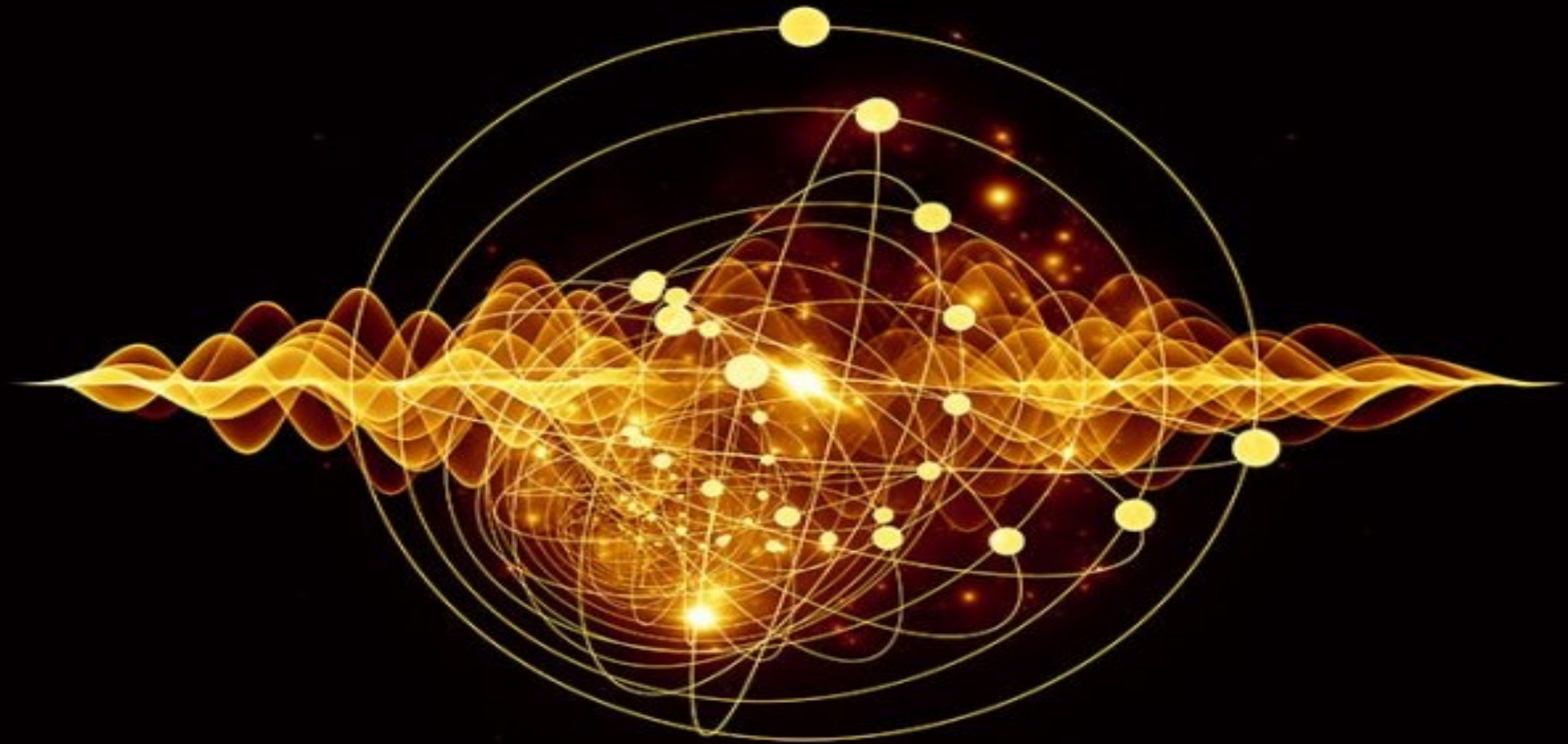




Particle Physics I

Lecture 6: Quantum mechanics, the Klein-Gordon and Dirac equations

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Today's learning targets

- Reminder of non-relativistic Quantum Mechanics – wavefunction, Schrödinger equation
- Probability density and flux (continuity equation)
- The Klein-Gordon equation for relativistic particles
- The Dirac equation and antiparticles

Quantum mechanics: reminder

- **Wavefunction:**

- Non-relativistic quantum mechanics (QM) postulates that free particles are described by wave packets which can be decomposed into a Fourier integral of plane waves $\Rightarrow$ wavefunction

$$\vec{x}(t) \Rightarrow \Psi(\vec{x}, t) \text{ or } \Psi(\vec{p}, E)$$

- QM takes into account wave-particle duality implying that one can never predict the exact particle position and momentum at the same time
- Dynamical variables (e.g. E, p) of a QM state are obtained from the time-dependent wavefunction by acting on it with time-independent operators

- **Interpretation of the wave function:**

- the concept of a precise trajectory is replaced by a probability density to find the particle at a given position at a given time:

$$\rho(\vec{x}, t) = |\Psi(\vec{x}, t)|^2 = \Psi^*(\vec{x}, t)\Psi(\vec{x}, t)$$

Quantum mechanics: reminder

- **Observables:**

- any measurable physics quantity A can be associated to a linear operator $\hat{A}$ such that if one knows $\Psi(x)$ the expectation value of that quantity can be obtained using

$$\langle \hat{A} \rangle = \int \Psi^*(\vec{x}, t) \hat{A} \Psi(\vec{x}, t) d^3\vec{x}$$

- for position, momentum (in 1D) and energy the corresponding operators and expectation values are

$$x \Rightarrow \hat{X} = x \Rightarrow \langle \hat{x} \rangle = \int \Psi^*(x, t) x \Psi(x, t) dx$$

$$p_x \Rightarrow \hat{P}_x = -i\hbar \frac{\partial}{\partial x} \Rightarrow \langle \hat{P}_x \rangle = \int \Psi^*(x, t) \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi(x, t) dx$$

$$E \Rightarrow \hat{E} = i\hbar \frac{\partial}{\partial t} \Rightarrow \langle \hat{E} \rangle = \int \Psi^*(x, t) \left(i\hbar \frac{\partial}{\partial t} \right) \Psi(x, t) dx$$

Quantum mechanics: reminder

- **Heisenberg's uncertainty principle:**

- for two physics quantities to be simultaneously measurable their operators should commute

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0$$

- examples:

$$[\hat{X}, \hat{Y}] = [\hat{Y}, \hat{Z}] = [\hat{Z}, \hat{X}] = 0$$

$$[\hat{P}_x, \hat{P}_y] = [\hat{P}_y, \hat{P}_z] = [\hat{P}_z, \hat{P}_x] = 0$$

$$[\hat{X}, \hat{P}_y] = [\hat{X}, \hat{P}_z] = 0$$

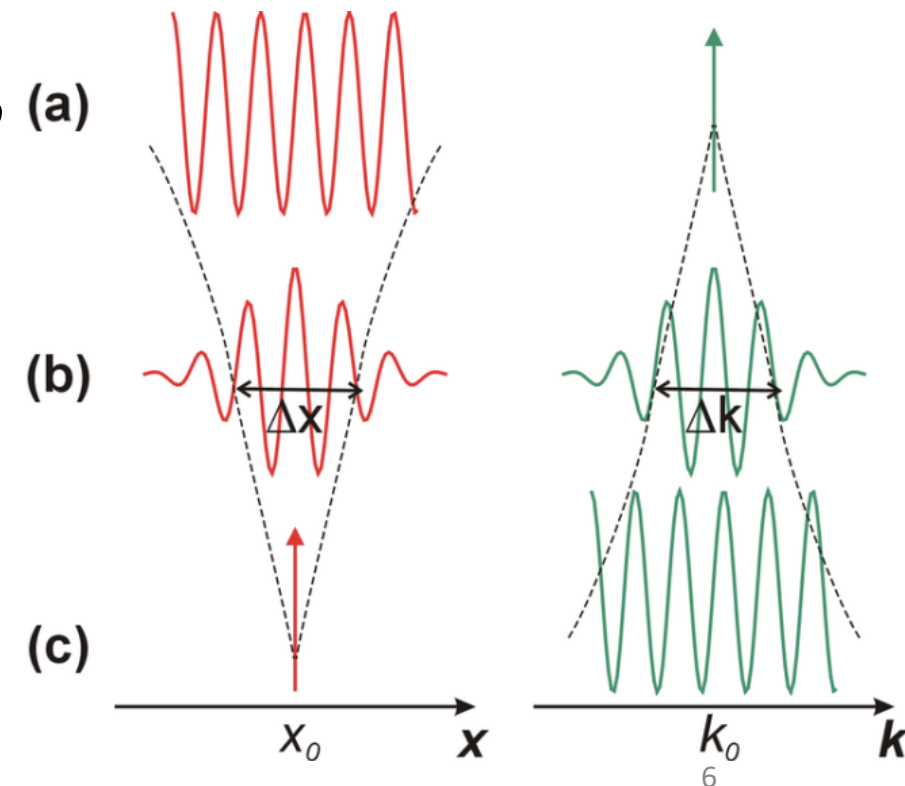
$$[\hat{X}, \hat{P}_x] = [\hat{Y}, \hat{P}_y] = [\hat{Z}, \hat{P}_z] = i\hbar$$

Cross section: example

- The last equation leads to the Heisenberg uncertainty principle:

$$\sigma_x \sigma_{p_x} \geq \frac{\hbar}{2}$$

- Arises due to particle-wave nature of all quantum objects
- (a) a pure wave of fixed frequency has no spatial localisation but p is well-defined as $p \propto k \propto 1/\lambda \propto \nu$
- (b) a wave packet with spatial dispersion Δx and frequency dispersion Δk – the spatial dispersion is inversely proportional to the frequency dispersion $\sigma_x \sigma_{p_x} \geq \hbar/2$
- (c) a particle is fully localised but has no determined frequency



Schrödinger equation (1926)

- The equation governing the dynamics of a quantum system was established by Schrödinger for non-relativistic particles. He assumed the solution to be of the same form as an electromagnetic wave:

$$\Psi = Ne^{i(kx - \omega t)} \text{ or } Ne^{i(px - Et)/\hbar} \text{ (using } E = \hbar\omega, p = \hbar k)$$

- Start with non-relativistic relation between energy and momentum

$$E = \frac{p^2}{2m} + V \quad | \times \Psi \quad \Rightarrow \quad E\Psi = \frac{p^2}{2m} \Psi + V\Psi$$

- Take the derivative of the wavefunction Ψ :

$$\begin{aligned} \frac{\partial^2 \Psi}{\partial x^2} &= -k^2 \Psi = -\frac{p^2}{\hbar^2} \Psi \Rightarrow p^2 \Psi = -\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} \\ \frac{\partial \Psi}{\partial t} &= -i\omega \Psi = -i \frac{E}{\hbar} \Psi \Rightarrow E\Psi = i\hbar \frac{\partial \Psi}{\partial t} \end{aligned}$$

- Giving the **Schrödinger equation for a non-relativistic particle with no spin:**

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

Schrödinger equation (1926)

- **Continuity equation in the context of QM:**

- in electromagnetism charge conservation in a volume V where no particles are created or destroyed is given by:

$$\vec{\nabla} \cdot \vec{j}(\vec{x}, t) + \frac{\partial \rho(\vec{x}, t)}{\partial t} = 0$$

$\vec{\nabla} \cdot \vec{j}(\vec{x}, t)$ → N of particles leaving volume V

$\frac{\partial \rho(\vec{x}, t)}{\partial t}$ ← decrease in N of particles in a volume V

$\rho(\vec{x}, t)$ – charge density
 $\vec{j}(\vec{x}, t)$ – current (flux) of ρ

- What is the connection between the continuity equation in electrodynamics and the QM description
- Need to find what ρ and j are in the QM formalism
- Start with Schrödinger equation for a non-relativistic free particle ($V = 0$)

$$i\hbar \frac{\partial \Psi}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = 0 \quad (1)$$

- Multiply Eq.1 by Ψ^* , multiply the complex conjugate of Eq.1 by Ψ and subtract the two

Schrödinger equation (1926)

- Result:

$$\frac{\partial(\Psi^*\Psi)}{\partial t} + \vec{\nabla} \cdot \left(\frac{i\hbar}{2m} (\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) \right) = 0$$

- Resembles a lot the continuity equation:

$$\vec{\nabla} \cdot \vec{j}(\vec{x}, t) + \frac{\partial \rho(\vec{x}, t)}{\partial t} = 0$$

- From here we can extract the probability density ρ and the probability current (flux) j

$$\rho(\vec{x}, t) = |\Psi(\vec{x}, t)|^2 = \Psi^*(\vec{x}, t)\Psi(\vec{x}, t)$$

$$\vec{j}(\vec{x}, t) = -\frac{i\hbar}{2m} (\Psi^*(\vec{x}, t)\nabla\Psi(\vec{x}, t) - \Psi(\vec{x}, t)\nabla\Psi^*(\vec{x}, t))$$

Plane wave example

$$\rho(\vec{x}, t) = |\Psi(\vec{x}, t)|^2 = \Psi^*(\vec{x}, t)\Psi(\vec{x}, t)$$

$$\vec{j}(\vec{x}, t) = -\frac{i\hbar}{2m}(\Psi^*(\vec{x}, t)\nabla\Psi(\vec{x}, t) - \Psi(\vec{x}, t)\nabla\Psi^*(\vec{x}, t))$$

- Switching to natural units ($c = \hbar = 1$)

$$\Psi = Ne^{i(\vec{p}\cdot\vec{x}-Et)/\hbar} \Rightarrow \rho = |N|^2 \text{ and } \vec{j} = |N|^2 \frac{\vec{p}}{m} = |N|^2 \vec{v}$$

- The number of particles per unit volume is $|N|^2$
- For $|N|^2$ particles per unit volume moving at velocity $\vec{v}$, we have $|N|^2 \vec{v}$ passing through a unit area per unit time (particle flux)
- We can conclude that $\vec{j}$ as a vector in the particle's direction with magnitude equal to the **flux**

Klein-Gordon equation (1926)

- Following the same spirit, Oscar Klein and Walter Gordon attempted to find a QM equation describing a relativistic electron by using the relativistic relation between energy and momentum for a free particle

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

- Replace E and p with the corresponding operators

$$(\hat{E})^2\Psi = (\hat{P})^2\Psi + m^2\Psi$$

$$\hat{E} = i\frac{\partial}{\partial t}, \hat{P}_x = -i\hbar\frac{\partial}{\partial x}, \hat{P}_y = -i\hbar\frac{\partial}{\partial y}, \hat{P}_z = -i\hbar\frac{\partial}{\partial z}$$

$$\left(i\frac{\partial}{\partial t}\right)^2\Psi = (-i\nabla)^2\Psi + m^2\Psi$$

- Klein-Gordon equation for a relativistic particle with no spin

$$\frac{\partial^2\Psi}{\partial t^2} = \nabla^2\Psi - m^2\Psi \tag{2}$$

Klein-Gordon equation (1926)

- Using $\partial_\mu = \frac{\partial}{\partial x^\mu} = \left(\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$ and $\partial_\mu \partial^\mu = \partial_t^2 - \partial_x^2 - \partial_y^2 - \partial_z^2$, one can write the KG equation as:

$$(\partial_\mu \partial^\mu + m^2)\Psi = 0$$

- **Problems with the KG equation:**

- for a plane wave solution $\Psi = Ne^{i(\vec{p}\cdot\vec{x}-Et)}$, the KG equation gives

$$-E^2\Psi = -|\vec{p}|^2\Psi - m^2\Psi \Rightarrow E = \pm\sqrt{|\vec{p}|^2 + m^2}$$

- historically, the negative solutions were viewed as problematic
 - it implied no ground state in the atoms
 - transition to lower energy states is always possible

Klein-Gordon equation (1926)

- **Problems with the KG equation:**

- compute the probability density and probability current (flux)

$$\rho = -i(\Psi^* \partial_t \Psi - \Psi \partial_t \Psi^*)$$

$$\vec{j}(\vec{x}, t) = -i(\Psi^* \nabla \Psi - \Psi \nabla \Psi^*)$$

- for a plane wave: $\Psi = N e^{i(\vec{p} \cdot \vec{x} - Et)}$

$$\rho = 2E|N|^2 \text{ and } \vec{j} = 2|N|^2 \vec{p}$$

- $\Rightarrow$ particle densities are proportional to E , which can also be negative
- How can a probability be negative? No interpretation can be made at that time.

The Dirac equation (1928)

- There were two main problems with the KG equation:
 - negative energy solutions
 - negative particle densities associated with these solutions
- Nowadays in Quantum Field Theory (QFT) these problems are overcome
 - the KG equation is used to describe spin-0 particles (e.g. pions)



- These problems led to new developments
 - motivated Dirac to search for a different formulation of relativistic QM in which all particle densities are positive
 - the resulting wave equation had solutions which not only solved this problem but also fully described the intrinsic spin and magnetic moment of the electron!

The Dirac equation (1928)

- Schrödinger equation:

$$i \frac{\partial \Psi}{\partial t} + \frac{1}{2m} \frac{\partial^2 \Psi}{\partial x^2} = 0$$

- first order in ∂_t , second order in $\partial_x, \partial_y, \partial_z$

- Klein-Gordon equation:

$$(\partial_\mu \partial^\mu + m^2) \Psi = 0$$

- second order in $\partial_t, \partial_x, \partial_y, \partial_z$

- Dirac looked for an alternative, which has first order in $\partial_t, \partial_x, \partial_y, \partial_z$:

$$\hat{H}\Psi = (\vec{\alpha} \cdot \vec{p} + \beta m)\Psi = i \frac{\partial \Psi}{\partial t} \quad (3)$$

Hamiltonian operator

$-i\nabla$

The Dirac equation (1928)

- Squaring Eq.3 we should get:

$$-\frac{\partial^2 \Psi}{\partial t^2} = -\frac{\partial^2 \Psi}{\partial x^2} - \frac{\partial^2 \Psi}{\partial y^2} - \frac{\partial^2 \Psi}{\partial z^2} + m^2 \Psi \quad (4)$$

- For this to be a reasonable formulation of QM, Dirac's equation must be compatible with KG:

$$\begin{aligned} \alpha_x^2 &= \alpha_y^2 = \alpha_z^2 = \beta^2 = 1 \\ \alpha_j \beta + \beta \alpha_j &= 0 \\ \alpha_i \alpha_j + \alpha_j \alpha_i &= 0 \quad (j \neq i) \end{aligned} \quad (5)$$

- Obviously α_i and β can not be numbers: require 4 mutually anti-commuting matrices
- Must be at least 4×4 matrices

The Dirac equation (1928)

- Consequently, the wavefunction must be a four-component Dirac spinor
- The wavefunction has new degrees of freedom as a result of introducing an equation that is first order in time/space derivatives

$$\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \end{pmatrix}$$

- For the Hamiltonian $\hat{H}\Psi = (\vec{\alpha} \cdot \vec{p} + \beta m)\Psi = i \frac{\partial \Psi}{\partial t}$ to be Hermitian:

$$\alpha_x = \alpha_x^\dagger, \alpha_y = \alpha_y^\dagger, \alpha_z = \alpha_z^\dagger, \beta = \beta^\dagger$$

- It is convenient to introduce an explicit representation for α, β
- It should be noted that physical results do not depend on the particular representation: everything is in the commutation relations

Pauli spin matrices

- A convenient choice is to use Pauli (spin) matrices $\sigma_x, \sigma_y, \sigma_z$:

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad \alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}$$

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- The matrices are Hermitian and anti-commute with each other

The Dirac equation: Probability density and current

- Let's get back to the probability density and current that were problematic in the KG equation
- Dirac equation:

$$\left(-i\alpha_x \frac{\partial}{\partial x} - i\alpha_y \frac{\partial}{\partial y} - i\alpha_z \frac{\partial}{\partial z} + \beta m\right) \Psi = \left(i \frac{\partial}{\partial t}\right) \Psi \quad (6)$$

- It's Hermitian conjugate

$$+i \frac{\partial \Psi^\dagger}{\partial x} \alpha_x^\dagger + i \frac{\partial \Psi^\dagger}{\partial y} \alpha_y^\dagger + i \frac{\partial \Psi^\dagger}{\partial z} \alpha_z^\dagger + m \Psi^\dagger \beta^\dagger = -i \frac{\partial \Psi^\dagger}{\partial t} \quad (7)$$

- Compute $\Psi^\dagger \times \text{Eq. 6} - \text{Eq. 7} \times \Psi$ taking into account that α and β are Hermitian and the relation

$$\Psi^\dagger \alpha_x \frac{\partial \Psi}{\partial x} + \frac{\partial \Psi^\dagger}{\partial x} \alpha_x \Psi = \frac{\partial (\Psi^\dagger \alpha_x \Psi)}{\partial x}$$

The Dirac equation: Probability density and current

- We get the continuity equation:

$$\nabla \cdot (\Psi^\dagger \vec{\alpha} \Psi) + \frac{\partial (\Psi^\dagger \Psi)}{\partial t} = 0 \quad (8)$$

- Where $\Psi^\dagger = (\Psi_1^*, \Psi_2^*, \Psi_3^*, \Psi_4^*)$
- The probability density and current are

$$\rho = \Psi^\dagger \Psi, \quad \mathbf{j} = \Psi^\dagger \vec{\alpha} \Psi \quad (9)$$

- where $\rho = \Psi^\dagger \Psi = |\Psi_1^*|^2 + |\Psi_2^*|^2 + |\Psi_3^*|^2 + |\Psi_4^*|^2 > 0$
- Unlike the KG equation, the Dirac equation has probability density which are **always positive!**
- The solutions of the Dirac equation are the four-component Dirac spinors
- The great success of the Dirac equation is that these components naturally describe the property of intrinsic spin of particles

Covariant notation: the Dirac γ matrices

- The Dirac equation can be written more elegantly by introducing the four Dirac gamma matrices

$$\gamma^0 = \beta, \quad \gamma^1 = \beta\alpha_x, \quad \gamma^2 = \beta\alpha_y, \quad \gamma^3 = \beta\alpha_z$$

- The probability density and current are

$$\left(i\beta\alpha_x \frac{\partial}{\partial x} + i\beta\alpha_y \frac{\partial}{\partial y} + i\beta\alpha_z \frac{\partial}{\partial z} - \beta^2 m \right) \Psi = - \left(i\beta \frac{\partial}{\partial t} \right) \Psi$$

$$\Rightarrow \left(i\gamma^1 \frac{\partial}{\partial x} + i\gamma^2 \frac{\partial}{\partial y} + i\gamma^3 \frac{\partial}{\partial z} - m \right) \Psi = -i\gamma^0 \frac{\partial \Psi}{\partial t}$$

- Using $\partial_\mu = \frac{\partial}{\partial x^\mu} = \left(\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$ we can rewrite it as

$$(i\gamma^\mu \partial_\mu - m)\Psi = 0 \tag{10}$$

- The Dirac gamma matrices are not four-vectors: they are constant matrices that remain invariant under Lorentz transformations

The Dirac equation: solutions

- Consider a particle at rest, $p = 0$:

$$\left(i\gamma^0 \frac{\partial}{\partial t} - m\right) \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \end{pmatrix} = 0, \quad \text{where } \gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

- Spinor Ψ splits into two 2-component bi-spinors: $\Psi \equiv \begin{pmatrix} \Psi_A \\ \Psi_B \end{pmatrix}$

$$\begin{aligned} i \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \frac{\partial}{\partial t} \begin{pmatrix} \Psi_A \\ \Psi_B \end{pmatrix} &= m \begin{pmatrix} \Psi_A \\ \Psi_B \end{pmatrix} \\ \Rightarrow i \frac{\partial \Psi_A}{\partial t} &= m \Psi_A, \quad i \frac{\partial \Psi_B}{\partial t} = -m \Psi_B \end{aligned} \tag{10}$$

- The solutions are written as a function of the bi-spinors u_A and u_B :

$$\Psi_A(t) = u_A e^{-imt}, \quad E > 0: \text{positive energy solutions}$$

$$\Psi_B(t) = u_B e^{imt}, \quad E < 0: \text{negative energy solutions}$$

The Dirac equation: solutions

- Going back to Eq. 10

$$\begin{pmatrix} mI & 0 \\ 0 & -mI \end{pmatrix} \begin{pmatrix} u_A \\ u_B \end{pmatrix} = m \begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

- Left-hand side is diagonal $\Rightarrow$ we can find decoupled solutions for u_A and u_B , and choose a set of eigenvector

$$u_A = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ or } u_A = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \text{ with } E = +m$$

$$u_B = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ or } u_A = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \text{ with } E = -m$$

The Dirac equation: solutions

- Putting everything together, for a particle at rest we find:

$$\Psi_0^{(1)} = N \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} e^{-imt}, \quad \Psi_0^{(2)} = N \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} e^{-imt}, \text{ with positive energy}$$

$$\Psi_0^{(3)} = N \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} e^{+imt}, \quad \Psi_0^{(4)} = N \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} e^{+imt}, \text{ with negative energy}$$

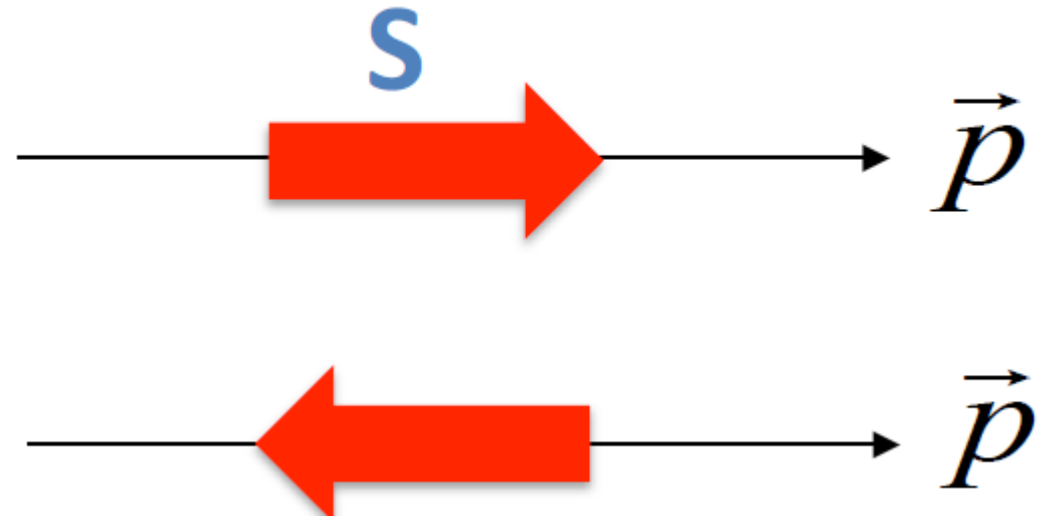
- Four solutions: two with positive energy and two with negative energy

The Dirac equation: solutions

- The fact that there are two identical fermions with the same energy implies that there is another quantum number that should allow to distinguish them, the helicity
- The corresponding operator is the operator projecting the spin on the direction of motion

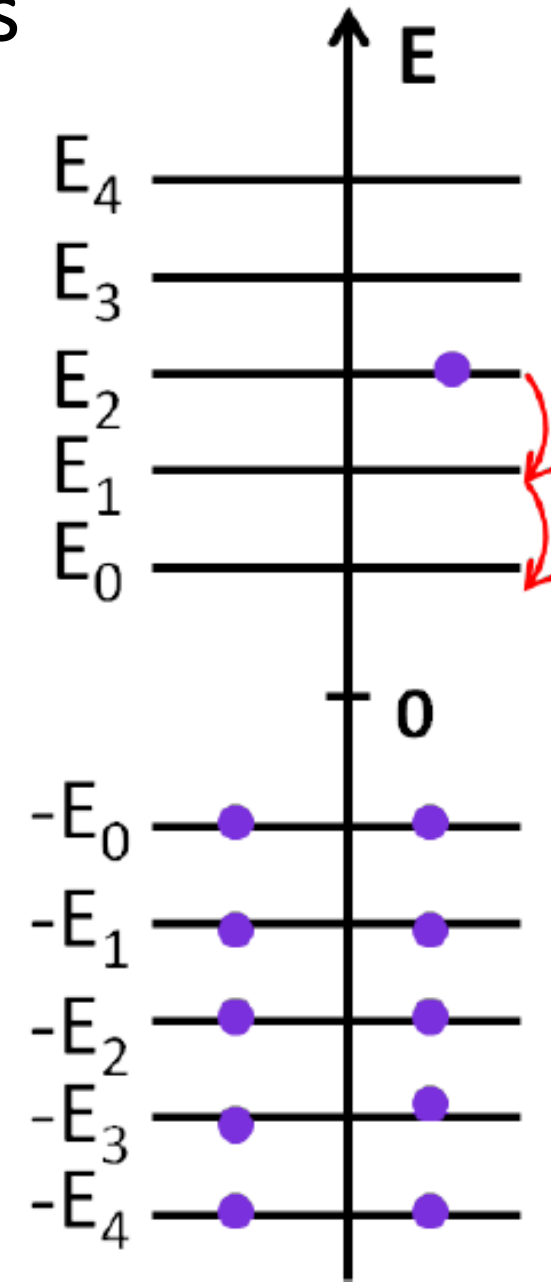
$h = +1$, positive helicity

$h = -1$, negative helicity



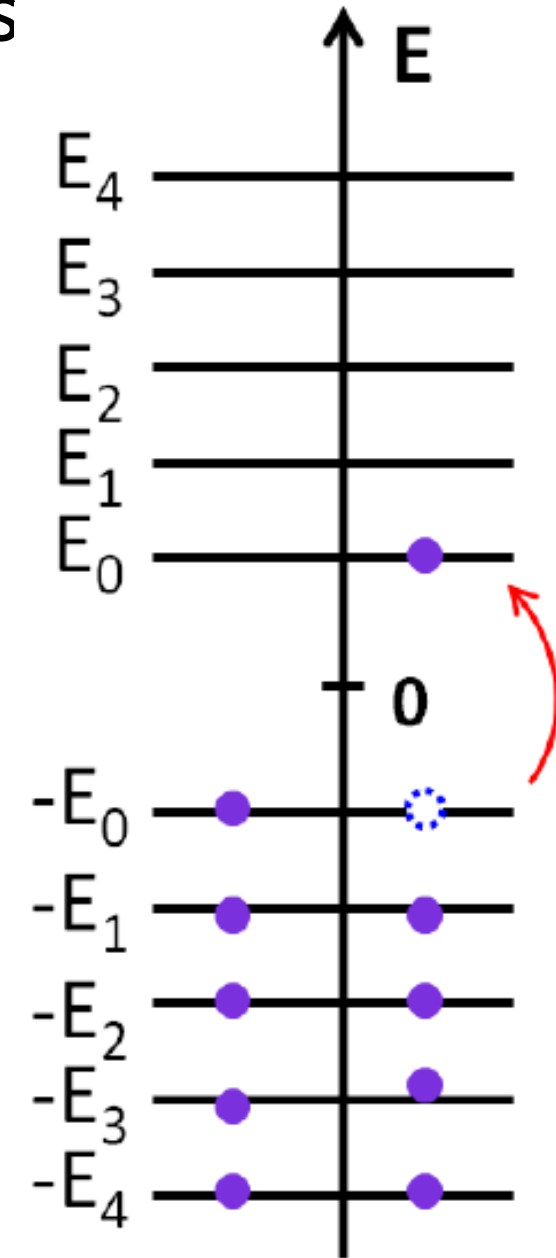
Dirac's explanation of the negative energy solutions

- Atoms are observed to be stable
- When an electron occupies a high energy level, it undergoes transition down to the state of lowest energy not yet occupied by two electrons
- To save his equation, Dirac makes a hypothesis
 - all states of negative energy are occupied by two electrons, preventing another electron to reach these states
- All the electron filling the negative energy states form what was called the Dirac sea



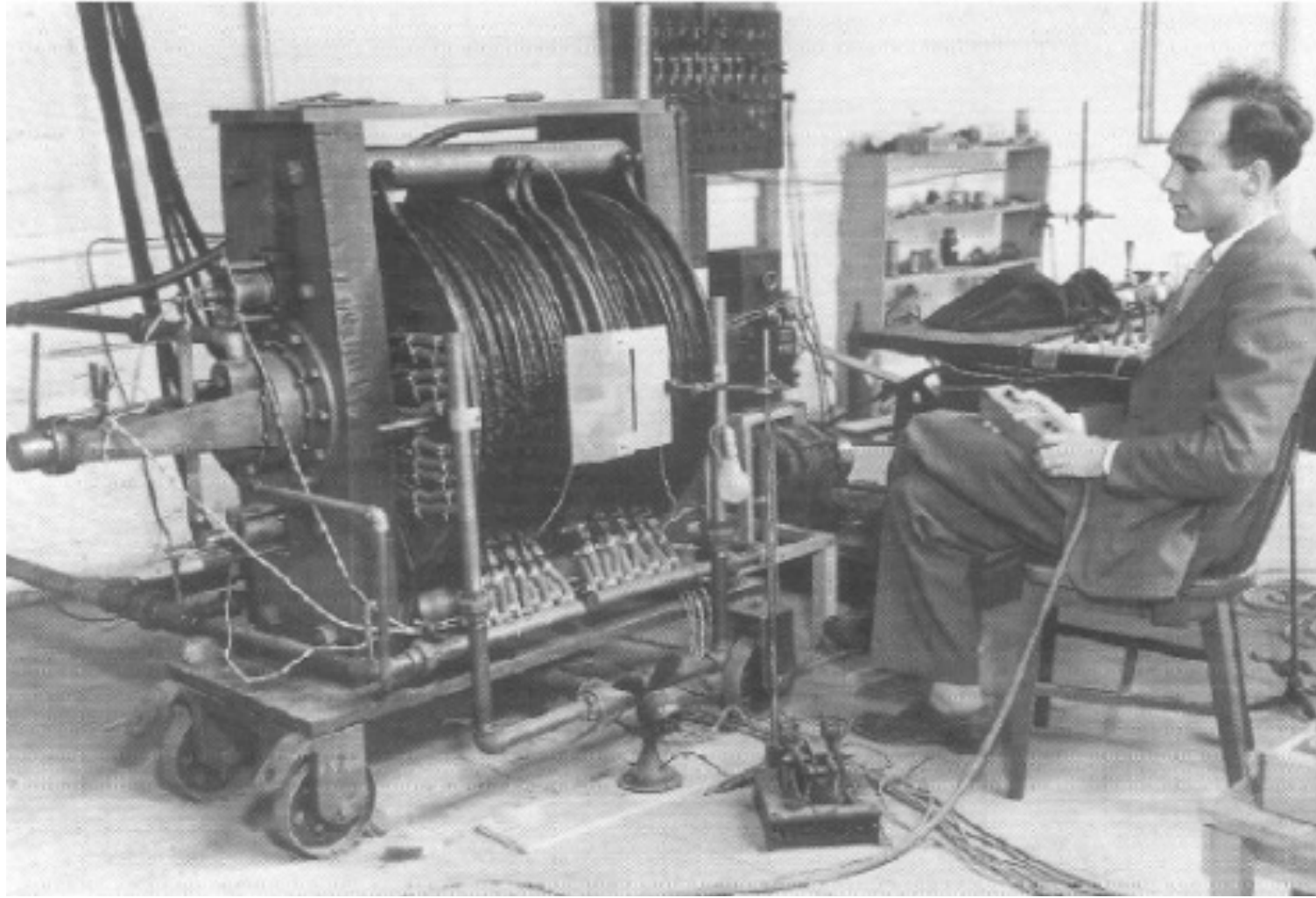
Dirac's explanation of the negative energy solutions

- What happens if sufficient energy is provided to an electron of the sea?
- It will appear like a hole in the sea
 - missing $q = -e \Rightarrow$ presence of $q = +e$
 - missing $E < 0 \Rightarrow$ presence of $E > 0$
- A hole in the electron sea at energy level $E < 0$ looks like an ordinary particle with charge $q = +e$ and energy $-E > 0$!
- Would such positive electrons exist?
- If yes, then they will be identical to the electron except for their charge



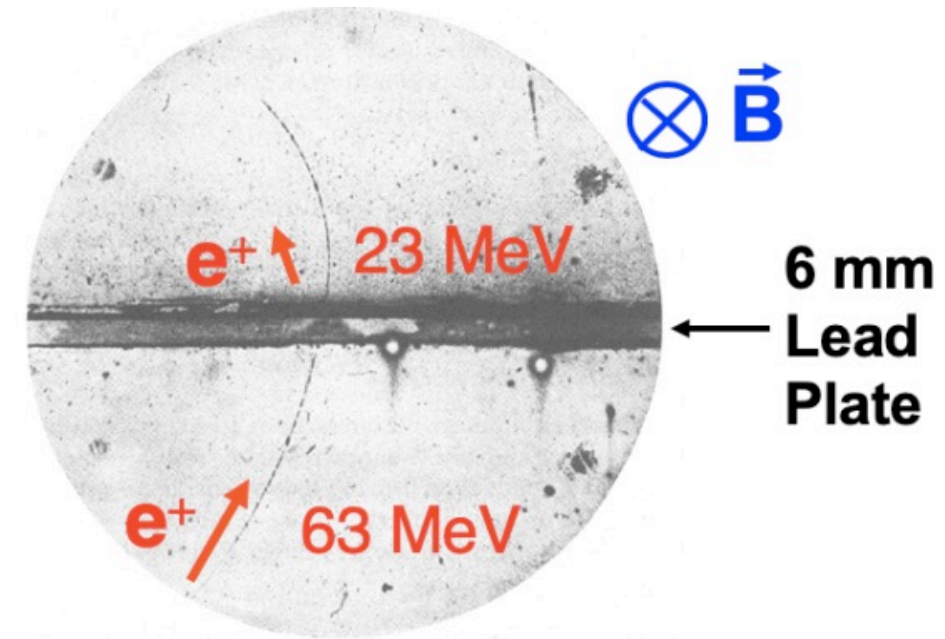
Discovery of the anti-electron (1932)

- The mystery of negative energy solutions of Dirac's equation persisted until 1932, when C. Anderson discovered a new particle seemingly identical to the electron but with opposite charge



Discovery of the anti-electron (1932)

- He used a cloud chamber – a tube filled with supersaturated vapour
- Charged particles passing through the vapour ionise it, which then seed an ion trail that can be photographed
- Uniform magnetic field was applied
- He observed the tracks of a positively charged particle for which the energy losses in the Pb –plate were not compatible with those of a proton
- On the contrary, the track looked exactly like an electron



This was the observation of the first antiparticle, the anti-electron, called positron

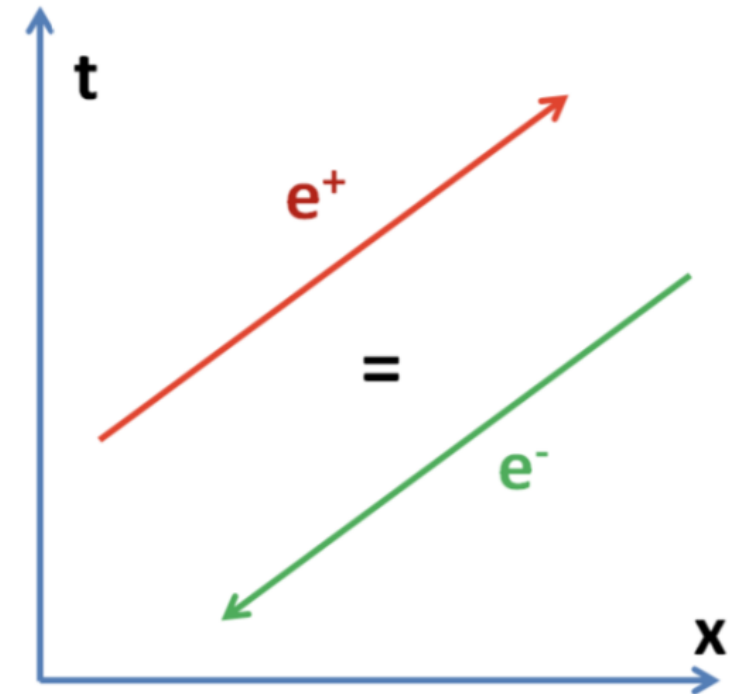
Discovery of the anti-electron



- 1933 – Dirac, together with Schrödinger, receive the Nobel prize
- 1936 – Anderson, at the age of 31, becomes the second youngest Nobel prize winner

The antiparticles

- Feynman-Stücklenberg interpretation for $E < 0$ (1940):
 - the story of the sea of electrons was not very satisfactory (infinite negative charge in the Universe)
 - new hypothesis supported by the positron observation
 - **each particle of mass m and charge q has a corresponding antiparticle of mass m and charge $-q$**
- Indeed, the $E < 0$ solution can be written as $E(-t)$ instead of $-Et$
- Corresponds to a particle of positive energy E with time inversed
- Nowadays, we know that for each particle that we know there exists an anti-particle
- The discovery of the positron was an important milestone that contributed significantly to our understanding of particle physics



Summary of Lecture 6

Main learning outcomes

- Reminder of non-relativistic Quantum Mechanics – wavefunction interpretation, Schrödinger equation
- The Klein-Gordon equation for relativistic particles: derivation, solution and resulting problems
- The Dirac equation and antiparticles: derivation and solution
- How to compute probability density and flux using the continuity equation for Schrödinger, Klein-Gordon and Dirac equations
- Antiparticle interpretation and the discovery of the positron