Klein-Gordon equation, a closer look

Non-relativistic Schrödinger mechanics probability density

$$P(x+dx) = |\psi(x)|^2 > 0$$

and flux density

$$\boldsymbol{S} = -i\hbar/2m(\psi^*\nabla\psi - \psi\nabla\psi^*)$$

satisfy the continuity equation

$$\partial P/\partial t + \nabla\cdot\boldsymbol{S} = 0.$$

We want to generalize this in 4-dimensions such that the 4-current

$$\partial^\mu s_\mu = 0 \quad \text{where} \quad s_\mu = (icP, \boldsymbol{S})$$

Physical requirements are:
P is the fourth component of a 4-vector, thus transforms like $P \to \gamma P$
P, being probability density is positive definitive.
Let

$$s_\mu = C(\phi^*\frac{\partial\phi}{\partial x_\mu} - \frac{\partial\phi^*}{\partial x_\mu}\phi)$$

in which ϕ is a solution to the free particle K-G eq.
Now

$$\begin{aligned}\frac{\partial s_\mu}{\partial x_\mu} &= C(\frac{\partial\phi^*}{\partial x_\mu}\frac{\partial\phi}{\partial x_\mu} + \phi^*\frac{\partial^2\phi}{\partial x_\mu^2} - \frac{\partial\phi^*}{\partial x_\mu}\frac{\partial\phi}{\partial x_\mu} - \frac{\partial^2\phi^*}{\partial x_\mu^2}\phi) \\ &= \phi^*\mu^2\phi - \mu^2\phi^*\phi = 0\end{aligned}$$

For a non-relativistic particle (slow), $E \approx m_0c^2$ and

$$\phi \sim \psi e^{-imc^2t/\hbar}$$

Setting $C = -i\hbar/2m$ leads to $\boldsymbol{s} = \boldsymbol{S}$ and

$$s_0 = -is_4 = (2imc/\hbar)A|\psi|^2 = c|\psi|^2.$$

To sum up so far, relativistic current density: satisfies the continuity equation, and
components of the current density coincide with non-relativistic flux density with zeroth component being the probability density times c
Problems arise since

$$P = \frac{i\hbar}{2mc^2}\left(\phi^*\frac{\partial\phi}{\partial x_\mu} - \frac{\partial\phi^*}{\partial x_\mu}\phi\right)$$

is not positive definitive in the relativistic case.

Explicitely, both

$$\psi = u(x)e^{-iEt/\hbar} \quad \text{and} \quad \psi = u^*(x)e^{iEt/\hbar}$$

are solutions to the Klein-Gordon equation since the time derivative is of the second order (compare in Shrödinger eq. d/dt is 1st order).
we get negative probability solutions!
omitting solutions $\psi = u(x)e^{-iEt/\hbar}$ $(E < 0)$ does not help, since
$\psi = u(x)e^{-iEt/\hbar}$ $(E > 0)$ do not form a complete basis
we are in trouble, either we must abandon Klein-Gordon equation and derive something better, i.e. find a relativistic wave equation linear in time-derivatives
or
interpret the equation in another way
Instead of associating the s_μ with probability, we should look at s_μ as the charge-current density like before when dealing with a complex scalar fields.
The treatment for a classical scalar field generalizes to the QM by replacing the classical fields with (non-hermitian) operators:

$$\phi = \frac{\phi_1 + i\phi_2}{\sqrt{2}} \quad ; \quad \phi^\dagger = \frac{\phi_1 - i\phi_2}{\sqrt{2}}$$

The probability component of a 4-current operator

$$j_\mu = q\left(\phi^\dagger \frac{\partial \phi}{\partial x_\mu} - \frac{\partial \phi^\dagger}{\partial x_\mu}\phi\right)$$

can be shown to satisfy

$$\int \frac{j_4}{ic} d^3x = q \sum_{\boldsymbol{k}} \left(N_{\boldsymbol{k}}^{(+)} - N_{\boldsymbol{k}}^{(-)}\right) \qquad (*)$$

where $N_{\boldsymbol{k}}^{(\pm)} = a_{\boldsymbol{k}\pm}^\dagger a_{\boldsymbol{k}\pm}$ and

$$a_{\boldsymbol{k}\pm} = \frac{1}{\sqrt{2}}(a_{\boldsymbol{k}}^{(1)} \pm i a_{\boldsymbol{k}}^{(2)}) \quad ; \quad a_{\boldsymbol{k}\pm}^\dagger = \frac{1}{\sqrt{2}}(a_{\boldsymbol{k}}^{(1)} \mp i a_{\boldsymbol{k}}^{(2)}).$$

$N_{\boldsymbol{k}}^{(+)}$ and $N_{\boldsymbol{k}}^{(-)}$ are the number operators for a Klein-Gordon particle of charge q and its antiparticle (w charge $-q$)
The eigenvalue of (*) is the total charge of the field.
In other words, the probability to find a particle is not conserved (as in non-relativistic QM), instead the net charge is conserved quantity.
This is cool since now we take into account also the possibility for particle creation/annihilation, e.g.

$$\gamma \to \pi^+ + \pi^-.$$

To emphasize once more: there is nothing wrong with Klein-Gordon as long as it is read in appropriate way.

Dirac's equation

We construct relativistically covariant equation that takes into account also the spin.
The kinetic energy operator is

$$H^{(\mathrm{KE})} = \frac{\boldsymbol{p}^2}{2m}.$$

Previously we derived for Pauli spin matrices the relation

$$(\boldsymbol{\sigma} \cdot \boldsymbol{a})^2 = |\boldsymbol{a}|^2,$$

so we can also write

$$H^{(\mathrm{KE})} = \frac{(\boldsymbol{\sigma} \cdot \boldsymbol{p})(\boldsymbol{\sigma} \cdot \boldsymbol{p})}{2m}.$$

However, when the particle moves under the influence of a vector potential these expressions differ. Substituting

$$\boldsymbol{p} \mapsto \boldsymbol{p} - e\boldsymbol{A}/c$$

the latter takes the form

$$\begin{aligned}
&\frac{1}{2m}\boldsymbol{\sigma} \cdot \left(\boldsymbol{p} - \frac{e\boldsymbol{A}}{c}\right) \boldsymbol{\sigma} \cdot \left(\boldsymbol{p} - \frac{e\boldsymbol{A}}{c}\right) \\
&\quad = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e\boldsymbol{A}}{c}\right)^2 \\
&\qquad + \frac{i}{2m}\boldsymbol{\sigma} \cdot \left[\left(\boldsymbol{p} - \frac{e\boldsymbol{A}}{c}\right) \times \left(\boldsymbol{p} - \frac{e\boldsymbol{A}}{c}\right)\right] \\
&\quad = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e\boldsymbol{A}}{c}\right)^2 - \frac{e\hbar}{2mc}\boldsymbol{\sigma} \cdot \boldsymbol{B},
\end{aligned}$$

where we have used the identities

$$(\boldsymbol{\sigma} \cdot \boldsymbol{a})(\boldsymbol{\sigma} \cdot \boldsymbol{b}) = \boldsymbol{a} \cdot \boldsymbol{b} + i\boldsymbol{\sigma} \cdot (\boldsymbol{a} \times \boldsymbol{b})$$

and

$$\boldsymbol{p} \times \boldsymbol{A} = -i\hbar(\nabla \times \boldsymbol{A}) - \boldsymbol{A} \times \boldsymbol{p}.$$

Let us suppose that for the relativistically invariant expression

$$(E^2/c^2) - \boldsymbol{p}^2 = (mc)^2$$

the operator analogy

$$\frac{1}{c^2}{E^{(\mathrm{op})}}^2 - \boldsymbol{p}^2 = (mc)^2$$

holds. Here

$$E^{(\mathrm{op})} = i\hbar\frac{\partial}{\partial t} = i\hbar c\frac{\partial}{\partial x_0}$$

and

$$\boldsymbol{p} = -i\hbar\nabla.$$

We write the operator equation into the form

$$\left(\frac{E^{(\mathrm{op})}}{c} - \boldsymbol{\sigma}\cdot\boldsymbol{p}\right)\left(\frac{E^{(\mathrm{op})}}{c} + \boldsymbol{\sigma}\cdot\boldsymbol{p}\right) = (mc)^2$$

or

$$\left(i\hbar\frac{\partial}{\partial x_0} + \boldsymbol{\sigma}\cdot i\hbar\nabla\right)\left(i\hbar\frac{\partial}{\partial x_0} - \boldsymbol{\sigma}\cdot i\hbar\nabla\right)\phi = (mc)^2\phi.$$

Here ϕ is a two component wave function (spinor).
We define new two component wave functions

$$\begin{aligned}
\phi^{(R)} &= \frac{1}{mc}\left(i\hbar\frac{\partial}{\partial x_0} - i\hbar\boldsymbol{\sigma}\cdot\nabla\right)\phi \\
\phi^{(L)} &= \phi.
\end{aligned}$$

It is easy to see that these satisfy the set of simultaneous equations

$$\begin{aligned}
\left[i\hbar\boldsymbol{\sigma}\cdot\nabla - i\hbar\frac{\partial}{\partial x_0}\right]\phi^{(L)} &= -mc\phi^{(R)} \\
\left[-i\hbar\boldsymbol{\sigma}\cdot\nabla - i\hbar\frac{\partial}{\partial x_0}\right]\phi^{(R)} &= -mc\phi^{(L)}.
\end{aligned}$$

We define yet new two component wave functions

$$\begin{aligned}
\psi_A &= \phi^{(R)} + \phi^{(L)} \\
\psi_B &= \phi^{(R)} - \phi^{(L)}.
\end{aligned}$$

These in turn satisfy the matrix equation

$$\begin{pmatrix} -i\hbar\frac{\partial}{\partial x_0} & -i\hbar\boldsymbol{\sigma}\cdot\nabla \\ i\hbar\boldsymbol{\sigma}\cdot\nabla & i\hbar\frac{\partial}{\partial x_0} \end{pmatrix}\begin{pmatrix}\psi_A \\ \psi_B\end{pmatrix} = -mc\begin{pmatrix}\psi_A \\ \psi_B\end{pmatrix}.$$

We now define the four component wave function

$$\psi = \begin{pmatrix}\psi_A \\ \psi_B\end{pmatrix} = \begin{pmatrix}\phi^{(R)} + \phi^{(L)} \\ \phi^{(R)} - \phi^{(L)}\end{pmatrix}$$

and the 4×4-matrices

$$\begin{aligned}
\gamma_k &= \begin{pmatrix} 0 & -i\sigma_k \\ i\sigma_k & 0 \end{pmatrix} \\
\gamma_4 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\end{aligned}$$

We end up with the *Dirac's equation*

$$\left(\boldsymbol{\gamma}\cdot\nabla+\gamma_4\frac{\partial}{\partial(ix_0)}\right)\psi+\frac{mc}{\hbar}\psi=0$$

for free spin-$\frac{1}{2}$ particles. Employing the four vector notation the equation takes the form

$$\left(\gamma_\mu\frac{\partial}{\partial x_\mu}+\frac{mc}{\hbar}\right)\psi=0.$$

reminder:

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

Note The Dirac equation is in fact a set of *four* coupled linear differential equations. The wave function ψ is the four component vector

$$\psi=\begin{pmatrix}\psi_1\\\psi_2\\\psi_3\\\psi_4\end{pmatrix}.$$

This kind of a four component object is called *bispinor* or Dirac's spinor. Explicitely written down the Dirac equation is

$$\sum_{\mu=1}^{4}\sum_{\beta=1}^{4}\left[(\gamma_\mu)_{\alpha\beta}\frac{\partial}{\partial x_\mu}+\left(\frac{mc}{\hbar}\right)\delta_{\alpha\beta}\right]\psi_\beta=0.$$

Note The fact that the Dirac spinor happens to have four components has nothing to do with our four dimensional space-time; ψ_β does not transform like a four vector under Lorentz transformations.
It is easy to verify that the *gamma-matrices* (*Dirac matrices*) γ_μ satisfy the anticommutation rule

$$\{\gamma_\mu,\gamma_\nu\}=\gamma_\mu\gamma_\nu+\gamma_\nu\gamma_\mu=2\delta_{\mu\nu}.$$

Furthermore, every γ_μ is Hermitian,

$$\gamma_\mu^\dagger=\gamma_\mu,$$

and traceless, i.e.

$$\mathrm{Tr}\,\gamma_\mu=0.$$

Let's multiply the equation

$$\left(\boldsymbol{\gamma}\cdot\nabla+\gamma_4\frac{\partial}{\partial(ix_0)}\right)\psi+\frac{mc}{\hbar}\psi=0$$

on both sides by the matrix γ_4 and we get

$$\left(c\hbar\gamma_4\boldsymbol{\gamma}\cdot\nabla - i\hbar\frac{\partial}{\partial t}\right)\psi + \gamma_4 mc^2\psi = 0.$$

Denote

$$\begin{aligned}\beta &= \gamma_4 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ \alpha_k &= i\gamma_4\gamma_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix},\end{aligned}$$

which satisfy the relations

$$\begin{aligned}\{\alpha_k, \beta\} &= 0 \\ \beta^2 &= 1 \\ \{\alpha_k, \alpha_l\} &= 2\delta_{kl}.\end{aligned}$$

When we now write

$$H = -ic\hbar\boldsymbol{\alpha}\cdot\nabla + \beta mc^2,$$

the Dirac equation takes the familiar form

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

We define the *adjungated* spinor $\bar{\psi}$ like:

$$\bar{\psi} = \psi^\dagger\gamma_4.$$

Explicitely, if ψ is a column vector

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix},$$

then $\psi^\dagger$ and $\bar{\psi}$ are row vectors

$$\begin{aligned}\psi^\dagger &= (\psi_1^*, \psi_2^*, \psi_3^*, \psi_4^*) \\ \bar{\psi} &= (\psi_1^*, \psi_2^*, -\psi_3^*, -\psi_4^*).\end{aligned}$$

Forming the Hermitean conjugate of the Dirac equation

$$\left(\gamma_\mu\frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar}\right)\psi = 0$$

we get

$$\frac{\partial}{\partial x_k}\psi^\dagger\gamma_k + \frac{\partial}{\partial x_4^*}\psi^\dagger\gamma_4 + \frac{mc}{\hbar}\psi^\dagger = 0.$$

We multiply this from right by the matrix γ_4 and end up with the *adjungated equation*

$$-\frac{\partial}{\partial x_\mu}\bar{\psi}\gamma_\mu + \frac{mc}{\hbar}\bar{\psi} = 0.$$

Here we have used the relations

$$\begin{aligned}\frac{\partial}{\partial x_4^*} &= \frac{\partial}{\partial (ict)^*} = -\frac{\partial}{\partial x_4}\\ \gamma_k\gamma_4 &= -\gamma_4\gamma_k.\end{aligned}$$

Let's multiply the original Dirac equation

$$\left(\gamma_\mu\frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar}\right)\psi = 0$$

from left with the adjungated spinor $\bar{\psi}$ and the adjungated equation

$$-\frac{\partial}{\partial x_\mu}\bar{\psi}\gamma_\mu + \frac{mc}{\hbar}\bar{\psi} = 0$$

from right with the spinor ψ and subtract the resulting equations. We then get

$$\frac{\partial}{\partial x_\mu}(\bar{\psi}\gamma_\mu\psi) = 0.$$

The quantity

$$s_\mu = ic\bar{\psi}\gamma_\mu\psi = (c\psi^\dagger\boldsymbol{\alpha}\psi, ic\psi^\dagger\psi)$$

thus satisfies a continuity equation. According to Green's theorem we have

$$\int \bar{\psi}\gamma_4\psi\, d^3x = \int \psi^\dagger\psi\, d^3x = \text{constant},$$

where the constant can be taken to be 1 with a suitable normalization of ψ. Because

$$\bar{\psi}\gamma_4\psi = \psi^\dagger\psi = \sum_{\beta=1}^{4}\psi_\beta^*\psi_\beta$$

is positively definite it can be interpreted as a probability density. Then

$$s_k = ic\bar{\psi}\gamma_k\psi = c\psi^\dagger\alpha_k\psi$$

can be identified as the density of the probability current.
Note It can be shown that s_μ transforms like a four vector, so the continuity equation is relativistically covariant.
Note 2 We assume that the solution ψ to the Dirac equation is a single particle wave function subjected to the normalization above. This interpretation encounters problems which we will resolve later.

It can be proved that any sets of four matrices γ_μ and γ'_μ satisfying the anticommutation relations

$$\begin{aligned}\{\gamma_\mu, \gamma_\nu\} &= 2\delta_{\mu\nu} \\ \{\gamma'_\mu, \gamma'_\nu\} &= 2\delta_{\mu\nu},\end{aligned}$$

are related to each other through a similarity transformation with a non-singular 4×4-matrix S:

$$S\gamma_\mu S^{-1} = \gamma'_\mu.$$

With the help of the matrices γ'_μ the original Dirac equation can be written as

$$\left(S^{-1}\gamma'_\mu S \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar}\right) S^{-1} S\psi = 0.$$

Multiplying this from left with the matrix S we get

$$\left(\gamma'_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar}\right) \psi' = 0,$$

where

$$\psi' = S\psi.$$

Thus Dirac's equation is independent on the explicit form of the matrices γ_μ; only the anticommutation of the matrices is relevant. If the matrices γ'_μ are Hermitean the transformation matrix S can be taken to be unitary. It is easy to show that then the probability density and current, for example, are independent on the representation:

$$\bar{\psi}'\gamma'_\mu\psi' = \bar{\psi}\gamma_\mu\psi.$$

Vector potential

When the system is subjected to a vector potential

$$A_\mu = (\boldsymbol{A}, iA_0),$$

we make the ordinary substitutions

$$-i\hbar(\partial/\partial x_\mu) \mapsto -i\hbar(\partial/\partial x_\mu) - eA_\mu/c.$$

The Dirac equation takes now the form

$$\left(\frac{\partial}{\partial x_\mu} - \frac{ie}{\hbar c}A_\mu\right)\gamma_\mu\psi + \frac{mc}{\hbar}\psi = 0.$$

Assuming that A_μ does not depend on time the time dependence of the spinor ψ can be written as

$$\psi = \psi(\boldsymbol{x}, t)\big|_{t=0}\, e^{-iEt/\hbar}.$$

Let us write now the Dirac equation for the components ψ_A and ψ_B:

$$\begin{aligned}
\left[\boldsymbol{\sigma}\cdot\left(\boldsymbol{p}-\frac{e\boldsymbol{A}}{c}\right)\right]\psi_B &= \frac{1}{c}(E-eA_0-mc^2)\psi_A \\
-\left[\boldsymbol{\sigma}\cdot\left(\boldsymbol{p}-\frac{e\boldsymbol{A}}{c}\right)\right]\psi_A &= -\frac{1}{c}(E-eA_0+mc^2)\psi_B.
\end{aligned}$$

With the help of the latter equation we eliminate ψ_B from the upper equation and get

$$\left[\boldsymbol{\sigma}\cdot\left(\boldsymbol{p}-\frac{e\boldsymbol{A}}{c}\right)\right]\left[\frac{c^2}{E-eA_0+mc^2}\right]\left[\boldsymbol{\sigma}\cdot\left(\boldsymbol{p}-\frac{e\boldsymbol{A}}{c}\right)\right]\psi_A = (E-eA_0-mc^2)\psi_A.$$

Suppose now that

$$E\approx mc^2,\quad |eA_0|\ll mc^2$$

and measure the energy starting from the rest energy:

$$E^{(\mathrm{NR})}=E-mc^2.$$

We expand

$$\begin{aligned}
\frac{c^2}{E-eA_0+mc^2} &= \frac{1}{2m}\left[\frac{2mc^2}{2mc^2+E^{(\mathrm{NR})}-eA_0}\right] \\
&= \frac{1}{2m}\left[1-\frac{E^{(\mathrm{NR})}-eA_0}{2mc^2}+\cdots\right].
\end{aligned}$$

This can be taken to be the power series in $(v/c)^2$ since

$$E^{(\mathrm{NR})}-eA_0\approx[\boldsymbol{p}-(e\boldsymbol{A}/c)]^2/2m\approx mv^2/2.$$

Taking into account only the leading term we get

$$\frac{1}{2m}\boldsymbol{\sigma}\cdot\left(\boldsymbol{p}-\frac{e\boldsymbol{A}}{c}\right)\boldsymbol{\sigma}\cdot\left(\boldsymbol{p}-\frac{e\boldsymbol{A}}{c}\right)\psi_A=(E^{(\mathrm{NR})}-eA_0)\psi_A.$$

This can be written as

$$\left[\frac{1}{2m}\left(\boldsymbol{p}-\frac{e\boldsymbol{A}}{c}\right)^2-\frac{e\hbar}{2mc}\boldsymbol{\sigma}\cdot\boldsymbol{B}+eA_0\right]\psi_A=E^{(\mathrm{NR})}\psi_A.$$

Up to the zeroth order of $(v/c)^2$ the component ψ_A is thus the two component Schrödinger-Pauli wave function (multiplied with the factor e^{-imc^2t}) familiar from the non-relativistic quantum mechanics. The equation

$$-\left[\boldsymbol{\sigma}\cdot\left(\boldsymbol{p}-\frac{e\boldsymbol{A}}{c}\right)\right]\psi_A=-\frac{1}{c}(E-eA_0+mc^2)\psi_B$$

tells us that the component ψ_B is roughly by the factor

$$|\boldsymbol{p} - (e\boldsymbol{A}/c)|/2mc \approx v/2c$$

"less" than ψ_A. Due to this, provided that $E \approx mc^2$, ψ_A is known as the *big* and ψ_B as the *small* component of the Dirac wave function ψ.
We obtain relativistic corrections only when we consider the second or higher order terms of the expansion

$$\begin{aligned} \frac{c^2}{E - eA_0 + mc^2} &= \frac{1}{2m}\left[\frac{2mc^2}{2mc^2 + E^{(\mathrm{NR})} - eA_0}\right] \\ &= \frac{1}{2m}\left[1 - \frac{E^{(\mathrm{NR})} - eA_0}{2mc^2} + \cdots\right]. \end{aligned}$$

Let us suppose now that

$$\boldsymbol{A} = 0.$$

The wave equation is then

$$H_A\psi_A = E^{(\mathrm{NR})}\psi_A,$$

where

$$H_A = (\boldsymbol{\sigma}\cdot\boldsymbol{p})\frac{1}{2m}\left(1 - \frac{E^{(\mathrm{NR})} - eA_0}{2mc^2}\right)(\boldsymbol{\sigma}\cdot\boldsymbol{p}) + eA_0.$$

This wave equation looks like a time independent Schrödinger equation for the wave function ψ_A.
However,

- evaluating corrections up to the order $(v/c)^2$ the wave function ψ_A is not normalized because the probability interpretation of Dirac's theory requires that

  $$\int (\psi_A^\dagger\psi_A + \psi_B^\dagger\psi_B)\, d^3x = 1,$$

  where ψ_B already of the order v/c.
- explicitely writing down the expression for the operator H_A we see that it contains the non-Hermitian term $i\hbar\boldsymbol{E}\cdot\boldsymbol{p}$.
- the equation is not an eigenvalue equation since H_A itself contains the term $E^{(\mathrm{NR})}$.

Up to the order $(v/c)^2$ the normalization condition can now be written as

$$\int \psi_A^\dagger\left(1 + \frac{\boldsymbol{p}^2}{4m^2c^2}\right)\psi_A\, d^3x \approx 1,$$

because according to the equation

$$-\left[\boldsymbol{\sigma}\cdot\left(\boldsymbol{p} - \frac{e\boldsymbol{A}}{c}\right)\right]\psi_A = -\frac{1}{c}(E - eA_0 + mc^2)\psi_B$$

we have

$$\psi_B \approx \frac{\boldsymbol{\sigma}\cdot\boldsymbol{p}}{2mc}\psi_A.$$

It is worthwhile to define the new two component wave function Ψ:

$$\Psi = \Omega\psi_A,$$

where

$$\Omega = 1 + \frac{\boldsymbol{p}^2}{8m^2c^2}.$$

Now Ψ is up to the order $(v/c)^2$ normalized correctly because

$$\int \Psi^\dagger\Psi\, d^3x \approx \int \psi_A^\dagger\left(1+\frac{\boldsymbol{p}^2}{4m^2c^2}\right)\psi_A\, d^3x.$$

We multiply the equation

$$H_A\psi_A = E^{(\mathrm{NR})}\psi_A,$$

on both sides with the operator

$$\Omega^{-1} = 1 - (\boldsymbol{p}^2/8m^2c^2),$$

and get

$$\Omega^{-1}H_A\Omega^{-1}\Psi = E^{(\mathrm{NR})}\Omega^{-2}\Psi.$$

Explicitely, up to the order $(v/c)^2$ this can be written as

$$\begin{aligned}\Bigg[\frac{\boldsymbol{p}^2}{2m} + eA_0 - \left\{\frac{\boldsymbol{p}^2}{8m^2c^2}, \left(\frac{\boldsymbol{p}^2}{2m}+eA_0\right)\right\}\\ - \frac{(\boldsymbol{\sigma}\cdot\boldsymbol{p})}{2m}\left(\frac{E^{(\mathrm{NR})}-eA_0}{2mc^2}\right)(\boldsymbol{\sigma}\cdot\boldsymbol{p})\Bigg]\Psi\\ = E^{(\mathrm{NR})}\left(1-\frac{\boldsymbol{p}^2}{4m^2c^2}\right)\Psi.\end{aligned}$$

Writing $E^{(\mathrm{NR})}\boldsymbol{p}^2$ in the form $\frac{1}{2}\{E^{(\mathrm{NR})},\boldsymbol{p}^2\}$ we get

$$\begin{aligned}\Bigg[\frac{\boldsymbol{p}^2}{2m} + eA_0 - \frac{\boldsymbol{p}^4}{8m^3c^2}\\ + \frac{1}{8m^2c^2}\Big(\{\boldsymbol{p}^2,(E^{(\mathrm{NR})}-eA_0)\}\\ -2(\boldsymbol{\sigma}\cdot\boldsymbol{p})(E^{(\mathrm{NR})}-eA_0)(\boldsymbol{\sigma}\cdot\boldsymbol{p})\Big)\Bigg]\Psi\\ = E^{(\mathrm{NR})}\Psi.\end{aligned}$$

Because for arbitrary operators A and B

$$\{A^2,B\} - 2ABA = [A,[A,B]]$$

holds we can, by setting

$$
\begin{aligned}
\boldsymbol{\sigma}\cdot\boldsymbol{p} &= A \\
E^{(\mathrm{NR})} - eA_0 &= B,
\end{aligned}
$$

reduce the equation into the form

$$
\begin{aligned}
&\left[\frac{\boldsymbol{p}^2}{2m} + eA_0 - \frac{\boldsymbol{p}^4}{8m^3c^2}\right. \\
&\qquad\left. - \frac{e\hbar\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p})}{4m^2c^2} - \frac{e\hbar^2}{8m^2c^2}\nabla\cdot\boldsymbol{E}\right]\Psi \\
&\qquad = E^{(\mathrm{NR})}\Psi.
\end{aligned}
$$

In the derivation of the equation we have employed the relations

$$
\begin{aligned}
[\boldsymbol{\sigma}\cdot\boldsymbol{p}, (E^{(\mathrm{NR})} - eA_0)] &= -ie\hbar\boldsymbol{\sigma}\cdot\boldsymbol{E} \\
[\boldsymbol{\sigma}\cdot\boldsymbol{p}, -ie\hbar\boldsymbol{\sigma}\cdot\boldsymbol{E}] &= -e\hbar^2\nabla\cdot\boldsymbol{E} \\
&\quad -2e\hbar\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p}),
\end{aligned}
$$

the validity of which can be verified by noting that

$$
\begin{aligned}
\nabla A_0 &= -\boldsymbol{E} \\
\nabla\times\boldsymbol{E} &= 0.
\end{aligned}
$$

The resulting equation is a proper Schrödinger equation for a two component wave function.

Physical interpretation

We look at the meaning of the terms in the equation

$$
\begin{aligned}
&\left[\frac{\boldsymbol{p}^2}{2m} + eA_0 - \frac{\boldsymbol{p}^4}{8m^3c^2}\right. \\
&\qquad\left. - \frac{e\hbar\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p})}{4m^2c^2} - \frac{e\hbar^2}{8m^2c^2}\nabla\cdot\boldsymbol{E}\right]\Psi \\
&\qquad = E^{(\mathrm{NR})}\Psi.
\end{aligned}
$$

1. The term $\frac{\boldsymbol{p}^2}{2m} + eA_0$ gives the non-realtivistic Schrödinger equation.

2. The term $-\frac{\boldsymbol{p}^4}{8m^3c^2}$ is a relativistic correction to the kinetic energy as can be seen from the expansion

$$
\sqrt{(mc^2)^2 + |\boldsymbol{p}|^2c^2} - mc^2 = \frac{|\boldsymbol{p}|^2}{2m} - \frac{|\boldsymbol{p}|^4}{8m^3c^2} + \cdots.
$$

3. The term $-\frac{e\hbar\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p})}{4m^2c^2}$ describes the interaction between the spin of a moving electron and electric field. Intuitively this, so called *Thomas term*, is

due to the fact that the moving electron experiences an apparent magnetic field $\boldsymbol{E} \times (\boldsymbol{v}/c)$. If the electric field is a central field,

$$eA_0 = V(r),$$

it can be written in the form

$$\begin{aligned} -\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p}) &= -\frac{\hbar}{4m^2c^2}\left(-\frac{1}{r}\frac{dV}{dr}\right)\boldsymbol{\sigma}\cdot(\boldsymbol{x}\times\boldsymbol{p}) \\ &= \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\boldsymbol{S}\cdot\boldsymbol{L}, \end{aligned}$$

where we have substituted

$$\boldsymbol{S} = \hbar\boldsymbol{\sigma}/2.$$

So we actually have a spin orbit interaction.
4. The term $-\frac{e\hbar^2}{8m^2c^2}\nabla\cdot\boldsymbol{E}$ is known as the *Darwin term*. Its meaning can be deduced when we note that $\nabla\cdot\boldsymbol{E}$ is the charge density. For example, in the hydrogen atom where $\nabla\cdot\boldsymbol{E} = -e\delta(\boldsymbol{x})$ it causes the energy shift

$$\int \frac{e^2\hbar^2}{8m^2c^2}\delta(\boldsymbol{x})|\psi^{(\mathrm{Schrö})}|^2\, d^3x = \frac{e^2\hbar^2}{8m^2c^2}|\psi^{(\mathrm{Schrö})}|^2\bigg|_{\boldsymbol{x}=0},$$

which differs from zero only in the s-state.
Considering the 2nd, 3rd and 4th term as a perturbation of hydrogen atom Hamiltonian and taking the wave functions of non-perturbed non-relativistic hydrogen atom wave functions, the lowest order correction ΔE can be calculated as we have learned before

$$E = E^{(0)} - \left(\frac{e^2}{4\pi\hbar c}\right)\left(\frac{e^2}{8\pi a_0}\right)\frac{1}{n^3}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right)$$

The j-fold degeneracy of shell n is now lifted when
    $j \neq n$ while
    $j = n$, degeneracy persists

Free particle at rest
Multiply Dirac equation from left as

$$\begin{aligned} \gamma_\nu\frac{\partial}{\partial x_\nu}\times(\gamma_\mu\frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar})\psi &= 0 \\ \frac{\partial}{\partial x_\nu}\frac{\partial}{\partial x_\mu}\gamma_\nu\gamma_\mu\psi - (\frac{mc}{\hbar})^2\psi &= 0 \\ \frac{\partial}{\partial x_\nu}\frac{\partial}{\partial x_\mu}(\gamma_\nu\gamma_\mu + \gamma_\mu\gamma_\nu)\psi - 2(\frac{mc}{\hbar})^2\psi &= 0 \\ \frac{\partial}{\partial x_\nu}\frac{\partial}{\partial x_\mu}(2\delta_{\mu\nu})\psi - 2(\frac{mc}{\hbar})^2\psi &= 0 \\ \frac{\partial}{\partial x_\mu}\frac{\partial}{\partial x_\mu}\psi - (\frac{mc}{\hbar})^2\psi &= 0 \end{aligned}$$

This is a set of 4 *uncoupled* Klein-Gordon equations, i.e. each of the components of ψ satisfy K-G independently.
The solutions are

$$\psi \sim u(\boldsymbol{p})e^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar - iEt/\hbar}$$

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

and u is a 4-component spinor independent on x, t
Setting $\boldsymbol{p}$=0, we get

$$\psi \sim u(\boldsymbol{p})e^{\pm imc^2t/\hbar}$$

to be solved with

$$\gamma_4 \frac{\partial}{\partial(ict)}\psi = -\frac{mc}{\hbar}\psi$$

The solutions are

$$\begin{array}{ll} (1,0,0,0)^T e^{-imc^2t/\hbar} & (0,1,0,0)^T e^{-imc^2t/\hbar} \\ (0,0,1,0)^T e^{+imc^2t/\hbar} & (0,0,0,1)^T e^{+imc^2t/\hbar} \end{array}$$

If we stick in the picture that $H = i\hbar\frac{\partial}{\partial t}$ we have 2 solutions (spin up/down) with $E > 0$ and 2 with $E < 0$.

Free particle on the run
Set $\boldsymbol{p} \neq 0$, but $A_\mu = 0$

$$\psi = (\psi_A, \psi_B)^T = (u_a(\boldsymbol{p}), u_b(\boldsymbol{p}))^T \exp(i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar - iEt/\hbar)$$

with

$$\begin{aligned} u_A(\boldsymbol{p}) &= \frac{c}{E - mc^2}(\boldsymbol{\sigma}\cdot\boldsymbol{p})u_B(\boldsymbol{p}) \\ u_B(\boldsymbol{p}) &= \frac{c}{E + mc^2}(\boldsymbol{\sigma}\cdot\boldsymbol{p})u_A(\boldsymbol{p}) \end{aligned}$$

Again we may try $u_A(\boldsymbol{p})$ =(1,0) or (0,1) and the same for $u_B(\boldsymbol{p})$.
Using

$$\boldsymbol{\sigma}\cdot\boldsymbol{p} = \begin{pmatrix} p_3 & p_1 - ip_2 \\ p_1 + ip_2 & -p_3 \end{pmatrix}$$

we find the solutions

$$
\begin{aligned}
u^{(1)} &= N\begin{pmatrix} 1 \\ 0 \\ p_3c/E' \\ (p_1+ip_2)c/E' \end{pmatrix} \\
u^{(2)} &= N\begin{pmatrix} 0 \\ 1 \\ (p_1-ip_2)c/E' \\ -p_3c/E' \end{pmatrix} \\
u^{(3)} &= N\begin{pmatrix} -p_3c/E' \\ -(p_1+ip_2)c/E' \\ 1 \\ 0 \end{pmatrix} \\
u^{(4)} &= N\begin{pmatrix} -(p_1-ip_2)c/E' \\ p_3c/E' \\ 0 \\ 1 \end{pmatrix}
\end{aligned}
$$

with

$$E' = |E| + mc^2 \quad \text{and} \quad N = \sqrt{E'/2mc^2}$$

Two first are $E > 0$ solutions while 3 and 4 $E < 0$. These are to be combined with the plane wave parts $\exp[i/\hbar(\boldsymbol{p}\cdot\boldsymbol{x} \mp Et)]$.
We notice that there is a gap between allowed energy values:
$-\infty \leq E \leq -mc^2$ and $mc^2 \leq E \leq \infty$.
Now an atom can make a radiative transition to the ground state.
From the ground state, transition with $\Delta E > 2mc^2$ should lead to a negative energy state and finally to $E = -\infty$
This way normal atoms would evaporate within fractions of a second.
Obviously something is incorrect.

Dirac's way out
Dirac proposed that all the negative energy states are filled and thus only positive energy states can be occupied. This works "fine" for electrons since they obey Pauli's exclusion principle and thus start filling the energy levels from the bottom.
Note There is no such Dirac sea for bosons and so this explanation can not be used for Klein-Gordon particles for example.
We may ask, how come this explanation still persists in the literature?
The reason:

- it predicted the existence of antiparticles
- it can incorporate positrons in a neat way

Let us assume a negative energy electron absorbs a photon with $\hbar\omega > mc^2$. Now the negative energy electron can "materialize" into normal positive energy electron while it leaves a hole to the sea. This hole is identified as a positive energy positron with charge $|e|$.
The source of the problem is the same as in the Klein-Gordon case. Dirac equation is an equation written for a single particle wave function and so it can not, even in a principle level, take into account particle creation/annihilation without introducing such exotic mechanisms.
To emphasize once more, this is *not* the way to do relativistic quantum mechanics...

The modern way out
We need to lean on field theory to describe spin half particles in a transparent way. For this we need to introduce similar number operators acting on state vectors as in the case of radiation field.
This time, however, we need to take into account the Pauli's exclusion principle.
We introduce fermionic operators b_r and $b_r^\dagger$ analogic to the bosonic a and $a^\dagger$. Collective index r provides description of all the mutually commuting observables present.
We demand

$$\{b_r, b_{r'}^\dagger\} = \delta_{r,r'} \quad \text{and} \quad \{b_r, b_{r'}\} = \{b_r^\dagger, b_{r'}^\dagger\} = 0$$

These are the creation and annihilation operators.
A single particle state is

$$|1_r\rangle = b_r^\dagger|0\rangle$$

while two (or more) particle state

$$|2_r\rangle = b_r^\dagger b_r^\dagger|0\rangle = \frac{1}{2}\{b_r^\dagger, b_r^\dagger\}|0\rangle = 0$$

disappears as it should according to Pauli.
We also see that two particle state

$$|1_{r'}\rangle|1_r\rangle = b_{r'}^\dagger b_r^\dagger|0\rangle = -b_r^\dagger b_{r'}^\dagger|0\rangle = -|1_r\rangle|1_{r'}\rangle$$

is necessarily antisymmetric.
The Hermitian occupation number operator is as before

$$N_r = b_r^\dagger b_r$$

for whom

$$\begin{aligned} N_r|0\rangle &= b_r^\dagger b_r|0\rangle = 0 \\ N_r b_r^\dagger|0\rangle &= b_r^\dagger(1 - b_r^\dagger b_r)|0\rangle = b_r^\dagger|0\rangle \end{aligned}$$

More over

$$N_r^2 = b_r^\dagger b_r b_r^\dagger b_r = b_r^\dagger(-b_r^\dagger b_r + 1)b_r = N_r$$

leading to

$$N_r(N_r - 1) = 0.$$

We see that the allowed eigenvalues of the occupation number operator are zero and one.
Simple representation can be found.

$$b_r = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad b_r^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad N_r = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

acting on

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$