Quantum Physics 2006/07

Lecture 15: Special Relativity Review; the Klein Gordon Equation

A Review of Special Relativity

Four-Vector Notation: The coordinates of an object or 'event' in four-dimensional space-time, Minkowski space, form a *contravariant* four-vector whose components have 'upper' indices:

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

Similarly, we define a *covariant* four-vector whose components have 'lower' indices:

$$x_\mu \equiv (x_0,\, x_1,\, x_2,\, x_3) \equiv (ct,\, -\underline{x})$$

A general four-vector a^μ is defined in the same way:

$$\begin{aligned} a^\mu &\equiv (a^0,\, a^1,\, a^2,\, a^3) \equiv (a^0,\, \underline{a}) \\ a_\mu &\equiv (a_0,\, a_1,\, a_2,\, a_3) \equiv (a^0,\, -\underline{a}) \end{aligned}$$

so that $a^0 = a_0$ and $a^i = -a_i,\ i = 1, 2, 3$. Upper and lower indices are related by the *metric tensor* $g^{\mu\nu}$:

$$a^\mu = g^{\mu\nu}\, a_\nu \qquad\qquad a_\mu = g_{\mu\nu}\, a^\nu$$

where

$$g^{\mu\nu} = g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

and we use the Einstein summation convention where there is an implicit sum over the *repeated index*: $\nu = 0, 1, 2, 3$.

The *scalar product* in Minkowski space is defined, for general 4-vectors a^μ and b^μ by

$$\begin{aligned} a \cdot b &\equiv a^\mu b_\mu = a_\mu b^\mu = a_\mu b_\nu g^{\mu\nu} = a^\mu b^\nu g_{\mu\nu} \\ &= a^0 b^0 - \underline{a} \cdot \underline{b} \end{aligned}$$

where $\underline{a}$ and $\underline{b}$ are ordinary 3-vectors.

NB we **do *not* underline** 4-vectors; every pair of repeated indices is implicitly summed over and each pair consists of one upper & one lower index. An expression with two identical upper (or lower) indices (eg $a^\mu b^\mu$) is simply **wrong**!

Lorentz transformations: Lorentz transformations are linear transformations on the components of 4-vectors which leave invariant this scalar product:

$$a'^{\,\mu} = \Lambda^\mu{}_\nu\, a^\nu \quad \text{eg} \quad x'^{\,\mu} = \Lambda^\mu{}_\nu\, x^\nu$$

Strictly, these are *homogeneous* Lorentz transformations – translations are not included.

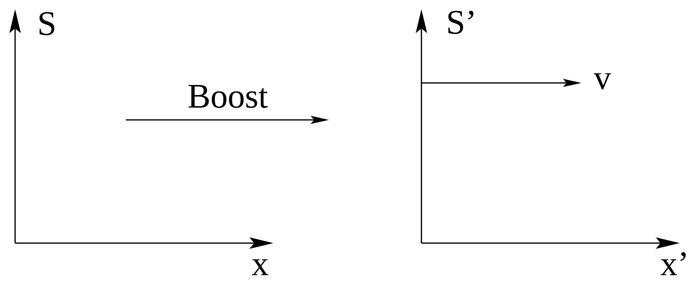
The 'standard' Lorentz transformation is a 'boost' along the x direction

$$\Lambda^\mu{}_\nu \;=\; \begin{pmatrix} \cosh\omega & -\sinh\omega & 0 & 0 \\ -\sinh\omega & \cosh\omega & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

where

$$\begin{aligned} \tanh\omega &\equiv \beta \equiv v/c \\ \cosh\omega &\equiv \gamma = (1-\beta^2)^{-1/2} \;=\; (1-(v/c)^2)^{-1/2} \\ \sinh\omega &= \gamma\,\beta \end{aligned}$$

Hence $ct' = \gamma\,(ct - (v/c)x)$ and $x' = \gamma\,(x - vt)$ as usual, relating the time and space co-ordinates of a given event in two inertial frames in relative motion:



Differential operators

$$\begin{aligned} \partial_\mu &\equiv \frac{\partial}{\partial x^\mu} = \left(\frac{1}{c}\frac{\partial}{\partial t},\, \underline{\nabla}\right) \\ \partial^\mu &\equiv \frac{\partial}{\partial x_\mu} \;=\; \left(\frac{1}{c}\frac{\partial}{\partial t},\, -\underline{\nabla}\right) \end{aligned}$$

d'Alembertian: $$\partial_\mu\,\partial^\mu \;=\; \partial^\mu\,\partial_\mu \;=\; \partial^2 \;=\; \frac{1}{c^2}\frac{\partial^2}{\partial t^2} \;-\; \nabla^2 \qquad (\;=\;\Box)$$

(NB sometimes $\Box$ is called $\Box^2$, so we will almost always use ∂^2.)

Momentum and energy: The conserved 4-momentum is denoted by:

$$\begin{aligned} p^\mu &\equiv \left(\frac{E}{c},\, \underline{p}\right) \\ p^2 &= \frac{E^2}{c^2} \;-\; \underline{p}\cdot\underline{p} \;=\; m^2c^2 \quad \text{for a free particle} \\ \text{or}\quad E^2 &= |\underline{p}|^2c^2 \;+\; m^2c^4 \end{aligned}$$

where m is the mass of the particle.

The Klein-Gordon equation

Recall that the Schrödinger equation for a free particle

$$\left\{-\frac{\hbar^2}{2m}\nabla^2\right\}\Psi(\underline{r},t) \;=\; i\hbar\frac{\partial}{\partial t}\Psi(\underline{r},t)$$

can be obtained from the (non-relativistic) classical total energy

$$E \;=\; \frac{|\underline{p}|^2}{2m} \;=\; H$$

by means of the operator substitution prescriptions

$$E \rightarrow i\hbar\frac{\partial}{\partial t} \qquad \text{and} \qquad \underline{p} \rightarrow -i\hbar\underline{\nabla}$$

The relativistic expression for the total energy of a free particle is

$$E^2 \;=\; |\underline{p}|^2c^2 \;+\; m^2c^4$$

Schrödinger (& Klein, Gordon, & Fock) suggested this as a starting point, thus obtaining

$$-\hbar^2\frac{\partial^2}{\partial t^2}\phi(\underline{r},t) \;=\; -\,\hbar^2\,c^2\nabla^2\phi(\underline{r},t) \;+\; m^2c^4\phi(\underline{r},t) \tag{1}$$

which is the Klein Gordon (KG) equation for a free relativistic particle.[1] We can write the KG equation in a manifestly covariant form as

$$\left(\Box \;+\; \frac{m^2c^2}{\hbar^2}\right)\phi(x) \;=\; 0 \qquad \text{or} \qquad \left(\partial^2 \;+\; \frac{m^2c^2}{\hbar^2}\right)\phi(x) \;=\; 0$$

where x is the usual four-vector $(ct,\, x^1,\, x^2,\, x^3)$. Thus, in covariant form, the operator prescription is

$$\hat{p}^\mu \;\rightarrow\; i\hbar\frac{\partial}{\partial x_\mu} \;=\; i\hbar\left\{\frac{1}{c}\frac{\partial}{\partial t},\; -\underline{\nabla}\right\}$$

Note: for a *massless* particle, $m = 0$, the KG equation reduces to the classical wave equation.

Free particle solutions: By substitution into the KG equation (**??**) we see it has plane-wave solutions

$$\phi(\underline{r},t) \;=\; \exp\{i\underline{k}\cdot\underline{r} \;-\; i\omega\, t\}$$

provided that ω, $\underline{k}$ & m are related by

$$\hbar^2\omega^2 \;=\; \hbar^2c^2|\underline{k}|^2 \;+\; m^2c^4$$

Taking the square-root, we obtain: $\hbar\omega \;=\; \pm\left\{\hbar^2c^2|\underline{k}|^2 \;+\; m^2c^4\right\}^{1/2}$.

Such solutions are readily seen to be eigenfunctions of the momentum operator and of the energy operator, with eigenvalues $\underline{p} \equiv \hbar\underline{k}$ and $E \equiv \hbar\omega$ respectively.

[1] The KG equation was first written down by Schrödinger but, due to the problems we will discover below, he discarded it in favour of the non-relativistic equation that bears his name.

Thus, if we interpret $\hbar\omega$ as an allowed total energy of the free particle solution, there is an ambiguity in the *sign* of the total energy: there are both +ve and −ve energy solutions, and these have energy

$$E \;=\; \pm\sqrt{|\underline{p}|^2c^2 + m^2c^4}$$

The positive-energy eigenvalues are in agreement with the classical relation betwen energy, mass, and momentum, but what are we to make of particles with negative total energy?

If we define the four-vector $\quad k^\mu \equiv (\frac{\omega}{c}, \underline{k}) \quad$ then we can write the solution in covariant form

$$\phi(x) \;\equiv\; \exp(-ik\cdot x) \;\equiv\; \exp(-ik^\mu x_\mu) \;\equiv \exp(-ip^\mu x_\mu/\hbar)$$

and thus interpret the four-momentum as $p^\mu = \hbar k^\mu$.

Continuity equation and probability interpretation

Denote the Schrödinger equation by (SE) and its complex-conjugate by (SE)*. By considering

$$\Psi^*\,(\mathrm{SE}) \;-\; \Psi\,(\mathrm{SE})^*\,,$$

we get a continuity equation $\qquad \frac{\partial}{\partial t}\rho \;+\; \underline{\nabla}\cdot\underline{j} \;=\; 0$

where $\qquad \rho \;=\; \Psi^*\,\Psi \qquad$ and $\qquad \underline{j} \;=\; -\frac{i\hbar}{2m}\,(\Psi^*\underline{\nabla}\Psi \;-\; \Psi\underline{\nabla}\Psi^*)$

are the probability density and probability current respectively. (Integrate over any volume, and use the divergence theorem to see why.) We can repeat this for the Klein Gordon equation, and obtain the quantities

$$\rho \;=\; \frac{i\hbar}{2mc^2}\left(\phi^*\frac{\partial\phi}{\partial t} \;-\; \phi\frac{\partial\phi^*}{\partial t}\right)$$

$$\underline{j} \;=\; -\frac{i\hbar}{2m}\,(\phi^*\underline{\nabla}\phi \;-\; \phi\underline{\nabla}\phi^*)$$

1. $\underline{j}$ is *identical* in form to the non-relativistic Schrödinger current (we have *chosen* to normalise $\underline{j}$ so that this is the case.).
2. ρ can be shown to reduce to $\phi^*\phi$ in the non-relativistic limit.
3. The candidate for the probability density, $\rho(x)$, is no longer positive definite (negative energy solutions have $\rho < 0$ (exercise). Therefore there is no obvious probability-density interpretation.

Summary: The Klein Gordon (KG) equation is the simplest relativistically-covariant generalisation of the Schrödinger equation. Its solutions have the usual desirable properties for the description of a relativistic quantum particle, but they also describe particles of negative total energy, together with negative probabilities for finding them!

Considering the positive energy solutions only, the KG equation with a Coulomb potential can be solved exactly for the energy levels of the hydrogen atom. The non-relativistic expansion reproduces exactly the relativistic kinetic energy correction ΔE_{KE} obtained in perturbation theory in Lecture 6, page 2, but it doesn't account for either the spin-orbit correction or the Darwin term, so something else is required...