Relativistic Quantum Mechanics

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❑ OUTLINE

- **The Schrodinger equation**
  - Non-relativistic quantum mechanics (revisited)
- **A quick review of special theory of relativity**
- **Klein-Gordon Equation**
  - A relativistic wave equation for bosons
- **The Dirac Equation**
  - A relativistic wave equation for fermions

Non-Relativistic QM (Revision)

- For particle physics need a relativistic formulation of quantum mechanics. But first take a few moments to review the non-relativistic formulation QM
- Take as the starting point non-relativistic energy:

$$E = T + V = \frac{\vec{p}^2}{2m} + V$$

- In QM we identify the energy and momentum operators:

$$\hat{p} = -i\hbar\nabla \qquad \hat{E} = i\hbar\frac{\partial}{\partial t}$$

which gives the time dependent Schrödinger equation (take V=0 for simplicity)

$$-\frac{\hbar^2}{2m}\nabla^2\psi = i\hbar\frac{\partial\psi}{\partial t}$$

with plane wave solutions: $\psi = Ne^{-\frac{i}{\hbar}(Et-\vec{p}\cdot\vec{x})}$ where $\begin{cases} \hat{p}\psi = -i\hbar\nabla\psi \\ \hat{E}\psi = i\hbar\frac{\partial\psi}{\partial t} \end{cases}$

- Time dependent Schrödinger equation

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

- **But how we do interpret the SE and associated wave function ?**

The best way is to see what it conserves. What are the conserved currents and densities?

$$\psi^* \times \text{S.E.} : \quad \psi^* \, i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \psi^* \nabla^2 \psi + V \psi^* \psi \qquad (1)$$

$$\psi \times \text{S.E.}^* : \quad -\psi \, i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \psi \nabla^2 \psi^* + V \psi^* \psi \qquad (2)$$

Now using Eq. (1)- Eq.(2)

$$\Rightarrow i\hbar \frac{\partial [\psi^* \psi]}{\partial t} = \frac{\hbar^2}{2m} \left[-\psi^* \nabla^2 \psi + \psi \nabla^2 \psi^* \right] = \frac{\hbar^2}{2m} \vec{\nabla} . \left[\psi^* \vec{\nabla} \psi + \psi \vec{\nabla} \psi^* \right]$$

$$\left(\vec{\nabla} . \left[\psi^* \vec{\nabla} \psi \right] = \vec{\nabla} \psi^* . \vec{\nabla} \psi + \psi^* \nabla^2 \psi \right)$$

$\rho = \psi^* \psi$ satisfies a **continuity equation**

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0$$

with

$$\vec{J} = \frac{\hbar}{2im}\left[\psi^*(\vec{\nabla}\psi) - (\vec{\nabla}\psi^*)\psi\right]$$

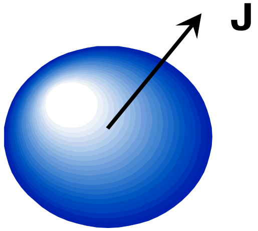
conserved current

Now, integrating over a volume V:

$$\int_V \frac{\partial \rho}{\partial t} dV = -\int_V \vec{\nabla} \cdot \vec{J}\, dV$$

and using Gauss' Theorem

$$\frac{\partial}{\partial t}\int_V \rho\, dV = -\int_A \vec{J}.d\vec{A}$$



Volume V enclosed by Area A

Any change in the total ρ in the volume must come about through a current **J** through the surface of the volume.

$\rho = \psi^* \psi$ is a conserved density and we interpret it as the **probability density** for finding a particle at a particular position.

- For a plane wave $\psi = N e^{i(\vec{p}.\vec{r} - Et)}$

$$\rho = |N|^2 \quad \text{and} \quad \vec{j} = |N|^2 \frac{\vec{p}}{m} = |N|^2 \vec{v}$$

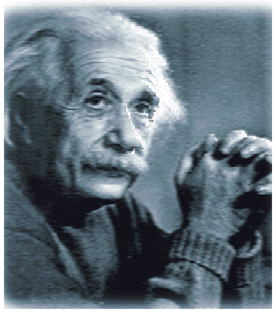
★ The number of particles per unit volume is $|N|^2$

★ For $|N|^2$ particles per unit volume moving at some velocity, have passing through a unit area per unit time (particle flux). Therefore is a vector in the particle's direction with magnitude equal to the flux.

❖ The SE is first order in the time derivatives and second order in spatial derivatives – and is manifestly not Lorentz invariant.

❖ The Schrodinger Equation only describes particles in the non relativistic limit. To describe the particle at particle colliders we need to incorporate special theory of relativity

❑ A Quick Review of Special Theory of Relativity



We construct a position *four-vector* as

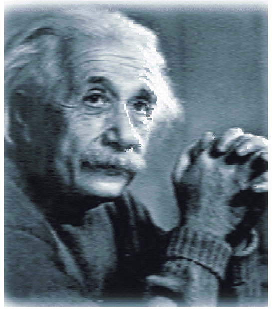
$$x^\mu \equiv (x^0, x^1, x^2, x^3) \equiv (ct, \vec{x}) \qquad (\mu = \{0,1,2,3\})$$

An observer in a frame S′ will instead observe a four-vector $x'^\mu = \Lambda^\mu{}_\nu x^\nu$ where Λ denotes a Lorentz transformation.

e.g. under a Lorentz boost by v in the positive x direction:

$$\begin{pmatrix} ct' \\ x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \gamma & -\frac{v}{c}\gamma & 0 & 0 \\ -\frac{v}{c}\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix} \qquad \gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$$

- The quantity $x^\mu x_\mu$ is **invariant** under a Lorentz transformation



$$x^\mu x_\mu \equiv g_{\mu\nu} x^\mu x^\nu = (ct)^2 - |\vec{x}|^2$$

[note the definition of a covector $x_\mu \equiv g_{\mu\nu} x^\nu$]

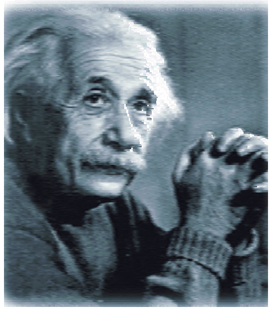
Here $g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$ is the **metric tensor** of Minkowski space-time.

- This invariance implies that the Lorentz transformation is orthogonal:

$$\left. \begin{aligned} x'^\mu x'_\mu &= g_{\mu\nu} x'^\mu x'^\nu = g_{\mu\nu} \Lambda^\mu{}_\alpha x^\alpha \Lambda^\mu{}_\beta x^\beta \\ x^\mu x_\mu &= g_{\mu\nu} x^\mu x^\nu \end{aligned} \right\}$$

$$x'^\mu x'_\mu = x^\mu x_\mu \Leftrightarrow g_{\mu\nu} \Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta = g_{\alpha\beta} \Leftrightarrow \left[\Lambda^{-1}\right]_{\mu\nu} = \Lambda_{\nu\mu}$$

- A particle's **four-momentum** is defined by $p^\mu = m\frac{dx^\mu}{d\tau}$



τ is **proper time**, the time in the particle's own rest frame.

It is related to an observer's time via $t = \gamma\tau$

Its four-momentum's time component is the particle's energy, while the space components are its three-momentum

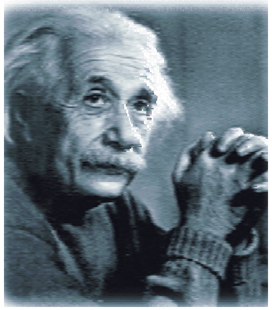
$$p^\mu = \left(\frac{E}{c}, \vec{p}\right)$$

and its length is an invariant, its **mass^2** (times c^2):

$$p^\mu p_\mu = \frac{E^2}{c^2} - |\vec{p}|^2 = m^2c^2$$

Finally, I define the derivative

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



This is a covector (index down).

You will sometimes use the vector expression

$$\partial^\mu = \left(\frac{1}{c}\frac{\partial}{\partial t}, -\nabla\right)$$

← Watch the minus sign!

∂_μ transforms as $\partial_\mu \rightarrow \partial'_\mu = \left[\Lambda^{-1}\right]^\nu{}_\mu \partial_\nu$

$$\left[\partial x'^\mu = \frac{\partial x'^\mu}{\partial x^\nu} \partial x^\nu = \Lambda^\mu{}_\nu \partial x^\nu \quad \text{so} \quad \frac{\partial}{\partial x'^\mu} = \frac{\partial x^\nu}{\partial x'^\mu} \frac{\partial}{\partial x^\nu} = \left[\Lambda^{-1}\right]^\nu{}_\mu \frac{\partial}{\partial x^\nu} \right]$$

Klein-Gordon Equation

- A relativistic wave equation for bosons
- Feynman-stuckelberg Interpretation
- Normalization of KG Solutions

❑ Klein-Gordon Equation

Oskar Klein

- Klein Gordon (KG) Equation was the first relativistic (Lorentz covariant) quantum mechanical model.
- To the best of my knowledge, KGE is not being used now a days in either physics or quantum chemistry except for some work with pions.
- It nonetheless serve as an excellent pedagogical tool for the introduction of concepts.
- Disparaged shortly after introduction, it was resurrected and vindicated a decade later when Pauli and his postdoc Victor Weisskopf showed that it is really an important equation I relativistic quantum field theory.

The invariant of four vector-momentum's length provides us a relation between energy, momentum and mass

$$p^{\mu} p_{\mu} = \frac{E^2}{c^2} - \left|\vec{p}\right|^2 = m^2 c^2$$

Replacing energy and momentum with $E \rightarrow i\hbar \frac{\partial}{\partial t}, \quad p \rightarrow -i\hbar \nabla$ gives the Klien-Gordon equation

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{m^2 c^2}{\hbar^2} \right) \phi = 0$$

❖ I have put V=0 for simplicity (free particle)

- The plane wave solution for above equation is $\phi(t, \vec{x}) = N e^{-\frac{i}{\hbar}(Et - \vec{p}.\vec{x})}$

Normalization

- This is relativistic wave equation for spin zero particles, which is conventionally denoted by ϕ

- Is the Klein-Gordon equation the same in all reference frames?

  Under a Lorentz transformation the Klein-Gordon operator is invariant, so:

$$\left(\frac{\partial}{\partial x'^{\mu}}\frac{\partial}{\partial x'_{\mu}} + m^2\right)\phi'(x') = \left(\frac{\partial}{\partial x^{\mu}}\frac{\partial}{\partial x_{\mu}} + m^2\right)\phi'(\Lambda x) = 0$$

- Since $|\phi|$ is invariant, then $|\phi|^2$ does not change with a Lorentz transformation.
- This sound good – the probability does not change with reference frame

Unfortunately, the probability **should** change with reference frame!

Remember that $|\phi|^2$ is a probability density:

Length contraction changes volumes $V' = \frac{1}{\gamma} V$

The probability $P = \rho V$ so for P to be invariant we need $\rho' = \gamma \rho$

Probability and current densities

We know that K-G equation is

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \phi = \frac{m^2 c^2}{\hbar^2} \phi \qquad (1)$$

Complex conjugate of K-G Equation K-G equation is

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \phi^* = \frac{m^2 c^2}{\hbar^2} \phi^* \qquad (2)$$

Multiply equation (1) by ϕ^* from left and equation (2) by ϕ from right, we get

$$\phi^*\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\phi = \frac{m^2c^2}{\hbar^2}\phi^*\phi \tag{3}$$

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\phi^*\phi = \frac{m^2c^2}{\hbar^2}\phi^*\phi \tag{4}$$

Then subtract Eq.(2) From Eq.(1)

$$[\phi^*(\nabla^2\phi) - (\nabla^2\phi^*)\phi] + \frac{1}{c^2}[\frac{\partial^2\phi^*}{\partial t^2}\phi - \phi^*\frac{\partial^2\phi}{\partial t^2}] = 0 \tag{5}$$

$$\Downarrow$$

$$\nabla[\phi^*(\nabla\phi) - (\nabla\phi^*)\phi] + \frac{1}{c^2}\frac{\partial}{\partial t}[\frac{\partial\phi^*}{\partial t}\phi - \phi^*\frac{\partial\phi}{\partial t}] = 0 \tag{6}$$

Multiply Eq. (6) by $\frac{\hbar}{2im}$, we get

$$\nabla\frac{\hbar}{2im}[\phi^*(\nabla\phi) - (\nabla\phi^*)\phi] + \frac{\partial}{\partial t}\frac{\hbar}{2imc^2}[\frac{\partial\phi^*}{\partial t}\phi - \phi^*\frac{\partial\phi}{\partial t}] = 0 \tag{7}$$

Eq. (6) can be written as

$$\nabla\cdot J + \frac{\partial\rho}{\partial t} = 0 \tag{8}$$

where

$J = \frac{\hbar}{2im}[\phi^*(\nabla\phi) - (\nabla\phi^*)\phi]$ Current density

$\rho = \frac{\hbar}{2imc^2}[\frac{\partial\phi^*}{\partial t}\phi - \phi^*\frac{\partial\phi}{\partial t}]$ probability density

Exercise: Derive the continuity equation above, in a non-covariant notation (just as we did for the Schrödinger equation). Now derive it using a covariant notation.

Consider a plane wave solution: $\phi(t,\vec{x}) = Ne^{-\frac{i}{\hbar}(Et-\vec{p}.\vec{x})}$ Of K-G Equation

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\phi = \frac{m^2c^2}{\hbar^2}\phi \implies E^2 = p^2c^2 + m^2c^4$$

$$\implies E = \pm\sqrt{p^2c^2 + m^2c}$$

★ Not surprisingly, the KG equation has negative energy solutions

★Historically –ve energy solutions were viewed as problematic but for KG, there is also a problem with probability density

$$\rho = \frac{\hbar}{2imc^2}[\frac{\partial\phi^*}{\partial t}\phi - \phi^*\frac{\partial\phi}{\partial t}] = 2|N|^2 E$$

- So these –ve energy states have negative probability distributions
- We can not just ignore these solutions since they will crop up in any Fourier decomposition

This is why Schrödinger abandoned this equation and developed the non-relativistic Schrödinger equation instead – he (implicitly) took the positive sign of the square root so that he could ignore the negative energy solutions.

Feynman-stuckelberg Interpretation

- Quantum field theory tells us that positive energy states must propagate forwards in time in order to preserve causality
- Feynman an Stuckelburge suggested that –ve energy states propagate backwards in time

Our negative energy solution (E<0) plane wave solution are

$$\phi_{E,\vec{p}}(t,\vec{x}) = N e^{-\frac{i}{\hbar}\left(|E|(-t)-\vec{p}\cdot\vec{x}\right)} = \phi_{|E|,-\vec{p}}(-t,\vec{x})$$

Negative sign moved to time

Remember

$$\vec{p} = m\frac{d\vec{x}}{dt} = -m\frac{d\vec{x}}{d(-t)}$$

✧ Particles flowing backwards in time are then reinterpreted as anti-particles flowing in the forward direction

If field is charged, we may interpret j^μ as a charge density, instead of a probability density

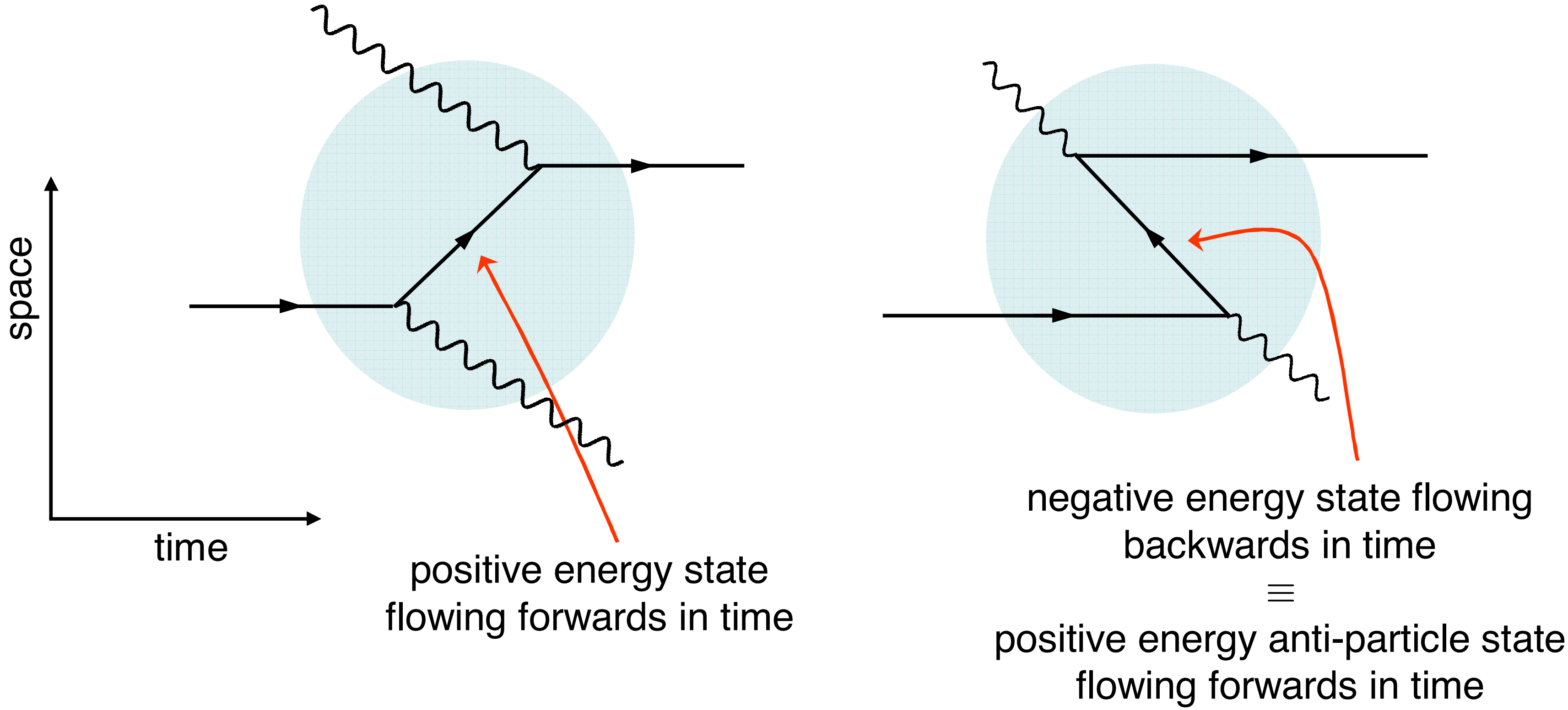
$$j^\mu = -ie\left[\phi^*(\partial^\mu \phi) - (\partial^\mu \phi^*)\phi\right]$$

Now $\rho = j^0$, so for a particle of energy E: $j^0 = -2e|N|^2 E$

while for an anti-particle of energy E: $j^0 = +2e|N|^2 E = -2e|N|^2(-E)$

which is the same as the charge density for an electron of energy -E

In reality, we only ever see the final state particles, so we must include these anti-particles anyway.



Quantum mechanics does not adequately handle the creation of particle—anti-particle pairs out of the vacuum. For that you will need **Quantum Field Theory**.

◆ Normalization of KG Solutions

The particle (or charge) density allows us to normalize the KG solutions in a box

$\rho = 2|N|^2 E$ so in a box of volume V the number of particles is:

$$\int_V \rho dV = \int_V 2|N|^2 E dV = 2|N|^2 EV$$

If we normalize to 2E particles per unit volume, then N=1

Notice that this is a covariant choice. Since the number of particles in a box should be independent of reference frame, but the volume of the box changes with a Lorentz boost, the density must also change with a boost. In fact, the density is the time component of a four-vector j^0.