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Optical properties of two new Dirac semimetals: 8-Pmmn borophene and Kekulé-Y modulated graphene

Saúl A. Herrera and Gerardo G. Naumis
Depto. de Sistemas Complejos, Instituto de Física, Universidad Nacional Autónoma de México (UNAM)

Instituto de Física UNAM

CONACYT

INTRODUCTION

We present results obtained from theoretical studies on the electronic and optical properties of two Dirac semimetals of recent interest: 8-Pmmn borophene [1] and Kekulé-Y modulated graphene [2,3]. The former exhibits an anisotropic Fermi velocity and a strong electron-hole asymmetry [4,5], while the latter presents a valley-momentum coupling and two species of Dirac fermions [6,7]. We show that the electron-hole asymmetry in borophene and the valley coupling in Kekulé modulated graphene introduce a similar split in the interband conductivity of both materials. Furthermore, in Kekulé modulated graphene the valley coupling introduces a second plasmonic branch and a tunable absorption peak originating from low energy intervalley transitions.

I. Optical conductivity of 8-Pmmn borophene

8-Pmmn borophene exhibits:

- Semimetallic energy dispersion
- Anisotropic Fermi velocity
- Strong electron-hole asymmetry

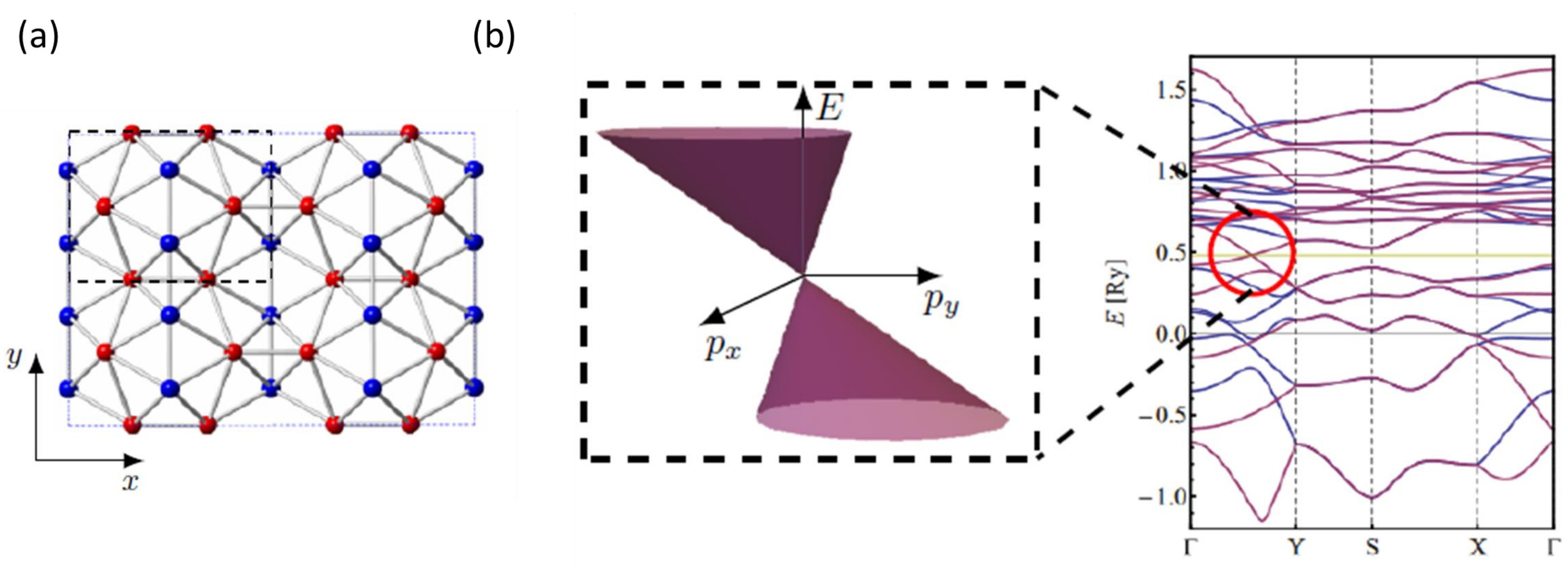

Fig. 1. (a) Atomic structure of 8-Pmmn borophene. (b) Electronic spectrum: the low-energy semimetallic dispersion exhibits an anisotropic Fermi velocity and strong electron-hole asymmetry. Figures taken from [1,2].

Anisotropic optical conductivity

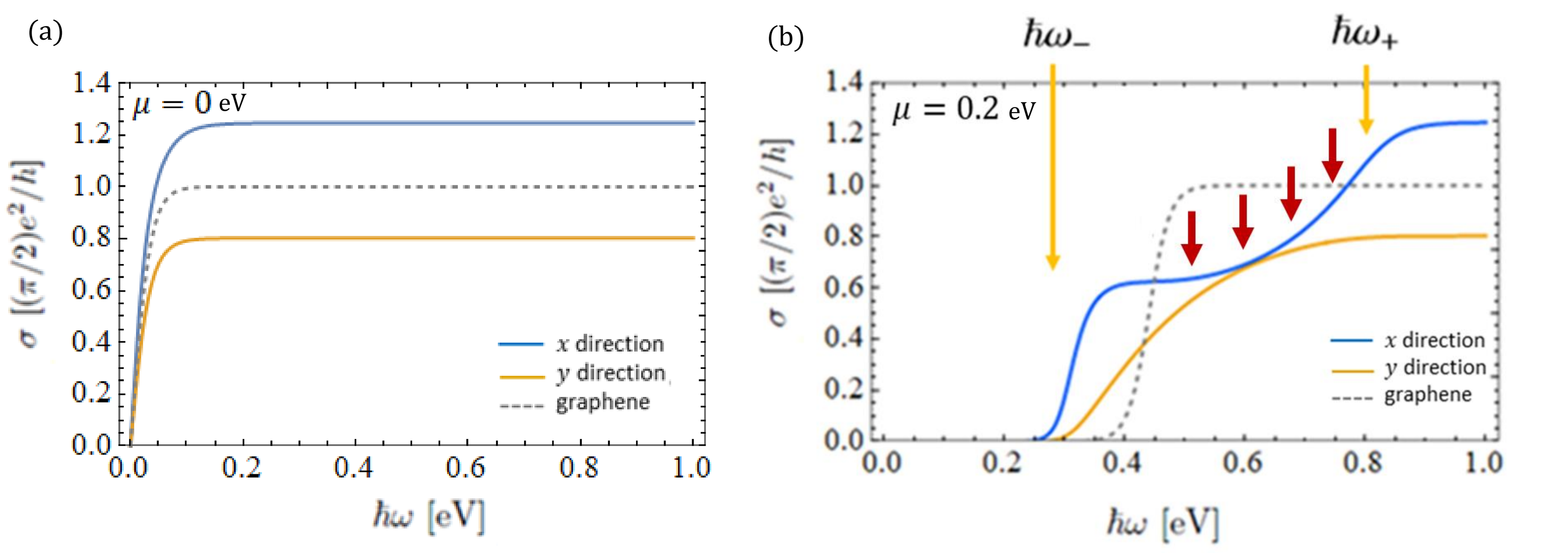

Fig. 2. Interband conductivity of borophene compared to that of graphene. (a) At $\mu = 0$, the anisotropic Fermi velocity scales the conductivity in a direction-dependent manner, while maintaining the overall step-like shape. (b) At $\mu > 0$, the electron-hole asymmetry γ in borophene becomes important, reducing the optical absorption in the x component around $\hbar\omega \sim 2\mu$, splitting the step-like conductivity into two half steps.

Interband transitions

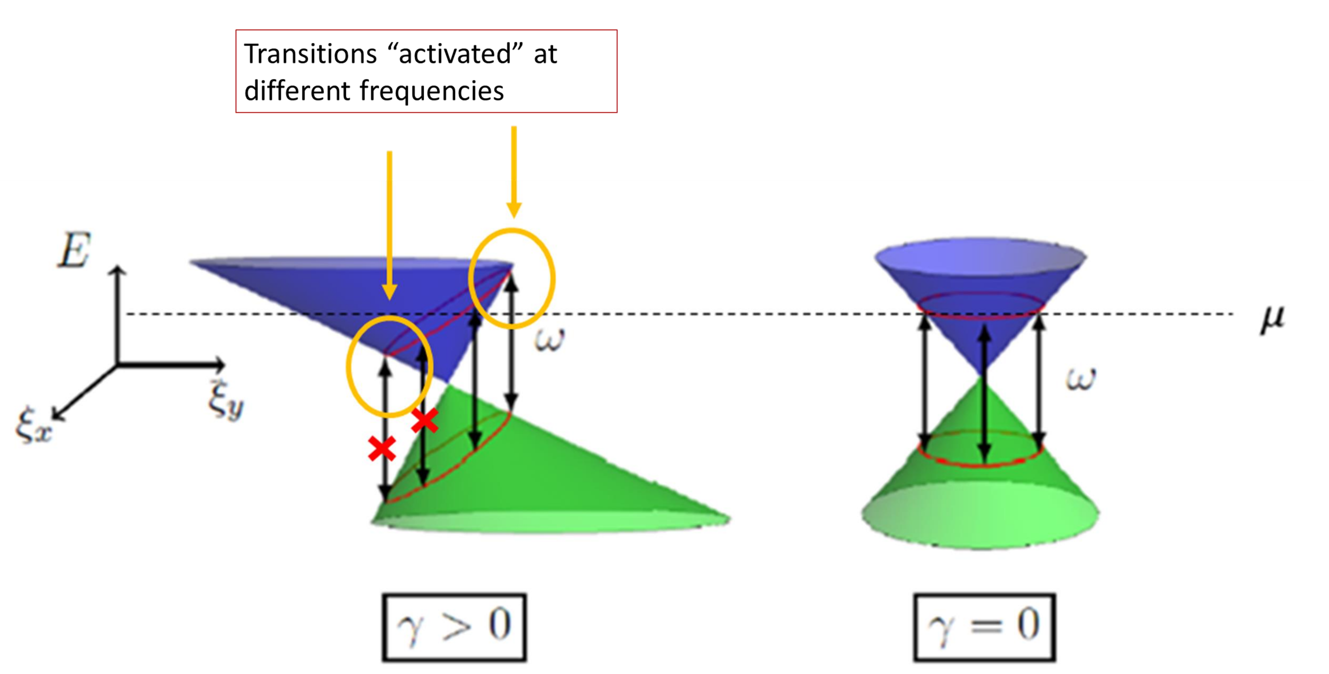

Fig. 3. Optical transitions in semimetallic borophene compared to those in graphene. Due to borophene's electron-hole asymmetry (γ>0), optical transitions are shifted in energy. At finite doping the transitions on one side of the dispersion are forbidden due to Pauli blocking, occurring only at higher frequencies and leading the step-like conductivity to split into two half steps.

II. Dynamic polarization and plasmons in Kekulé-Y modulated graphene

Kekulé modulated graphene exhibits:

- Valley-momentum coupling
- Two species of Dirac fermions
- Tunable optical absorption

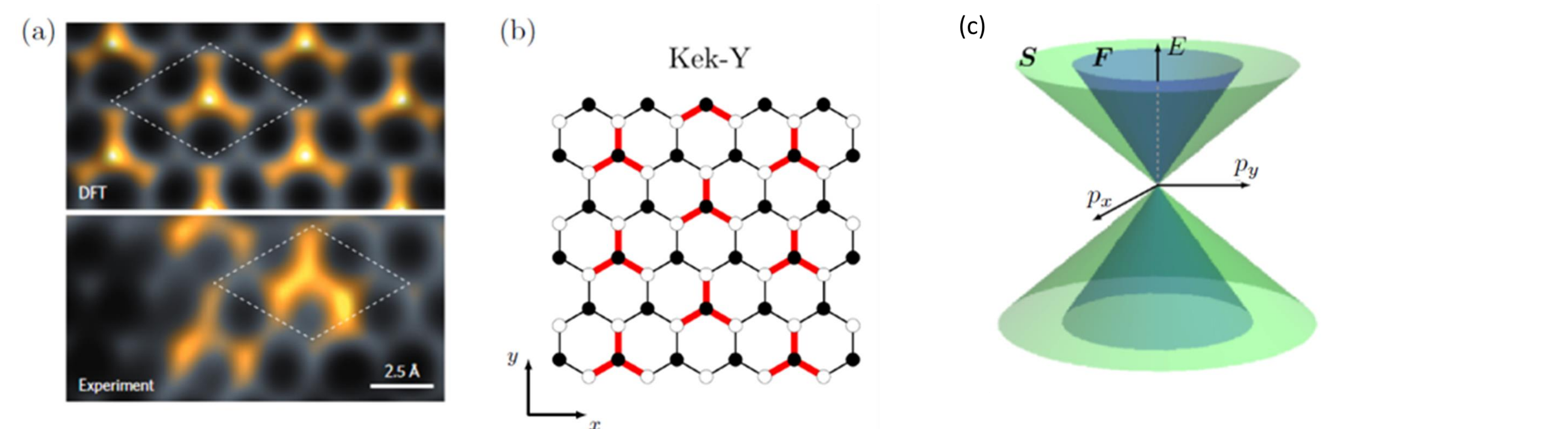

Fig. 4. (a) Graphene layer grown over Cu(111) exhibiting Kekulé-Y modulation. Taken from [3]. (b) The atomic lattice of Kekulé-Y modulated graphene. (c) Low-energy electronic dispersion: the K and K' valleys in graphene fold onto the Γ point and the Fermi velocity splits $v_0 \to v_0(1 \pm \Delta_0)$ due to the valley-coupling amplitude Δ_0.

"Splitting" of the polarizability

Tunable intervalley conductivity

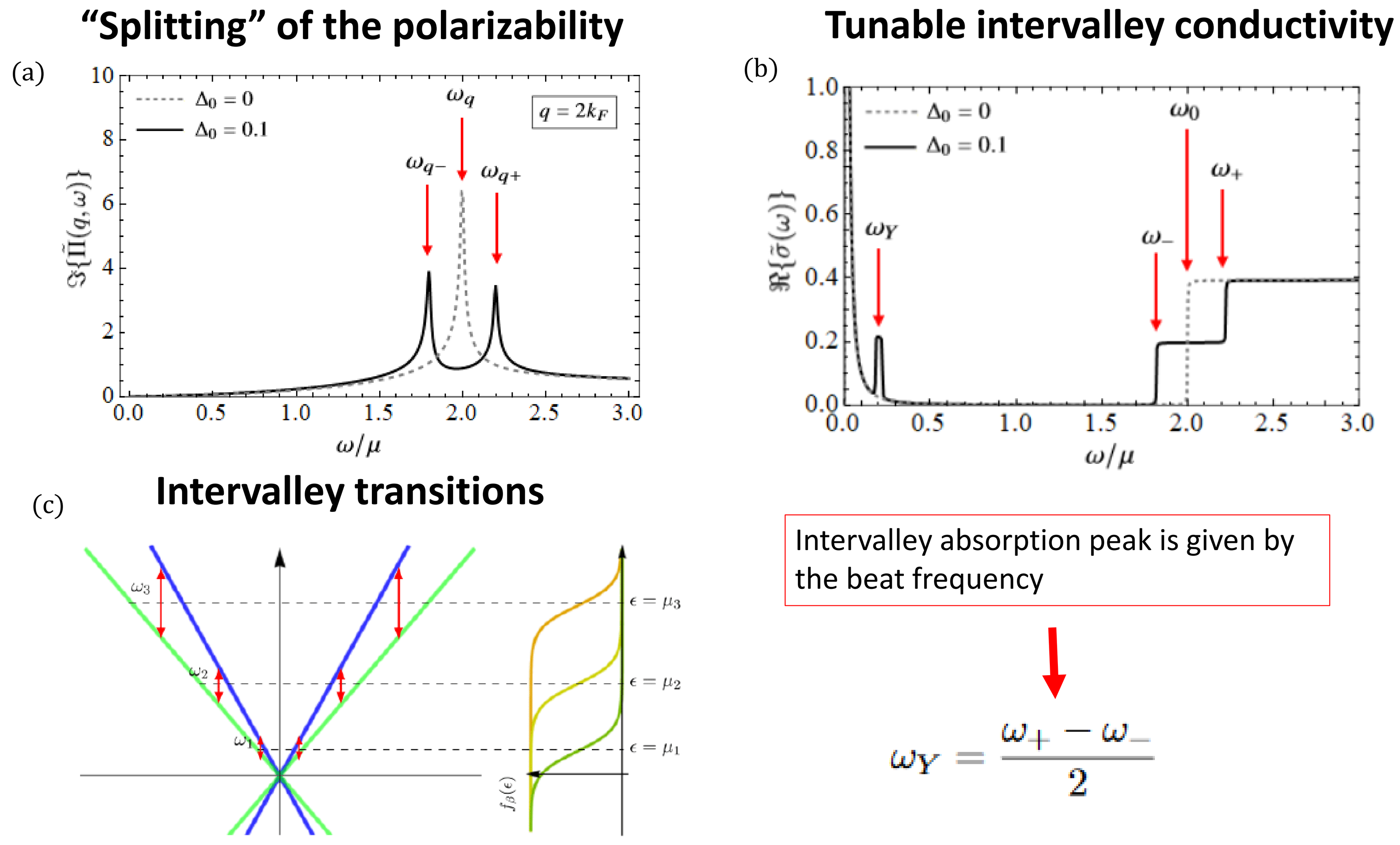

Fig. 5. (a) Imaginary part of the dynamic polarization of graphene with ($\Delta_0 > 0$) and without ($\Delta_0 = 0$) Kekulé modulation: the Kekulé modulation "splits" graphene's spectrum, making evident the broken valley degeneracy. (b) Optical conductivity of Kekulé modulated graphene: an absorption peak due to intervalley transitions appears at low frequencies and the step-like interband conductivity of graphene splits into two half steps. (c) Intervalley optical transitions in Kek-Y graphene.

Second plasmonic branch

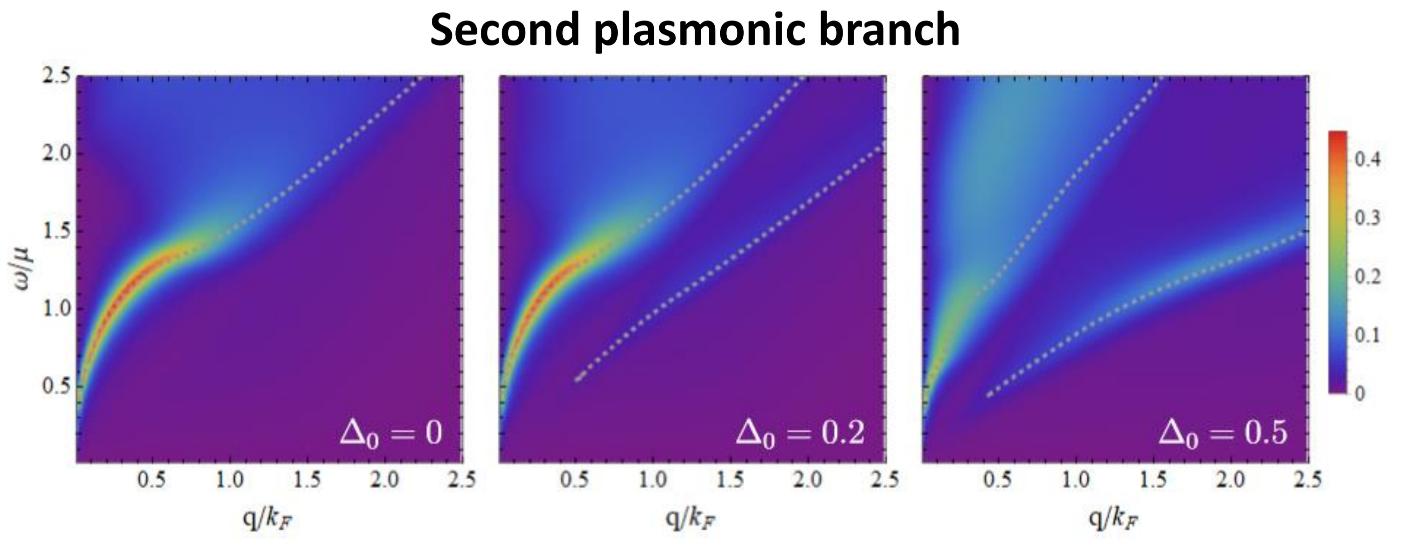

Fig. 6. Plasmon dispersion (dashed lines) and loss function (color plot) for graphene with different values of the Kekulé-Y valley coupling Δ_0. The valley coupling introduces a second plasmonic branch in the diffusive regime.

CONTACT PERSON

Saúl A. Herrera
herrera.st.lp@gmail.com
Depto. de Sistemas Complejos, Instituto de Física, Apdo. Postal 01000, Ciudad de México, México

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