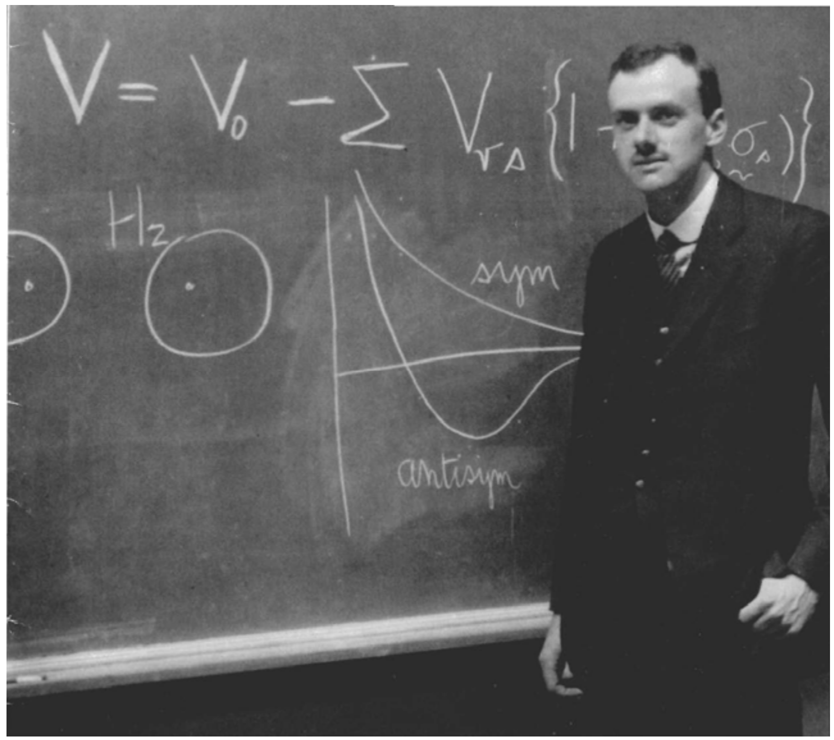
Advanced Quantum Physics

Lecture 11



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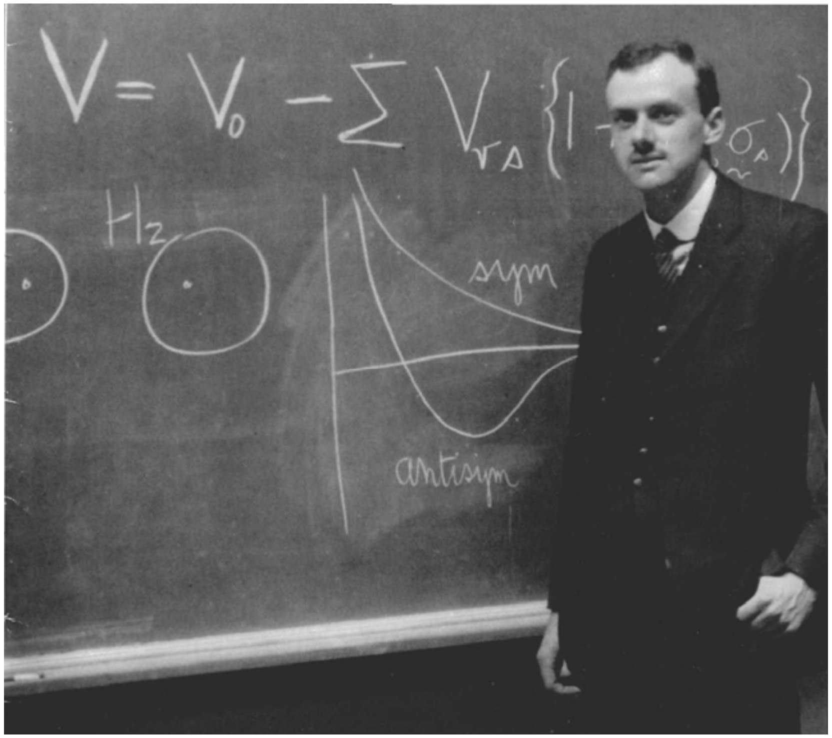
www.sp.phy.cam.ac.uk/~dar11/pdf

Section 3:Relativity and Magnetic fields

Paul Dirac

- Combined special relativity with quantum mechanics to produce the ‘Dirac equation’ – predicting the electron spin, corrections to the Hamiltonian for the hydrogen atom, antiparticles.
- Theory of magnetic monopoles – suggesting quantization of electric charge if they exist – never found...
- Quantization of electromagnetic field leading to theory of photons.
- Prediction that particles could be scattered by light – currently used to manipulate atoms by laser beams.
- Nobel prize 1933 – shared with Schrodinger



“I have trouble with Dirac. This balancing on the dizzying path between genius and madness is awful”

Albert Einstein.

The Dirac equation (recap)

- In the last lecture we showed that a wave equation of first order in position and time would allow invariance under a Lorentz transformation.

$$i\hbar\frac{\partial\psi}{\partial t}=\left[c\alpha_1\hat{p}_x+c\alpha_2\hat{p}_y+c\alpha_3\hat{p}_z+\beta mc^2\right]\psi=\left[c\boldsymbol{\alpha}\cdot\hat{\mathbf{p}}+\beta mc^2\right]\psi$$

- To allow for this the equation contains a set of 4x4 matrices and the wavefunction must be a 4 component column vector.
- The first two components of the column vector correspond to positive energy solutions to the Dirac equation, the last two to negative energy solutions.
- The pairs of components are not independent.
- This wavefunction can represent the spatial and spin states of both electrons and positrons.

Solutions of the Dirac equation

•For a particle travelling along the z-axis there are four time independent orthonormal solutions of the Dirac equation.

N normalization factor

•Positive energy:

$(E=+E_0)$

$$\chi = N\begin{bmatrix} 1 \\ 0 \\ \frac{cp_z}{mc^2+E_0} \\ 0 \end{bmatrix}\exp(ikz), \qquad \chi = N\begin{bmatrix} 0 \\ 1 \\ 0 \\ \frac{-cp_z}{mc^2+E_0} \end{bmatrix}\exp(ikz)$$

•Negative energy:

$(E=-E_0)$

$$\chi = N\begin{bmatrix} \frac{-cp_z}{mc^2+E_0} \\ 0 \\ 1 \\ 0 \end{bmatrix}\exp(ikz), \qquad \chi = N\begin{bmatrix} 0 \\ \frac{cp_z}{mc^2+E_0} \\ 0 \\ 1 \end{bmatrix}\exp(ikz)$$

where $E_0 = +\left(p^2c^2 + m^2c^4\right)^{1/2}$ is positive.

Probability and current densities

- The wavefunction ψ may be represented as a 4 component vector: $\psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$
- We can define $\psi^\dagger$ to be a row vector: $\psi^\dagger = \begin{bmatrix} \psi_1^* & \psi_2^* & \psi_3^* & \psi_4^* \end{bmatrix}$
- We can write the Dirac equation in the form:

$$i\hbar \frac{\partial \psi}{\partial t} = \left[c\boldsymbol{\alpha} \cdot \hat{\mathbf{p}} + \beta mc^2 \right] \psi$$

- Now $\boldsymbol{\alpha}, \beta, \hat{\mathbf{p}}$ are all Hermitian and with $\hat{\mathbf{p}} = -i\hbar\nabla$ we can write:

$$-i\hbar \frac{\partial \psi^\dagger}{\partial t} = \psi^\dagger \left[c\boldsymbol{\alpha} \cdot \left(-i\hbar\nabla \right) + \beta mc^2 \right] = \left(i\hbar c\nabla \right) \psi^\dagger \cdot \boldsymbol{\alpha} + mc^2 \psi^\dagger \beta$$

- Multiply on the right by ψ $\quad -i\hbar \frac{\partial \psi^\dagger}{\partial t} \psi = \left(i\hbar c\nabla \right) \psi^\dagger \cdot \boldsymbol{\alpha}\,\psi + mc^2 \psi^\dagger \beta \psi$

- Multiply the Dirac equation on the left by $\psi^\dagger$ $\quad i\hbar \psi^\dagger \frac{\partial \psi}{\partial t} = -i\hbar c \psi^\dagger \boldsymbol{\alpha} \cdot \nabla \psi + \psi^\dagger \beta \psi mc^2$

- Taking the difference and dividing by $-i\hbar$:

$$\frac{\partial}{\partial t}\left(\psi^\dagger \psi \right) = -\left(c\nabla \right) \psi^\dagger \cdot \boldsymbol{\alpha}\,\psi - c\psi^\dagger \boldsymbol{\alpha} \cdot \nabla \psi = -\nabla \cdot \left(\psi^\dagger c\boldsymbol{\alpha}\,\psi \right)$$

Probability and current densities

- From the last slide: $$\frac{\partial}{\partial t}\left(\psi^{\dagger}\psi\right) = -\nabla\cdot\left(\psi^{\dagger}c\boldsymbol{\alpha}\,\psi\right)$$

- The quantity $\psi^{\dagger}\psi = |\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + |\psi_4|^2$ is positive and can be interpreted as a position probability density $P(\mathbf{r},t)$.

- The equation at the top of the slide is of the form of a continuity equation:

$$\frac{\partial P}{\partial t} + \nabla\cdot\mathbf{j} = 0$$

which implies that the vector,

$$\mathbf{j}(\mathbf{r},t) = \psi^{\dagger}c\boldsymbol{\alpha}\,\psi$$

can be regarded as a probability current density and $c\boldsymbol{\alpha}$ can be interpreted as a velocity operator.

The Dirac Equation in an electromagnetic field

- As for the Schrodinger equation we replace $\hat{\mathbf{p}}$ by $-i\hbar\nabla - q\mathbf{A}$ and add $q\phi$ to the energy, so;

$$i\hbar\frac{\partial\psi}{\partial t} = \left[c\boldsymbol{\alpha}\cdot\left(-i\hbar\nabla - q\mathbf{A}\right) + \beta mc^2 + q\phi\right]\psi$$

where $\mathbf{A}$ is the magnetic vector potential and ϕ the scalar potential.

- As before we express the Dirac equation as two coupled equations with time independent solutions χ_+, χ_- :

$$\boldsymbol{\sigma}\cdot\left(-i\hbar\nabla - q\mathbf{A}\right)c\chi_- + mc^2\chi_+ + q\phi\chi_+ = E\chi_+$$

$$\boldsymbol{\sigma}\cdot\left(-i\hbar\nabla - q\mathbf{A}\right)c\chi_+ - mc^2\chi_- + q\phi\chi_- = E\chi_-$$

- Writing χ_- as the subject in the second equation:

$$\chi_- = \frac{1}{\left(E + mc^2 - q\phi\right)}\boldsymbol{\sigma}\cdot\left(-i\hbar\nabla - q\mathbf{A}\right)c\chi_+$$

and substituting into the first:

$$\boldsymbol{\sigma}\cdot\left(-i\hbar\nabla - q\mathbf{A}\right)c\frac{1}{\left(E + mc^2 - q\phi\right)}\boldsymbol{\sigma}\cdot\left(-i\hbar\nabla - q\mathbf{A}\right)c\chi_+ + q\phi\chi_+ = \left(E - mc^2\right)\chi_+$$

The Dirac Equation in a magnetic field (1)

- From the last slide:

$$\boldsymbol{\sigma}\cdot\left(-i\hbar\nabla-q\mathbf{A}\right)c\frac{1}{\left(E+mc^2-q\phi\right)}\boldsymbol{\sigma}\cdot\left(-i\hbar\nabla-q\mathbf{A}\right)c\chi_+ + q\phi\chi_+ = \left(E-mc^2\right)\chi_+$$

- If $\phi=0$ we can write:

$$\left[\boldsymbol{\sigma}\cdot\left(-i\hbar\nabla-q\mathbf{A}\right)\right]^2 c^2\chi_+ = \left(E+mc^2\right)\left(E-mc^2\right)\chi_+ = \left(E^2-m^2c^4\right)\chi_+$$

- We use the following identity for the Pauli spin matrices:

$$\left(\boldsymbol{\sigma}\cdot\mathbf{a}\right)\left(\boldsymbol{\sigma}\cdot\mathbf{b}\right) = \mathbf{a}\cdot\mathbf{b} + \mathbf{i}\boldsymbol{\sigma}\cdot\left(\mathbf{a}\times\mathbf{b}\right)$$

where $\mathbf{a},\mathbf{b}$ are vectors or vector operators whose components commute with those of $\boldsymbol{\sigma}$. For the first term in the equation above we can write:

$$=\left(-i\hbar\nabla-q\mathbf{A}\right)^2 c^2\chi_+ + i\boldsymbol{\sigma}\cdot\left[\left(-i\hbar\nabla-q\mathbf{A}\right)\times\left(-i\hbar\left(\nabla\chi_+\right)-q\mathbf{A}\chi_+\right)\right]c^2$$

$$=\left(-i\hbar\nabla-q\mathbf{A}\right)^2 c^2\chi_+ - q\hbar\boldsymbol{\sigma}\cdot\left[\mathbf{A}\times\left(\nabla\chi_+\right)+\nabla\times\left(\mathbf{A}\chi_+\right)\right]c^2$$

$$\boxed{\nabla\times\nabla\chi_+ = \mathbf{A}\times\mathbf{A}\chi_+ = 0}$$

- Given that $\nabla\times\left(\mathbf{A}\chi_+\right)=\nabla\chi_+\times\mathbf{A}+\chi_+\nabla\times\mathbf{A}$ and $\nabla\chi_+\times\mathbf{A}=-\mathbf{A}\times\nabla\chi_+$
- We have:

$$\left(-i\hbar\nabla-q\mathbf{A}\right)^2 c^2\chi_+ - q\hbar\boldsymbol{\sigma}\cdot\left[\nabla\times\mathbf{A}\right]c^2\chi_+ = \left(E^2-m^2c^4\right)\chi_+$$

The Dirac Equation in a magnetic field (2)

- From the last slide and since $\mathbf{B} = \nabla \times \mathbf{A}$ we have:

$$\left(-i\hbar\nabla - q\mathbf{A}\right)^2 c^2 \chi_+ - q\hbar\boldsymbol{\sigma}\cdot\mathbf{B}c^2\chi_+ = \left(E^2 - m^2c^4\right)\chi_+$$

- If we have $E = E' + mc^2$, in the non-relativistic limit $E' \ll mc^2 \simeq E$ then:

$$E^2 - m^2c^4 = \left(E - mc^2\right)\left(E + mc^2\right) \simeq 2E'mc^2$$

- And so:

$$\left(\frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}\right)^2 - \frac{q\hbar}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}\right)\chi_+ = E'\chi_+$$

- The first term is expected (see lecture 9).
- The second term has the form of an interaction $-\boldsymbol{\mu}_{\mathbf{s}}\cdot\mathbf{B}$ between a magnetic field and a particle with magnetic moment $\boldsymbol{\mu}_{\mathbf{s}} = \frac{q\hbar\boldsymbol{\sigma}}{2m}$
- Can be written in terms of the spin operator $\hat{\mathbf{S}} = \frac{\hbar}{2}\boldsymbol{\sigma}$ giving $\boldsymbol{\mu}_{\mathbf{s}} = \frac{q}{m}\hat{\mathbf{S}}$
- For an electron where $q = -|e|$ we have $\boldsymbol{\mu}_{\mathbf{s}} = -\frac{e}{m}\hat{\mathbf{S}} = -\frac{g_s\mu_B\hat{\mathbf{S}}}{\hbar}$ where the *Bohr magneton* $\mu_B = \frac{e\hbar}{2m}$ and the gyromagnetic ratio $g_s = 2$
- So the Dirac equation predicts the existence of the *intrinsic* magnetic moment of the electron as well as its magnitude.

The Dirac Equation in an electric field (1)

- From slide 8:

$$\boldsymbol{\sigma}\cdot\left(-i\hbar\nabla - q\mathbf{A}\right)c\frac{1}{\left(E+mc^2-q\phi\right)}\boldsymbol{\sigma}\cdot\left(-i\hbar\nabla - q\mathbf{A}\right)c\chi_+ + q\phi\chi_+ = \left(E-mc^2\right)\chi_+$$

- If we now assume $\mathbf{A}=0$ and $E = E' + mc^2$

$$-c^2\hbar^2\left(\boldsymbol{\sigma}\cdot\nabla\right)\frac{1}{\left(E'+2mc^2-q\phi\right)}\left(\boldsymbol{\sigma}\cdot\nabla\right)\chi_+ + q\phi\chi_+ = E'\chi_+$$

- If we expand

$$\frac{1}{\left(E'+2mc^2-q\phi\right)} \simeq \frac{1}{2mc^2}\left[1-\frac{E'-q\phi}{2mc^2}\right]$$

$$E'-q\phi \ll mc^2$$

we have:

$$-c^2\hbar^2\left(\boldsymbol{\sigma}\cdot\nabla\right)\frac{1}{2mc^2}\left[1-\frac{E'-q\phi}{2mc^2}\right]\left(\boldsymbol{\sigma}\cdot\nabla\right)\chi_+ + q\phi\chi_+ = E'\chi_+$$

- Giving

$$-\frac{\hbar^2}{2m}\left[1-\frac{E'-q\phi}{2mc^2}\right]\left(\boldsymbol{\sigma}\cdot\nabla\right)^2\chi_+ - \frac{q\hbar^2}{4m^2c^2}\left(\boldsymbol{\sigma}\cdot\nabla\phi\right)\left(\boldsymbol{\sigma}\cdot\nabla\chi_+\right) + q\phi\chi_+ = E'\chi_+$$

The Dirac Equation in an electric field (2)

- From the last slide:

$$-\frac{\hbar^2}{2m}\left[1-\frac{E'-q\phi}{2mc^2}\right](\boldsymbol{\sigma}\cdot\nabla)^2\chi_+ - \frac{q\hbar^2}{4m^2c^2}(\boldsymbol{\sigma}\cdot\nabla\phi)(\boldsymbol{\sigma}\cdot\nabla\chi_+) + q\phi\chi_+ = E'\chi_+$$

- Using the identity: $(\boldsymbol{\sigma}\cdot\mathbf{a})(\boldsymbol{\sigma}\cdot\mathbf{b}) = \mathbf{a}\cdot\mathbf{b} + \mathbf{i}\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b})$ we have $(\boldsymbol{\sigma}\cdot\nabla)^2 = \nabla^2$ and: $(\boldsymbol{\sigma}\cdot\nabla\phi)(\boldsymbol{\sigma}\cdot\nabla\chi_+) = (\nabla\phi)\cdot(\nabla\chi_+) + i\boldsymbol{\sigma}\cdot[(\nabla\phi)\times(\nabla\chi_+)]$
- If we assume that $\phi(r)$ is spherically symmetric:

$$\nabla\phi(r) = \frac{d\phi}{dr}\hat{\mathbf{r}}, \qquad (\nabla\phi)\cdot(\nabla\chi_+) = \frac{d\phi}{dr}\frac{\partial\chi_+}{\partial r}$$

- The orbital angular momentum operator is given by: $\hat{\mathbf{L}} = \mathbf{r}\times(-i\hbar\nabla)$
- The Pauli spin operator by: $\hat{\mathbf{S}} = (\hbar/2)\boldsymbol{\sigma}$
- So $\quad i\boldsymbol{\sigma}\cdot[(\nabla\phi)\times(\nabla\chi_+)] = -\frac{2}{\hbar^2}\frac{1}{r}\frac{d\phi}{dr}\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}\chi_+$
- Hence

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + q\phi + \frac{\hbar^2}{2m}\left[\frac{E'-q\phi}{2mc^2}\right]\nabla^2 + \frac{q}{2m^2c^2}\frac{1}{r}\frac{d\phi}{dr}\hat{\mathbf{L}}\cdot\hat{\mathbf{S}} - \frac{q\hbar^2}{4m^2c^2}\frac{d\phi}{dr}\frac{\partial}{\partial r}\right]\chi_+ = E'\chi_+$$

The Dirac Equation in an electric field (3)

- This equation has been derived using relativistic quantum theory and then taking the non-relativistic limit:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + q\phi + \frac{\hbar^2}{2m}\left[\frac{E'-q\phi}{2mc^2}\right]\nabla^2 + \frac{q}{2m^2c^2}\frac{1}{r}\frac{d\phi}{dr}\hat{\mathbf{L}}\cdot\hat{\mathbf{S}} - \frac{q\hbar^2}{4m^2c^2}\frac{d\phi}{dr}\frac{\partial}{\partial r}\right]\chi_+ = E'\chi_+$$

- The first and second terms are in the non-relativistic Hamiltonian for a particle of mass m and charge q in a central potential $\phi(r)$.
- Since $\hat{\mathbf{p}} = -i\hbar\nabla, \quad E' - q\phi(r) \simeq \hat{\mathbf{p}}^2/2m$ the third term can be written:

$$\frac{\hbar^2}{2m}\left[\frac{E'-q\phi}{2mc^2}\right]\nabla^2 \simeq \frac{\hat{\mathbf{p}}^4}{8m^3c^2}$$

This is a relativistic correction to the kinetic energy operator.

- Fourth term is the spin orbit interaction.
- The fifth term is non-Hermitian due to normalization difficulties with the Dirac spinor wavefunction. C G Darwin showed it could be written as:

$\frac{q\hbar^2}{8m^2c^2}\nabla^2\phi(r)$ and for a Coulomb potential for a hydrogenic atom as:

$$\frac{\pi\hbar^2}{2m^2c^2}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)\delta(\mathbf{r})$$ -really only affects the s states.

Dirac Equation – the hydrogen atom Hamiltonian

- Substituting $q\phi(r) = V(r),\ \hat{\mathbf{p}} = -i\hbar\nabla$ and using the following expression for the potential:

$$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}$$

we can write the Hamiltonian for the hydrogenic atom, correct to terms in v^2/c^2 as:

$$\hat{H} = \underbrace{\frac{\hat{\mathbf{p}}^2}{2m} + V(r)}_{\text{non- relativistic Hamiltonian}} \underbrace{- \frac{\hat{\mathbf{p}}^4}{8m^3c^2}}_{\text{relativistic K.E.}} + \underbrace{\frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}}_{\text{Spin-orbit coupling}} + \underbrace{\frac{\pi\hbar^2}{2m^2c^2}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)\delta(\mathbf{r})}_{\text{The 'Darwin' term – only affects s-states}}$$

- This expression will be used in discussions of atomic physics later in the course.

Dirac Equation – the hydrogen atom eigenenergies

•The Dirac equation can be solved exactly for the hydrogen atom. The energy eigenvalues are given by:

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

A rather complicated derivation – see Quantum Mechanics Bransden & Joachin p 702-710

•Expanding this result in powers of $(Z\alpha)^2$ we obtain:

$$E_{nj}^{D} = mc^2\left[1-\frac{(Z\alpha)^2}{2n^2}-\frac{(Z\alpha)^4}{2n^4}\left(\frac{n}{j+\tfrac{1}{2}}-\frac{3}{4}\right)+....\right]$$

and so

$$E_{nj} = E_{nj}^{D}-mc^2 = E_n^{(0)}\left[1+\frac{(Z\alpha)^2}{2n^2}\left(\frac{n}{j+\tfrac{1}{2}}-\frac{3}{4}\right)+....\right]$$

Shows the effect on the energy eigenvalues of different j values.

where

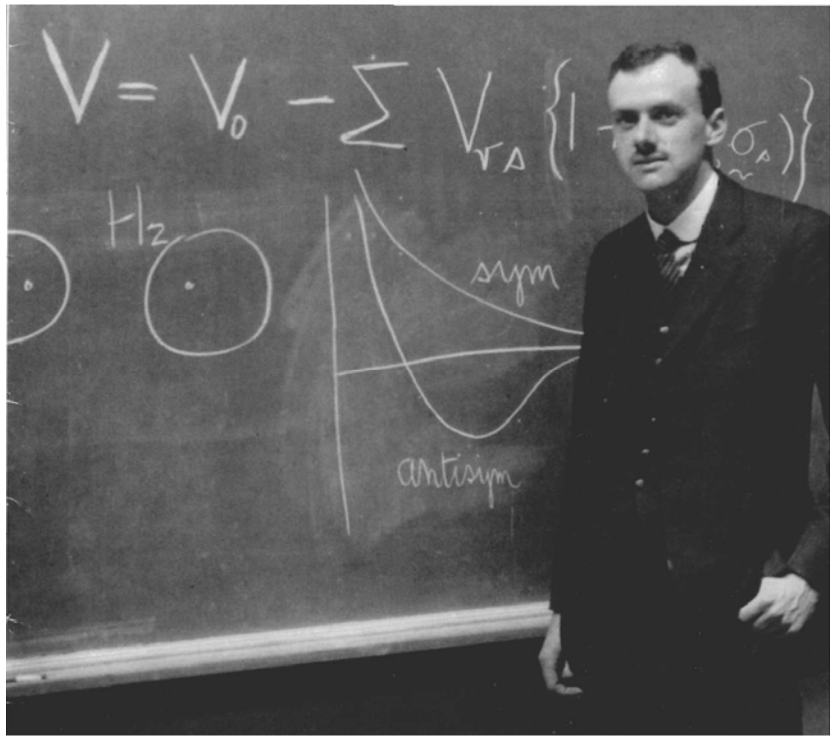
$$E_n^{(0)} = \frac{1}{2}mc^2\frac{(Z\alpha)^2}{n^2}, \qquad \left[\alpha=\frac{e^2}{4\pi\varepsilon_0\hbar c}\simeq\frac{1}{137}\right]$$

are the energy eigenvalues obtained with the (non-relativistic) Schrodinger equation.

Lecture 11 - Summary

- Recap of the Dirac equation and it’s solutions.
- Probability and current densities - the continuity equation.
- The Dirac equation in a magnetic field – emergence of an energy of interaction between the magnetic field and an intrinsic magnetic moment with a gyromagnetic ratio $g_s = 2$.
- The Dirac equation in an electric field – giving rise to additional terms in the Hamiltonian calculated at low enegies. These terms are - a contribution to the kinetic energy, the spin-orbit coupling and the Darwin term.
- The hydrogen atom eigenenergies taking into account relativistic effects.

Lecture 11



The End!!

(www.sp.phy.cam.ac.uk/~dar11/pdf)