PHYSICAL REVIEW B **78**, 201406(R) (2008)

Analytic solution for electrons and holes in graphene under electromagnetic waves: Gap appearance and nonlinear effects

F. J. López-Rodríguez[1] and G. G. Naumis[1,2,3]
[1]*Departamento de Física-Química, Instituto de Física, Universidad Nacional Autónoma de México (UNAM), Apartado Postal 20-364, 01000 México D.F., Mexico*
[2]*Facultad de Ciencias, Universidad Autónoma del Estado de Morelos, Av. Universidad 10001, 62210, Cuernavaca, Morelos, Mexico*
[3]*Departamento de Física-Matemática, Universidad Iberoamericana, Prolongación Paseo de la Reforma 880, Col. Lomas de Santa Fe, 01210 México D.F., Mexico*
(Received 22 September 2008; published 17 November 2008)

We find the exact solution of graphene carriers dynamics under electromagnetic radiation. To obtain the solution of the corresponding Dirac equation, we combine Floquet theory with a trial solution. Then the energy spectrum is obtained without using any approximation. We also prove that the energy spectrum presents a gap opening, which depends on the radiation frequency and electric wave intensity, whereas the current shows a strongly nonlinear behavior.

DOI: 10.1103/PhysRevB.78.201406 PACS number(s): 73.22.−f, 73.21.−b, 81.05.Uw

Graphene, a two-dimensional allotrope of carbon, has been the center of much research since its experimental discovery four years ago.[1] It has amazing properties.[2–4] For instance, electrons in graphene behave as massless relativistic fermions.[5,6] Such property is a consequence of its bipartite crystal structure,[7] in which a conical dispersion relation appears near the K,K' points of the first Brillouin zone.[8] Among other properties one can cite the high mobility that remains higher even at high electric fields and translates into ballistic transport on a submicron scale[9] at 300 K. Graphene is therefore a promising material for building electronic devices, but there are some obstacles to overcome. One is the transmission probability of electrons in graphene, which can be unity irrespective of the height and width of a given potential barrier.[2] As a result, conductivity cannot be changed by an external gate voltage, a feature required to build a field-effect transistor (FET), although a quantum dot can be used. In a previous paper, we have shown that a possible way to induce a pseudogap around the Fermi energy consists of doping graphene.[10] On the other hand, much effort has been devoted to understanding the electrodynamic properties of graphene as well as its frequency dependent conductivity.[11–15] In this Rapid Communication, we solve without the need of any approximation, the problem of graphene's electron behavior in the presence of an electromagnetic plane wave. As a result, we are able to find a gap opening. This is like if electrons in graphene acquire an effective mass under electromagnetic radiation. We also calculate the current and show that there is a strongly nonlinear electromagnetic response, as was claimed before by Mikhailov[16] using a semiclassical approximation.

Consider an electron in a graphene lattice subject to an electromagnetic plane wave as shown in Fig. 1. The plane wave propagates along the two-dimensional space where electrons move. In this Rapid Communication we take $\mathbf{k}=(0,k)$. The generalization to any direction of $\mathbf{k}$ is straightforward. It has been proved that a single-particle Dirac Hamiltonian can be used as a very good approximation to describe charge carriers dynamics in graphene.[17] For wave vectors close to the K point of the first Brillouin zone, the Hamiltonian is[18]

$$H(x,y,t)=v_F\begin{pmatrix} 0 & \hat{\pi}_x - i\hat{\pi}_y \\ \hat{\pi}_x + i\hat{\pi}_y & 0 \end{pmatrix}, \tag{1}$$

where v_F is the Fermi velocity $v_F \approx c/300$, $\hat{\pi}=\hat{\mathbf{p}}-e\mathbf{A}/c$ with $\hat{\mathbf{p}}$ being the electron momentum operator, and $\mathbf{A}$ is the vector potential of the applied electromagnetic field, given by $\mathbf{A}=[\frac{E_0}{\omega}\cos(ky-\omega t),0]$, where E_0 is the amplitude of the electric field and ω is the frequency of the wave. E_0 is taken as a constant since screening effects are weak in graphene.[19] For the valley K' the signs before π_y are the opposite.[18] The dynamics is governed by

$$H(x,y,t)\mathbf{\Psi}(x,y,t)=i\hbar\frac{\partial \mathbf{\Psi}(x,y,t)}{\partial t}, \tag{2}$$

where

$$\mathbf{\Psi}(x,y,t)=\begin{pmatrix} \Psi_A(x,y,t) \\ \Psi_B(x,y,t) \end{pmatrix}$$

is a two component spinor. Here A and B stand for each sublattice index of the bipartite graphene lattice.[7] To find the eigenstates and eigenenergies we adapt a method developed

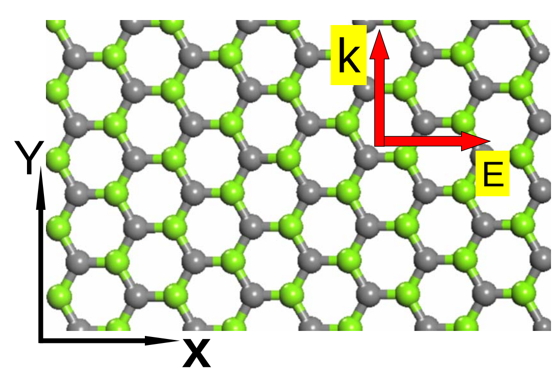

FIG. 1. (Color online) Graphene lattice. Atoms in the A sublattice are shown with different color than those in the B sublattice. The vector $\mathbf{k}$ in which the electromagnetic field propagates and the electric-field vector $\mathbf{E}$ are shown.

by Volkov in 1935 (Ref. 20) to study the movement of relativistic particles under an electromagnetic field. Volkov considered bispinors and Dirac matrices. We use instead Pauli matrices and spinors. First we write the equations of motion for each component of the spinor

$$v_F(\hat{\pi}_x - i\hat{\pi}_y)\Psi_B(x,y,t) = i\hbar\frac{\partial\Psi_A(x,y,t)}{\partial t}, \quad (3)$$

$$v_F(\hat{\pi}_x + i\hat{\pi}_y)\Psi_A(x,y,t) = i\hbar\frac{\partial\Psi_B(x,y,t)}{\partial t}. \quad (4)$$

Considering the magnetic field as $\mathbb{B}$, the commutation rules for $\hat{\pi}_x$ and $\hat{\pi}_y$ are

$$[\hat{\pi}_i,\hat{\pi}_j] = \frac{i\hbar e}{c}\varepsilon_{ijk}\mathbb{B}_k, \quad i,j = x,y, \quad (5)$$

$$\left[\frac{\partial}{\partial t},\hat{\pi}_x \pm i\hat{\pi}_y\right] = -\frac{eE_o}{c}\sin(ky-\omega t), \quad (6)$$

and using that $k_\mu A^\mu=0$, we find the following equation of motion for the spinor:

$$-\hbar^2\left[v_F^2\left(\frac{\partial^2\mathbf{\Psi}}{\partial x^2}+\frac{\partial^2\mathbf{\Psi}}{\partial y^2}\right)-\frac{\partial^2\mathbf{\Psi}}{\partial t^2}\right]+2i\hbar\xi v_F\cos\phi\frac{\partial\mathbf{\Psi}}{\partial x} + [\xi^2\cos^2\phi - \xi v_F\hbar\sigma_z k\sin\phi - i\hbar\omega\xi\sigma_x\sin\phi]\mathbf{\Psi} = \mathbf{0}, \quad (7)$$

where we have defined the phase ϕ of the electromagnetic wave as $\phi=ky-\omega t$. The parameter ξ is defined as $\xi=\frac{eE_0v_F}{c\omega}$, and σ_μ is the set of Pauli matrices. To solve this equation, we follow Volkov's suggestion to use a trial function that depends upon the phase ϕ of the wave with the following form:

$$\mathbf{\Psi}(x,y,t) = e^{ip_xx/\hbar+ip_yy/\hbar-i\epsilon t/\hbar}\mathbf{F}(\phi), \quad (8)$$

where $\epsilon=v_F\sqrt{p_x^2+p_y^2}$ and $\mathbf{F}(\phi)$ is a spinor. Inserting Eq. (8) into Eq. (7), it yields an equation for $\mathbf{F}(\phi)$. The resulting differential equation is

$$2i\hbar\epsilon\eta\frac{d\mathbf{F}(\phi)}{d\phi} + [-2\xi v_F p_x\cos\phi - \xi v_F\hbar\sigma_z k\sin\phi + \xi^2\cos^2\phi - i\hbar\omega\xi\sigma_x\sin\phi]\mathbf{F}(\phi) = 0, \quad (9)$$

and $\eta=\epsilon\omega - v_F^2kp_y$. The previous equation can be solved to give

$$\mathbf{F}(\phi) = \exp[G(\phi)]\mathbf{u}, \quad (10)$$

where $\mathbf{u}$ is a two component spinor and,

$$G(\phi) = \frac{i\xi^2}{4\hbar\eta}\phi - \frac{i\xi v_F}{\hbar\eta}p_x\sin\phi - i\frac{\xi v_F\sigma_z k}{2\eta}\cos\phi + \frac{i\xi^2}{8\hbar\eta}\sin 2\phi - \frac{\xi\omega}{2\eta}\sigma_x\cos\phi. \quad (11)$$

In the important case of a field with a long wavelength compared with the system size ($\lambda\to\infty$), $G(\phi)$ is reduced to

$$G_\infty(t) \equiv \lim_{\lambda\to\infty} G(\phi) = -\frac{i\xi^2}{4\hbar\epsilon}t - \frac{i\xi v_F}{\hbar\epsilon\omega}p_x\sin\omega t + \frac{i\xi^2}{8\hbar\epsilon\omega}\sin 2\omega t - \frac{\xi}{2\epsilon}\sigma_x\cos\omega t, \quad (12)$$

where ϕ is now equal to ωt. The complete solution is

$$\mathbf{\Psi}(\mathbf{x},\mathbf{y},\mathbf{t}) = \exp[ip_xx/\hbar + ip_yy/\hbar - i\epsilon t/\hbar]\exp[G(\phi)]\mathbf{u}, \quad (13)$$

where $\mathbf{u}$ must be taken as a two component spinor, which satisfies the requirement that when $\mathbf{A}\to 0$, $\mathbf{\Psi}(x,y,t)$ should be the solution of the free Dirac equation to avoid strange solutions. Thus $\mathbf{u}$ is given by

$$\mathbf{u} = \frac{1}{\sqrt{2}}\begin{pmatrix}\pm e^{-i\varphi/2}\\ e^{i\varphi/2}\end{pmatrix}, \quad \varphi = \tan\left(\frac{p_y}{p_x}\right), \quad (14)$$

where the plus sign stands for electrons and the minus sign stands for holes. The eigenvalues are $\epsilon+\xi^2\omega/4\eta$. But now we need to take into account the time periodicity of the electromagnetic field, which means that the solution must be written in the following way:[21]

$$\mathbf{\Psi} = \exp(-i\chi t/\hbar)\mathbf{\Phi}(x,y,t), \quad (15)$$

where $\mathbf{\Phi}(x,y,t)$ is periodic in time, i.e., $\mathbf{\Phi}(x,y,t) = \mathbf{\Phi}(x,y,t+T)$, and χ is a real parameter, being unique up to multiples of $\hbar\omega$, $\omega=2\pi/\tau$. In fact, such property is very well known within the so-called Floquet theory,[21] developed for time-dependent fields. This time periodicity of the field leads to the formation of bands. Our solution [Eq. (13)] satisfies the requisite form Eq. (15). However, to obtain the Floquet states[21] for this problem, we need to consider that $\epsilon+\xi^2\omega/4\eta$ is unique up to multiples of $\hbar\omega$. Thus $E=\epsilon+\xi^2\omega/4\eta+n\hbar\omega$, where n is an integer such that $n=0,\pm1,\pm2,\ldots$, while $\mathbf{\Phi}(x,y,t)$ is the Floquet mode given by

$$\mathbf{\Phi}(x,y,t) = \exp[in\omega t + ip_xx/\hbar + ip_yy/\hbar]\exp[F(\phi)]\mathbf{u}, \quad (16)$$

where $F(\phi)=G(\phi)+i\xi^2\omega t/4\hbar\eta$. The Floquet modes of the problem must satisfy the equation[21]

$$\left[H(x,y,t) - i\hbar\frac{\partial}{\partial t}\right]\mathbf{\Phi}(x,y,t) = E\mathbf{\Phi}(x,y,t). \quad (17)$$

The final eigenenergies for electron and holes are the following:

$$E_n(p) = n\hbar\omega \pm v_F\|p\| \pm \left[\frac{e^2E_0^2v_F}{4c^2\omega^2\|p\|\left[1-\left(\frac{v_Fkp_y}{\omega\|p\|}\right)\right]}\right], \quad (18)$$

where $n=0,\pm1,\ldots$, and the wave function is

$$\mathbf{\Psi}_{n,p}(x,y,t) = \exp[-iE_n(p)t/\hbar]\mathbf{\Phi}(x,y,t), \tag{19}$$

and $\mathbf{\Phi}(x,y,t)$ is the Floquet mode Eq. (16). If the two smallest terms are neglected in Eq. (12), our solution can be reduced to one found in Ref. 22. The spectrum given by Eq. (18) is made of bands, where the electromagnetic field bends the linear dispersion relationship due to the last term. In the important limit of long wavelengths, such term becomes

$$\Delta(p) = \frac{e^2E_0^2 v_F}{4c^2\|p\|\omega^2} = \frac{\xi^2}{4\epsilon}. \tag{20}$$

Thus, around the Fermi energy, holes and electron bands are separated by a gap of size $\Delta = 2\Delta(p_F)$. To estimate the magnitude of the gap, we consider electrons near the Fermi energy, thus $\epsilon = v_F\|p\| \approx \epsilon_F$, where ϵ_F is approximately[12] $\epsilon_F = 86$ meV. For a typical microwave frequency $\omega = 50$ GHz with an intensity $E_0 = 3$ V/cm of the electric field, the gap size is around $\Delta \approx 0.2$ meV. Due to the gap opening, the particles are no longer massless. The mass acquired by the carriers due to the field is therefore around $10^{-4}m_e$. Since this is a time-dependent problem, one cannot measure the gap directly from the density of states. Instead, one can look for jumps in the dc conductance, using, for example, the device proposed in Ref. 22. Finally, the solution can be used to evaluate the current using the collisionless Boltzmann equation,[16] neglecting interband transitions. However, this approach turns out to give the same results as considering the velocity of the particles as time dependent while the distribution function $[f_{\mathbf{p}}(t)]$ remains static.[23] Such equivalence is the result of the trivial statement that in the Boltzmann approach, the electric field induces a displacement of the Fermi surface.[23] In fact, the current obtained below is equal to the one obtained using a Boltzmann equation semiclassical approach for graphene under an electric adiabatic field,[16] which also reproduces the intraband Drude conductivity.[16] The electric current is given by $\mathbf{j}(t) = 4S^{-1}\Sigma_{\mathbf{p}}\mathbf{j}_{\mathbf{p}}(t)f_{\mathbf{p}}(t)$, where S^{-1} is the sample area and the factor 4 comes for the spin and valley degeneracies. $\mathbf{j}_{\mathbf{p}}(t)$ denotes the contribution to the current of particles with momentum $\mathbf{p}$ at time t. Let us first calculate the μ component of the current vector, given by $j_{\mu,\mathbf{p}}(t) = ev_F\mathbf{\Psi}^*_{n,p}\sigma_\mu\mathbf{\Psi}_{n,p}$. We use Eq. (19) in the long-wavelength limit to obtain the components of j in the x and y directions,

$$j_{x,p}(t) = ev_F \sinh\left(\frac{\xi}{\epsilon}\cos\omega t\right) + \cosh\left(\frac{\xi}{\epsilon}\cos\omega t\right)\cos\varphi, \tag{21}$$

and $j_{y,p} = ev_F\sin\varphi$. In j_x we observe a very important nonlinear behavior. In fact, $j_{x,p}(t)$ can be written as a combination of harmonics by using a Fourier series development of the hyperbolic functions[24]

$$j_{x,p}(t) = ev_F\sum_{s=0}^{\infty} J_{2s+1}\left(\frac{\xi}{\epsilon}\right)\cos[(2s+1)\omega t] + ev_F\left[J_0\left(\frac{\xi}{\epsilon}\right) + 2\sum_{s=1}^{\infty} J_{2s}\left(\frac{\xi}{\epsilon}\right)\cos(2s\omega t)\right]\cos\varphi, \tag{22}$$

where $J_s(\xi/\epsilon)$ is a Bessel function. Our result is similar to the current obtained using a semiclassical approximation,[16] except for the last term, which eventually cancels out in the thermodynamical limit. Now we include such limit by using the distribution function $f(\mathbf{p})$. In this case, we are dealing with quasiparticles with an effective dispersion relation. Using Eq. (22), and by summing over the phase space we get

$$j_x(t) = \frac{4ev_F}{(2\pi\hbar)^2}\sum_{s=0}^{\infty} A(s)\cos[(2s+1)\omega t],$$

$$A(s) \equiv \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} J_{2s+1}\left(\frac{\xi}{v_F p}\right) n(p)\,dp_x dp_y, \tag{23}$$

where $n(p) = [1+\exp(E_n(p)-\epsilon_F)/k_BT]^{-1}$ is the occupation factor. For $\epsilon_F \gg k_BT$, $n(p)$ can be replaced by a step function. Using Eq. (18), $v_Fp_F = \epsilon_f[1+\sqrt{1-(\xi/\epsilon_f)^2}]/2$ for $n=0$, $A(s)$ is

$$A(s) = 2\pi p_F^2\alpha^2\int_0^1 J_{2s+1}\left(\frac{Q_0}{\alpha x}\right)x\,dx,$$

$$\alpha \equiv \left(\frac{(1+\sqrt{1-Q_0^2})}{2}\right) \approx \left\{1 - \frac{1}{4}Q_0^2\right\}, \tag{24}$$

where $Q_0 = \xi/\epsilon_F = eE_0/(c\omega p_F)$. For $s=0$ we obtain,

$$A(0) \approx \pi p_F^2\alpha Q_0\left[1 + \frac{1}{8}\left(\frac{Q_0}{\alpha}\right)^2 - \frac{1}{576}\left(\frac{Q_0}{\alpha}\right)^4 + \cdots\right], \tag{25}$$

and for $s>0$, the integral can be approximated as $A(s) \approx 2\pi p_F^2(Q_0/2)^3\Gamma(s-\frac{1}{2})/\alpha\Gamma(s+\frac{5}{2})$. The first terms of the current are

$$j_x(t) \approx en_ev_FQ_0\left\{\left(1-\tfrac{1}{8}Q_0^2\right)\cos(\omega t) + \tfrac{2}{15}Q_0^2\cos(3\omega t) + \cdots\right\},$$

where n_e is the density of electrons $n_e = p_F^2/\pi\hbar^2$. In conclusion, we solved the Dirac equation for graphene charge carriers under an electromagnetic field.

We acknowledge DGAPA-UNAM Projects No. IN-117806 and No. IN-111906, and CONACyT Grants No. 48783-F and No. 50368.

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, Science **306**, 666 (2004).
[2] M. I. Katsnelson, Mater. Today **10**, 20 (2007).
[3] K. S. Novoselov, Z. Jiang, Y. Zhang, S. V. Morozov, H. L. Stormer, U. Zeitler, J. C. Maan, G. S. Boebinger, P. Kim, and A. K. Geim, Science **315**, 1379 (2007).
[4] K. S. Novoselov, E. McCann, S. V. Morozov, V. I. Fal'ko, M. I. Katsnelson, U. Zeitler, D. Jiang, F. Schedin, and A. K. Geim, Nat. Phys. **2**, 177 (2006).
[5] G. W. Semenoff, Phys. Rev. Lett. **53**, 2449 (1984).
[6] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, Nature (London) **438**, 197 (2005).
[7] J. C. Slonczewski and P. R. Weiss, Phys. Rev. **109**, 272 (1958).
[8] P. R. Wallace, Phys. Rev. **71**, 622 (1947).
[9] A. K. Geim and K. S. Novoselov, Nature Mater. **6**, 183 (2007).
[10] G. G. Naumis, Phys. Rev. B **76**, 153403 (2007).
[11] N. M. R. Peres, F. Guinea, and A. H. Castro Neto, Phys. Rev. B **73**, 125411 (2006).
[12] V. P. Gusynin and S. G. Sharapov, Phys. Rev. B **73**, 245411 (2006).
[13] V. P. Gusynin, S. G. Sharapov, and J. P. Carbotte, Phys. Rev. Lett. **96**, 256802 (2006).
[14] S. A. Mikhailov and K. Ziegler, Phys. Rev. Lett. **99**, 016803 (2007).
[15] V. Lukose, R. Shankar, and G. Baskaran, Phys. Rev. Lett. **98**, 116802 (2007).
[16] S. A. Mikhailov, Europhys. Lett. **79**, 27002 (2007).
[17] S. Das Sarma, E. H. Hwang, and W.-K. Tse, Phys. Rev. B **75**, 121406(R) (2007).
[18] M. I. Katsnelson, Eur. Phys. J. B **57**, 225 (2007).
[19] D. P. DiVincenzo and E. J. Mele, Phys. Rev. B **29**, 1685 (1984).
[20] V. B. Berestetskii, E. M. Lifshitz, and L. P. Pitaevskii, *Quantum Electrodynamics*, Course of Theoretical Physics Vol. 4, 2nd ed. (Mir, Moscow, 1982).
[21] T. Dittrich, P. Hänggi, G. Ingold, B. Kramer, Gerd Schön, and W. Zwerger, *Quantum Transport and Dissipation* (Wiley, New York, 1998).
[22] B. Trauzettel, Ya. M. Blanter, and A. F. Morpurgo, Phys. Rev. B **75**, 035305 (2007).
[23] M. Torres and A. Kunold, Phys. Rev. B **71**, 115313 (2005).
[24] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products*, 5th ed. (Academic, San Diego, 1994).