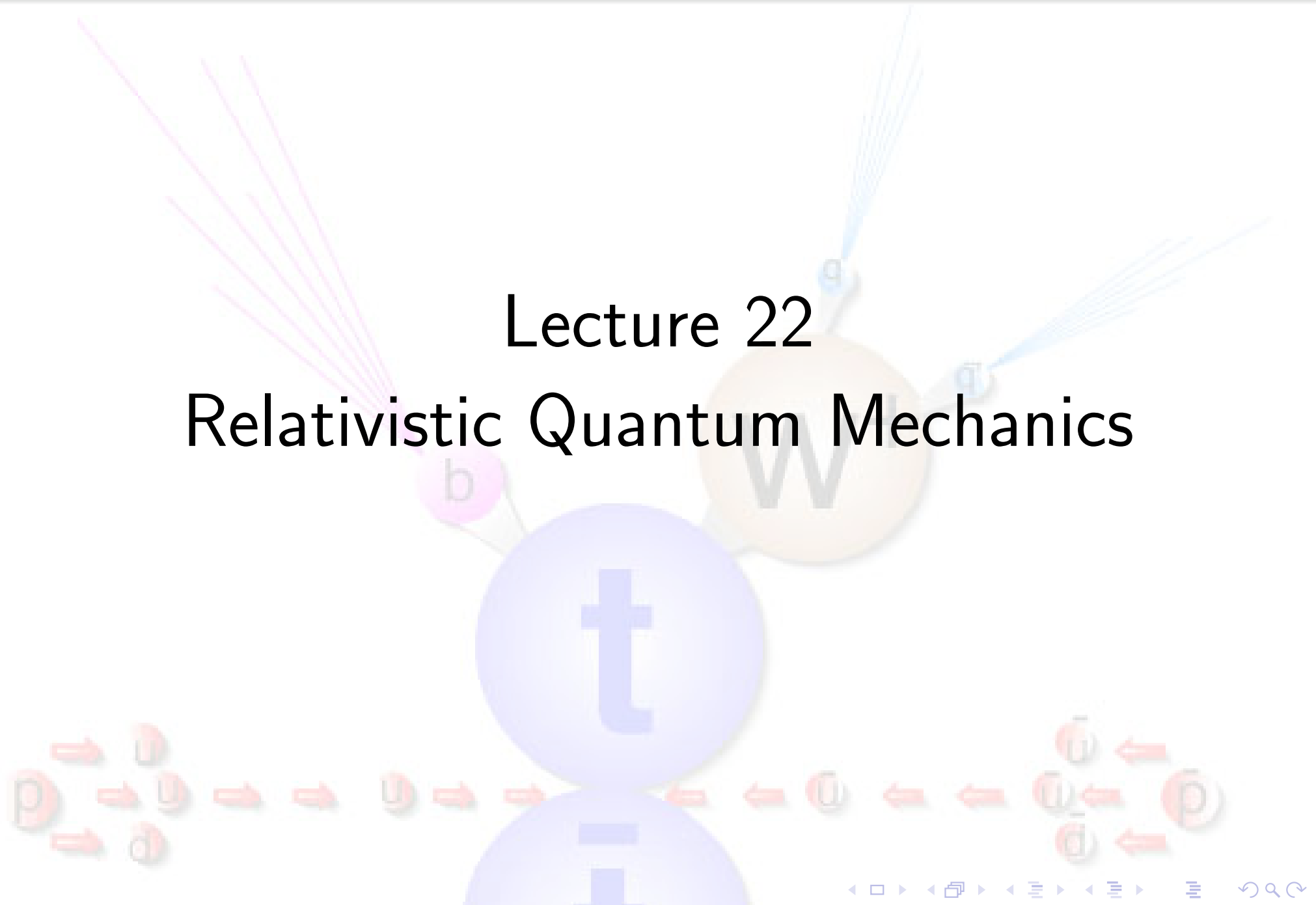


# Lecture 22

## 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

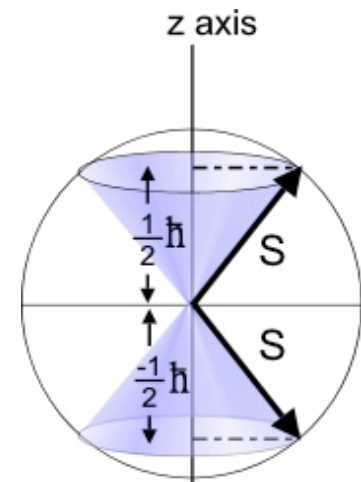
e.g. electron-positron pairs by energetic  $\gamma$ -rays in matter.

## 2 Vacuum instability: If binding energy of electron

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

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  $E_{\text{kin}} \sim mc^2$ , i.e.  $p \sim mc$

- 2 From uncertainty relation,  $\Delta x \Delta p > h$ , this translates to a length

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

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**

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

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

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

- **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,  $\Lambda$ , 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  $x_1$

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

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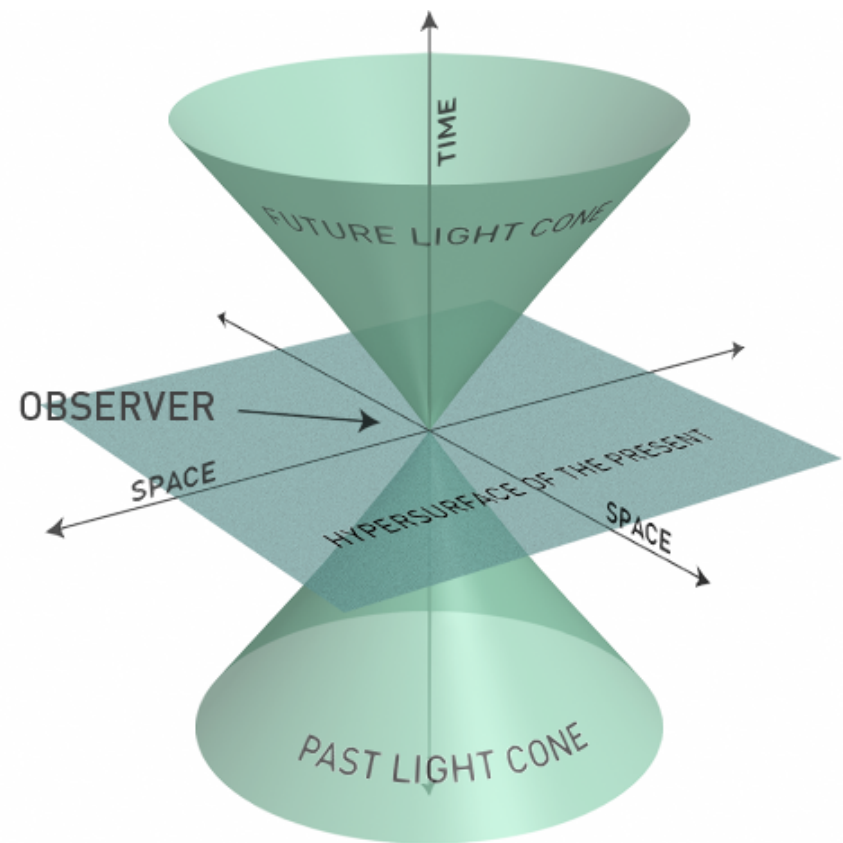
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# Special relativity (revision and notation)

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

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

- 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**

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

- 5 Remaining components of group generated by

$$\mathcal{L}^\downarrow_- = T\mathcal{L}^\uparrow_+, \quad \mathcal{L}^\uparrow_- = P\mathcal{L}^\uparrow_+, \quad \mathcal{L}^\downarrow_+ = TP\mathcal{L}^\uparrow_+.$$

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# Special relativity (revision and notation)

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

$$\Lambda^\mu_\nu = \delta^\mu_\nu + \omega^\mu_\nu, \quad \omega^\mu_\nu \ll 1$$

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

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.  $\partial_\mu x^\mu = 1$

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

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

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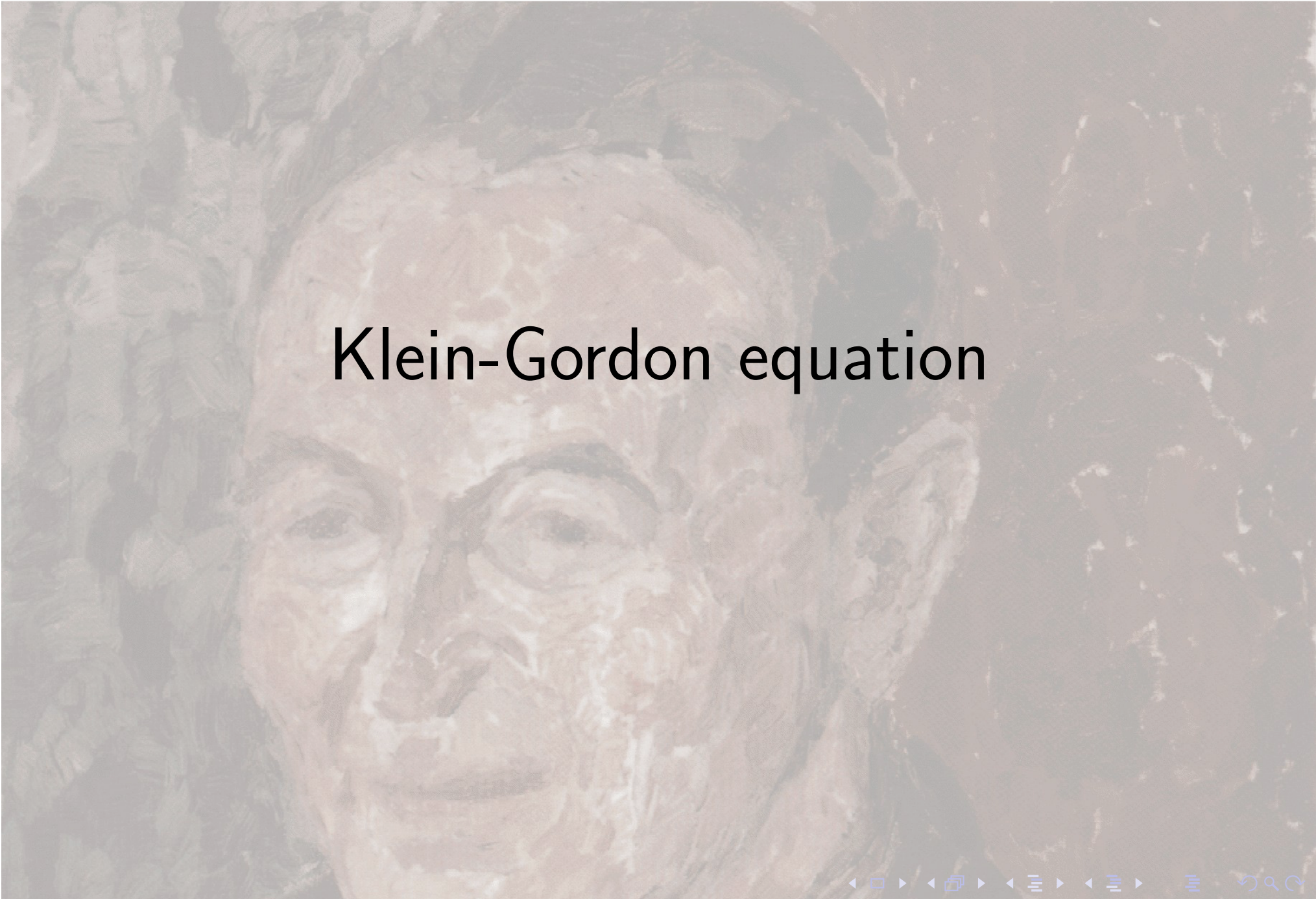
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# Klein-Gordon equation

# Klein-Gordon equation

How to make wave equation relativistic?

- According to canonical quantization procedure in NRQM:

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

transforms as a 4-vector under LT

- What if we apply quantization procedure to energy?

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

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

- Meaning of square root? Taylor expansion:

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

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

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

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

- Klein-Gordon equation is local and manifestly Lorentz covariant.
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# Klein-Gordon equation: Probabilities

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

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

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

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

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

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# Klein-Gordon equation: Probabilities

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

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

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

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# Klein-Gordon equation: viability?

But is Klein-Gordon equation acceptable?

- Density  $\rho = i \frac{\hbar}{2mc^2} (\psi^* \partial_t \psi - \psi \partial_t \psi^*)$  is not positive definite.
- Klein-Gordon equation is not first order in time derivative  
therefore we must specify  $\psi$  **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

$$\begin{aligned} (\partial^2 + k_c^2) \psi &= F(\psi) && \text{self – interaction} \\ \left[ (\partial + iqA/\hbar c)^2 + k_c^2 \right] \psi &= 0 && \text{interaction with EM field} \end{aligned}$$

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# 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**,

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

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.

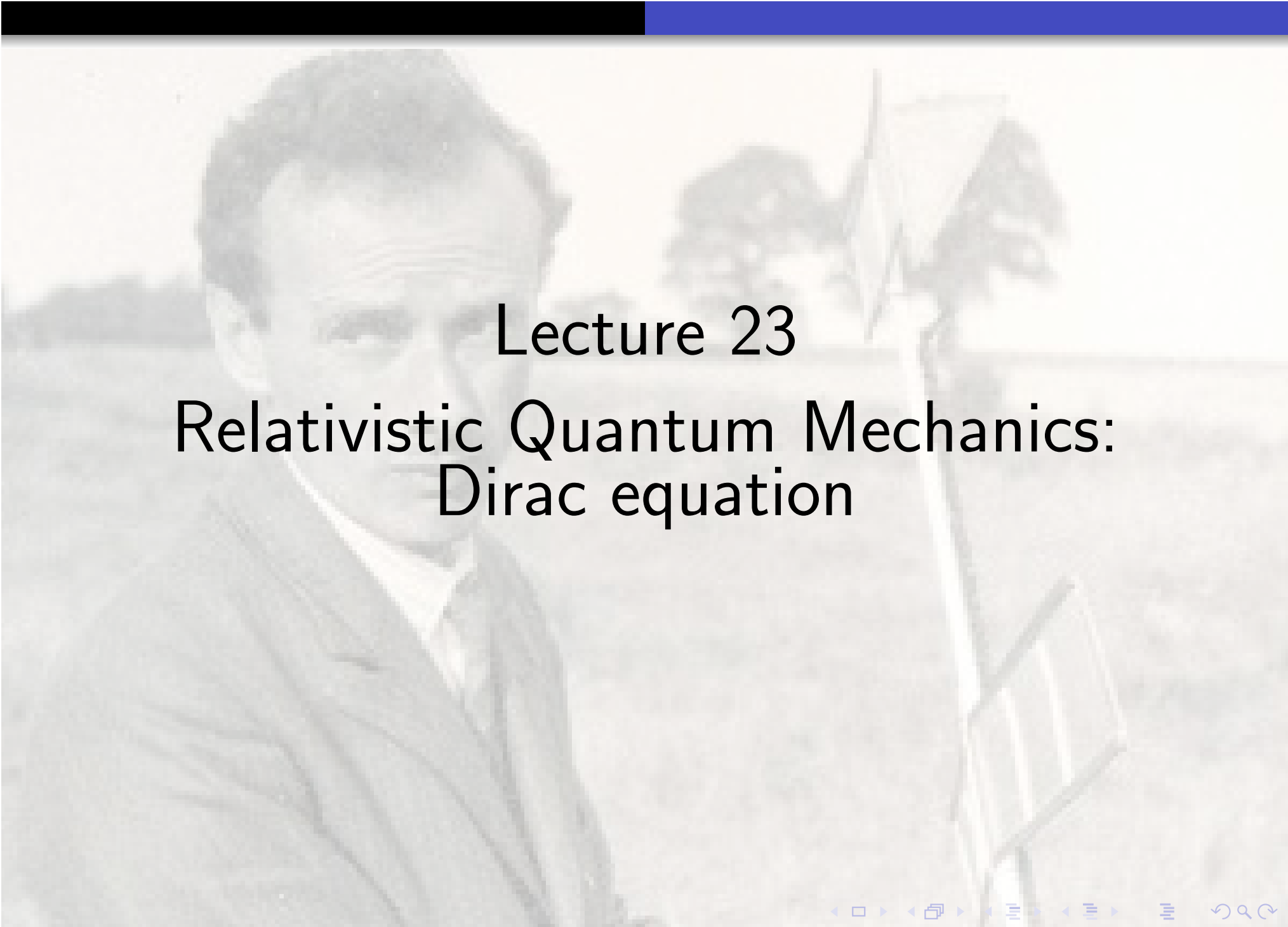
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# Lecture 23

## Relativistic Quantum Mechanics: 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
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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  $\hbar = c = 1$ )

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

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- Equation is acceptable if:
  - 1  $\psi$  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  $\psi$  does not have to satisfy any auxiliary boundary conditions.
- From condition (1) we require (assuming  $[\gamma^\mu, \hat{p}_\nu] = 0$ )

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

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i.e. obeys Klein-Gordon if  $\{\gamma^\mu, \gamma^\nu\} \equiv \gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\nu\mu}$   
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  - 1  $\psi$  satisfies Klein-Gordon equation,  $(\partial^2 + m^2)\psi = 0$ ;
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i.e. obeys Klein-Gordon if  $\{\gamma^\mu, \gamma^\nu\} \equiv \gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\nu\mu}$   
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# Dirac Equation: Hamiltonian formulation

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

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

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

- So we obtain the defining properties of Dirac  $\gamma$  matrices,

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

- Since space-time is four-dimensional,  $\gamma$  must be of dimension at least  $4 \times 4$  –  $\psi$  has at least four components.
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$\boldsymbol{\sigma}$  – **Pauli spin matrices**

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

- Applying complex conjugation to Dirac equation

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- So, in contrast to the Klein-Gordon equation, the density  $\rho = j^0 = \psi^\dagger \psi$  is, as required, positive definite.
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# 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,

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

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

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

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- 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  $\Sigma_{\mu\nu} = \frac{i}{2} [\gamma_\mu, \gamma_\nu]$ .

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# Relativistic covariance

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

- 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,

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

- This equation is satisfied by (exercise)

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

- 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  $\Sigma_{\mu\nu} = \frac{i}{2} [\gamma_\mu, \gamma_\nu]$ .

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

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

- 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?

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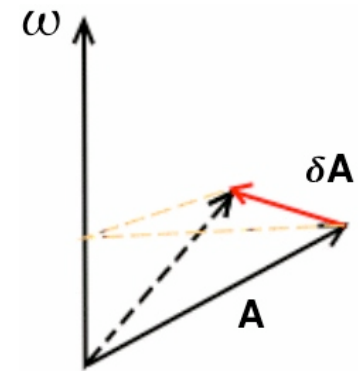
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# Angular momentum and spin

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

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

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



- In non-relativistic quantum mechanics:

$$\psi'(\mathbf{x}') = \psi(\mathbf{x}) = \psi(\Lambda^{-1} \mathbf{x}') \simeq \psi((\mathbb{I} - \omega) \cdot \mathbf{x}')$$

$$\simeq \psi(\mathbf{x}') - \omega \cdot \mathbf{x}' \cdot \nabla \psi(\mathbf{x}') + \dots$$

$$= \psi(\mathbf{x}') - i(\mathbf{n} \times \mathbf{x}') \cdot (\nabla) \psi(\mathbf{x}') + \dots$$

$$= (1 - i(\mathbf{n} \cdot \mathbf{L}) \theta) \psi(\mathbf{x}') \simeq U \psi(\mathbf{x}')$$

$$\Rightarrow \text{rotation operator } U = e^{-i\theta \mathbf{n} \cdot \mathbf{L}}$$

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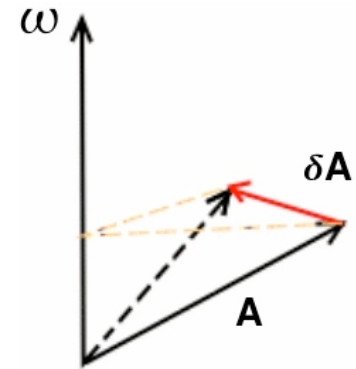
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cf. generator of rotations:  $\hat{U} = e^{-i\theta \mathbf{n} \cdot \hat{\mathbf{L}}}$ .



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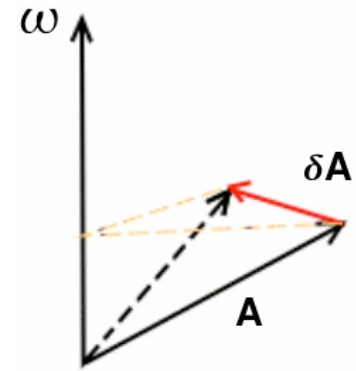
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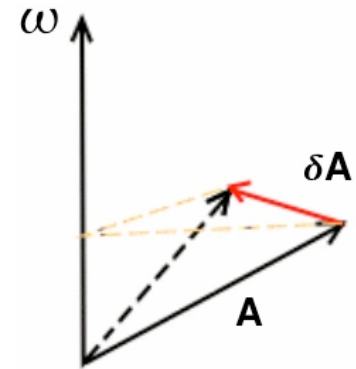
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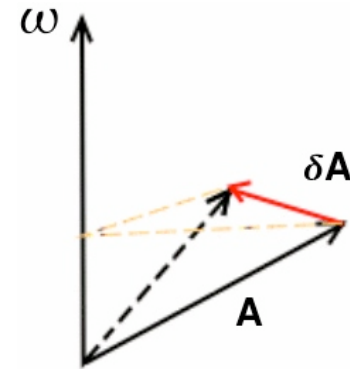
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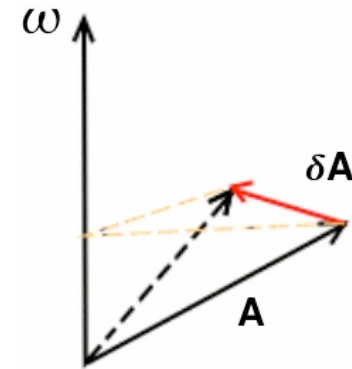
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$$\Sigma_{ij} = \frac{i}{2} [\gamma_i, \gamma_j] = \epsilon_{ijk} \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}, \quad \gamma_i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}$$

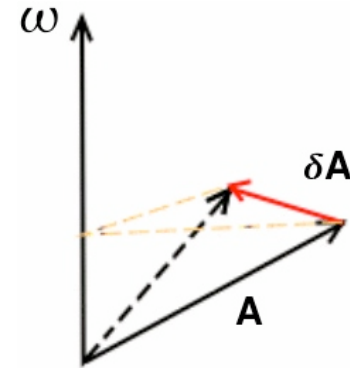
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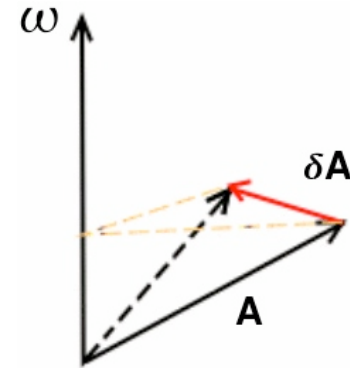
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$$\psi'(x') = S(\Lambda)\psi(\Lambda^{-1}x') \simeq (1 - i\theta \mathbf{n} \cdot \hat{\mathbf{J}})\psi(x')$$

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- 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  $S(\Lambda)\gamma^\nu S^{-1}(\Lambda) = (\Lambda^{-1})^\nu_\mu \gamma^\mu$

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

achieved if  $S(P) = \gamma^0 e^{i\phi}$ , where  $\phi$  denotes arbitrary phase.

- But since  $P^2 = \mathbb{I}$ ,  $e^{i\phi} = 1$  or  $-1$

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## Lecture 24

# Relativistic Quantum Mechanics: Solutions of the Dirac equation

electron

positron

electron

photon

# 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

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

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

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

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

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

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

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

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

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:

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

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

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

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

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

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- 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...

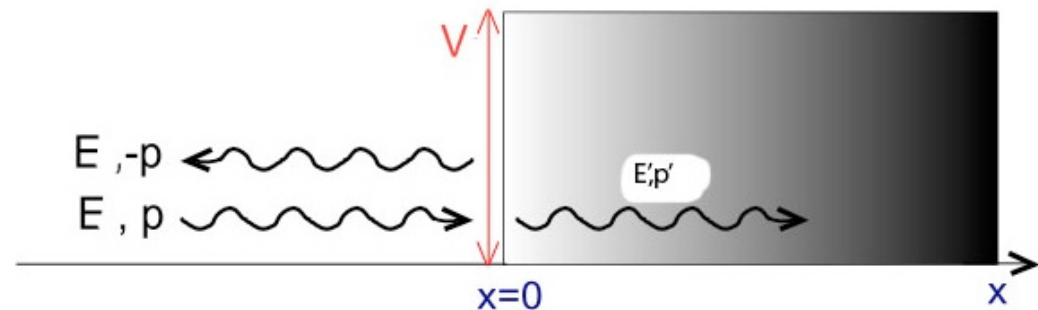
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# Klein paradox and antiparticles

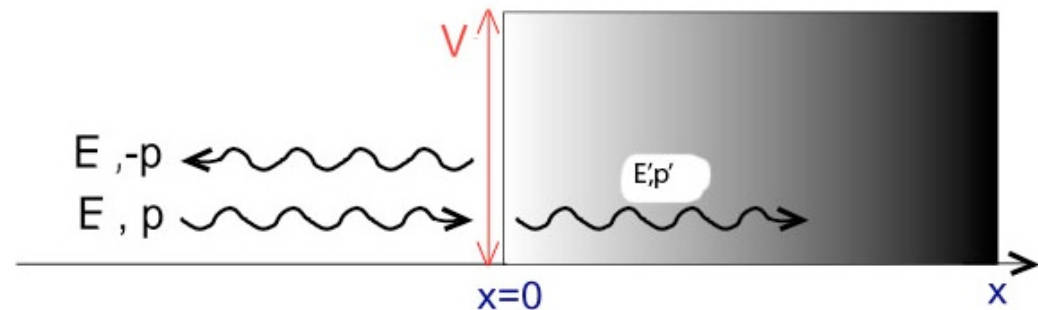


- Consider plane wave, unit amplitude, energy  $E$ , momentum  $p \hat{e}_3$ , and spin  $\uparrow$  ( $\chi = (1, 0)$ ) incident on potential barrier  $V(\mathbf{x}) = V\theta(x_3)$

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

- At barrier, spin is conserved, component  $r$  is reflected ( $E, -p \hat{e}_3$ ), and component  $t$  is transmitted ( $E' = E - V, p' \hat{e}_3$ )
- 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



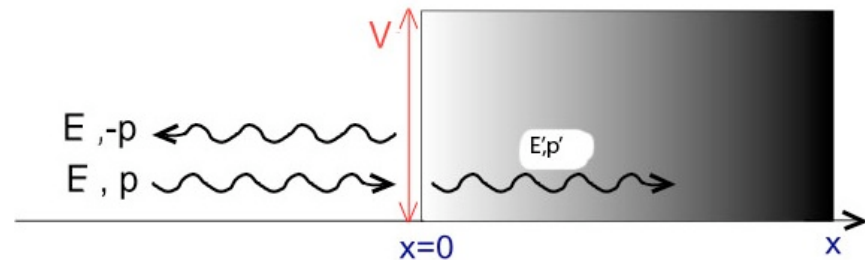
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- Boundary conditions: since Dirac equation is first order, require only continuity of  $\psi$  at interface (cf. Schrodinger eqn.)

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

(helicity conserved in reflection)

- Equating (generically complex) coefficients:

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

# Klein paradox and antiparticles

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

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

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

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

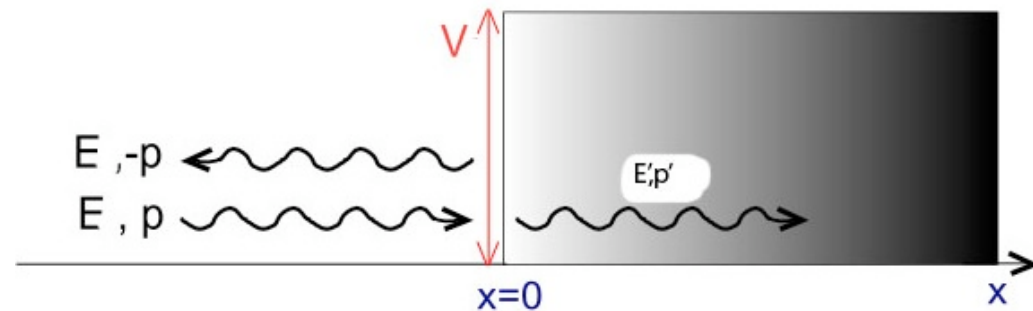
$$t = \frac{2}{1 + \zeta}, \quad \frac{1 + r}{1 - r} = \frac{1}{\zeta}, \quad r = \frac{1 - \zeta}{1 + \zeta}$$

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

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

# 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,

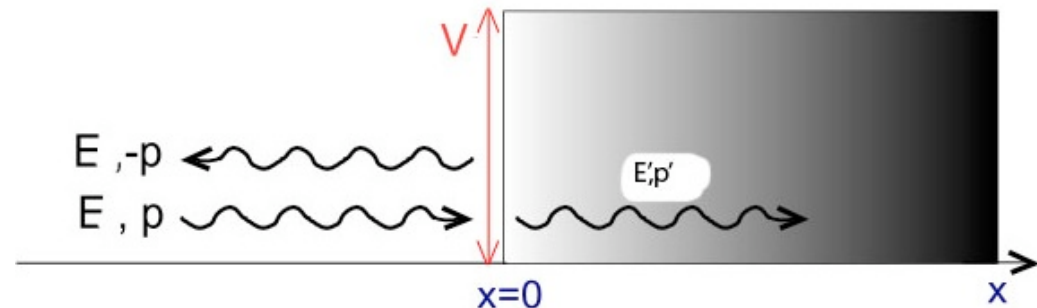
$$j_3^{(i)} = \begin{pmatrix} 1 & 0 & \frac{p}{E+m} & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ \frac{p}{E+m} \\ 0 \end{pmatrix} = \frac{2p}{E+m},$$

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

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,

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

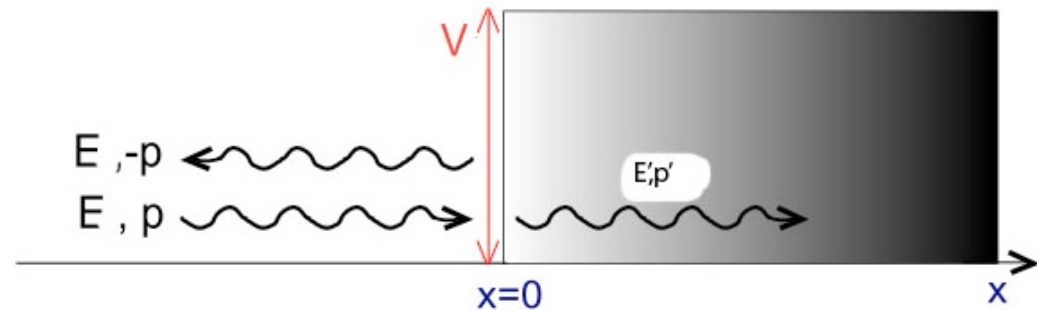
$$\frac{j_3^{(t)}}{j_3^{(i)}} = |t|^2 \frac{(p' + p'^*)}{2p} \frac{E + m}{E' + m} = \frac{4}{|1 + \zeta|^2} \frac{1}{2} (\zeta + \zeta^*) = \frac{2(\zeta + \zeta^*)}{|1 + \zeta|^2}$$

- 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

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



Three distinct regimes in energy:

①  $E' \equiv (E - V) > m$ :

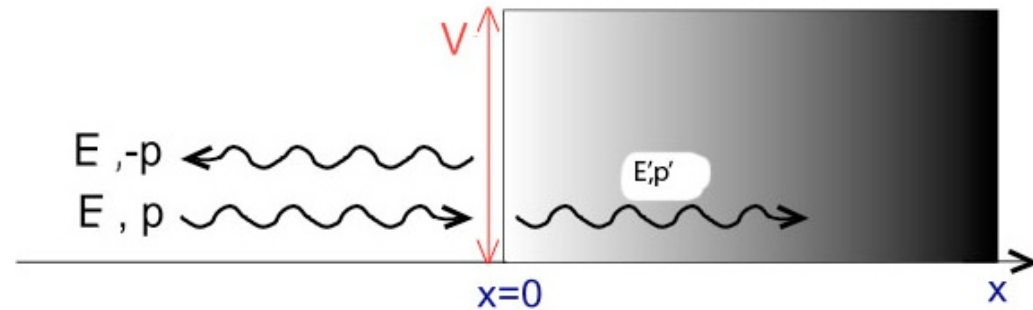
i.e.  $p'^2 = E'^2 - m^2 > 0$ ,  $p' > 0$  (beam propagates to right).

Therefore  $\zeta \equiv \frac{p'}{p} \frac{E+m}{E'+m} > 0$  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.

# Klein paradox and antiparticles

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



Three distinct regimes in energy:

②  $m > E' > -m$ :

i.e.  $p'^2 = E'^2 - m^2 < 0$ ,  $p'$  pure imaginary.

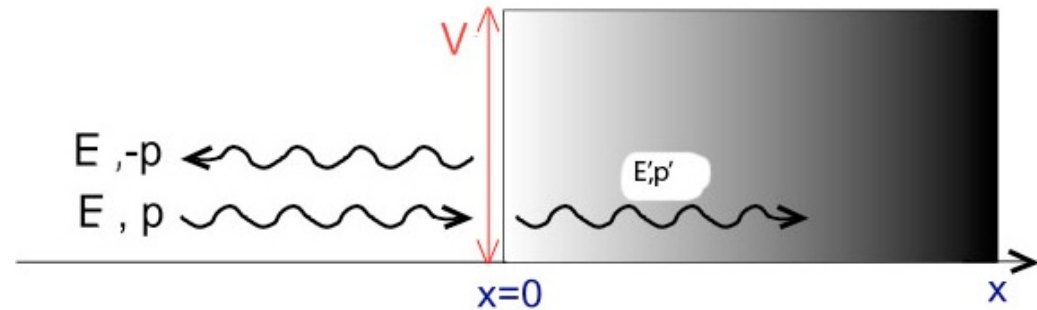
Particles have insufficient energy to surmount potential barrier.

Therefore,  $\zeta \equiv \frac{p'}{p} \frac{E+m}{E'+m}$  pure imaginary,  $|j_3^{(r)}| = |j_3^{(i)}|$ .

i.e. all beam is reflected;  $\psi$  has evanescent decays on the right hand side of the barrier (cf. NRQM).

# Klein paradox and antiparticles

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



Three distinct regimes in energy:

③  $E' = E - V < -m$ :

i.e. step height  $V > E + m \geq 2m$  larger than twice rest mass energy.

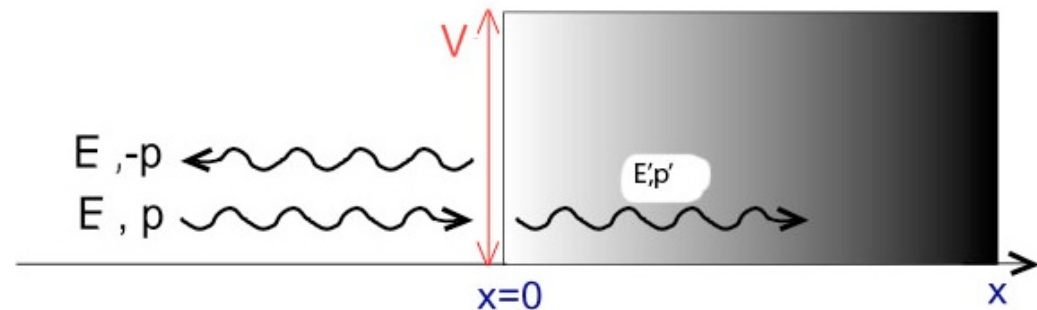
$p'^2 = E'^2 - m^2 > 0$ ,  $p' > 0$  (beam propagates to the right)

But  $\zeta = \frac{p'}{p} \frac{(E+m)}{(E'+m)} < 0$  real!

Therefore  $|j_3^{(r)}| > |j_3^{(i)}|$ !! – more current is reflected than is incident  
– **Klein Paradox** (also holds for Klein-Gordon equation).

But particle current conserved – it is as though an additional beam of particles were incident from right.

# Klein paradox and antiparticles

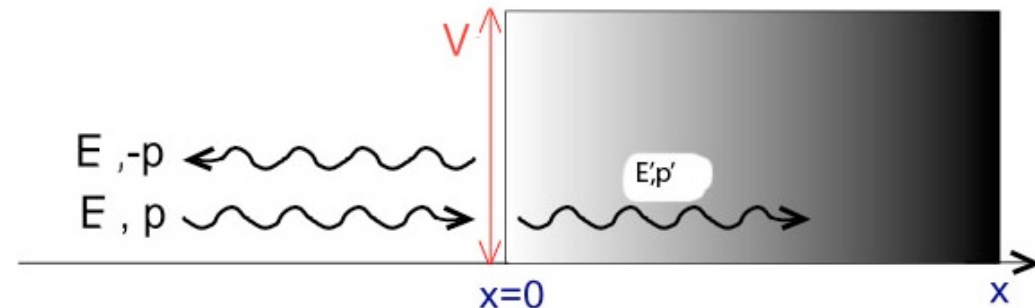


## Physical Interpretation:

- “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

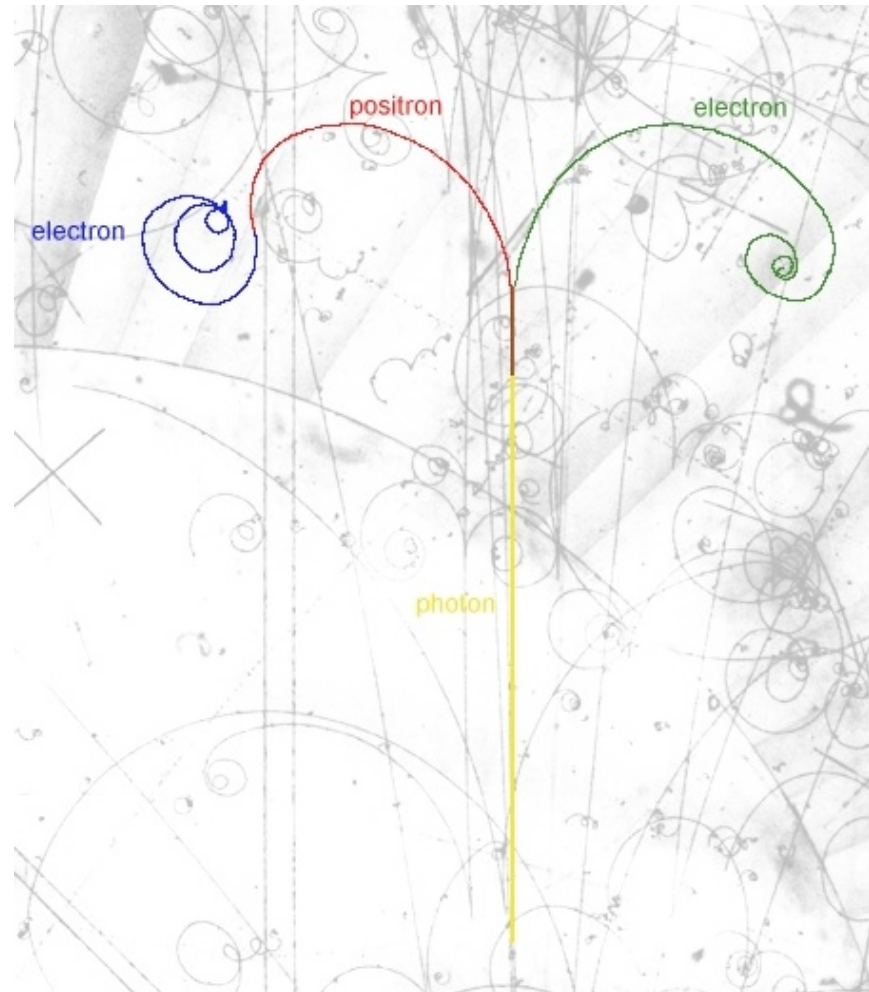
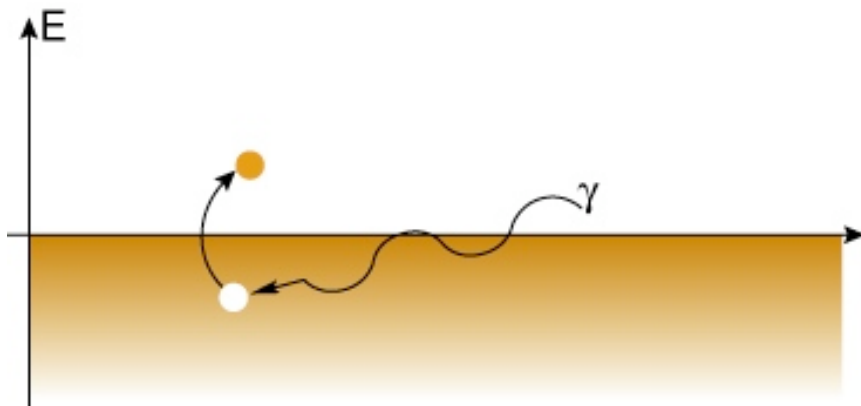
## Negative energy states



- 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. “+”)

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

- But Dirac equation was constructed on premise that  $\psi$  associated with “single particle” (cf. Schrödinger equation). However, for  $V > 2m$ , theory describes creation of particle/antiparticle pairs.
- $\psi$  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)...

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

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

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

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

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

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- 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!)

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

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

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

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# Quantization of Dirac field

- Dirac equation associated with Lagrangian density,

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

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

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- 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,

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

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

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

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

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

- 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**,  $p^\mu \mapsto p^\mu - qA^\mu$ , where  $A^\mu = (\phi, \mathbf{A})$ , i.e.

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- 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  $c$ ,

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

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

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

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

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

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

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

- 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

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- 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**  
 $\hat{H}_{\text{NR}}\psi_a = W\psi_a$  where, defining  $V = q\phi$ ,

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

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

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

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

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

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# 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

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

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# 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,  $\delta$ -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;  $\text{H}_2^+$  ion;  $\text{H}_2$  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 coefficients; 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\*.