A Wave Equation for Electrons in Graphene

Ron Bourgoin

Edgecombe Community College

Rocky Mount, North Carolina, USA

Abstract

We accept the statement that "carriers in graphene are described not by the Schrödinger equation"[1] as a challenge to show that electrons in graphene can be described by the Schrödinger equation.

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We begin our discussion with the wave equation in rectangular coordinates,

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}=\frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} \qquad (1)$$

which we transform to cylindrical coordinates r,θ,z, because we model the electron as a cylindrical element of mass energy that translates longitudinally along the *z* axis,

$$\frac{\partial^2\psi}{\partial r^2}+\frac{1}{r}\frac{\partial\psi}{\partial r}+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2}+\frac{\partial^2\psi}{\partial z^2}=\frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} \qquad (2)$$

We now define the wave function as a product of four separate functions, each of which has one variable only,

$$\psi = R\Theta ZT \qquad (3)$$

Use of (3) in equation (2) provides

$$\frac{1}{R}\frac{\partial^2 R}{\partial r^2}+\frac{1}{Rr}\frac{\partial R}{\partial r}+\frac{1}{r^2\Theta}\frac{\partial^2\Theta}{\partial\theta^2}+\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}=\frac{1}{v^2}\frac{1}{T}\frac{\partial^2 T}{\partial t^2} \qquad (4)$$

after we have taken the indicated derivatives in (2), and then divided each term by the product (3). This allows a separation into four separate functions. Each function is equal to a constant.[2] We begin by isolating the time function,

$$\frac{1}{T}\frac{d^2 T}{dt^2}=-\omega^2 \qquad (5)$$

where ordinary derivative notation is used since there is only one variable that applies. This has solution

$$T=e^{\pm i\omega t} \qquad (6)$$

where ω is angular frequency. We refer to this as the time part. The equation in z is isolated also,

$$\frac{1}{Z}\frac{d^2 Z}{dz^2}=-k^2 \qquad (7)$$

with solution

$$Z=e^{\pm ikz} \qquad (8)$$

where z is the axis of electron translation, and *k* is wave number. We refer to this as the space part. We now insert the results of (5) and (7) into equation (4) to obtain,

$$\frac{1}{R}\frac{\partial^2 R}{\partial r^2}+\frac{1}{Rr}\frac{\partial R}{\partial r}+\frac{1}{r^2\Theta}\frac{\partial^2\Theta}{\partial\theta^2}-k^2=-\frac{\omega^2}{v^2} \qquad (9)$$

We now revisit the psi-function (3) and insert in it the results of (6) and (8),

$$\psi=R\Theta e^{\pm i\omega t}e^{\pm ikz} \qquad (10)$$

We observe here that if we select

$$e^{+i\omega t} \qquad (11)$$

and

$$e^{-ikz} \qquad (12)$$

we can collect the time part and the space part into one exponential expression,[3]

$$e^{i\omega t - ikz} \tag{13}$$

which is observed to describe a travelling wave, which can further be written as

$$e^{i\omega(t - kz/\omega)} \tag{14}$$

and also

$$e^{i\omega(t - z/v)} \tag{15}$$

from which we deduce that

$$\frac{kz}{\omega} = \frac{z}{v} \tag{16}$$

which reduces to a dispersion relation for electrons in graphene

$$k = \frac{\omega}{v} \tag{17}$$

the square of which provides

$$k^2 = \frac{\omega^2}{v^2} \tag{18}$$

which now allows equation (9) to be written in the form

$$\frac{1}{R}\frac{\partial^2 R}{\partial r^2} + \frac{1}{Rr}\frac{\partial R}{\partial r} + \frac{1}{r^2 \Theta}\frac{\partial^2 \Theta}{\partial \theta^2} = 0 \tag{19}$$

We isolate the angle function,

$$\frac{1}{\Theta}\frac{d^2 \Theta}{d\theta^2} = -1 \tag{20}$$

which has solution

$$\Theta = e^{i\theta} \tag{21}$$

which indicates a cycle of 2π radians. We take this to represent the electron spin. We insert the integer value from (20) and insert it into equation (19) to obtain

$$\frac{1}{R}\frac{d^2R}{dr^2}+\frac{1}{Rr}\frac{dR}{dr}-\frac{1}{r^2}=0 \tag{22}$$

We then multiply through by R to arrive at the potential equation

$$\frac{d^2R}{dr^2}+\frac{1}{r}\frac{dR}{dr}-\frac{R}{r^2}=0 \tag{23}$$

We observe that we can factor this equation into the form

$$\frac{d}{dr}\left[\frac{dR}{dr}+\frac{R}{r}\right]=0 \tag{24}$$

Since the function and its derivative are both zero at infinity, we conclude that

$$\frac{dR}{dr}+\frac{R}{r}=0 \tag{25}$$

which has solution

$$R=\frac{a}{r} \tag{26}$$

where *a* is a constant. Electron-electron interaction is therefore

$$F=-\frac{dR}{dr}=\frac{a}{r^2} \tag{27}$$

where a is the square of the electrostatic charge divided by the dielectric constant, and F is force. In graphene the dielectric constant is 2.5[4], which means the Coulomb force between electrons in graphene is weak.[5] Electron motion in graphene, therefore, is not correlated by Coulomb repulsion,[6] a finding which coincides with experimental measurement.

We summarize by saying that we have described the electron in monolayer graphene by use of the Schrödinger equation. We have also discovered a dispersion relation, and we have shown that electrons in graphene are not correlated by Coulomb repulsion.

References

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