Lecture 22
Relativistic Quantum Mechanics

Background

- Why study relativistic quantum mechanics?

1. Many experimental phenomena cannot be understood within purely non-relativistic domain.

   e.g. quantum mechanical spin, emergence of new sub-atomic particles, etc.

2. New phenomena appear at relativistic velocities.

   e.g. particle production, antiparticles, etc.

3. Aesthetically and intellectually it would be profoundly unsatisfactory if relativity and quantum mechanics could not be united.

Background

- When is a particle relativistic?

1. When velocity approaches speed of light c or, more intrinsically, when energy is large compared to rest mass energy, mc^2.

   e.g. protons at CERN are accelerated to energies of ca. 300GeV (1GeV$= 10^9$eV) much larger than rest mass energy, 0.94 GeV.

2. Photons have zero rest mass and always travel at the speed of light – they are never non-relativistic!

Background

- What new phenomena occur?

1. **Particle production**

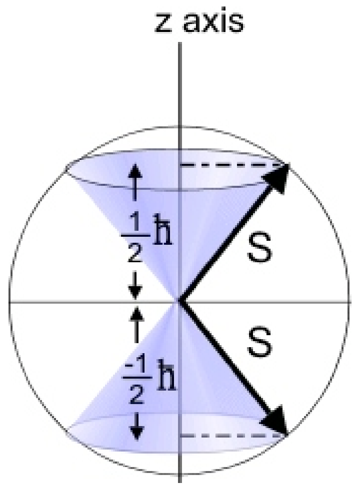
   e.g. electron-positron pairs by energetic γ-rays in matter.

2. **Vacuum instability:** If binding energy of electron

$$E_{\rm bind} = \frac{Z^2 e^4 m}{2\hbar^2} > 2mc^2$$

   a nucleus with initially no electrons is instantly screened by creation of electron/positron pairs from vacuum

3. **Spin**: emerges naturally from relativistic formulation



Background

- When does relativity intrude on QM?

1. When $E_{\mathrm{kin}} \sim mc^2$, i.e. $p \sim mc$
2. From uncertainty relation, $\Delta x \Delta p > h$, this translates to a length

$$\boxed{\Delta x > \frac{h}{mc} = \lambda_c}$$

the **Compton wavelength**.

3. for massless particles, $\lambda_c = \infty$, i.e. relativity always important for, e.g., photons.

Relativistic quantum mechanics: outline

1. Special relativity (revision and notation)
2. Klein-Gordon equation
3. Dirac equation
4. Quantum mechanical spin
5. Solutions of the Dirac equation
6. Relativistic quantum field theories
7. Recovery of non-relativistic limit

Special relativity (revision and notation)

Space-time is specified by a 4-vector

- A **contravariant 4-vector**

$$\boxed{x = (x^\mu) \equiv (x^0, x^1, x^2, x^3) \equiv (ct, \mathbf{x})}$$

transformed into covariant 4-vector $x_\mu = g_{\mu\nu} x^\nu$ by Minkowskii metric

$$(g_{\mu\nu}) = (g^{\mu\nu}) = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}, \qquad g^{\mu\nu} g_{\nu\lambda} = g^\mu_{\ \lambda} \equiv \delta^\mu_{\ \lambda},$$

- **Scalar product**: $x \cdot y = x_\mu y^\mu = x^\mu y^\nu g_{\mu\nu} = x^\mu y_\mu$

Special relativity (revision and notation)

- **Lorentz group**: consists of linear transformations, Λ, preserving $x \cdot y$, i.e. for $x^\mu \mapsto x'^\mu = \Lambda^\mu{}_\nu x^\nu = x \cdot y$

$$x' \cdot y' = g_{\mu\nu} x'^\mu y'^\nu = \underbrace{g_{\mu\nu} \Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta}_{= g_{\alpha\beta}} x^\alpha y^\beta = g_{\alpha\beta} x^\alpha y^\beta$$

e.g. Lorentz transformation along x_1

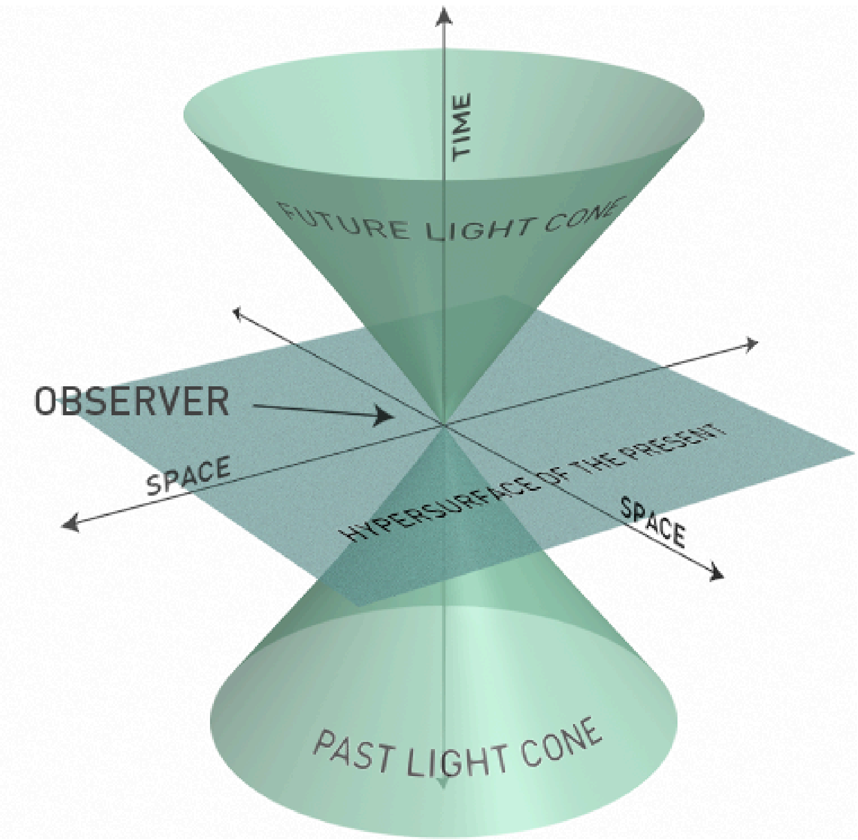
$$\boxed{\Lambda^\mu{}_\nu = \begin{pmatrix} \gamma & -\gamma v/c & & \\ -\gamma v/c & \gamma & & \\ & & 1 & 0 \\ & & 0 & 1 \end{pmatrix}, \qquad \gamma = \frac{1}{(1 - v^2/c^2)^{1/2}}}$$

Special relativity (revision and notation)

- 4-vectors classified as time-like or space-like

$$\boxed{x^2 = (ct)^2 - \mathbf{x}^2}$$

1. forward time-like: $x^2 > 0$, $x^0 > 0$
2. backward time-like: $x^2 > 0$, $x^0 < 0$
3. space-like: $x^2 < 0$



Special relativity (revision and notation)

- Lorentz group splits up into four components:

1. Every LT maps time-like vectors ($x^2 > 0$) into time-like vectors
2. **Orthochronous transformations** $\Lambda^0{}_0 > 0$, preserve forward/backward sign
3. **Proper**: $\det \Lambda = 1$ (as opposed to -1)
4. Group of proper orthochronous transformation: $\mathcal{L}_+^\uparrow$ – subgroup of Lorentz group – excludes **time-reversal** and **parity**

$$T = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}, \qquad P = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}$$

5. Remaining components of group generated by

$$\mathcal{L}_-^\downarrow = T\mathcal{L}_+^\uparrow, \qquad \mathcal{L}_-^\uparrow = P\mathcal{L}_+^\uparrow, \qquad \mathcal{L}_+^\downarrow = TP\mathcal{L}_+^\uparrow.$$

Special relativity (revision and notation)

1. Special relativity requires theories to be invariant under LT or, more generally, **Poincaré transformations**: $x^\mu \longrightarrow \Lambda^\mu{}_\nu x^\nu + a^\mu$
2. Generators of proper orthochronous transformations, $\Lambda \in \mathcal{L}_+^\uparrow$, can be reached by infinitesimal transformations

$$\Lambda^\mu{}_\nu = \delta^\mu{}_\nu + \omega^\mu{}_\nu, \qquad \omega^\mu{}_\nu \ll 1$$

$$g_{\mu\nu}\Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta = g_{\alpha\beta} + \omega_{\alpha\beta} + \omega_{\beta\alpha} + O(\omega^2) \overset{!}{=} g_{\alpha\beta}$$

i.e. $\omega_{\alpha\beta} = -\omega_{\beta\alpha}$, $\omega_{\alpha\beta}$ has six independent components

$\mathcal{L}_+^\uparrow$ has six independent generators: three rotations and three boosts

3. covariant and contravariant derivative, chosen s.t. $\partial_\mu x^\mu = 1$

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = \left(\frac{1}{c}\frac{\partial}{\partial t}, \nabla\right), \qquad \partial^\mu = \frac{\partial}{\partial x_\mu} = \left(\frac{1}{c}\frac{\partial}{\partial t}, -\nabla\right).$$

4. d'Alembertian operator: $\partial^2 = \partial_\mu \partial^\mu = \dfrac{1}{c^2}\dfrac{\partial^2}{\partial t^2} - \nabla^2$

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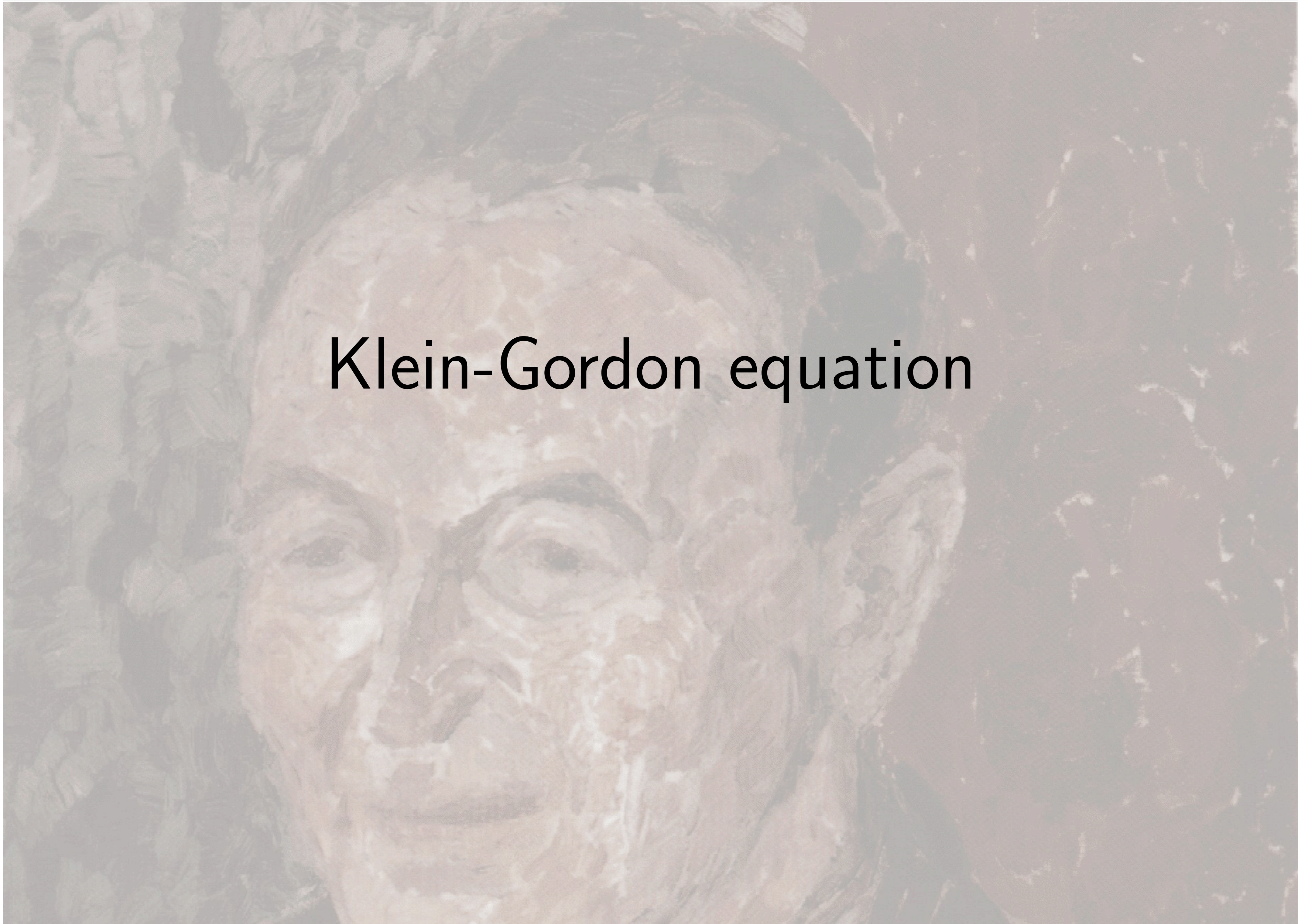
Klein-Gordon equation



Klein-Gordon equation

How to make wave equation relativistic?

- According to canonical quantization procedure in NRQM:

$$\hat{\mathbf{p}} = -i\hbar\nabla, \qquad \hat{E} = i\hbar\partial_t, \qquad \text{i.e. } p^\mu \equiv (E/c, \mathbf{p}) \mapsto \hat{p}^\mu$$

transforms as a 4-vector under LT

- What if we apply quantization procedure to energy?

$$p^\mu p_\mu = (E/c)^2 - \mathbf{p}^2 = m^2c^2, \qquad m - \text{rest mass}$$

$$E(p) = +\left(m^2c^4 + \mathbf{p}^2c^2\right)^{1/2} \quad \longmapsto \quad i\hbar\partial_t\psi = \left[m^2c^4 - \hbar^2c^2\nabla^2\right]^{1/2}\psi$$

- Meaning of square root? Taylor expansion:

$$i\hbar\partial_t\psi = mc^2\psi - \frac{\hbar^2\nabla^2}{2m}\psi - \frac{\hbar^4(\nabla^2)^2}{8m^3c^2}\psi + \cdots$$

i.e. time-evolution of ψ specified by infinite number of boundary conditions $\mapsto$ non-locality, and space/time asymmetry – suggests that this equation is a poor starting point...

Klein-Gordon equation

- Alternatively, apply quantization to energy-momentum invariant:

$$E^2 = \mathbf{p}^2 c^2 + m^2 c^4, \qquad -\hbar^2 \partial_t^2 \psi = \left(-\hbar^2 c^2 \nabla^2 + m^2 c^4\right) \psi$$

- Setting $k_c = \frac{2\pi}{\lambda_c} = \frac{mc}{\hbar}$, leads to **Klein-Gordon equation**,

$$\boxed{\left(\partial^2 + k_c^2\right) \psi = 0}$$

- Klein-Gordon equation is local and manifestly Lorentz covariant.
- Invariance of ψ under rotations means that, if valid at all, Klein-Gordon equation limited to spinless particles

- But can $|\psi|^2$ be interpreted as probability density?

Klein-Gordon equation: Probabilities

- Probabilities? Take lesson from non-relativistic quantum mechanics:

$$\psi^* \overbrace{\left(i\hbar\partial_t + \frac{\hbar^2\nabla^2}{2m}\right)\psi = 0,}^{\text{Schrodinger eqn.}} \qquad \overbrace{\psi\left(-i\hbar\partial_t + \frac{\hbar^2\nabla^2}{2m}\right)\psi^* = 0}^{\text{c.c.}}$$

$$\text{i.e.} \qquad \partial_t|\psi|^2 - i\frac{\hbar}{2m}\nabla\cdot(\psi^*\nabla\psi - \psi\nabla\psi^*) = 0$$

- cf. continuity relation – conservation of probability: $\partial_t\rho + \nabla\cdot\mathbf{j} = 0$

$$\boxed{\rho = |\psi|^2, \qquad \mathbf{j} = -i\frac{\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*)}$$

Klein-Gordon equation: Probabilities

- Applied to KG equation: $\psi^* \left(\frac{1}{c^2} \partial_t^2 - \nabla^2 + k_c^2 \right) \psi = 0$

$$\hbar^2 \partial_t \left(\psi^* \partial_t \psi - \psi \partial_t \psi^* \right) - \hbar^2 c^2 \nabla \cdot \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right) = 0$$

cf. continuity relation – conservation of probability: $\partial_t \rho + \nabla \cdot \mathbf{j} = 0$.

$$\boxed{\rho = i \frac{\hbar}{2mc^2} \left(\psi^* \partial_t \psi - \psi \partial_t \psi^* \right), \qquad \mathbf{j} = -i \frac{\hbar}{2m} \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right)}$$

- With 4-current $j^\mu = (\rho c, \mathbf{j})$, continuity relation $\partial_\mu j^\mu = 0$.

i.e. Klein-Gordon density is the time-like component of a 4-vector.

Klein-Gordon equation: viability?

But is Klein-Gordon equation acceptable?

- Density $\rho = i\dfrac{\hbar}{2mc^2}\left(\psi^*\partial_t\psi - \psi\partial_t\psi^*\right)$ is not positive definite.
- Klein-Gordon equation is not first order in time derivative therefore we must specify ψ **and** $\partial_t\psi$ everywhere at $t = 0$.
- Klein-Gordon equation has both positive and negative energy solutions.

Could we just reject negative energy solutions? Inconsistent – local interactions can scatter between positive and negative energy states

$$\left(\partial^2 + k_c^2\right)\psi = F(\psi) \qquad \text{self} - \text{interaction}$$

$$\left[\left(\partial + iqA/\hbar c\right)^2 + k_c^2\right]\psi = 0 \qquad \text{interaction with EM field}$$

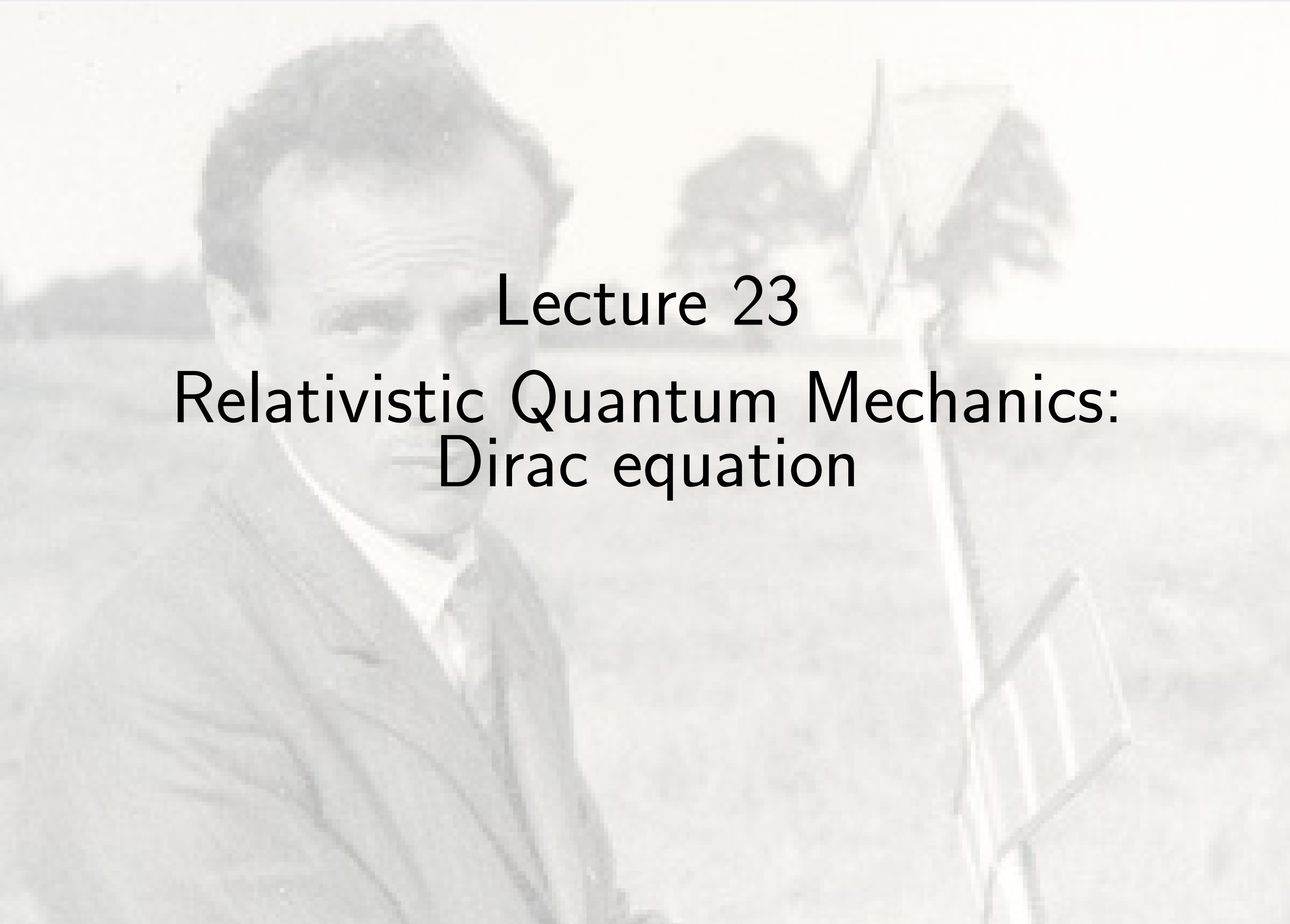
Relativistic quantum mechanics: summary

- When the kinetic energy of particles become comparable to rest mass energy, $p \sim mc$ particles enter regime where relativity intrudes on quantum mechanics.
- At these energy scales qualitatively new phenomena emerge:

  e.g. particle production, existence of antiparticles, etc.
- By applying canonical quantization procedure to energy-momentum invariant, we are led to the **Klein-Gordon equation**,

$$\boxed{(\partial^2 + k_c^2)\psi = 0}$$

  where $\lambda = \frac{\lambda_c}{2\pi} = \frac{\hbar}{mc}$ denotes the Compton wavelength.
- However, the Klein-Gordon equation does not lead to a positive definite probability density and admits positive and negative energy solutions – these features led to it being abandoned as a viable candidate for a relativistic quantum mechanical theory.



Lecture 23
Relativistic Quantum Mechanics: Dirac equation

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Dirac Equation

- Dirac placed emphasis on two constraints:
  1. Relativistic equation must be first order in time derivative (and therefore proportional to $\partial_\mu = (\partial_t/c, \nabla)$).
  2. Elements of wavefunction must obey Klein-Gordon equation.
- Dirac's approach was to try to factorize Klein-Gordon equation: $(\partial^2 + m^2)\psi = 0$ (where henceforth we set $\hbar = c = 1$)

$$(-i\gamma^\nu \partial_\nu - m)(i\gamma^\mu \partial_\mu - m)\psi = 0$$

i.e. with $\hat{p}_\mu = i\partial_\mu$

$$\boxed{(\gamma^\mu \hat{p}_\mu - m)\,\psi = 0}$$

Dirac Equation

$$\boxed{(\gamma^\mu \hat{p}_\mu - m)\,\psi = 0}$$

- Equation is acceptable if:
  1. ψ satisfies Klein-Gordon equation, $(\partial^2 + m^2)\psi = 0$;
  2. there must exist 4-vector current density which is conserved and whose time-like component is a positive density;
  3. ψ does not have to satisfy any auxiliary boundary conditions.
- From condition (1) we require (assuming $[\gamma^\mu, \hat{p}_\nu] = 0$)

$$0 = (\gamma^\nu \hat{p}_\nu + m)\,(\gamma^\mu \hat{p}_\mu - m)\,\psi = (\underbrace{\gamma^\nu\gamma^\mu}_{(\gamma^\nu\gamma^\mu + \gamma^\mu\gamma^\nu)/2}\ \hat{p}_\nu \hat{p}_\mu - m^2)\psi$$

$$= \left(\frac{1}{2}\{\gamma^\nu, \gamma^\mu\}\hat{p}_\nu \hat{p}_\mu - m^2\right)\psi = (g^{\nu\mu}\hat{p}_\nu \hat{p}_\mu - m^2)\psi = (p^2 - m^2)\psi$$

i.e. obeys Klein-Gordon if $\{\gamma^\mu, \gamma^\nu\} \equiv \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\nu\mu}$

$\Rightarrow \gamma^\mu$, and therefore ψ, can not be scalar.

Dirac Equation: Hamiltonian formulation

$$\boxed{(\gamma^\mu \hat{p}_\mu - m)\,\psi = 0, \qquad \{\gamma^\mu, \gamma^\nu\} = 2g^{\nu\mu}}$$

- To bring Dirac equation to the form $i\partial_t \psi = \hat{H}\psi$, consider

$$\gamma^0(\gamma^\mu \hat{p}_\mu - m)\psi = \gamma^0(\gamma^0 \hat{p}_0 - \boldsymbol{\gamma} \cdot \hat{\mathbf{p}} - m)\psi = 0$$

- Since $(\gamma^0)^2 \equiv \frac{1}{2}\{\gamma^0, \gamma^0\} = g^{00} = \mathbb{I}$,

$$\gamma^0(\gamma^\mu \hat{p}_\mu - m)\psi = i\partial_t \psi - \gamma^0 \boldsymbol{\gamma} \cdot \hat{\mathbf{p}}\psi - m\gamma^0 \psi = 0$$

- i.e. Dirac equation can be written as $i\partial_t \psi = \hat{H}\psi$ with

$$\boxed{\hat{H} = \boldsymbol{\alpha} \cdot \hat{\mathbf{p}} + \beta m, \qquad \boldsymbol{\alpha} = \gamma^0 \boldsymbol{\gamma}, \qquad \beta = \gamma^0}$$

- Using identity $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$,

$$\beta^2 = \mathbb{I}, \qquad \{\boldsymbol{\alpha}, \beta\} = 0, \qquad \{\alpha_i, \alpha_j\} = 2\delta_{ij} \quad \text{(exercise)}$$

Dirac Equation: γ matrices

$$\boxed{i\partial_t \psi = \hat{H}\psi, \qquad \hat{H} = \boldsymbol{\alpha}\cdot\hat{\mathbf{p}} + \beta m, \qquad \boldsymbol{\alpha} = \gamma^0 \boldsymbol{\gamma}, \qquad \beta = \gamma^0}$$

- Hermiticity of $\hat{H}$ assured if $\boldsymbol{\alpha}^\dagger = \boldsymbol{\alpha}$, and $\beta^\dagger = \beta$, i.e.

$$(\gamma^0 \boldsymbol{\gamma})^\dagger \equiv \boldsymbol{\gamma}^\dagger \gamma^{0\dagger} = \gamma^0 \boldsymbol{\gamma}, \qquad \text{and } \gamma^{0\dagger} = \gamma^0$$

- So we obtain the defining properties of Dirac γ matrices,

$$\boxed{\gamma^{\mu\dagger} = \gamma^0 \gamma^\mu \gamma^0, \qquad \{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}}$$

- Since space-time is four-dimensional, γ must be of dimension at least 4×4 – ψ has at least four components.
- However, 4-component wavefunction ψ does not transform as 4-vector – it is known as a **spinor (or bispinor)**.

Dirac Equation: γ matrices

$$\boxed{\gamma^{\mu\dagger} = \gamma^0\gamma^\mu\gamma^0, \qquad \{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}}$$

- From the defining properties, there are several possible representations of γ matrices. In the **Dirac/Pauli representation:**

$$\gamma^0 = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix}, \qquad \boldsymbol{\gamma} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & 0 \end{pmatrix}$$

$\boldsymbol{\sigma}$ – **Pauli spin matrices**

$$\boxed{\sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k, \qquad \sigma_i{}^\dagger = \sigma_i}$$

e.g., $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

- So, in Dirac/Pauli representation,

$$\boldsymbol{\alpha} = \gamma^0\boldsymbol{\gamma} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \qquad \beta = \gamma^0 = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix}$$

Dirac Equation: conjugation, density and current

$$\boxed{(\gamma^\mu \hat{p}_\mu - m)\,\psi = 0, \qquad \gamma^{\mu\,\dagger} = \gamma^0\gamma^\mu\gamma^0}$$

- Applying complex conjugation to Dirac equation

$$[(\gamma^\mu \hat{p}_\mu - m)\psi]^\dagger = \psi^\dagger\left(-i\gamma^{\dagger\,\mu}\overleftarrow{\partial}_\mu - m\right) = 0, \qquad \psi^\dagger\overleftarrow{\partial}_\mu \equiv (\partial_\mu\psi)^\dagger$$

- Since $(\gamma^0)^2 = \mathbb{I}$, we can write,

$$0 = \underbrace{\psi^\dagger\gamma^0}_{\bar{\psi}}(-i\underbrace{\gamma^0\gamma^{\dagger\,\mu}}_{\gamma^\mu\gamma^0}\overleftarrow{\partial}_\mu - m\gamma^0) = -\bar{\psi}\left(i\gamma^\mu\overleftarrow{\partial}_\mu + m\right)\gamma^0$$

- Introducing **Feynman 'slash' notation** $\not{a} \equiv \gamma^\mu a_\mu$, obtain conjugate form of Dirac equation

$$\boxed{\bar{\psi}(i\overleftarrow{\not{\partial}} + m) = 0}$$

Dirac Equation: conjugation, density and current

$$\boxed{\bar{\psi}(i\overleftarrow{\not{\partial}} + m) = 0, \qquad \not{\partial} = \gamma^\mu \partial_\mu}$$

- The, combining the Dirac equation, $(i\overrightarrow{\not{\partial}} - m)\psi = 0$ with its conjugate, we have $\bar{\psi}(i\overleftarrow{\not{\partial}} + m)\psi = 0 = -\bar{\psi}(i\overrightarrow{\not{\partial}} - m)\psi$, i.e.

$$\boxed{\bar{\psi}\left(\overleftarrow{\not{\partial}} + \overrightarrow{\not{\partial}}\right)\psi = \partial_\mu(\underbrace{\bar{\psi}\gamma^\mu\psi}_{j^\mu}) = 0}$$

- We therefore identify $j^\mu = (\rho, \mathbf{j}) = (\psi^\dagger\psi, \psi^\dagger\boldsymbol{\alpha}\psi)$ as the 4-current.
- So, in contrast to the Klein-Gordon equation, the density $\rho = j^0 = \psi^\dagger\psi$ is, as required, positive definite.
- Motivated by this triumph(!), let us now consider what constraints relativistic covariance imposes and what consequences follow.

Relativistic covariance

- If $\psi(x)$ obeys the Dirac equation its counterpart $\psi'(x')$ in a LT frame $x'^{\nu} = \Lambda^{\nu}{}_{\mu}x^{\mu}$, must obey the Dirac equation,

$$\left(i\gamma^{\nu}\frac{\partial}{\partial x'^{\nu}} - m\right)\psi'(x') = 0$$

- If observer can reconstruct $\psi'(x')$ from $\psi(x)$ there must exist a local (linear) transformation,

$$\boxed{\psi'(x') = S(\Lambda)\psi(x)}$$

where $S(\Lambda)$ is a 4×4 matrix, i.e.

$$S(\Lambda)\left(i\gamma^{\mu}\frac{\partial x^{\nu}}{\partial x'^{\mu}}(\Lambda^{-1})^{\nu}{}_{\mu}S(\Lambda)\gamma^{\nu}S^{-1}(\Lambda)\gamma^{\nu}\frac{\partial}{\partial x^{\nu}} - m\right)S(\Lambda)\psi(x) = 0$$

- Compatible with Dirac equation if $\boxed{S(\Lambda)\gamma^{\nu}S^{-1}(\Lambda) = (\Lambda^{-1})^{\nu}{}_{\mu}\gamma^{\mu}}$

Relativistic covariance

$$\boxed{\psi'(x') = S(\Lambda)\psi(x), \qquad S(\Lambda)\gamma^\nu S^{-1}(\Lambda) = (\Lambda^{-1})^\nu{}_\mu \gamma^\mu}$$

- **But how do we determine $S(\Lambda)$?** For an infinitesimal (i.e. proper orthochronous) LT

$$\Lambda^\mu{}_\nu = \delta^\mu{}_\nu + \omega^\mu{}_\nu, \qquad (\Lambda^{-1})^\mu{}_\nu = \delta^\mu{}_\nu - \omega^\mu{}_\nu + \cdots$$

(recall that generators, $\omega_{\mu\nu} = -\omega_{\nu\mu}$, are antisymmetric).

- This allows us to form the Taylor expansion of $S(\Lambda)$:

$$S(\Lambda) \equiv S(\mathbb{I} + \omega) = \underbrace{S(\mathbb{I})}_{\mathbb{I}} + \underbrace{\left(\frac{\partial S}{\partial \omega}\right)_{\mu\nu}}_{-\frac{i}{4}\Sigma_{\mu\nu}} \omega^{\mu\nu} + O(\omega^2)$$

where $\Sigma_{\mu\nu} = -\Sigma_{\nu\mu}$ (follows from antisymmetry of ω) is a matrix in bispinor space, and $\omega_{\mu\nu}$ is a number.

Relativistic covariance

$$\boxed{S(\Lambda) = \mathbb{I} - \frac{i}{4}\Sigma_{\mu\nu}\omega^{\mu\nu} + \cdots, \quad S^{-1}(\Lambda) = \mathbb{I} + \frac{i}{4}\Sigma_{\mu\nu}\omega^{\mu\nu} + \cdots}$$

- Requiring that $S(\Lambda)\gamma^\nu S^{-1}(\Lambda) = (\Lambda^{-1})^\nu{}_\mu \gamma^\mu$, a little bit of algebra (see problem set/handout) shows that matrices $\Sigma_{\mu\nu}$ must obey the relation,

$$[\Sigma_{\mu\eta}, \gamma^\nu] = 2i\left(\gamma_\mu \delta^\nu{}_\eta - \gamma_\eta \delta^\nu{}_\mu\right)$$

- This equation is satisfied by (exercise)

$$\boxed{\Sigma_{\alpha\beta} = \frac{i}{2}[\gamma_\alpha, \gamma_\beta]}$$

- In summary, under set of infinitesimal Lorentz transformation, $x' = \Lambda x$, where $\Lambda = \mathbb{I} + \omega$, relativistic covariance of Dirac equation demands that wavefunction transforms as $\psi'(x') = S(\Lambda)\psi$ where $S(\Lambda) = \mathbb{I} - \frac{i}{4}\Sigma_{\mu\nu}\omega^{\mu\nu} + O(\omega^2)$ and $\Sigma_{\mu\nu} = \frac{i}{2}[\gamma_\mu, \gamma_\nu]$.

Relativistic covariance

$$\boxed{S(\Lambda) = \mathbb{I} - \frac{i}{4}\Sigma_{\mu\nu}\omega^{\mu\nu} + \cdots}$$

- "Finite" transformations (i.e. non-infinitesimal) generated by

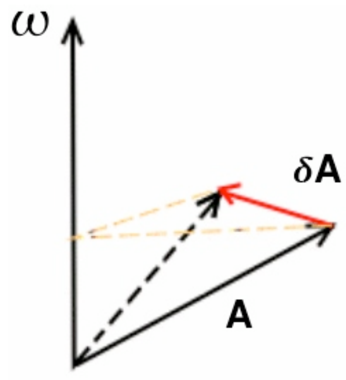
$$\boxed{S(\Lambda) = \exp\left[-\frac{i}{4}\Sigma_{\alpha\beta}\omega^{\alpha\beta}\right], \qquad \omega^{\alpha\beta} = \Lambda^{\alpha\beta} - g^{\alpha\beta}}$$

1. Transformations involving unitary matrices $S(\Lambda)$, where $S^\dagger S = \mathbb{I}$ translate to **spatial rotations**.
2. Transformations involving Hermitian matrices $S(\Lambda)$, where $S^\dagger = S$ translate to **Lorentz boosts**.

- **So what??** What are the consequences of relativistic covariance?

Angular momentum and spin

- For infinitesimal anticlockwise rotation by angle θ around $\mathbf{n}$



$$\mathbf{x}' \simeq \mathbf{x} + \theta\mathbf{n} \times \mathbf{x} \equiv \Lambda\,\mathbf{x}, \qquad \Lambda \simeq \mathbb{I} + \underbrace{\theta\,\mathbf{n}\,\times}_{\omega}$$

i.e. $\omega_{ij} = \theta\,\epsilon_{ikj} n_k$, $\omega_{0i} = \omega_{i0} = 0$.

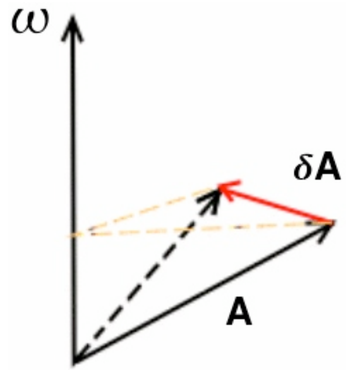
- In non-relativistic quantum mechanics:

$$\begin{aligned}
\psi'(\mathbf{x}') = \psi(\mathbf{x}) = \psi(\Lambda^{-1}\mathbf{x}') &\simeq \psi((\mathbb{I} - \omega)\cdot\mathbf{x}') \\
&\simeq \psi(\mathbf{x}') - \omega\cdot\mathbf{x}'\cdot\nabla\psi(\mathbf{x}') + \cdots \\
&= \psi(\mathbf{x}') - i\theta\mathbf{n}\times\mathbf{x}'\cdot(-i\nabla)\psi(\mathbf{x}') + \cdots \\
&= (1 - i\theta\mathbf{n}\cdot\hat{\mathbf{L}})\psi(\mathbf{x}') + \cdots \equiv \hat{U}\psi(\mathbf{x}')
\end{aligned}$$

cf. generator of rotations: $\hat{U} = e^{-i\theta\mathbf{n}\cdot\hat{\mathbf{L}}}$.

Angular momentum and spin

- But relativistic covariance of Dirac equation demands that $\psi'(x') = S(\Lambda)\psi(x)$



- With $\omega_{ij} = \theta\,\epsilon_{ijk} n_k$, $\omega_{0i} = \omega_{i0} = 0$,

$$S(\Lambda) \simeq \mathbb{I} - \frac{i}{4}\Sigma_{\alpha\beta}\omega^{\alpha\beta} = \mathbb{I} - \frac{i}{4}\Sigma_{ij}\epsilon_{ikj} n_k \theta$$

- In Dirac/Pauli representation $\qquad \sigma_k$ – Pauli spin matrices

$$\Sigma_{ij} = \frac{i}{2}[\gamma_i, \gamma_j] = \epsilon_{ijk} \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}, \qquad \gamma_i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}$$

- i.e. $\boxed{S(\Lambda) = \mathbb{I} - i\theta\mathbf{n}\cdot\mathbf{S}}$ where

$$S_k = \frac{1}{4}\epsilon_{ijk}\Sigma_{ij} = \frac{1}{4}\underbrace{\epsilon_{ijk}\epsilon_{ijl}}_{\delta_{jj}\delta_{kl} - \delta_{jl}\delta_{jk} = 2\delta_{kl}}\sigma_l \otimes \mathbb{I} = \frac{1}{2}\begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}$$

Angular momentum and spin

- Altogether, combining components of transformation,

$$\psi'(x') = \overbrace{S(\Lambda)}^{\mathbb{I} - i\theta\mathbf{n}\cdot\mathbf{S}} \underbrace{\psi(x\Lambda^{-1}x')}_{(\mathbb{I} - i\theta\mathbf{n}\cdot\hat{\mathbf{L}})\psi(x')} \simeq (\mathbb{I} - i\theta\mathbf{n}\cdot(\mathbf{S} + \hat{\mathbf{L}}))\psi(x')$$

  we obtain

$$\boxed{\psi'(x') = S(\Lambda)\psi(\Lambda^{-1}x') \simeq (1 - i\theta\mathbf{n}\cdot\hat{\mathbf{J}})\psi(x')}$$

  where $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \mathbf{S}$ represents **total angular momentum.**

- Intrinsic contribution to angular momentum known as **spin**.

$$\boxed{[S_i, S_j] = i\epsilon_{ijk}S_k, \qquad (S_i)^2 = \frac{1}{4} \qquad \text{for each } i}$$

- Dirac equation is relativistic wave equation for spin 1/2 particles.

Parity

- So far we have only dealt with the subgroup of proper orthochronous Lorentz transformations, $\mathcal{L}_+^\uparrow$.
- Taking into account Parity, $P^{\mu\nu} = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}$

  relativistic covariance demands $S(\Lambda)\gamma^\nu S^{-1}(\Lambda) = (\Lambda^{-1})^\nu{}_\mu \gamma^\mu$

$$\boxed{S^{-1}(P)\gamma^0 S(P) = \gamma^0, \qquad S^{-1}(P)\gamma^i S(P) = -\gamma^i}$$

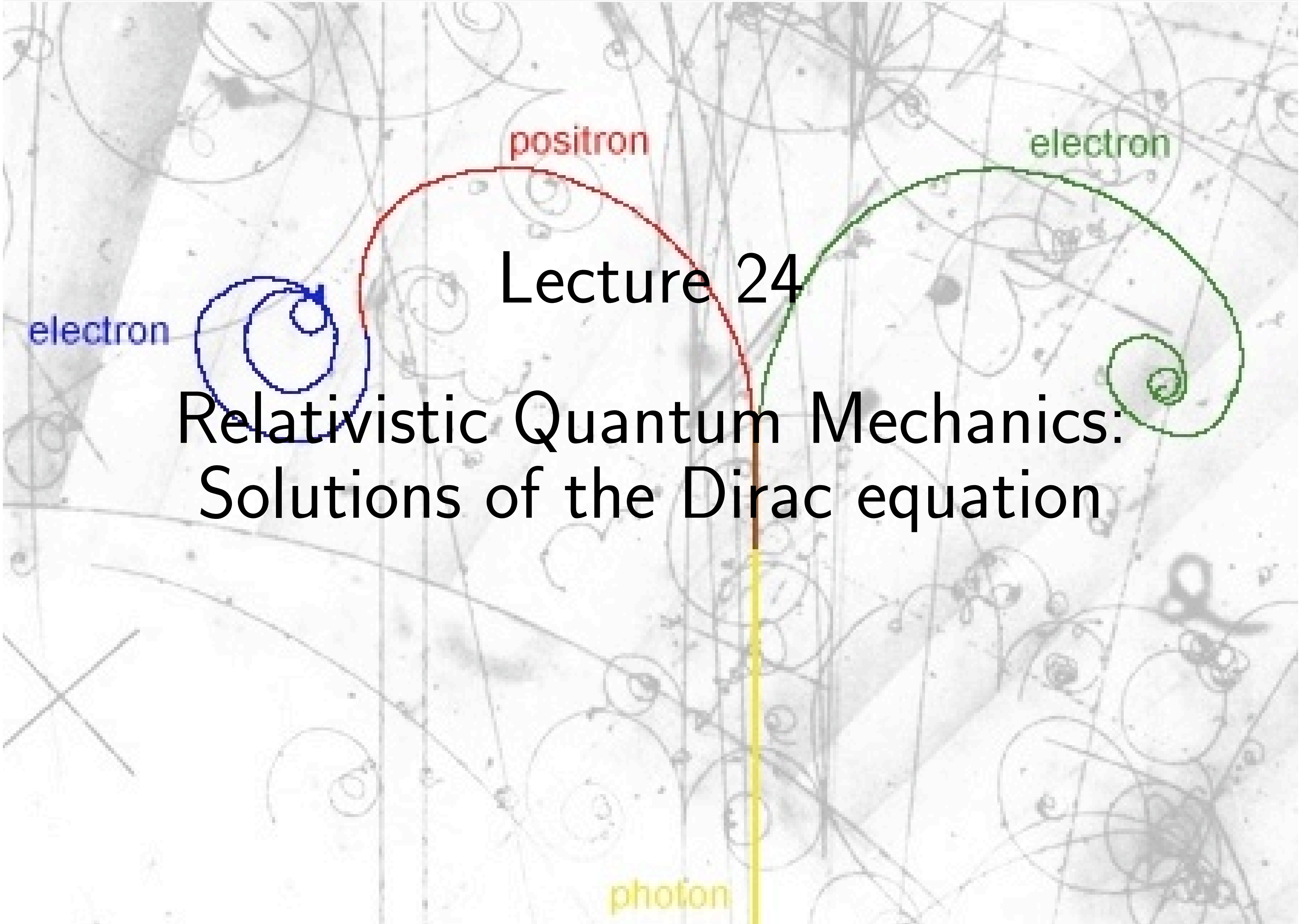
  achieved if $S(P) = \gamma^0 e^{i\phi}$, where ϕ denotes arbitrary phase.
- But since $P^2 = \mathbb{I}$, $e^{i\phi} = 1$ or -1

$$\boxed{\psi'(x') = S(P)\psi(\Lambda^{-1}x') = \eta\gamma^0\psi(Px')}$$

where $\eta = \pm 1$ — intrinsic parity of the particle

Lecture 24

Relativistic Quantum Mechanics: Solutions of the Dirac equation



Relativistic quantum mechanics: outline

1. Special relativity (revision and notation)
2. Klein-Gordon equation
3. Dirac equation
4. Quantum mechanical spin
5. Solutions of the Dirac equation
6. Relativistic quantum field theories
7. Recovery of non-relativistic limit

Free particle solutions of Dirac Equation

$$\boxed{(\not{p} - m)\psi = 0, \qquad \not{p} = i\gamma^\mu \partial_\mu}$$

- Free particle solution of Dirac equation is a plane wave:

$$\boxed{\psi(x) = e^{-ip\cdot x}u(p) = e^{-iEt + i\mathbf{p}\cdot\mathbf{x}}u(p)}$$

where $u(p)$ is the bispinor amplitude.

- Since components of ψ obey KG equation, $(p^\mu p_\mu - m^2)\psi = 0$,

$$(p_0)^2 - \mathbf{p}^2 - m^2 = 0, \qquad E \equiv p_0 = \pm\sqrt{\mathbf{p}^2 + m^2}$$

So, once again, as with Klein-Gordon equation we encounter positive and negative energy solutions!!

Free particle solutions of Dirac Equation

$$\boxed{\psi(x) = e^{-ip\cdot x}u(p) = e^{-iEt+i\mathbf{p}\cdot\mathbf{x}}u(p)}$$

- **What about bispinor amplitude, $u(p)$?**
- In Dirac/Pauli representation,

$$\gamma^0 = \begin{pmatrix} \mathbb{I}_2 & \\ & -\mathbb{I}_2 \end{pmatrix}, \qquad \boldsymbol{\gamma} = \begin{pmatrix} & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & \end{pmatrix}$$

the components of the bispinor obeys the condition,

$$(\gamma^\mu p_\mu - m)u(p) = \begin{pmatrix} p^0 - m & -\boldsymbol{\sigma}\cdot\mathbf{p} \\ \boldsymbol{\sigma}\cdot\mathbf{p} & -p^0 - m \end{pmatrix} u(p) = 0$$

- i.e. bispinor elements:

$$u(p) = \begin{pmatrix} \xi \\ \eta \end{pmatrix}, \qquad \begin{cases} (p^0 - m)\xi = \sigma\cdot\mathbf{p}\eta \\ \sigma\cdot\mathbf{p}\xi = (p^0 + m)\eta \end{cases}$$

Free particle solutions of the Dirac Equation

$$u(p) = \begin{pmatrix} \xi \\ \eta \end{pmatrix}, \qquad \begin{cases} (p^0 - m)\xi = \sigma \cdot \mathbf{p}\eta \\ \sigma \cdot \mathbf{p}\xi = (p^0 + m)\eta \end{cases}$$

- Consistent when $(p^0)^2 = \mathbf{p}^2 + m^2$ and $\eta = \dfrac{\boldsymbol{\sigma} \cdot \mathbf{p}}{p^0 + m}\xi$

$$\boxed{u^{(r)}(p) = N(p) \begin{pmatrix} \chi^{(r)} \\ \dfrac{\boldsymbol{\sigma} \cdot \mathbf{p}}{p_0 + m}\chi^{(r)} \end{pmatrix}}$$

  where $\chi^{(r)}$ are a pair of orthogonal two-component vectors with index $r = 1, 2$, and $N(p)$ is normalization.

- **Helicity:** Eigenvalue of spin projected along direction of motion

$$\boxed{\frac{1}{2}\boldsymbol{\sigma} \cdot \frac{\mathbf{p}}{|\mathbf{p}|}\chi^{(\pm)} \equiv \mathbf{S} \cdot \frac{\mathbf{p}}{|\mathbf{p}|}\chi^{(\pm)} = \pm\frac{1}{2}\chi^{(\pm)}}$$

  e.g. if $\mathbf{p} = p\,\hat{\mathbf{e}}_3$, $\chi^{(+)} = (1, 0)$, $\chi^{(-)} = (0, 1)$

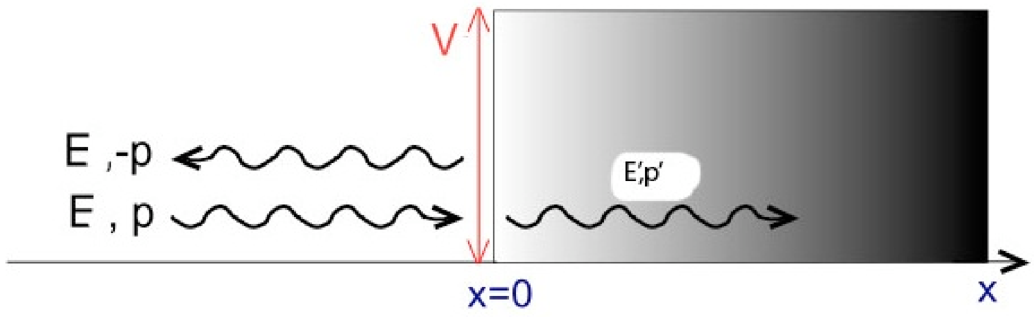
Free particle solutions of the Dirac Equation

- So, general *positive* energy plane wave solution written in eigenbasis of helicity,

$$\boxed{\psi_p^{(\pm)}(x) = N(p)e^{-ip\cdot x}\begin{pmatrix} \chi^{(\pm)} \\ \pm\dfrac{|\mathbf{p}|}{p_0+m}\chi^{(\pm)} \end{pmatrix}}$$

- But how to deal with the problem of negative energy states? Must we reject the Dirac as well as the Klein-Gordon equation?
- In fact, the existence of negative energy states provided the key that led to the discovery of **antiparticles**.
- To understand why, let us consider the problem of scattering from a potential step...

Klein paradox and antiparticles



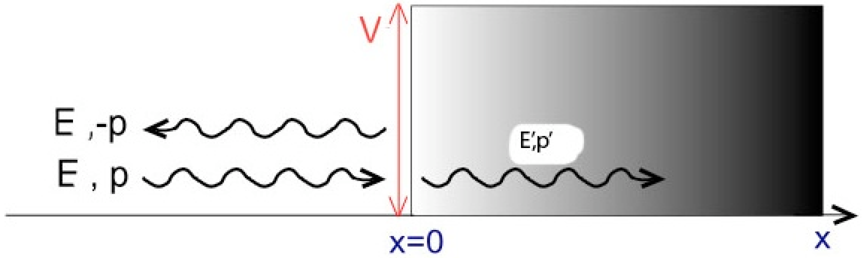
- Consider plane wave, unit amplitude, energy E, momentum $p\,\hat{\mathrm{e}}_3$, and spin $\uparrow$ ($\chi = (1,0)$) incident on potential barrier $V(\mathbf{x}) = V\theta(x_3)$

$$\psi_{\mathrm{in}} = e^{-ip_0 t + ipx_3}\begin{pmatrix} \chi^{(+)} \\ \dfrac{p}{p_0+m}\chi^{(+)} \end{pmatrix}$$

- At barrier, spin is conserved, component r is reflected $(E,\ -p\,\hat{\mathrm{e}}_3)$, and component t is transmitted $(E' = E - V,\ p'\,\hat{\mathrm{e}}_3)$
- From Klein-Gordon condition (energy-momentum invariant): $p_0^2 \equiv E^2 = p^2 + m^2$ and ${p_0'}^2 \equiv E'^2 = p'^2 + m^2$

Klein paradox and antiparticles

$$\psi_{\rm in} = e^{-ip_0 t + ipx_3} \begin{pmatrix} \chi^{(+)} \\ \dfrac{p}{p_0+m}\chi^{(+)} \end{pmatrix}$$



- Boundary conditions: since Dirac equation is first order, require only continuity of ψ at interface (cf. Schrodinger eqn.)

$$\begin{pmatrix} 1 \\ 0 \\ p/(E+m) \\ 0 \end{pmatrix} + r \begin{pmatrix} 1 \\ 0 \\ -p/(E+m) \\ 0 \end{pmatrix} = t \begin{pmatrix} 1 \\ 0 \\ p'/(E'+m) \\ 0 \end{pmatrix}$$

(helicity conserved in reflection)

- Equating (generically complex) coefficients:

$$1 + r = t, \qquad \frac{p}{E+m}(1-r) = \frac{p'}{E'+m} t$$

Klein paradox and antiparticles

$$1 + r = t \quad (1), \qquad \frac{p}{E+m}(1-r) = \frac{p'}{E'+m}t \quad (2)$$

- From (2), $1 - r = \zeta t$ where

$$\boxed{\zeta = \frac{p'}{p}\frac{(E+m)}{(E'+m)}}$$

- Together with (1), $(1+\zeta)t = 2$

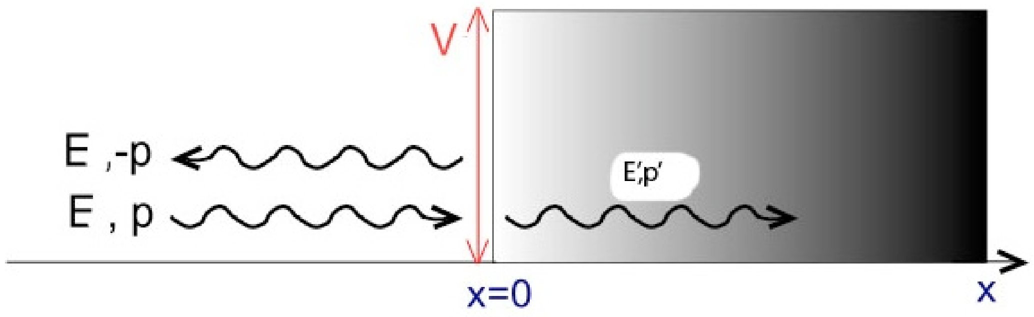
$$\boxed{t = \frac{2}{1+\zeta}, \qquad \frac{1+r}{1-r} = \frac{1}{\zeta}, \qquad r = \frac{1-\zeta}{1+\zeta}}$$

- Interpret solution by studying vector current: $\mathbf{j} = \bar{\psi}\boldsymbol{\gamma}\psi = \psi^\dagger \boldsymbol{\alpha}\psi$

$$j_3 = \psi^\dagger \alpha_3 \psi, \qquad \alpha_3 = \gamma_0\gamma_3 = \begin{pmatrix} & \sigma_3 \\ \sigma_3 & \end{pmatrix}$$

Klein paradox and antiparticles

$$j_3 = \psi^\dagger \begin{pmatrix} & \sigma_3 \\ \sigma_3 & \end{pmatrix} \psi$$



- (Up to overall normalization) the incident, transmitted and reflected currents given by,

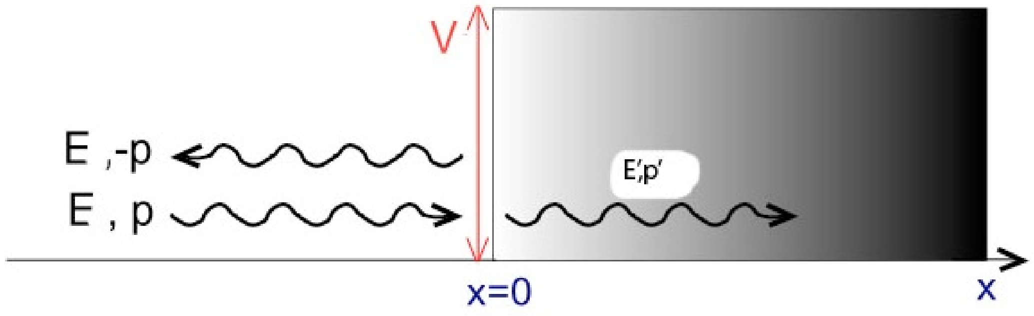
$$j_3^{(i)} = \begin{pmatrix} 1 & 0 & \frac{p}{E+m} & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ \frac{p}{E+m} \\ 0 \end{pmatrix} = \frac{2p}{E+m},$$

$$j_3^{(t)} = \frac{1}{E'+m}(p' + p'^*)|t|^2, \qquad j_3^{(r)} = -\frac{2p}{E+m}|r|^2$$

where we note that, depending on height of the potential, p' may be complex (cf. NRQM).

Klein paradox and antiparticles

$$\zeta = \frac{p'}{p}\frac{E+m}{E'+m}$$



- Therefore, ratio of reflected/transmitted to incident currents,

$$\frac{j_3^{(r)}}{j_3^{(i)}} = -|r|^2 = -\left|\frac{1-\zeta}{1+\zeta}\right|^2$$

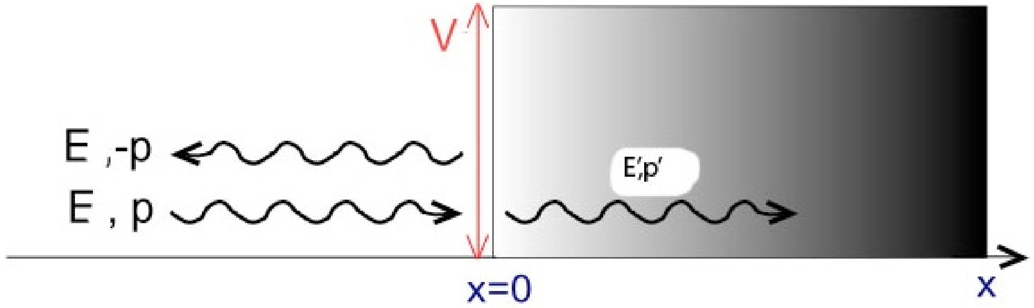
$$\frac{j_3^{(t)}}{j_3^{(i)}} = |t|^2 \frac{(p'+p'^*)}{2p}\frac{E+m}{E'+m} = \frac{4}{|1+\zeta|^2}\frac{1}{2}(\zeta+\zeta^*) = \frac{2(\zeta+\zeta^*)}{|1+\zeta|^2}$$

- From which we can confirm current conservation, $j_3^{(i)} = j_3^{(r)} + j_3^{(t)}$:

$$1 + \frac{j_3^{(r)}}{j_3^{(i)}} = \frac{|1+\zeta|^2 - |1-\zeta|^2}{|1+\zeta|^2} = \frac{2(\zeta+\zeta^*)}{|1+\zeta|^2} = \frac{j_3^{(t)}}{j_3^{(i)}}$$

Klein paradox and antiparticles

$$\boxed{\frac{j_3^{(r)}}{j_3^{(i)}} = -|r|^2 = -\left|\frac{1-\zeta}{1+\zeta}\right|^2}$$



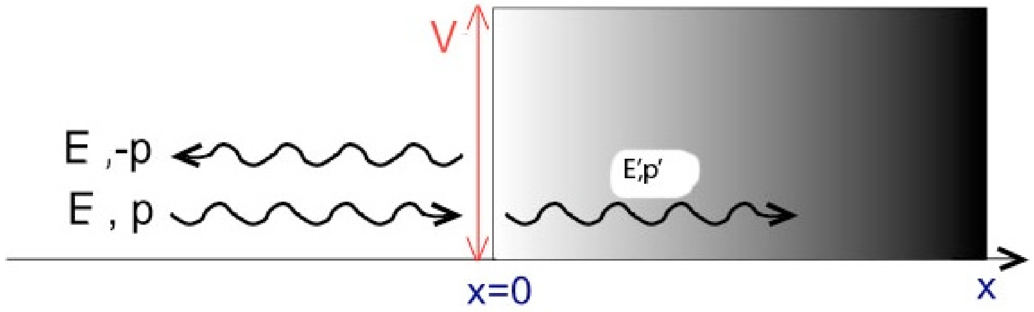
Three distinct regimes in energy:

1. $E' \equiv (E - V) > m$:
   i.e. $p'^2 = E'^2 - m^2 > 0$, $p' > 0$ (beam propagates to right).

   Therefore $\zeta \equiv \dfrac{p'}{p}\dfrac{E+m}{E'+m} > 0$ and real; $|j_3^{(r)}| < |j_3^{(i)}|$ as expected,
   i.e. for $E' > m$, as in non-relativistic quantum mechanics, some of the beam is reflected and some transmitted.

2. $m > E' > -m$:
   i.e. $p'^2 = E'^2 - m^2 < 0$, p' pure imaginary.
   Particles have insufficient energy to surmount potential barrier.

Klein paradox and antiparticles



Physical Interpretation:

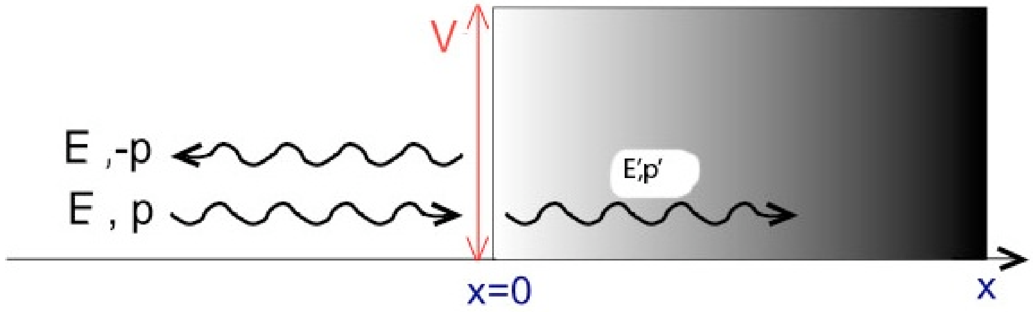
- "Particles" from right should be interpreted as **antiparticles** propagating to right

  i.e. incoming beam stimulates emission of particle/antiparticle pairs at barrier.

- Particles combine with reflected to beam to create current to left that is larger than incident current while antiparticles propagate to the right in the barrier region.

Klein paradox and antiparticles

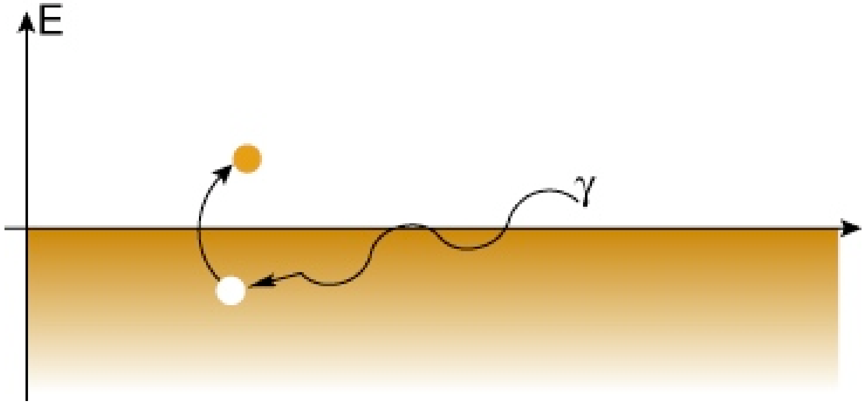
Negative energy states

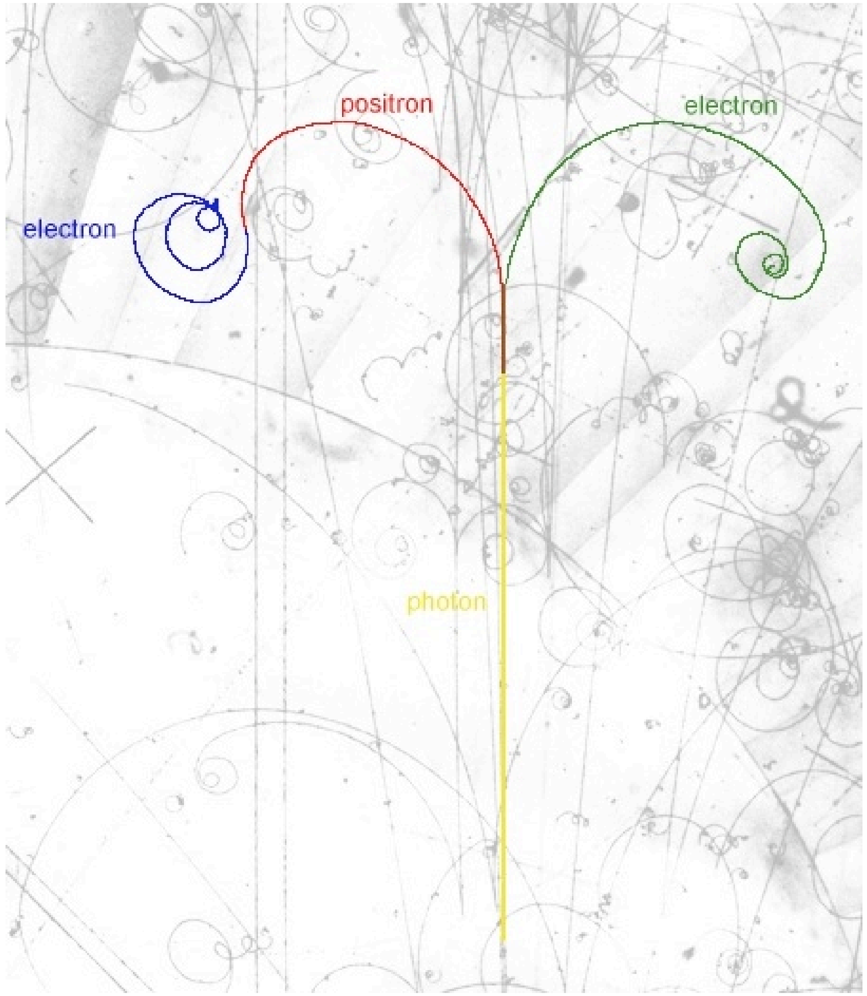


- Existence of antiparticles suggests redefinition of plane wave states with $E < 0$: Dirac particles are, in fact, **fermions** and Pauli exclusion applies.
- Dirac vacuum corresponds to infinite sea of filled negative energy states.
- When $V > 2m$ the potential step is in a precarious situation: It becomes energetically favourable to create particle/antiparticle pairs – cf. vacuum instability.
- Incident beam stimulates excitation of a positive energy particle from negative energy sea leaving behind positive energy "hole" – an **antiparticle**.

Klein paradox and antiparticles

cf. creation of electron-positron pair vacuum due to high energy photon.





Klein paradox and antiparticles

- Therefore, for $E < 0$, we should set $p_0 = +\sqrt{\mathbf{p}^2 + m^2}$ and $\psi(x) = e^{+ip\cdot x} v(p)$ where $(\not{p} + m)v(p) = 0$ *(N.B. "+")*

$$\boxed{v^{(r)}(p) = N(p) \begin{pmatrix} \dfrac{\boldsymbol{\sigma}\cdot\mathbf{p}}{p_0 + m}\chi^{(r)} \\ \chi^{(r)} \end{pmatrix}}$$

- But Dirac equation was constructed on premace that ψ associated with "single particle" (cf. Schrödinger equation). However, for $V > 2m$, theory describes creation of particle/antiparticle pairs.
- ψ must be viewed as a **quantum field** capable of describing an indefinite number of particles!!
- In fact, Dirac equation must be viewed as **field equation**, cf. wave equation for harmonic chain. As with chain, quantization of theory leads to positive energy quantum particles (cf. phonons).
- Allows reinstatement of Klein-Gordon theory as a relativistic theory for scalar (spin 0 particles)...

Quantization of Klein-Gordon field

- Klein-Gordon equation abandoned as candidate for relativistic theory on basis that (i) it admitted negative energy solutions, and (ii) probability density was not positive definite.

- But Klein paradox suggests reinterpretation of Dirac wavefunction as a quantum field.

- If ϕ were a classical field, Klein-Gordon equation, $(\partial^2 - m^2)\phi = 0$ would be associated with Lagrangian density,

$$\boxed{\mathcal{L} = \frac{1}{2}\partial_\mu \phi \partial^\mu \phi - \frac{1}{2} m^2 \phi^2}$$

- Defining canonical momentum, $\pi(x) = \partial_{\dot{\phi}} \mathcal{L} = \dot{\phi}(x)$

$$\mathcal{H} = \pi\dot{\phi} - \mathcal{L} = \frac{1}{2}\left[\pi^2 + (\nabla\phi)^2 + m^2\phi^2\right]$$

$\mathcal{H}$ is +ve definite! i.e. if quantized, only +ve energies appear.

Quantization of Klein-Gordon field

- Promoting fields to operators $\pi \mapsto \hat{\pi}$ and $\phi \mapsto \hat{\phi}$, with "equal time" commutation relations, $[\hat{\phi}(\mathbf{x}, t), \hat{\pi}(\mathbf{x}', t)] = i\delta^3(\mathbf{x} - \mathbf{x}')$, (for $m = 0$, cf. harmonic chain!)

$$\boxed{\hat{H} = \int d^3x \left[\frac{1}{2}\left(\hat{\pi}^2 + (\nabla\hat{\phi})^2 + m^2\hat{\phi}^2\right)\right]}$$

- Turning to Fourier space (with $k_0 \equiv \omega_{\mathbf{k}} = \sqrt{\mathbf{k}^2 + m^2}$)

$$\hat{\phi}(x) = \int \frac{d^3k}{(2\pi)^3 2\omega_{\mathbf{k}}} \left(a(\mathbf{k})e^{-ik\cdot x} + a^\dagger(\mathbf{k})e^{ik\cdot x}\right), \qquad \hat{\pi}(x) \equiv \partial_0\hat{\phi}(x)$$

where $\left[a(\mathbf{k}), a^\dagger(\mathbf{k}')\right] = (2\pi)^3 2\omega_{\mathbf{k}}\delta^3(\mathbf{k} - \mathbf{k}')$,

$$\boxed{\hat{H} = \int \frac{d^3k}{(2\pi)^3 2\omega_{\mathbf{k}}}\omega_{\mathbf{k}}\left[a^\dagger(\mathbf{k})a(\mathbf{k}) + \frac{1}{2}\right]}$$

- Bosonic operators $a^\dagger$ and a create and annihilate relativistic scalar (bosonic, spin 0) particles

Quantization of Dirac field

- Dirac equation associated with Lagrangian density,

$$\boxed{\mathcal{L} = \bar{\psi}\,(i\gamma^\mu\partial_\mu - m)\,\psi, \qquad \text{i.e. } \partial_{\bar{\psi}}\mathcal{L} = (i\gamma^\mu\partial_\mu - m)\,\psi = 0}$$

- With momentum $\pi = \partial_{\dot{\psi}}\mathcal{L} = i\bar{\psi}\gamma^0 = i\psi^\dagger$, Hamiltonian density

$$\mathcal{H} = \pi\dot{\psi} - \mathcal{L} = \bar{\psi}i\gamma^0\partial_0\psi - \mathcal{L} = \bar{\psi}\,(-i\gamma\cdot\nabla + m)\,\psi$$

- Once again, we can follow using canonical quantization procedure, promoting fields to operators – but, in this case, one must impose equal time **anti-commutation** relations,

$$\begin{aligned}\{\hat{\psi}_\alpha(\mathbf{x},t), \hat{\pi}(\mathbf{x}',t)\} &\equiv \hat{\psi}_\alpha(\mathbf{x},t)\hat{\pi}_\beta(\mathbf{x}',t) + \hat{\pi}_\beta(\mathbf{x},t)\hat{\psi}_\alpha(\mathbf{x}',t) \\ &= i\delta^3(\mathbf{x}-\mathbf{x}')\delta_{\alpha\beta}\end{aligned}$$

Quantization of Dirac field

- Turning to Fourier space (with $k_0 \equiv \omega_{\mathbf{k}} = \sqrt{\mathbf{k}^2 + m^2}$)

$$\psi(x) = \sum_{r=1}^{2} \int \frac{d^3k}{(2\pi)^3 2\omega_{\mathbf{k}}} \left[a_r(\mathbf{k}) u^{(r)}(\mathbf{k}) e^{-ik\cdot x} + b_r^\dagger(\mathbf{k}) v^{(r)}(\mathbf{k}) e^{ik\cdot x} \right]$$

with equal time anti-commutation relations (hallmark of **fermions!**)

$$\{a_r(\mathbf{k}), a_s^\dagger(\mathbf{k}')\} = \{b_r(\mathbf{k}), b_s^\dagger(\mathbf{k}')\} = (2\pi)^3 2\omega_{\mathbf{k}} \delta_{rs} \delta^3(\mathbf{k} - \mathbf{k}')$$
$$\{a_r^\dagger(\mathbf{k}), a_s^\dagger(\mathbf{k}')\} = \{b_r^\dagger(\mathbf{k}), b_s^\dagger(\mathbf{k}')\} = 0$$

which accommdates Pauli exclusion $a_r^\dagger(\mathbf{k})^2 = 0(!)$, obtain

$$\boxed{\hat{H} = \sum_{r=1}^{2} \int \frac{d^3k}{(2\pi)^3 2\omega_{\mathbf{k}}} \omega_{\mathbf{k}} \left[a_r^\dagger(\mathbf{k}) a_r(\mathbf{k}) + b_r^\dagger(\mathbf{k}) b_r(\mathbf{k}) \right]}$$

- Physically $a(\mathbf{k}) u^{(r)}(\mathbf{k}) e^{-ik\cdot x}$ annihilates $+$ve energy fermion particle (helicity r), and $b^\dagger(\mathbf{k}) v^{(r)}(\mathbf{k}) e^{ik\cdot x}$ creates a $+$ve energy antiparticle.

Low energy limit of the Dirac equation

- Previously, we have explored the relativistic (fine-structure) corrections to the hydrogen atom. At the time, we alluded to these as the leading relativistic contributions to the Dirac theory.
- In the following section, we will explore how these corrections emerge from relativistic formulation.
- But first, we must consider interaction of charged particle with electromagnetic field.
- As with non-relativistic quantum mechanics, interaction of Dirac particle of charge q ($q = -e$ for electron) with EM field defined by **minimal substitution**, $p^\mu \longmapsto p^\mu - qA^\mu$, where $A^\mu = (\phi, \mathbf{A})$, i.e.

$$\boxed{(\not{p} - q\not{A} - m)\psi = 0}$$

Low energy limit of the Dirac equation

- For particle moving in potential $(\phi, \mathbf{A})$, stationary form of Dirac Hamiltonian given by $\hat{H}\psi = E\psi$ where, restoring factors of $\hbar$ and c,

$$\hat{H} = c\boldsymbol{\alpha}\cdot(\hat{\mathbf{p}} - q\mathbf{A}) + mc^2\beta + q\phi$$
$$= \begin{pmatrix} mc^2 + q\phi & c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} - q\mathbf{A}) \\ c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} - q\mathbf{A}) & -mc^2 + q\phi \end{pmatrix}$$

- To develop non-relativistic limit, consider bispinor $\psi^T = (\psi_a, \psi_b)$, where the elements obey coupled equations,

$$(mc^2 + q\phi)\psi_a + c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} - q\mathbf{A})\psi_b = E\psi_a$$
$$c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} - q\mathbf{A})\psi_a - (mc^2 - q\phi)\psi_b = E\psi_b$$

- If we define energy shift over rest mass energy, $W = E - mc^2$,

$$\psi_b = \frac{1}{2mc^2 + W - q\phi} c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} - q\mathbf{A})\psi_a$$

Low energy limit of the Dirac equation

$$\psi_b = \frac{1}{2mc^2 + W - q\phi} c\boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A})\psi_a$$

- In the non-relativistic limit, $W \ll mc^2$ and we can develop an expansion in v/c. At leading order, $\psi_b \simeq \frac{1}{2mc^2} c\boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A})\psi_a$.
- Substituted into first equation, obtain **Pauli equation** $\hat{H}_{\mathrm{NR}}\psi_a = W\psi_a$ where, defining $V = q\phi$,

$$\hat{H}_{\mathrm{NR}} = \frac{1}{2m} [\boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A})]^2 + V\,.$$

- Making use of Pauli matrix identity $\sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k$,

$$\boxed{\hat{H}_{\mathrm{NR}} = \frac{1}{2m}(\hat{\mathbf{p}} - q\mathbf{A})^2 - \frac{q\hbar}{2m}\boldsymbol{\sigma} \cdot (\nabla \times \mathbf{A}) + V}$$

i.e. **spin magnetic moment**,

$$\boldsymbol{\mu}_S = \frac{q\hbar}{2m}\boldsymbol{\sigma} = g\frac{q}{2m}\hat{\mathbf{S}}, \quad \text{with **gyromagnetic ratio**, } g = 2.$$

Low energy limit of the Dirac equation

$$\psi_b = \frac{1}{2mc^2 + W - V} c\boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A})\psi_a$$

- Taking into account the leading order (in v/c) correction (with $\mathbf{A} = 0$ for simplicity), we have

$$\psi_b \simeq \frac{1}{2mc^2}\left(1 - \frac{W - V}{2mc^2}\right) c\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}\psi_a$$

- Then substituted into the second bispinor equation (and taking into account correction from normalization) we find

$$\boxed{\hat{H} \simeq \frac{\hat{\mathbf{p}}^2}{2m} + V \underbrace{- \frac{\hat{\mathbf{p}}^4}{8m^3c^2}}_{\text{k.e.}} + \underbrace{\frac{1}{2m^2c^2}\mathbf{S} \cdot (\nabla V) \times \hat{\mathbf{p}}}_{\text{spin-orbit coupling}} + \underbrace{\frac{\hbar^2}{8m^2c^2}(\nabla^2 V)}_{\text{Darwin term}}}$$

Synopsis: (mostly revision) Lectures 1-4ish

1. **Foundations of quantum physics:**

   †Historical background; wave mechanics to Schrödinger equation.

2. **Quantum mechanics in one dimension:**

   Unbound particles: potential step, barriers and tunneling; bound states: rectangular well, δ-function well; †Kronig-Penney model .

3. **Operator methods:**

   Uncertainty principle; time evolution operator; Ehrenfest's theorem; †symmetries in quantum mechanics; Heisenberg representation; quantum harmonic oscillator; †coherent states.

4. **Quantum mechanics in more than one dimension:**

   Rigid rotor; angular momentum; raising and lowering operators; representations; central potential; atomic hydrogen.

† non-examinable *in this course*.

Synopsis: Lectures 5-10

5. **Charged particle in an electromagnetic field:**

   Classical and quantum mechanics of particle in a field; normal Zeeman effect; gauge invariance and the Aharonov-Bohm effect; Landau levels, †Quantum Hall effect.

6. **Spin:**

   Stern-Gerlach experiment; spinors, spin operators and Pauli matrices; spin precession in a magnetic field; parametric resonance; addition of angular momenta.

7. **Time-independent perturbation theory:**

   Perturbation series; first and second order expansion; degenerate perturbation theory; Stark effect; nearly free electron model.

8. **Variational and WKB method:**

   Variational method: ground state energy and eigenfunctions; application to helium; †Semiclassics and the WKB method.

† non-examinable *in this course*.

Synopsis: Lectures 11-15

9. **Identical particles:**

   Particle indistinguishability and quantum statistics; space and spin wavefunctions; consequences of particle statistics; ideal quantum gases; †degeneracy pressure in neutron stars; Bose-Einstein condensation in ultracold atomic gases.

10. **Atomic structure:**

    Relativistic corrections – spin-orbit coupling; Darwin term; Lamb shift; hyperfine structure. Multi-electron atoms; Helium; Hartree approximation †and beyond; Hund's rule; periodic table; LS and jj coupling schemes; atomic spectra; Zeeman effect.

11. **Molecular structure:**

    Born-Oppenheimer approximation; H_2^+ ion; H_2 molecule; ionic and covalent bonding; LCAO method; from molecules to solids; †application of LCAO method to graphene; molecular spectra; rotation and vibrational transitions.

† non-examinable *in this course*.

Synopsis: Lectures 16-19

12. **Field theory: from phonons to photons:**

    From particles to fields: classical field theory of harmonic atomic chain; quantization of atomic chain; phonons; classical theory of the EM field; †waveguide; quantization of the EM field and photons.

13. **Time-dependent perturbation theory:**

    Rabi oscillations in two level systems; perturbation series; sudden approximation; harmonic perturbations and Fermi's Golden rule.

14. **Radiative transitions:**

    Light-matter interaction; spontaneous emission; absorption and stimulated emission; Einstein's A and B coefficents; dipole approximation; selection rules; lasers.

† non-examinable *in this course*.

Synopsis: Lectures 20-24

15. **Scattering theory**

    †Elastic and inelastic scattering; †method of particle waves; †Born series expansion; Born approximation from Fermi's Golden rule; †scattering of identical particles.

16. **Relativistic quantum mechanics:**

    †Klein-Gordon equation; †Dirac equation; †relativistic covariance and spin; †free relativistic particles and the Klein paradox; †antiparticles; †coupling to EM field: †minimal coupling and the connection to non-relativistic quantum mechanics; †field quantization.

† non-examinable *in this course*.