Tuning laser-induced band gaps in graphene

Hernán L. Calvo,[1,2] Horacio M. Pastawski,[1] Stephan Roche,[3,4] and Luis E. F. Foa Torres[1,a)]
[1]*Instituto de Física Enrique Gaviola (IFEG)–CONICET, FaMAF, Universidad Nacional de Córdoba, Ciudad Universitaria, 5000 Córdoba, Argentina*
[2]*Institut für Theorie der Statistischen Physik, RWTH Aachen University, D-52056 Aachen, Germany*
[3]*CIN2 (ICN–CSIC), Catalan Institute of Nanotechnology, Universidad Autónoma de Barcelona, Campus UAB, 08193 Bellaterra (Barcelona), Spain*
[4]*Institució Catalana de Recerca i Estudis Avançats (ICREA), 08070 Barcelona, Spain*

(Received 6 March 2011; accepted 2 May 2011; published online 7 June 2011)

Could a laser field lead to the much sought-after tunable band gaps in graphene? By using Floquet theory combined with Green's functions techniques, we predict that a laser field in the mid-infrared range can produce observable band gaps in the electronic structure of graphene. Furthermore, we show how they can be tuned by using the laser polarization. Our results could serve as a guidance to design optoelectronic nanodevices. © *2011 American Institute of Physics*.
[doi:10.1063/1.3597412]

More than a century ago, the use of alternating currents (ac) sparked a revolution that changed our modern world. Today, the use of ac fields has reached the nanoscale.[1,2] Here, the interplay between the quantum coherence of the electrons, inelastic effects, and dynamical symmetry breaking offers fascinating opportunities for both basic research and applications. The coherent destruction of tunneling[3] and quantum charge pumping,[4–6] i.e., the generation of a dc current at zero bias voltage due to quantum interference,[7] are prominent examples of the wealth of phenomena driving this rapidly advancing area of research. By means of time-dependent gates,[8,9] surface acoustic waves,[10] or illumination with a laser field,[11] experiments have probed different facets of ac transport and light-matter interaction. On the other hand, theoretical insights keep opening exciting directions, from interaction-induced quantum pumping[12] to everlasting oscillations.[13]

Among many other benefits, the advent of graphene[14] and carbon nanotubes[15] provides an outstanding arena for the study of ac transport in highly coherent, low dimensional systems. Adiabatic quantum pumps,[16,17] ac controlled Fabry–Pérot resonators,[18] and photodetectors[19] are among the new breed of carbon-based devices. Furthermore, a few remarkable studies on Dirac fermions interacting with linearly[20,21] and circularly[22,23] polarized monochromatic light pointed out striking nonperturbative nonadiabatic effects; a laser field could lead to the opening of dynamical gaps[20] in graphene. For circularly polarized light, a further gap was shown to develop at the Dirac point.[22] Many open questions remain as follows: which experimental setup would unveil these phenomena and how could we tune them?

In this letter, we aim at elucidating these questions by analyzing the interaction between electrons and a monochromatic laser field of *arbitrary* polarization in graphene. Using a Floquet approach one finds that a laser of frequency Ω induces the lifting of degeneracies between (Floquet) states of the combined electron–photon system. Here, a careful analysis allows for the tuning of a feasible parameter range (laser frequency, power, and polarization). Our predictions show that these effects are within the reach of mid-infrared laser technology in a transport setup, thereby opening promising prospects for graphene-based optoelectronic devices.

In graphene, the low energy electronic states contributing to transport are close to the Dirac points **K** and **K′**. Since we consider a clean sample and given that the ac field does not introduce any intervalley coupling, we can describe both points separately. In the **K**-valley, those states can be accurately described by the $\mathbf{k}\cdot\mathbf{p}$ approximation through the envelope wave function $\Psi=(\Psi_A,\Psi_B)^{\mathrm{T}}$, where the two components refer to the interpenetrating sublattices A and B.[24] The time periodic electromagnetic field, with period $T=2\pi/\Omega$, is included as a monochromatic plane wave traveling along the z-axis, perpendicular to the plane defined by the graphene sheet. The magnetic vector potential is thus written as $\mathbf{A}(t)=\mathrm{Re}\{\mathbf{A}_0 e^{-i\Omega t}\}$, where $\mathbf{A}_0=A_0(1,e^{i\varphi})$ refers to the intensity and polarization φ of the field. For this choice of parameters, $\varphi=0$ yields a linearly polarized field $\mathbf{A}(t)=A_0\cos(\Omega t)(\hat{\mathbf{x}}+\hat{\mathbf{y}})$ while $\varphi=\pi/2$ results in a circularly polarized field $\mathbf{A}(t)=A_0(\cos(\Omega t)\hat{\mathbf{x}}+\sin(\Omega t)\hat{\mathbf{y}})$. Therefore, the graphene electronic states in the presence of the ac field are encoded in the Hamiltonian,

$$\mathcal{H}(t)=v_F\boldsymbol{\sigma}\cdot[\mathbf{p}-e\mathbf{A}(t)]. \tag{1}$$

Here $v_F\simeq 10^6$ m/s denotes the Fermi velocity and $\boldsymbol{\sigma}=(\sigma_x,\sigma_y)$ the Pauli matrices describing the pseudospin degree of freedom.

As will be made clear later on, a correct description of our problem crucially requires a solution valid beyond the adiabatic approximation. Hence, the Floquet theory[2] represents a suitable approach. The resulting picture is that of an effective time-independent Hamiltonian in a higher-dimensional space, the so-called Floquet space, defined as the direct product between the usual Hilbert space and the space of $2\pi/\Omega$-time periodic functions. This space is spanned by the states $\{|\mathbf{k},n\rangle_{\pm}\}$, where $\mathbf{k}$ is the electronic wave vector, n is the Fourier index, and the subindex refers to the alignment of the pseudospin with respect to the momentum. In this basis, the problem to solve is identical to the time-independent Schrödinger equation with Floquet Hamiltonian $H_F=H-i\hbar\partial_t$. The power of recursive Green's function techniques[25] can be exploited to obtain both the dc component of the conductance and density of states (DOS) from the so-called Floquet Green's functions.[26]

a)Electronic mail: lfoa@famaf.unc.edu.ar.

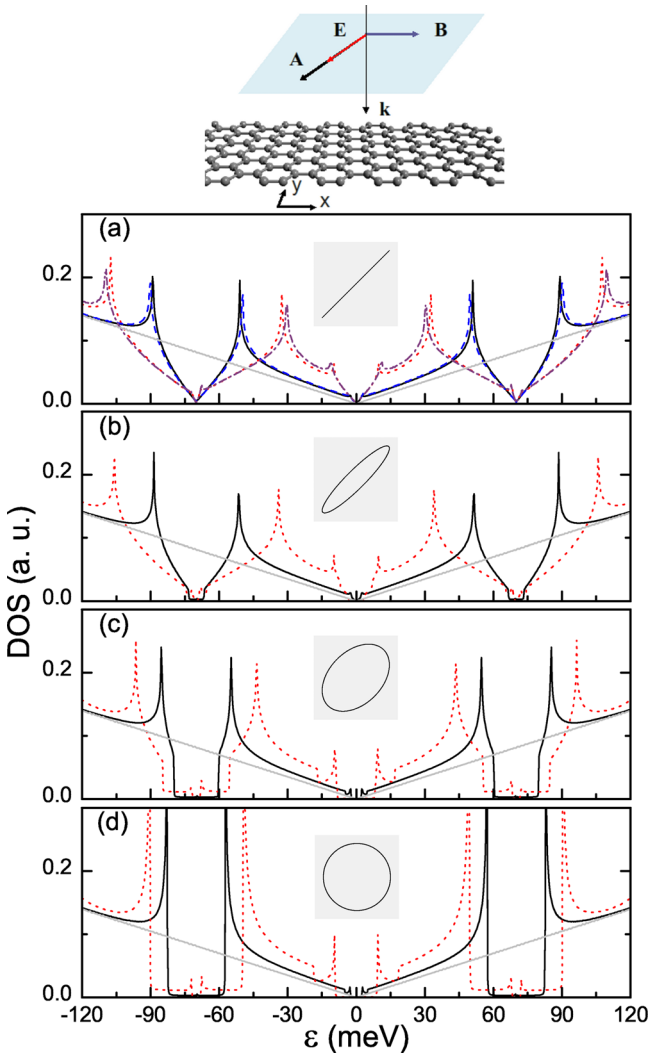

FIG. 1. (Color online) Scheme of the considered setup, where a laser field with $\hbar\Omega=140$ meV is applied perpendicular to a graphene monolayer. DOS for (a) linear, (b) $\varphi=0.125\pi$, (c) $\varphi=0.375\pi$, and (d) circular polarizations. The black solid line is for $I=32$ mW/μm^2 while the red dashed line corresponds to $I=130$ mW/μm^2. For linear polarization these results are compared with those of a tight-binding calculation for a system with 5×10^4 channels (blue dashed and purple dash-dotted lines). For reference the zero-field DOS is shown in solid gray.

Previous studies[20,22] have considered lasers either in the far infrared ($\hbar\Omega=29$ meV) (Ref. 20) or in the visible range.[22] In the first case, the predicted gaps were of about 6 meV and the authors considered the photocurrents generated in a p-n junction. On the other hand, for a laser in the visible range, the photon energy of about 2 eV is much larger than the typical optical phonon energies (170 meV), severe corrections to the transport properties due to dissipation of the excess energy via electron–(optical)phonon interactions are expected. Besides, appreciable effects in this last case required a power above 1 W/μm^2, which could compromise the material stability. To overcome both limitations we quantitatively explore the interaction with a laser in the mid-infrared range ($\lambda=5-10$ μm), where photon energies can be made smaller than the typical optical phonon energy while keeping a much lower laser power. Furthermore, we show that the polarization, whose role was overlooked, can be used as a control variable.

Figure 1 shows how the dc DOS (defined as in Ref. 22)

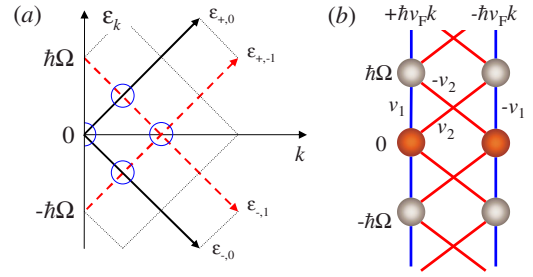

FIG. 2. (Color online) (a) Scheme of the quasienergies as a function of k. (b) Representation of the Floquet Hamiltonian for the $\mathbf{k}\cdot\mathbf{p}$ approach. Here, the direct hopping $v_1=eA_0v_F/2(\cos\alpha+e^{-i\varphi}\sin\alpha)$ sets the transition amplitude between Floquet states conserving pseudospin. In contrast, the off-diagonal term $v_2=i(eA_0v_F/2)(e^{-i\varphi}\cos\alpha-\sin\alpha)$ introduces an inelastic backscattering process that simultaneously enables both m and pseudospin transitions.

evolves as the polarization changes. Already for linear polarization (upper panel) one can find some surprises not reported before; (i) close to the Dirac point, the DOS is enhanced as compared to the case without laser (red dotted line). The DOS increases linearly but with a different slope. (ii) Close to $\pm\hbar\Omega/2$, stronger effects lead to a depletion of the states but without reaching a full gap. The counterpart of this depletion is given by the peaks in the DOS around the depletion area. More accurate calculations based on a tight-binding model in a micrometer-sized sample interacting with a linearly polarized field confirm these findings (top panel).

The panels in Fig. 1 show how these features change with the laser polarization; (i) close to the Dirac point a gap opens and the structure of the side peaks is severely modified. (ii) The depletion areas around $\pm\hbar\Omega/2$ transform into gaps whose widths are maximum for circular polarization.

To rationalize the behavior observed in Fig. 1 we resort to the Floquet picture explained above. A scheme with the relevant states close to the Dirac point is shown in Fig. 2. On the left panel, one can see the dispersion relation for the states $\{|\mathbf{k},n\rangle_{\pm}\}$ for $n=0$ (black solid lines) and $n=\pm1$ (red dashed lines), the scheme on the right panel shows the states represented by circles and their corresponding interactions with full lines. The effects of the ac field are expected to be stronger at the crossing points between these lines, leading to the opening of energy gaps at those points. From a geometrical argument one can see that the crossing of the states differing in one photon lies exactly at $\pm\hbar\Omega/2$. These degeneracies are lifted by the ac field leading to the gaps observed in Fig. 1. This mechanism is reminiscent of an inelastic Bragg reflection as found as a result of electron-phonon interaction in carbon nanotubes.[27] An estimation of the resulting gap gives:

$$\Delta_{k=\Omega/2v_F}\simeq eA_0v_F\sqrt{1-\cos(\varphi)\sin(2\alpha)}, \tag{2}$$

where $\alpha=\tan^{-1}(k_y/k_x)$. Equation (2) shows that the effect is linear in the field strength. Interestingly, after summing up over all directions in the two-dimensional (2D) $\mathbf{k}$-space, we see that no net gap opens in the linearly polarized case since in the orientation $\alpha=\pi/4$ both states become degenerate. However, as can be seen in Fig. 1, there is a strong modification in the DOS around $\hbar\Omega/2$. Changing the polarization away from the linear case, one sees that a *dynamical gap*[20] opens and reaches its maximum $\Delta_{\max}\simeq23$ meV (46 meV) for $I=32$ mW/μm^2 (130 mW/μm^2) in the circularly polarized case.

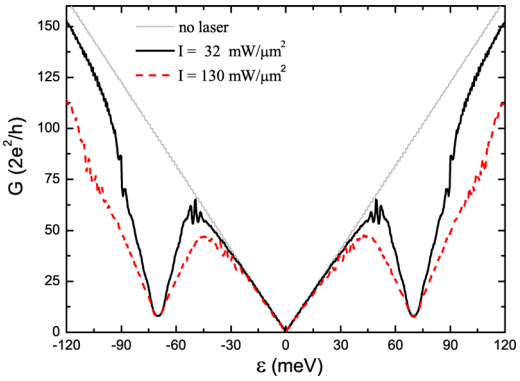

FIG. 3. (Color online) dc conductance through a graphene stripe of 1 μm $\times 1$ μm in the presence of a linearly polarized laser as a function of the Fermi energy.

Now, let us account for the phenomenon occurring at the Dirac point. Oka and Aoki (Ref. 22) predicted that circularly polarized light would induce a further gap around the Dirac point, in agreement with our Fig. 1(d). Here we see that these strong modifications extend all the way up to linear polarization. The leading contribution comes from the states connecting the degenerate ones at the Dirac point [there are four of these paths as can be seen by analyzing Fig. 2(b)]. The calculated gap reads

$$\Delta_{k=0} \simeq \frac{8}{\hbar\Omega}\mathrm{Re}\{v_1 v_2^*\} = 2\frac{(eA_0 v_F)^2}{\hbar\Omega}\sin\varphi, \tag{3}$$

which gives a quadratic dependence with the field strength and is inversely proportional to the frequency. Note also that there is no dependence of the gap with the orientation of the **k**-vector. The polarization yields a maximum gap for the circular polarization while no net gap opens for the linearly polarized case. However in Fig. 1(a) noticeable corrections around the Dirac point are observed even for linear polarization. A deeper analysis shows that this is due to the field-induced lifting of the degeneracies between the states $|\mathbf{k}, \pm 1\rangle_{\pm}$ around $\varepsilon = 0$.

Up to now, we have shown how the laser field modifies the electronic structure of 2D graphene that would be observed in any experiment carried out over a time much larger than the period T. A relevant question is if these effects would be observable in a transport experiment. To such end we compute the transport response at zero temperature using Floquet theory[26] applied to a π orbitals Hamiltonian. The electromagnetic field is accounted through the Peierls' substitution, which introduces an additional phase in the hopping γ_{ij} connecting adjacent sites $\mathbf{r}_i$ and $\mathbf{r}_j$; $\gamma_{ij} = \gamma_0 \exp[\mathrm{i}(2\pi/\Phi_0)\int_{\mathbf{r}_i}^{\mathbf{r}_j}\mathbf{A}(t)\cdot d\mathbf{r}]$, where $\gamma_0 \simeq 2.7$ eV is the hopping amplitude at zero field and Φ_0 is the quantum of magnetic flux. For computational convenience we use an armchair edge structure with the vector potential $\mathbf{A}(t) = A_x \cos(\Omega t)\hat{\mathbf{x}} + A_y \sin(\Omega t)\hat{\mathbf{y}}$.

Calculating the two-terminal dc component of the conductance as a function of Fermi energy is not, *a priori*, computationally easy. An efficient solution is achieved by decomposing the Hamiltonian into independent transversal channels as explained in Ref. 18. Although this decomposition is preserved by the interaction with the laser only for linear polarization ($A_y = 0$), it is already enough to give a flavor on the transport effects. Figure 3 gives the computed dc conductance[2,26] for a stripe 1 μm wide and 1 μm long. One can appreciate in Fig. 3 that the strong depletion areas observed in the DOS of Fig. 1 are indeed mirrored in the dc component of the conductance. Accordingly, the predicted dynamical gaps can be unveiled through transport measurements.

In summary, we have shown that it is possible to use a laser field in the mid-infrared range to tune the electronic structure of graphene and its electrical response. The modifications are predicted to arise both around the Dirac point and at $\pm\hbar\Omega/2$. Moreover, since the results are strongly dependent on the laser polarization, it may be used as a control parameter. We encourage experimentalists to pursue this exciting line of research.

We acknowledge correspondence with J. Kono, discussions with G. Usaj and support by SeCyT-UNC and ANPCyT. LEFFT acknowledges the support from the Alexander von Humboldt Foundation and ICTP, Trieste.

[1] G. Platero and R. Aguado, Phys. Rep. **395**, 1 (2004).
[2] S. Kohler, J. Lehmann, and P. Hänggi, Phys. Rep. **406**, 379 (2005).
[3] F. Grossmann, T. Dittrich, P. Jung, and P. Hänggi, Phys. Rev. Lett. **67**, 516 (1991).
[4] D. J. Thouless, Phys. Rev. B **27**, 6083 (1983).
[5] P. W. Brouwer, Phys. Rev. B **58**, R10135 (1998).
[6] B. L. Altshuler and L. I. Glazman, Science **283**, 1864 (1999).
[7] M. Büttiker and M. Moskalets, Lect. Notes Phys. **690**, 33 (2006), and references therein.
[8] M. Switkes, C. M. Marcus, K. Campman, and A. C. Gossard, Science **283**, 1905 (1999).
[9] M. D. Blumenthal, B. Kaestner, L. Li, S. Giblin, T. J. B. M. Janssen, M. Pepper, D. Anderson, G. Jones, and D. A. Ritchie, Nat. Phys. **3**, 343 (2007); B. Kaestner, V. Kashcheyevs, S. Amakawa, M. D. Blumenthal, L. Li, T. J. B. M. Janssen, G. Hein, K. Pierz, T. Weimann, U. Siegner, and H. W. Schumacher, Phys. Rev. B **77**, 153301 (2008).
[10] P. J. Leek, M. R. Buitelaar, V. I. Talyanskii, C. G. Smith, D. Anderson, G. A. C. Jones, J. Wei, and D. H. Cobden, Phys. Rev. Lett. **95**, 256802 (2005).
[11] A. Srivastava, R. Srivastava, J. Wang, and J. Kono, Phys. Rev. Lett. **93**, 157401 (2004).
[12] F. Reckermann, J. Splettstoesser, and M. R. Wegewijs, Phys. Rev. Lett. **104**, 226803 (2010).
[13] S. Kurth, G. Stefanucci, E. Khosravi, C. Verdozzi, and E. K. U. Gross, Phys. Rev. Lett. **104**, 236801 (2010).
[14] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. **81**, 109 (2009); N. M. R. Peres, *ibid.* **82**, 2673 (2010).
[15] R. Saito, G. Dresselhaus, and M. S. Dresselhaus, *Physical Properties of Carbon Nanotubes* (Imperial College Press, London, 1998); J.-C. Charlier, X. Blase, and S. Roche, Rev. Mod. Phys. **79**, 677 (2007).
[16] E. Prada, P. San-Jose, and H. Schomerus, Phys. Rev. B **80**, 245414 (2009).
[17] R. Zhu and H. Chen, Appl. Phys. Lett. **95**, 122111 (2009).
[18] C. G. Rocha, L. E. F. Foa Torres, and G. Cuniberti, Phys. Rev. B **81**, 115435 (2010); L. E. F. Foa Torres and G. Cuniberti, Appl. Phys. Lett. **94**, 222103 (2009).
[19] F. Xia, T. Mueller, Y.-m. Lin, A. Valdes-Garcia, and P. Avouris, Nat. Nanotechnol. **4**, 839 (2009).
[20] S. V. Syzranov, M. V. Fistul, and K. B. Efetov, Phys. Rev. B **78**, 045407 (2008).
[21] F. J. Lopez-Rodriguez and G. G. Naumis, Phys. Rev. B **78**, 201406(R) (2008).
[22] T. Oka and H. Aoki, Phys. Rev. B **79**, 081406(R) (2009).
[23] D. S. L. Abergel and T. Chakraborty, Appl. Phys. Lett. **95**, 062107 (2009).
[24] T. Ando, Semicond. Sci. Technol. **15**, R13 (2000); D. P. DiVincenzo and E. J. Mele, Phys. Rev. B **29**, 1685 (1984).
[25] H. M. Pastawski and E. Medina, Rev. Mex. Fis. **47**, 1 (2001).
[26] L. E. F. Foa Torres, Phys. Rev. B **72**, 245339 (2005).
[27] L. E. F. Foa Torres and S. Roche, Phys. Rev. Lett. **97**, 076804 (2006); Phys. Rev. B **78**, 035412 (2008).