Now we turn to relativistic quantum mechanics. We follow a roughly historical order in presenting this material, even though it involved some misconceptions at various stages. It would be possible to leapfrog directly to the modern point of view, but some important ideas would have to be badly unmotivated.

The first attempts at formulating a relativistic wave equation were made by Schrödinger. He was exploring the ideas of de Broglie, in which a classical energy and momentum E and $\vec{p}$ are associated with a frequency ω and wave number $\vec{k}$ by $E = \hbar\omega$, $\vec{p} = \hbar\vec{k}$, or, as operators acting on plane waves,

$$\left.\begin{aligned} E &\to i\hbar \frac{\partial}{\partial t} \\ \vec{p} &\to -i\hbar \nabla \end{aligned}\right\}.$$

Applied to the NR free particle for which $E = p^2/2m$, this yields the usual NR Schrödinger eqn,

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

For a relativistic free particle, the energy and momentum are related by

$$E = \sqrt{c^2 p^2 + m^2 c^4}.$$

Notice that the energy includes the rest mass mc^2, so for low velocities $v/c \ll 1$, the relativistic formula yields

$$E \approx mc^2 + \frac{p^2}{2m}.$$

In any case, the relativistic energy-momentum relation yields the wave equation,

$$i\hbar \frac{\partial \psi}{\partial t} = \sqrt{-\hbar^2 c^2 \nabla^2 + m^2 c^4}\, \psi$$

(still for a free particle.) The square root is hard to interpret. It makes sense in momentum space, but is nonlocal in real space, and it doesn't treat space and time on an equal footing so it's hard to see how it can be covariant. To fix this, Schrödinger squared the classical ~~eqn~~ energy-momentum relation,

$$E^2 = c^2 p^2 + m^2 c^4,$$

which implies a wave equ,

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = -\hbar^2 c^2 \nabla^2 \psi + m^2 c^4 \psi.$$

This is called the <u>Klein-Gordon eqn</u>. (Schrödinger never published it, and it was later discovered again by Klein and Gordon). An equivalent form is

$$\boxed{\frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} - \nabla^2 \psi = -\left(\frac{mc}{\hbar}\right)^2 \psi}$$

which shows the d'Alembertian or wave operator on the left. On the right appears the <u>Compton wavelength</u>

$$\lambda_c = \frac{\hbar}{mc}$$

of the particle. The Compton wavelength depends on the mass and it has the following interpretation. Let a particle of mass m be confined to a box of size L.

L.

By the uncertainty principle, the momentum ~~is~~ has the uncertainty

$$\Delta p = \frac{\hbar}{L}.$$

We ask, how small must L be such that Δp will reach relativistic values, say, mc? ~~the answer~~ (That is, $\frac{\hbar}{L} \sim mc$.) The answer is $L \sim \lambda_c$. Note for the photon ($m=0$) $\lambda_c = \infty$ and photons are always relativistic. For electrons, relativistic qu. mech. is necessary if the electron is examined on distance scales comparable to λ_c, which is $\frac{\hbar}{mc} = \alpha a_0 = 1/137 \times$ size of H-atom.

Notice for a photon $(m=0)$ the Klein ~~go~~-Gordon eqn. just becomes the wave eqn,

$$\frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} - \nabla^2 \psi = 0$$

which has no $\hbar$ and which of course comes out of the classical Maxwell eqns.

Let's look at plane-wave solutions of the K-G equ,

$$\psi = e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} \qquad (E, \vec{p} = \text{c-numbers, parameters of wave}).$$

Plugging into the K-G equ, we find a solution if

$$E = \pm\sqrt{c^2p^2 + m^2c^4}.$$

This of course is just the classical energy-momentum relation, but with the possibility of a minus sign, that is, $E<0$. The KG equ possesses <u>solutions of negative energy</u>. These have no analog in classical relativity theory or in the NR Sch. theory of QM, so we don't know what they mean. We ignore this interpretational difficulty and push on.

In the next step we introduce covariant notation. Let the space-time 4-vector be

$$x^\mu = (ct, \vec{x}) \qquad \text{i.e.,}\ x^0 = ct, \qquad \mu = 0,1,2,3.$$

The momentum 4-vector is

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

We use the metric

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

to raise and lower indices, so time-like vectors have + norm, and space-like vectors have − norm. Then

$$x_\mu = (ct, -\vec{x})$$

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

and

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

We also introduce the derivative operators,

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

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

Notice the positions of the indices. So far this is all classical.

Now we can write the de-Broglie – Einstein relations in covariant form,

$$\frac{E}{c} \rightarrow i\hbar \frac{\partial}{\partial(ct)} = i\hbar\,\partial^0$$

$$\vec{p} \rightarrow -i\hbar\,\nabla = i\hbar\,\partial^i \qquad i=1,2,3.$$

that is,

$$\boxed{p^\mu \rightarrow i\hbar\,\partial^\mu}$$

In terms of the 4-momentum operators, the KG equ can now be written

$$\boxed{\begin{aligned} & p^\mu p_\mu \psi = m^2c^2\psi \\ \text{or}\quad & \partial^\mu\partial_\mu \psi = -\left(\frac{mc}{\hbar}\right)^2\psi \end{aligned}}$$

Here of course the p^μ are operators, not c-numbers.

Next we look at the probability density and current. For the NR Sch. eqn., these are

$$\rho = |\psi|^2$$
$$\vec{J} = \frac{-i\hbar}{2m}\left(\psi^* \nabla\psi - \psi\nabla\psi^*\right) \qquad (\text{when } \vec{A}=0).$$

If ψ is a soln of the Sch. eqn, then

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

Sometimes the continuity eqn. can be put into covariant form. We define

$$J^\mu = (c\rho, \vec{J}),$$

whereupon

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{J} = \frac{\partial J^\mu}{\partial x^\mu} = \partial_\mu J^\mu .$$

We should not use such notation for the NR Sch. eqn. versions of ρ and $\vec{J}$, however. Just because we ~~define~~ write down 4 quantities and put a Greek index on them does not mean that they form a 4-vector. Instead they must transform as a 4-vector under Lorentz transformations. The quantities $(c\rho, \vec{J})$ defined for the NR Sch. eqn. do not transform as a 4-vector, even though they do satisfy the continuity eqn. Instead, they (and the continuity eqn) are specific to one Lorentz frame.

The KG eqn however does possess a conserved covariant 4-current.

It is

$$J^\mu = \frac{i\hbar}{2m}\left(\psi^*\partial^\mu\psi - \psi\,\partial^\mu\psi^*\right).$$

To show it is conserved, compute

$$\partial_\mu J^\mu = \frac{i\hbar}{2m}\left[(\partial_\mu\psi^*)(\partial^\mu\psi) + \psi^*(\partial_\mu\partial^\mu\psi) - (\partial_\mu\psi)(\partial^\mu\psi^*) - \psi(\partial_\mu\partial^\mu\psi^*)\right]$$

cancel.

The 1st + 3rd terms cancel. So do the 2nd and 4th if we use the KG eqn:

$$\partial_\mu\partial^\mu\psi = -\left(\frac{mc}{\hbar}\right)^2\psi$$

$$\partial_\mu\partial^\mu\psi^* = -\left(\frac{mc}{\hbar}\right)^2\psi^*$$

So, $\partial_\mu J^\mu = 0$. Moreover, this eqn. is covariant, since J^μ transforms as a 4-vector. This follows if we assume ψ transforms as a scalar (the simplest assumption for a scalar field).

Unfortunately, there is a problem with this 4-current. The density

$$\rho = \frac{1}{c}J^0 = \frac{i\hbar}{2mc^2}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right)$$

is not positive definite. It leads to "negative probabilities." We will not go into this in detail, except to remark that the negative probabilities can be seen to be related to the negative energy solutions, which are also related to the fact that the KG eqn is 2nd order in time.

For these reasons, the KG eqn. was abandoned for several years after its introduction, and regarded as unsatisfactory. Later it was revived, and it is now considered a respectible wave eqn. describing spin-0 bosons. But we need several new concepts to understand this. In fact, in this course we will not have much more to say about the KG eqn, for lack of time.

This was the state of affairs when Dirac began his investigations of relativistic wave eqns. To avoid negative probabilities, Dirac considered an eqn. that is first order in time,

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$

where H is some Hamiltonian operator to be determined. At first we take the case of a free particle.

Since the wave eqn. is 1st order in time, and since relativity theory is supposed to treat space and time on an equal footing, Dirac reasoned that the wave eqn. should be first order in space as well. (Of course the NR Sch. eqn. is 2nd order in space.) So using the momentum operators $p_k = -i\hbar \frac{\partial}{\partial x^k}$,

$k=1,2,3$, and introducing coefficients α_k, $k=1,2,3$ and another coefficient β, Dirac wrote

$$i\hbar \frac{\partial \psi}{\partial t} = -i\hbar c \sum_{k=1}^{3} \alpha_k \frac{\partial \psi}{\partial x_k} + mc^2 \beta \psi .$$ (free particle Dirac eqn)

The c in the α-term and the mc^2 in the β term are introduced to make α_k and β dimensionless. This is equivalent to the Hamiltonian,

$$H = c\, \vec{\alpha} \cdot \vec{p} + mc^2 \beta$$ (free particle Dirac Hamiltonian).

The quantities α_k or $\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ cannot be ordinary numbers because if they were they would specify a vector in ordinary space that would pick out a particular direction, which we don't expect for a free particle. Instead, Dirac assumed that ψ is a multi-component "spinor" wave function with N components,

$$\psi = \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_N \end{bmatrix}$$

where N is to be determined. Then α_k and β are interpreted as $N \times N$ matrices. We think of $\vec{\alpha}$ as a "vector of matrices" much like the Pauli matrices $\vec{\sigma}$. The matrices α_k and β must be constants (independent of $\vec{x}, t$) because the free particle Hamiltonian must be invariant under space or time translations. Thus $\vec{\alpha}\cdot\vec{p} = \vec{p}\cdot\vec{\alpha}$ (where $\vec{p} = -i\hbar\nabla$). Henceforth when looking at Dirac formalism you must remember that ψ is a spinor and $\vec{\alpha}, \beta$ are matrices.

To determine the form of the $\vec{\alpha}, \beta$ matrices Dirac required that every free particle solution of the Dirac eqn. should also be a solution of the KG eqn. This is so that the classical energy-momentum relations $E^2 = c^2p^2 + m^2c^4$ would be satisfied. Thus we take

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi = \left(c\sum_k \alpha_k p_k + mc^2\beta\right)\psi$$

and apply $i\hbar\frac{\partial}{\partial t}$ to both sides, getting

$$i\hbar\frac{\partial}{\partial t}\left(i\hbar\frac{\partial\psi}{\partial t}\right) = H\left(i\hbar\frac{\partial\psi}{\partial t}\right) = H^2\psi = \left(c\sum_k \alpha_k p_k + mc^2\beta\right)^2\psi$$

$$= -\hbar^2\frac{\partial^2\psi}{\partial t^2} = \left(c^2\sum_{k\ell}\alpha_k\alpha_\ell p_k p_\ell + mc^3\sum_k \alpha_k\beta + \beta\alpha_k + m^2c^4\beta^2\right)\psi.$$

To get the KG eqn, we must have:

$$\boxed{\begin{aligned} &\beta^2 = 1 \qquad \text{(the } N\times N \text{ identity matrix)} \\ &\alpha_k\beta + \beta\alpha_k = 0 \\ &\alpha_k^2 = 1 \quad , \quad k = 1,2,3 \\ &\alpha_k\alpha_\ell = -\alpha_\ell\alpha_k \quad (k \neq \ell). \end{aligned}}$$

Dirac algebra, version 1

If these are satisfied then

$$-\hbar^2 \frac{\partial^2\psi}{\partial t^2} = -\hbar^2 c^2 \nabla^2\psi + m^2c^4\psi \qquad \text{(KG eqn).}$$

The above equations constitute the <u>Dirac algebra</u> of the $\vec{\alpha}, \beta$ matrices. The Dirac algebra is more conveniently written in terms of <u>anticommutators</u>: (Note, $\{A,B\} = AB+BA$.)

$$\boxed{\begin{aligned} \{\alpha_k, \alpha_\ell\} &= 2\delta_{k\ell} \\ \{\alpha_k, \beta\} &= 0 \\ \{\beta, \beta\} &= 2 \end{aligned}}$$

Dirac algebra, anticommutator version.

To find the matrices that satisfy the Dirac algebra, first note that they must be Hermitian if we expect $H = c\vec{\alpha}\cdot\vec{p} + mc^2\beta$ to be Hermitian. Next, since $\alpha_k^2 = \beta^2 = 1$, their eigenvalues must be ± 1. Next, take $\alpha_k\beta + \beta\alpha_k = 0$, multiply by β, use $\beta^2 = 1$, and take traces, so that

$$\mathrm{tr}(\beta\alpha_k\beta) + \mathrm{tr}(\alpha_k) = 0.$$

But $\mathrm{tr}\,(\beta\alpha_k\beta) = \mathrm{tr}\,(\beta^2\alpha_k) = \mathrm{tr}\,(\alpha_k)$, so

$$2\,\mathrm{tr}(\alpha_k) = 0 \quad\Rightarrow\quad \mathrm{tr}\,\alpha_k = 0.$$

Similarly we can show that $\mathrm{tr}\,\beta = 0$. But since the trace is the sum of the eigenvalues, which must be ± 1, the number of $+1$'s and -1's must be equal, so <u>$N =$ even</u>.

Thus the simplest case to try is $N=2$. In this case all Hermitian matrices can be represented as a linear combination of $(I, \vec{\sigma})$, and with some computation one can show that it is impossible to satisfy the Dirac algebra with $N=2$. Instead we try $N=4$.

At $N=4$, Dirac was able to find matrices that satisfy his algebra. These are

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \begin{pmatrix}\text{Dirac-Pauli} \\ \text{representation}\end{pmatrix}.$$

Here all 4×4 matrices are partitioned into 4 2×2 matrices, and we use the Pauli matrices $\vec{\sigma}$ for the 2×2 subblocks. Also, 1 means identity matrix.

When we have a set of abstract algebraic relations that some objects satisfy, such as the Dirac algebra, and we find a concrete set of matrices that satisfy those relations, then we say that we have a <u>representation</u> of those relations. Thus, Dirac found a 4×4

matrix representation of his algebra (the Dirac-Pauli representation). However, that representation is not unique, because if we conjugate the matrices $\vec{\alpha}, \beta$ by any fixed 4×4 unitary matrix,

$$\vec{\alpha} \to U \vec{\alpha} U^{+}$$
$$\beta \to U \beta U^{+}$$

then the new $\vec{\alpha}, \beta$ are still Hermitian and still satisfy the same algebra. Any two representations that differ by such a conjugation (a change of basis) are said to be <u>equivalent</u>.

Another 4×4 representation of the Dirac algebra, equivalent to the Dirac-Pauli representation, is

$$\vec{\alpha} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & -\vec{\sigma} \end{pmatrix} \qquad \beta = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}. \qquad \left(\begin{array}{l}\text{Weyl} \\ \text{representation}\end{array}\right)$$

~~So there is no difference physically between~~ Any calculation that can be carried out in the Dirac-Pauli rep'n can also be carried out in the Weyl rep'n, with the same answers from a physical standpoint. But the calculation may be more or less convenient in one or the other. The Dirac-Pauli rep'n is especially useful when studying the NR limit of the Dirac eqn, while the Weyl rep'n is useful for ultra relativistic or massless particles (like neutrinos).

There is another equivalent representation of the Dirac algebra, due to Majorana, that is commonly used. We will not quote it, however.

It can be shown that all 4×4 representations of the Dirac algebra are equivalent to the one found by Dirac. Thus, apart from a change of basis (unitary conjugation), Dirac's solution by 4×4 matrices is <u>unique</u>.

The Dirac matrices are 4-dimensional, but this has nothing to do with the fact that there are 4 space-time dimensions. Instead, the Dirac matrices act on "spin space", while usual tensors in relativity theory $F_{\mu\nu}$ etc, act on space-time components.

The free particle Dirac eqn is

$$i\hbar\frac{\partial\psi}{\partial t} = -i\hbar c\,\vec{\alpha}\cdot\nabla\psi + mc^2\beta\psi$$
$$= H\psi$$

Dirac free particle Ham.

where $\boxed{H = c\,\vec{\alpha}\cdot\vec{p} + mc^2\beta.}$ To incorporate the interaction with the EM field, we use the <u>minimal</u> <u>coupling</u> prescription. This is the simplest method of coupling an otherwise free particle with the EM field which is Lorentz covariant. It amounts to replacing the 4-momentum of the particle p^μ by

$$p^\mu \rightarrow p^\mu - \frac{q}{c}A^\mu,$$

where q = charge and

$$A^\mu = (\Phi, \vec{A})$$

is the 4-vector potential (Φ = scalar potential, $\vec{A}$ = 3-vector potential).

In QM, the 4-momentum p^μ becomes the operator $i\hbar\partial^\mu$, so the minimal coupling prescription gives

$$i\hbar\frac{\partial}{\partial t} \rightarrow i\hbar\frac{\partial}{\partial t} - q\Phi,$$
$$-i\hbar\nabla \rightarrow -i\hbar\nabla - \frac{q}{c}\vec{A}.$$

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

With this change, the Dirac eqn becomes

$$i\hbar\frac{\partial\psi}{\partial t} = -i\hbar c\,\vec{\alpha}\cdot\nabla\psi - \frac{q}{c}(\vec{\alpha}\cdot\vec{A})\psi + mc^2\beta\psi + q\Phi\psi.$$

or
$$i\hbar \frac{\partial \psi}{\partial t} = H\psi,$$

where

Dirac Ham. for particle + EM field, minimal coupling.

$$\boxed{H = c\vec{\alpha}\cdot\left(\vec{p} - \frac{q}{c}\vec{A}\right) + mc^2\beta + q\Phi.}$$

It is a guess that this is correct. There are other Lorentz covariant couplings to the EM field, but these are not as simple as the minimal one, and they lead to more complicated equations.

Let us now look for a <u>conserved probability current</u>. Following the steps used in the NR Sch. eqn., we write down the wave eqn for ψ and then take the Hermitian conjugate, which maps the column spinor $\psi = \begin{bmatrix}\psi_1\\ \vdots \\ \psi_4\end{bmatrix}$ into the row spinor $\psi^+ = [\psi_1^* \dots \psi_4^*]$. Since matrices $\vec{\alpha}, \beta$ are Hermitian, they are not affected by the Herm. conj., but we must reverse the order of the spin matrix – spinor products:

$$i\hbar \frac{\partial \psi}{\partial t} = -i\hbar c\, \vec{\alpha}\cdot\nabla\psi - \frac{q}{c}(\vec{\alpha}\cdot\vec{A})\psi + mc^2\beta\psi + q\Phi\psi$$

$$-i\hbar \frac{\partial \psi^+}{\partial t} = i\hbar c\, \nabla\psi^+\cdot\vec{\alpha} - \frac{q}{c}\psi^+(\vec{\alpha}\cdot\vec{A}) + mc^2\psi^+\beta + q\Phi\psi^+$$

Now multiply 1st eqn by ψ^+ from the left and the 2nd by $-\psi$ from the right. Then all spin indices are contracted and we have a scalar insofar as spin indices are concerned. The quantities still depend on $\vec{x}, t$. The result is

$$i\hbar \frac{\partial}{\partial t}(\psi^+\psi) = -i\hbar c\, \nabla\cdot\left(\psi^+\vec{\alpha}\,\psi\right),$$

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

where
$$\rho = \psi^+ \psi, \qquad \vec{J} = c\,(\psi^+ \vec{\alpha}\, \psi).$$

To write this out explicitly, using $a, b = 1, \dots, 4$ for spinor indices,
$$\rho = \sum_{a=1}^{4} |\psi_a|^2$$

$$J_i = c \sum_{ab} \psi_a^* \, (\alpha_i)_{ab} \, \psi_b \, .$$

We see that $\rho \geq 0$, so ρ may be interpreted as a probability density. Dirac felt that in this way he had overcome the main difficulty of the Klein-Gordon eqn (negative probabilities). Thus we define $J^\mu = (c\rho, \vec{J})$, so the continuity eqn. is $\partial_\mu J^\mu = 0$. Of course we must show that J^μ transforms as a 4-vector to show that this eqn. is really covariant. That is a fairly large project that we defer until we have a better understanding of the physical meaning of the Dirac equation.

To develop the physics of the Dirac eqn, we consider the simplest possible exact solution, that of a free particle at rest, for which $\nabla \psi = 0$.

Then the Dirac eqn is

$$i\hbar \frac{\partial}{\partial t}\begin{pmatrix}\psi\end{pmatrix} = mc^2 \underbrace{\left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & -1 \end{array}\right)}_{\text{matrix } \beta \text{ (D-P rep'n)}}\begin{pmatrix}\psi\end{pmatrix}$$

There are 4 lin. indep. solns:

$$\underbrace{\begin{pmatrix}1\\0\\0\\0\end{pmatrix} e^{-imc^2t/\hbar}, \quad \begin{pmatrix}0\\1\\0\\0\end{pmatrix} e^{-imc^2t/\hbar}}_{E = mc^2}, \quad \underbrace{\begin{pmatrix}0\\0\\1\\0\end{pmatrix} e^{+imc^2t/\hbar}, \quad \begin{pmatrix}0\\0\\0\\1\end{pmatrix} e^{+imc^2t/\hbar}}_{E = -mc^2}$$

The energy of the solutions is given by the t-dependence. The first two have energies $E = +mc^2$. The time dependence $e^{-imc^2t/\hbar}$ would appear in the usual NR Sch. eqn, too, if we added the constant mc^2 to the Hamiltonian $p^2/2m$. Apart from this, the upper two components of the Dirac spior agree with the Pauli 2-component spinor for a NR spin ½ free particle at rest. The second pair of solutions have negative energies $E = -mc^2$, and we see that the Dirac eqn, like the KG eqn, has solutions of negative energy. The physical interpretation of these is not clear (ultimately we will see that they are related to the existence of antiparticles).

Next we turn to the Heisenberg eqns of motion for the Dirac equation. We use the ~~full~~ Hamiltonian that includes the interaction with the EM field: