

Dirac-Equation for Graphene with an Arbitrary Potential: Exact Analytical Results and General Proof of Bloch's Theorem

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Abstract

In this work, we reexamine the problem of the investigation of the electronic band structures of graphene using the Dirac-equation approach, with massless fermions (electrons). It is assumed that the charges experience a periodic external interaction potential of arbitrary form. First, we study all analytical properties of the wave-function that solves such an equation, and exactly solve the latter for normal incident wave-vectors, whatever is the potential expression. Second, we exactly determine the Dirac energy spectrum (at Dirac points). Thirdly, we give a general proof of the Bloch's theorem, usually encountered in Solid State Physics. Finally, the discussion is extended to nonzero gap monolayer-graphenes and to a finite number of parallel graphene layers.

Keywords: Graphene - Electronic band structures - Dirac equation - Bloch's theorem.

1. Introduction

Graphene is the first truly two-dimensional crystal ever observed in nature. It is a single plane of carbon atoms distributed regularly on a hexagonal lattice in the form of honeycomb. Graphene is considered as the mother of all other known carbon-rich materials, as graphite, diamond, fullerenes and carbon nanotubes. The graphene-terminology was introduced in 1986 for the first time by H.P. Boehm, R. Setton and E. Stumpp [1,2] to describe the graphite intercalation compounds. The first observation of a graphene sheet by *Electron Microscopy* was due in 1962 to H.P. Boehm and coworkers [3]. The microscopy images show graphite oxide flakes reduced with hydrazine of apparently atomic thickness, but this discovery remained a simple curiosity of laboratory. A real revolution in the field was marked by the isolation of graphene in 2004 by S.K. Novoselov and A.K. Geim [4] by an exfoliation of graphite using adhesive tape techniques. Due to its remarkable and exciting electronic and mechanical properties, the graphene has received a great deal of attention from both scientific community and industrials. As a matter of fact, the graphene possesses a very high electrical mobility and a great stability at the nano-scale [5-7]. Furthermore, contrarily to the carbon nanotubes, the graphene may be produced on large substrates. All these properties allow the manufacturing of graphene based-microelectronics systems that may treat information *ten* times more rapidly than the actual systems. Then, the graphene presents new features that may have some interest in Quantum Information.

From an electric point of view, the graphene is a special two-dimensional semi-conductor material possesses a *zero-gap* (semi-metal). The first theoretical investigation of the electronic band structures of the graphene has been done in 1947 by P.R. Wallace [8] who showed the unusual semi-metallic behavior in this material.

A pertinent remark is that, the electrons in graphene show a relativistic behavior. More precisely, electrons in graphene may be viewed as massless charged fermions living in two-dimensional space. This analogy makes the graphene as exciting bridge between condensed-matter and high energy physics. The essential conclusion is that, the behavior of electrons in graphene can be described solving a Dirac-like equation with an external potential [9-11]. The resolution of such an equation gives precious informations on the electronic band structures and other properties of graphene. We note that, in the Dirac-equation language, (i) the valence (VB) and conduction (CB) bands meet in two points in reciprocal space (*Dirac points*), (ii) the dispersion relation close to the Dirac points is linear and it has electronic-hole symmetry, and (iii) the VB is full and the CB is empty (the Fermi level is right at the Dirac points).

We emphasize that the Dirac equation has been exactly solved only for some class of the interaction potentials. In this work, however, we exactly solve this equation with arbitrary (periodic) potentials (for normal incident waves). In particular, we exactly determine the Dirac energy spectrum (at Dirac points) and give a general proof of the Bloch's theorem usually encountered in Solid

State Physics [12]. We also discuss the problem of graphene with gap and many parallel graphene-sheets.

The remaining of presentation proceeds as follows. In Section 2, we recall the useful basic equations. Exact analytic properties of the solution of Dirac-equation and the proof of the Bloch's theorem are presented in Section 3. We exactly determine, in Section 4, the Dirac energy spectrum (at Dirac points). Finally, some concluding remarks are drawn in the last section.

2. Basic equations

The Hamiltonian based on the Dirac-equation, is the following

$$\hat{H} = v_f(\sigma_x p_x + \sigma_y p_y) + V(x)\hat{I}, \tag{1}$$

with the momentum operators

$$p_x = \frac{\hbar}{i} \frac{\partial}{\partial x}, \quad p_y = \frac{\hbar}{i} \frac{\partial}{\partial y}, \tag{2}$$

along the x and y -directions, respectively. In definition (1), \hat{I} accounts for the 2×2 unit matrix and

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{2a}$$

for the standard Pauli matrices. There $v_f = 10^6$ m/s is the Fermi velocity.

The above Hamiltonian acts on two-component pseudospins $\Psi = (\Psi_A, \Psi_B)^T$, where $\Psi_A(x, y)$ and $\Psi_B(x, y)$ are the wave-functions relatively to the two sublattices A and B in graphene. We denote by E the associated energy. Since the Hamiltonian \hat{H} commutes with the momentum operator p_y , the wave-function, $\Psi(x, y)$, must have the form : $\Psi(x, y) = e^{ik_y y} \varphi(x, y) \equiv e^{ik_y y} (\varphi_A, \varphi_B)^T$, where k_y is the y -component of the incident wave-vector, $k = (k_x, k_y)$. Then, the basic equation to solve is

$$\frac{d\varphi}{dx} = A(x) \varphi, \tag{3}$$

where $A(x)$ is the following 2×2 matrix

$$A(x) = \begin{bmatrix} k_y & ik(x) \\ ik(x) & -k_y \end{bmatrix} = k_y \sigma_z + ik(x) \sigma_x, \tag{4}$$

with the third Pauli matrix

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4a}$$

We have used the notation

$$k(x) = (\hbar v_f)^{-1} [E - V(x)], \tag{4b}$$

where E is the energy and $V(x)$ is the interaction potential. It is assumed that such a potential is periodic in the x -variable. We denote by D its period, that is: $V(x + D) = V(x)$, for all $x \in \mathbf{R}$.

Mathematically speaking, Eq. (3) is a first-order linear differential system of (symmetric) matrix $A(x)$. The latter has the following trivial properties

$$\det[A(x)] = k_y^2 - k^2(x), \quad \text{Tr}[A(x)] = 0, \tag{5}$$

$$A^{-1}(x) = [k_y^2 - k^2(x)]^{-1} A(x). \tag{6}$$

Notice that the (stable) solution of differential system (3) is oscillatory if only if $k^2(x) > k_y^2$, for all $x \in \mathbf{R}$.

It will be convenient to introduce the Cauchy operator or *matriciant* we denote $M(x, x_0)$. The latter satisfies the following equation

$$\frac{dM}{dx} = A(x) M, \tag{7}$$

with the initial condition

$$M(x, x_0) = \hat{I}, \tag{7a}$$

where \hat{I} is the 2×2 identity matrix. The formal solution of Eq. (7) is

$$\varphi(x) = M(x, x_0) \varphi(x_0). \tag{8}$$

Here, x_0 is an arbitrary point. We note that the operator M can be related to the fundamental matrix, $X(x)$, by [13]

$$M(x, x_0) = X(x) X^{-1}(x_0). \tag{9}$$

The fundamental matrix $X(x)$ then solves the same differential equation as the matriciant $M(x, x_0)$. We recall that the matrix $X(x)$ is constructed with two fundamental solutions of Eq. (7). We recall that, any other fundamental matrix $X_1(x)$ can be written as [13]: $X_1(x) = X(x) C$, where C is a non-singular squared matrix.

It follows from the formal solution of equation (7) that the matriciant $M(x, x_0)$ must satisfy the following properties

$$M^{-1}(x, x_0) = M(x_0, x), \tag{10a}$$

$$M(x, y)M(y, z) = M(x, z), \text{(Multiplication property)}, \tag{10b}$$

$$\det[M(x)] = \det[M(0)] \times \exp\left\{\int_0^x \text{Tr}[A(y)] dy\right\}. \tag{10c}$$

Since $M(0) = \hat{I}$ and $\text{Tr}[A(x)] = 0$, the above equality becomes

$$\det[M(x)] = 1, \tag{11}$$

for all $x \in \mathbf{R}$. This relation is valid for all interaction potentials.

Remark that the matriciant M plays the role of the *evolution operator* of Quantum Mechanics and the matrix A is the analog of Hamiltonian, with the substitution $x \rightarrow t/i\hbar$, where t is time.

3. Analytical properties of the solution and proof of the Bloch's theorem

Assume that the interaction potential $V(x)$ is periodic in the x -variable, with period D . Then, the matrix $A(x)$ of the differential system is also periodic with the same period, that is: $A(x + D) = A(x)$. Without loss of generality, we shall set $x_0 = 0$ and use the notation $M(x, 0) \equiv M(x)$. We have the following properties:

Property 1: The matriciants $M(x + D)$ and $M(x)$ are related by

$$M(x + D) = M(x)G. \tag{12}$$

Putting $x = 0$ into this periodicity relation and using the property $M(0) = \hat{I}$ yields that the squared matrix G is simply $G = M(D)$. The latter is called *monodromy matrix* [13] that depends on electron energy E , the y -component of the incidence wave-vector, k_y , and parameters of the potential, $\{\lambda_i\}$. To show the above equality, we first note that the matriciant $M(x + D)$ is also solution to differential system (7). We write

$$A(x + D) = \frac{dM(x+D)}{dx} \cdot M^{-1}(x + D) = \frac{dM(x)}{dx} G G^{-1} M^{-1}(x) = A(x). \tag{13}$$

This ends the proof of property (12).

Property 2: The matriciant $M(x)$, with a periodic differential system matrix $A(x)$, satisfies the Floquet's theorem [13], according to which

$$M(x) = \varphi(x)e^{Kx}, \tag{14}$$

where $\varphi(x)$ is a periodic matrix, that is $\varphi(x + D) = \varphi(x)$. Combining equalities (12) and (14) gives the relation: $K = D^{-1} \ln M(D)$. We have used the identity $M(D) = \varphi(0) = \hat{I}$.

Property 3: There exists a (non-trivial) fundamental solution of differential system (3) such that

$$\varphi(x + D) = \rho\varphi(x). \tag{15}$$

This is the *Bloch's theorem*. Here, ρ is an eigenvalue (multiplier) of the monodromy matrix $G = M(D)$. To

show the above periodicity relation, we first apply Eq. (3) replacing x by $x + D$ and setting $x_0 = 0$, and combine it with relationship (12), to find

$$\varphi(x + D) = M(x)G\varphi(0). \tag{16}$$

On the other hand, we can choose a fundamental solution $\varphi(x)$ such that $\varphi(0)$ is an eigenvector of monodromy matrix G , that is $G\varphi(0) = \rho\varphi(0)$.

This completes the proof of Bloch's theorem.

Property 4: For a normal incidence, that is for $k_y = 0$, we *exactly* solve the differential system (7) and find

$$M(x) = \exp\{i\sigma_x \cdot \int_0^x k(y)dy\}. \tag{17}$$

This gives the *exact* pseudo-spinor

$$\varphi(x) = \exp\{i\sigma_x \cdot \int_0^x k(y)dy\}\varphi(0), \tag{18}$$

where the function $k(x)$ is that defined in Eq. (4b).

4. Exact Dirac energy spectrum

Now, come back to the monodromy matrix $G = M(D)$ and denote by ρ and ρ^* (complex conjugate of ρ) its eigenvalues. Then, we have

$$\rho + \rho^* = \text{Tr}G, \tag{19}$$

$$\rho\rho^* = \det G = 1. \tag{20}$$

The last equality means that the eigenvalue ρ belongs to the unit circle. Equality (19) implies that

$$-2 \leq \text{Tr}G \leq 2. \tag{21}$$

Inequalities $-2 < \text{Tr}G < 2$ define the domain in space of parameters $(E, k_y, \{\lambda_i\})$, where electron energy E makes sense. Equalities

$$\text{Tr}G = \pm 2 \tag{22}$$

then give the frontiers or energy band structures.

The monodromy matrix G is exactly given by

$$G = M(D) = \exp\{i\sigma_x \cdot \int_0^D k(y)dy\}. \tag{23}$$

This expression of G together with Eq. (22) yield the relation

$$2\cos\left((\hbar v_F)^{-1} \int_0^D [E - V(x)] dx\right) = \pm 2. \tag{24}$$

This implies the *exact* location of the *Dirac-points* of quantified energy

$$E_n = \hbar v_F \frac{n\pi}{D} + \frac{1}{D} \int_0^D V(x) dx, \quad n \in \mathbf{Z}, \quad (25)$$

whatever is the expression of the interaction potential, $V(x)$, provided that it is a periodic function of period D . The contribution of this potential to the Dirac energy is just its mean-value along a period D .

Remark that the difference between consecutive Dirac energies (gap) is

$$\Delta E = E_n - E_{n-1} = \hbar v_F \frac{\pi}{D}, \quad \forall n \in \mathbf{Z}, \quad (26)$$

independently of the value of the interaction potential. Let us compute the Dirac energy for some typical examples:

Example 1: Periodic rectangular potential.

In the interval $[0, D]$ of interest, it is defined by

$$V(x) = \begin{cases} V_A, & 0 \leq x \leq w_A, \\ V_B, & w_A \leq x \leq w_A + w_B. \end{cases} \quad (27)$$

For this case, the general Dirac energy expression becomes

$$E_n = \hbar v_F \frac{n\pi}{D} + \frac{w_A}{w_A+w_B} V_A + \frac{w_B}{w_A+w_B} V_B, \quad n \in \mathbf{Z}. \quad (28)$$

For $n = 0$, we recover the published result [14].

Example 2: Sawtooth potential

Its expression, in the interval $[0, D]$, is

$$V(x) = \left(\frac{V_0}{D}\right)x, \quad 0 < x < D, \quad (29)$$

where $V_0 > 0$ is the maximal value of the potential. For this case, we find that the Dirac energy is given by

$$E_n = \hbar v_F \frac{n\pi}{D} + \frac{V_0}{2D}, \quad n \in \mathbf{Z}. \quad (30)$$

Example 3: Oscillatory potential.

Its expression is

$$V(x) = V_0 \sin\left(\frac{2\pi}{D}x\right), \quad (31)$$

where $V_0 > 0$ is the potential amplitude. For such a potential, we find that

$$E_n = \hbar v_F \frac{n\pi}{D}, \quad n \in \mathbf{Z}, \quad (32)$$

independently on the potential characteristics.

Example 4: Periodic exponential potential.

In the interval $[0, D]$, its expression is

$$V(x) = \frac{V_0}{1-e^{-\alpha D}}(1 - e^{-\alpha x}), \quad 0 < x < D, \quad (33)$$

where the parameter α is positive. Here, $V_0 > 0$ denotes the maximal value of the potential. For this case, we find

$$E_n = \hbar v_F \frac{n\pi}{D} + \frac{V_0}{1-e^{-\alpha D}} \left[D + \frac{1}{\alpha}(e^{-\alpha D} - 1) \right], \quad n \in \mathbf{Z}. \quad (34)$$

5. Concluding remarks

In the present work, attention is paid to a reexamination of the analytical properties of the solution of the Dirac-like equation and its consequences on the electronic band structures. The originality of this investigation is that, the study was achieved for arbitrary periodic interaction potentials.

Firstly, we exactly studied all analytical properties of the wave-function. In particular, we determined the exact form of the solution for normal incident waves.

Secondly, we exactly determine the Dirac energy spectrum (at Dirac points).

Thirdly, we gave a general proof of the Bloch's theorem, usually encountered in Solid State Physics.

We emphasize that the above basic formulae can be extended to $n > 1$ parallel graphene-sheets. In this case, the wave-function φ is a generalized spinor of components φ_α ($1 \leq \alpha \leq n$) and the differential system matrix A is a squared matrix of order n . The coefficients of this matrix are constructed with the y -component of the incident wave-vector, k_y , the coupling constants between layers, $\{t_{\alpha\beta}\}$, and the interaction potential, $V(x)$ [15]. The latter is assumed to be periodic in the variable x , with period D . Then, the differential system matrix A is periodic, of period D . As main result, the above consequences (for a single graphene-sheet) remain the same in the case of many parallel graphene-sheets.

Also, the above obtained results can be extended, in a straightforward way, to the situation of graphene with gap (doped graphene). In this case, one must add to the Hamiltonian (1) some term, $\Delta\sigma_z$, where 2Δ is nothing else but the gap energy.

Further questions in relation with the subject are under investigation.

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