1.2 Some Quantum Mechanics
1.2.1 The Interpretation of the Wave Function

Before, used $\rho(\underline{x},t)d^3x = |\psi(\underline{x},t)|^2 d^3x$ to get the probability of finding a particle in volume d^3x at $\underline{x}$ at time t. (Assuming normalized ψ.) This requires:

1. $\rho(\underline{x},t) = |\psi|^2 \geq 0$
2. For a single particle, $\int \rho(\underline{x},t)d^3x = \int |\psi(\underline{x},t)|^2 d^3x = 1$ at any time t, and hence $\frac{\partial}{\partial t}\int \rho(\underline{x},t)d^3x = \frac{\partial}{\partial t}\int |\psi(\underline{x},t)|^2 d^3x = 0$ (1) to conserve probability.

Hence we need to show:

$$\frac{\partial \rho}{\partial t} + \underline{\nabla}\cdot\underline{j} = 0$$

(Equation of continuity), where $\underline{j}$ is a corresponding current density.

Consider the Schrödinger Equation.

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\underline{x})\psi \quad (1)$$

Taking its conjugate:

$$-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V(\underline{x})\psi^* \quad (2)$$

Multiply (1) by ψ^*, and then subtract (2) multiplied by ψ.

$$i\hbar\left(\psi^*\frac{\partial\psi}{\partial t} + \frac{\partial\psi^*}{\partial t}\psi\right) = -\frac{\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right)$$

i.e.

$$\frac{\partial}{\partial t}(\psi^*\psi) = \frac{i\hbar}{2m}\underline{\nabla}\cdot\left(\psi^*\underline{\nabla}\psi - \psi\underline{\nabla}\psi^*\right)$$

which is of the desired form, where $\rho(\underline{x},t) = |\psi(\underline{x},t)|^2 \geq 0$ and

$$\underline{j} = \frac{i\hbar}{2m}\left(\psi\underline{\nabla}\psi^* - \psi^*\underline{\nabla}\psi\right).$$

The continuity equation implies that

$$\frac{\partial}{\partial t}\int_{all\ space}|\psi(\underline{x},t)|^2 d^3x = 0$$

So the conditions for the Born interpretation are satisfied.

1.2.2 Minimal EM Interactions

Point particle with mass m and charge q at position $\underline{x}$ in an EM field $(\phi,\underline{A})$. We want to know what the QM equation of motion for this particle is.

Start from the classical Hamiltonian,

$$H(\underline{x},\underline{p}) = \frac{1}{2m}\left(\underline{p} - \frac{q}{c}\underline{A}\right)^2 + q\phi \quad (1)$$

To verify this, check Hamilton's Equations of Motion (using equations for many particles in places).

1. $\dot{x}_i = \frac{\partial H}{\partial p_i} = \frac{1}{2m} 2\left(p_i - \frac{q}{c} A_i \right)$

   i.e. the conjugate momentum $p_i = m\dot{x}_i + \frac{q}{c} A_i$, i.e. $\underline{p} = m\underline{\dot{x}} + \frac{q}{c}\underline{A}$ (2)

2. $\dot{p}_i = -\frac{\partial H}{\partial x_i}$ (somewhat tricky derivation)

   $m\underline{\ddot{x}} = q\underline{E} + \frac{q}{c}\underline{v} \times \underline{B}$

Note that (1) + (2) implies that the energy is

$$H\left(\underline{x}, \underline{p}\right) = E\left(\underline{x}, \underline{\dot{x}}\right) = \frac{1}{2} m\underline{\dot{x}}^2 + q\phi$$

Note that there is no contribution from the magnetic field, as it is at right angles to the particle and hence can't do any work on it.

Schrödinger Equation:

$$H\left(\underline{x}, \underline{\hat{p}}\right)\psi = i\hbar \frac{\partial \psi}{\partial t}$$

where $\underline{p} \to \underline{\hat{p}} = -i\hbar\underline{\nabla}$ (position operator is still $\underline{x}$).

$$-\frac{\hbar^2}{2m}\left(\underline{\nabla} - \frac{iq}{\hbar c}\underline{A}\right)^2 \psi\left(\underline{x}, t\right) = i\hbar\left(\frac{\partial}{\partial t} + \frac{iq}{\hbar}\phi\right)\psi\left(\underline{x}, t\right)$$

which is related to the "free" equation

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

by the minimal substitution

$$\underline{\nabla} \to \underline{\nabla} - \frac{iq}{\hbar c}\underline{A}$$

$$\frac{\partial}{\partial t} \to \frac{\partial}{\partial t} + \frac{iq}{\hbar}\phi .$$

Or in 4D notation,

$$\partial_\mu \to \partial_\mu + \frac{iq}{\hbar c} A_\mu\left(x\right) \quad (3)$$

(This combines the two substitutions before.)

The same argument works in the relativistic case.

$$H = \sqrt{\left(c\underline{p} - q\underline{A}\right)^2 + m^2c^4} + q\phi$$

Hence the "Schrödinger equation" is

$$\left(\sqrt{-\hbar^2c^2\left(\underline{\nabla} - \frac{iq}{\hbar c}\underline{A}\right)^2 + m^2c^4}\right)\psi\left(\underline{x}, t\right) = i\hbar\left(\frac{\partial}{\partial t} + \frac{iq}{\hbar}\phi\right)\psi\left(\underline{x}, t\right)$$

Again this is obtained from the free particle case by (3). Note that in the non-EM case, the first bit would form $\sqrt{p^2c^2 + m^2c^4}$.

Problem:- how do we interpret $\sqrt{\ }$, or in the free case $\sqrt{-\hbar^2 c^2 \nabla^2 + m^2 c^4}$?
We will come to this later.

1.3 Natural Units
Use natural units, such that $\hbar = c = 1$. So the unit of speed is the speed of light, and the unit of momentum is $\hbar$.

It's easy to put this in; the tricky bit is to get back to ordinary units. So use dimensions to restore $\hbar$, c, and then use

$$\hbar = 6.582 \times 10^{-22}\, MeV \text{ sec}$$
$$\hbar c = 1.973 \times 10^{-13}\, MeV\, m .$$

(See Martin & Shaw PP, section 1.5)

2. The Klein-Gorden Equation
Using free space, so $(\phi, \underline{A}) = 0$, and natural units. So the Schrödinger Equation is

$$H\phi(\underline{x},t) = i\frac{\partial \phi(\underline{x},t)}{\partial t} \quad (1)$$

where ϕ is now the wave function, and $H = \sqrt{-\underline{\nabla}^2 + m^2}$ (2). What does this mean?
In the Klein-Gordon (KG) equation, we avoid the problem by noting that H is independent of t, so we can multiply the equation by H again.

$$H^2\phi(\underline{x},t) = i\frac{\partial}{\partial t} H\phi = -\frac{\partial^2 \phi}{\partial t^2}$$

then using $H^2 = -\underline{\nabla}^2 + m^2$,

$$\left(\frac{\partial^2}{\partial t^2} - \underline{\nabla}^2 + m^2\right)\phi(\underline{x},t) = 0 \quad (3a)$$

$$\left(\Box + m^2\right)\phi(\underline{x},t) = 0 \quad (3b)$$

where $\Box = \partial_\mu \partial^\mu$. This is called the Klein-Gordon Equation. This is the correct equation, but what is its interpretation?

There are a whole series of problems.

2.1 Negative Energies
KG equation has solutions

$$\phi(\underline{x},t) = e^{i(\underline{p}\cdot\underline{x} - Et)}$$

with $\mathrm{E}^2 = \underline{p}^2 + m^2$, i.e. with energies $E = +\sqrt{\underline{p}^2 + m^2} \geq m^2 > 0$, and $E = -\sqrt{p^2 + m^2} \leq m^2 < 0$.
So we have a spectrum of energies available at $E > mc^2$ and $E < -mc^2$, with an energy gap in the middle. Classical particles can't jump this energy gap. Quantum mechanics say that interaction can cause quantum jumps releasing or absorbing quanta $\hbar\omega \geq 2mc^2$, either as radiation or as other particles.
So a particle can fall to negative energy states etc. releasing an infinite amount of energy. What stops it?