The effective mass in graphene

Among graphene's many interesting properties, its extremely high electrical conductivity and electron mobility are particularly remarkable [1]. In fact, the room temperature conductivity of graphene is higher than that of any other known material. There are two important factors contributing to this: The first is the high Debye temperature in graphene that suppresses phonon scattering and the second is the very special electric structure with the linear dispersion and density of states close to the Fermi energy, as shown in Figure 6.15. An apparent contradiction with these properties arises when we apply our usual definition of the effective mass to graphene. We have defined the effective mass as

$$m^* = \hbar^2 \left(\frac{d^2E(k)}{dk^2} \right)^{-1}. \tag{1}$$

Applying this to a linear dispersion with $E(k) \propto k$ clearly results in an diverging effective mass, something that appears to imply that it is impossible to drag the electrons through graphene by an external field, in contrast to the experimental observations. Matters are made even more confusing by the fact that the electrons in graphene are often called "massless", in drastic contrast to what (1) appears to suggest. The purpose of this note is to explain this. For a nice more in-depth discussion see also Refs. [2, 3].

The key-issue with the apparent contradiction is our semi-classical definition of the effective mass that implicitly assumes a parabolic band dispersion. In the following discussion, we show that the problem can be cured using an alternative expression for the effective mass.

In the following, we ignore the fact that the dispersion of graphene is linear around the K point of the two-dimensional Brillouin zone and not around the Γ point, i.e. around $\mathbf{k} = (0,0)$. This is not a problem because it could be taken care of by a simple coordinate transformation using $\mathbf{k}' = \mathbf{k} - \mathbf{K}$ instead of $\mathbf{k}$. In the following semi-classical picture, we also identify the momentum of the particle with $\hbar k$, something that we know is not strictly correct.

The problem of the diverging mass can be cured by an alternative definition of the effective mass as

$$m^* = \hbar^2 k \left(\frac{dE(k)}{dk} \right)^{-1}. \tag{2}$$

The motivation for this comes again from semi-classical arguments. We define the momentum of a particle as

$$p = \hbar k = m^* v_g \tag{3}$$

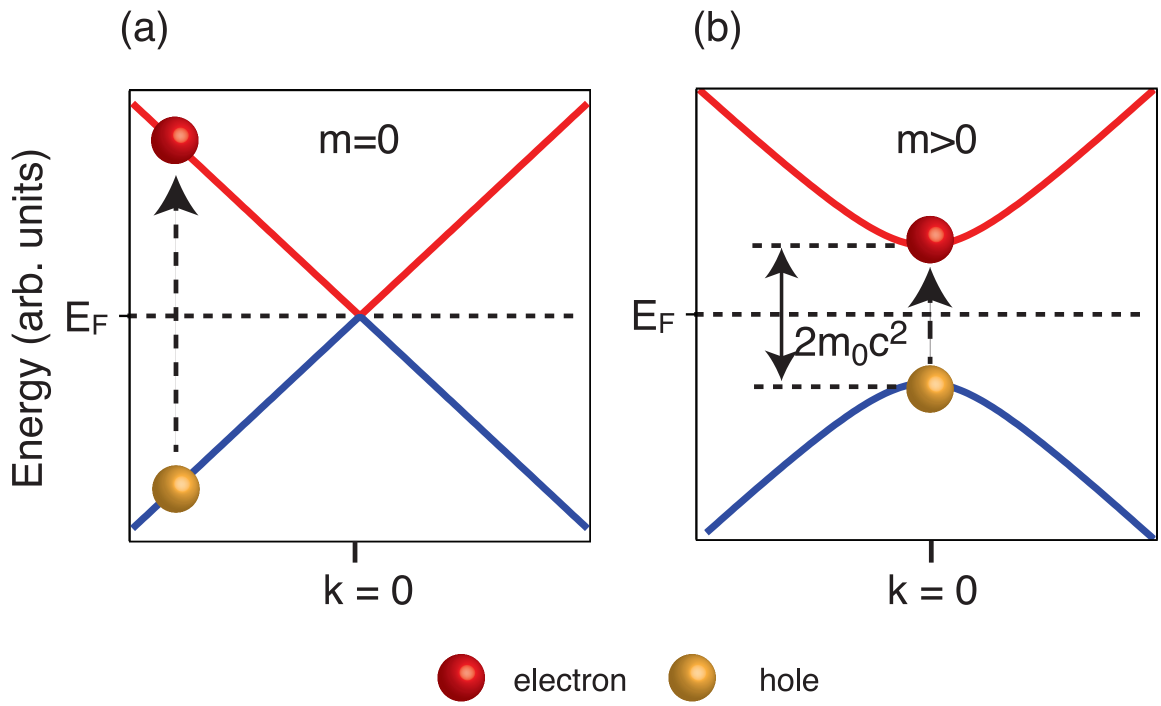

Figure 1: Relativistic dispersion for (a) massless and (b) massive particles.

with v_g being the usual group velocity

$$v_g = \frac{1}{\hbar}\frac{dE(k)}{dk}. \tag{4}$$

Substituting (4) into (3) gives the definition (2).

We try the new definition of the effective mass for a free electron with

$$E(k) = \frac{\hbar^2 k^2}{2m_e}. \tag{5}$$

Since

$$\frac{dE(k)}{dk} = \frac{\hbar^2 k}{m_e}, \tag{6}$$

using the definition (2) does indeed give m_e as the effective mass. The only thing that is not so pretty about the definition are the problems we run into when directly evaluating the expression (2) at $k = 0$ where both the energy and group velocity are zero.

We write the linear dispersion for graphene as $E(k) = \hbar c_g k$, where c_g is the speed of the electrons in graphene. Using this and (2) we obtain an effective mass of

$$m^* = \hbar\frac{1}{c_g}k, \tag{7}$$

which is k-dependent. For $k = 0$ the effective mass is also vanishing which at least partly appears to justify why the electrons in graphene are often called "massless" in the literature.

To really understand this, however, we have to consider the electrons in graphene in a relativistic sense. The energy-momentum relation for a relativistic particle is

$$E^2 = (pc)^2 + (m_0c^2)^2 = (\hbar kc)^2 + (m_0c^2)^2, \tag{8}$$

where m_0 is the rest mass of the particle. For a particle without a rest mass, such as a photon, we simply get that $E(k) = \pm\hbar kc$ with c being the speed of light. Fig. 1(a) shows a dispersion that corresponds to such a massless relativistic particle. It is exactly the dispersion that is observed fro graphene in the vicinity of the Fermi energy if we set $c = c_g$ and identify the blue part of the band with the bonding π-band and the red part with the anti-bonding π^*-band. It is in this sense that the electrons and holes in graphene are "massless". Indeed, the electrons in graphene are sometimes also called "relativistic". This is easy to understand in the picture presented here but not otherwise because c_g is much smaller than the speed of light.

If we excite an electron from the π-valence band to the π^*conduction band, this generates an electron and a hole that can be seen as a "particle" and its "anti-particle", respectively. All the excitation energy goes into kinetic energy of these two particles since there is no rest mass to overcome.

The situation for a finite rest mass m_0 is shown in Fig. 1(b). Here the excitation of an electron from the valence band to the conduction band also generates a particle and its anti-particle but we need at least $E = 2m_0c^2$ for the excitation (as shown in the figure) for the energy corresponding to the rest mass of the particles, without any kinetic energy. This would be the situation in a normal semiconductor with a finite band gap that, in this relativistic point of view, has a value of $E_g = 2m_0c^2$.

Finally, it is interesting to apply the definition of the effective mass (2) to the relativistic dispersion relation (8). This results in

$$m^* = \frac{\sqrt{(\hbar kc)^2 + (m_0c^2)^2}}{c^2}. \tag{9}$$

As expected, it returns the rest mass m_0 for $k = 0$.

Bibliography

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