Lecture X: The Dirac Equation and Graphene

Tuesday, November 21, 2017

Introduction: In light of Einstien's theory of relativity, energy and mass of a particle are related. The energy of a particle at rest (in motion) are given as:

$$E_o = m_o c^2 \qquad \text{Einstien's equation for particle at rest} \tag{1}$$

$$E = \sqrt{(m_o c^2)^2 + (cp)^2} \qquad \text{Einstien's equation for relativistic particle} \tag{2}$$

we can calculate the velocity v as:

$$v = \frac{\partial E}{\partial p} = c\frac{cp}{\sqrt{(m_o c^2)^2 + (cp)^2}} \tag{3}$$

From this expression, we can see the velocity v of massive particles as a function of momentum p approaches, but cannot exceed, the speed of light c:

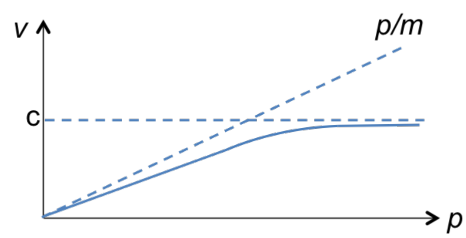

Figure 1: Velocity v of a massive particle as a function of momentum $\mathbf{p}$ according to equation 3.

Limiting cases of equation 2 for $m_o \to 0$ and $v \ll c$ yield:

$$E = c|\mathbf{p}| \qquad \text{Massless particle} \tag{4}$$

$$E \approx m_o c^2 + p^2/2m \qquad \text{Non-relativistic, massive particle} \tag{5}$$

which, as seen in figure 2, yield linear and parabolic dispersion relations for E vs. $\mathbf{p}$:

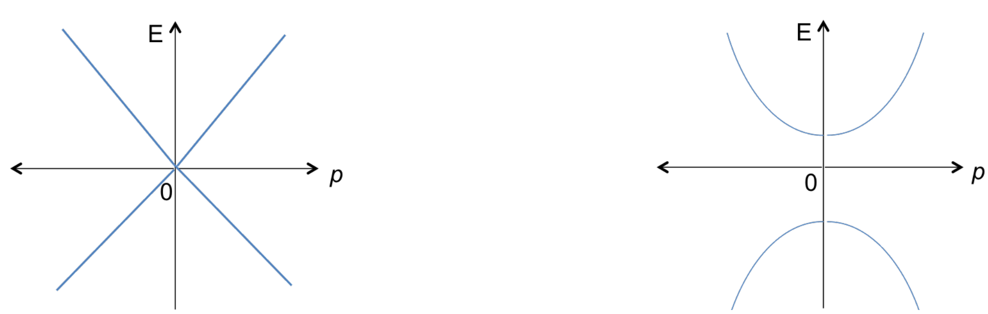

Figure 2: Energy E vs. momentum $\mathbf{p}$ for (left): a massless particle and (right): a massive particle according to equations 4-5.

To reconcile the relativistic energy equation 2 with quantum mechanics, we need to go back to the operator correspondence:

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

from which, we recall, we get Schrödingers equation for a free particle immediately from the definition of the Hamiltonian ($V = 0$ here):

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

For a relativistic particle, we need to take into account the rest mass. Following a similar recipe but using the expression for the energy of a relativistic free particle given by equation 2, we have (here, $m \equiv m_o$):

$$E^2 = c^2p^2 + m^2c^4 \qquad \longrightarrow \qquad -\hbar^2\frac{\partial^2\Psi}{\partial t^2} = \left(-\hbar^2c^2\nabla^2 + m^2c^4\right)\Psi \tag{6}$$

This is the Klein Gordon equation. However, we need a form which is first order in time. To this end, Dirac found the kinetic energy terms can be factored, and that the proper representation is based on a two dimensional basis, which treats spin up and spin down particles separately:

$$(p_x^2 + p_y^2 + m^2)\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \begin{pmatrix}m & p_x - ip_y\\ p_x + ip_y & -m\end{pmatrix}^2$$

Taking the square root of this expression gives a linear form for the energy operator, we can now use the same correspondence to write a first order quantum mechanical equation of motion for a relativistic particle:

$$i\hbar\frac{\partial\mathbf{\Psi}}{\partial t} = \left[-i\hbar\left(\sigma_x\frac{\partial}{\partial x} + \sigma_y\frac{\partial}{\partial y}\right) + \sigma_z m\right]\mathbf{\Psi} \tag{7}$$

which is the Dirac equation, where:

$$\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \qquad \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \qquad \sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \qquad \text{and} \qquad \mathbf{\Psi} = \begin{pmatrix}\Psi_\uparrow\\ \Psi_\downarrow\end{pmatrix}$$

The Dirac equation has several significant consequences, for instance, the existence of anti-particles and spin. As seen in the dispersion relation for graphene, for low energies near the Dirac point, electrons obey a Dirac equation with $m = 0$ and $c = v_F$, the Fermi velocity. We say the charge carriers in this case are "emergent" Dirac Fermions, with the two subtypes $A(B)$ corresponding to two spin spin states in the Dirac equation (termed "psuedo-spin"):

$$\mathbf{\Psi} = \begin{pmatrix}\Psi_\uparrow\\ \Psi_\downarrow\end{pmatrix} = \begin{pmatrix}\Psi_A\\ \Psi_B\end{pmatrix}$$

Because of these emergent properties, charge carriers in graphene are expected to have unique properties predicted by the theory, *e.g.* extraordinary transport properties, which have been borne out by experiments.