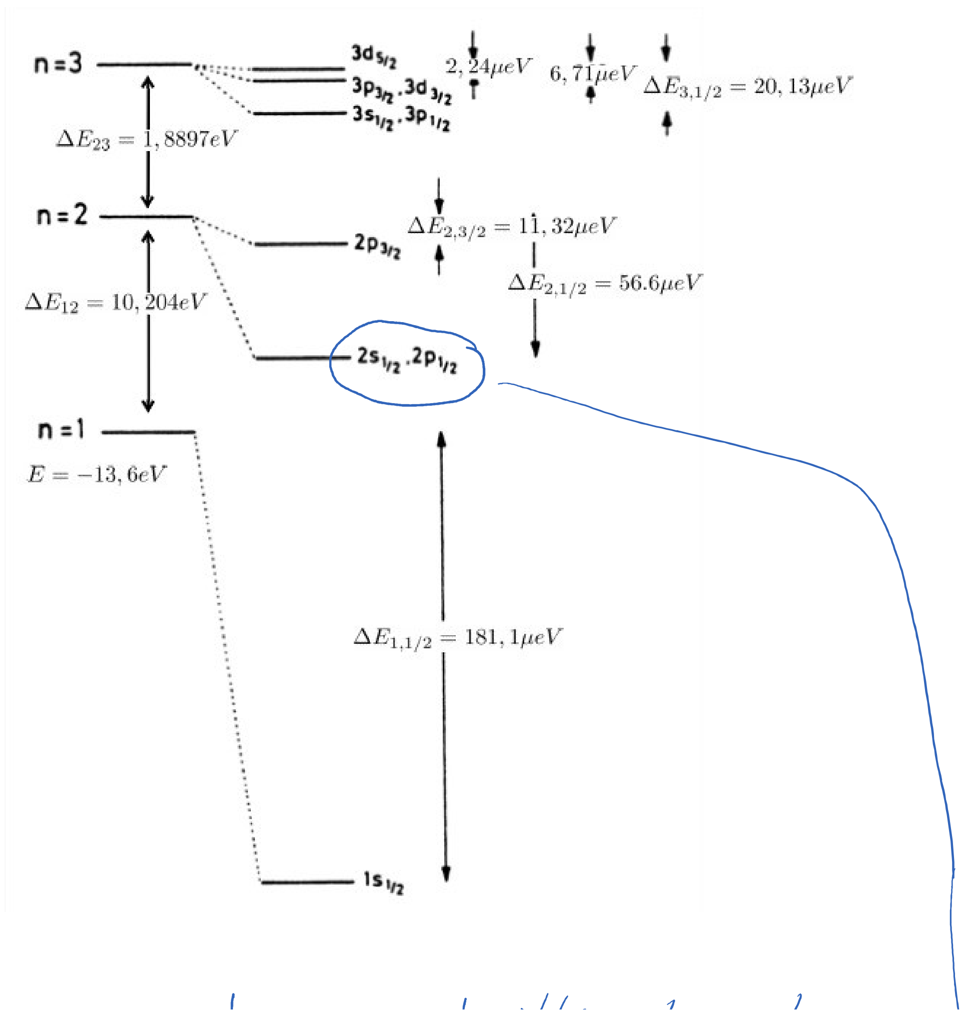
$\ell = 0, 1, 2, \ldots\ldots n-1$

j = total angular momentum

Schrödinger $\quad$ Dirac $\quad$ $n\ell$:


n=3
5/2
3/2
j = 1/2
3D5/2
3P3/2 3D3/2
3S1/2 3P1/2


n=2
10.2eV
j = 3/2
j = 1/2
2P3/2
l=0
2S1/2
2P1/2
l=1
j = l - 1/2
j = l + 1/2
-13.6eV
n=1
180μeV
l=0
1S1/2


n=3
3d5/2
3p3/2 ,3d3/2
3s1/2 ,3p1/2
2,24μeV
6,71μeV
ΔE3,1/2 = 20,13μeV
ΔE23 = 1,8897eV
n=2
2p3/2
ΔE2,3/2 = 11,32μeV
ΔE2,1/2 = 56.6μeV
ΔE12 = 10,204eV
2s1/2 ,2p1/2
n=1
E = −13,6eV
ΔE1,1/2 = 181,1μeV
1s1/2

measure!   Willis Lamb

→ Lamb shift ←

QED lifts degeneracy in j