Photoelectrons Unveil Topological Transitions in Graphen-like Systems

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Workshop on Next Generation Quantum Materials

http://fisica.cab.cnea.gov.ar/solidos/

Outline of the Talk

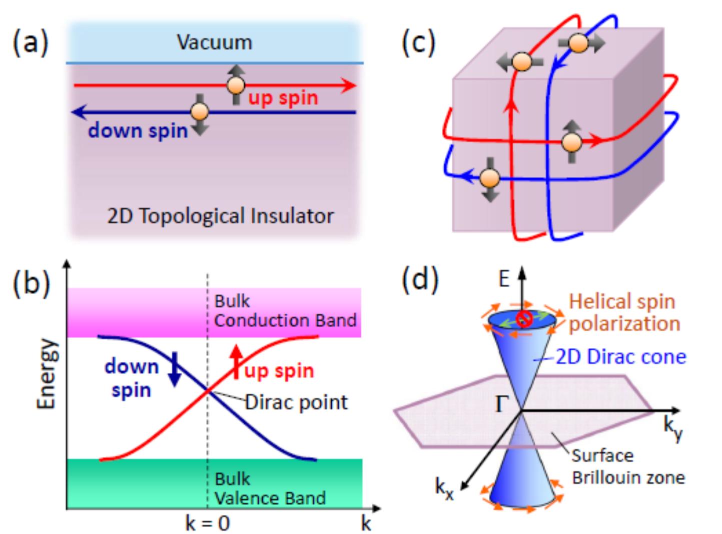
1.- INTRODUCTION
Topological Insulators
2.- FLOQUET TI – the case of GRAPHEN
4.- THEORY of Tr-ARPES
5.- RERULTS
5.- FINAL REMARCKS

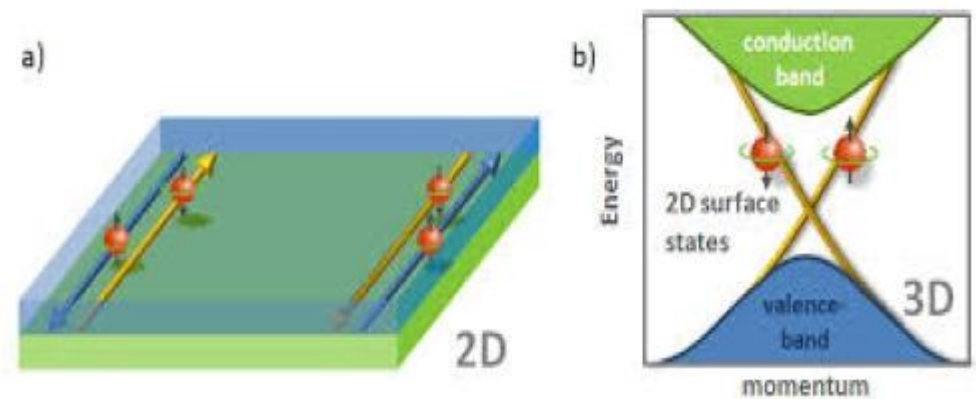
Lucila Peralta Gavensky

Gonzalo Usaj

Topological Insulator

In Topological Insulators the bulk gaps are bridged by surface states.



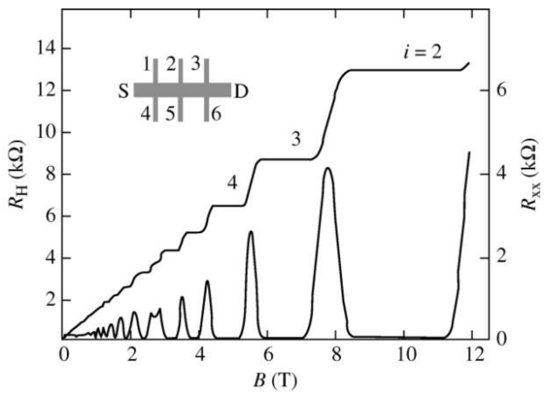


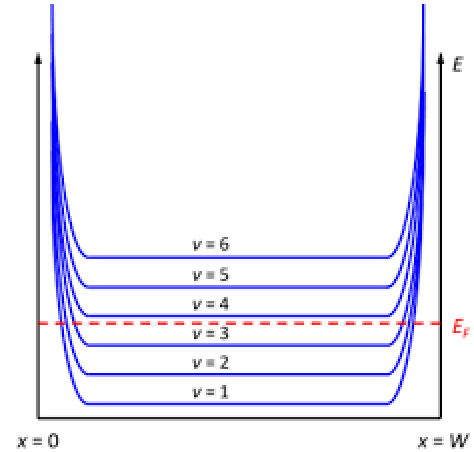
FROM: Y. Ando, J. Phys. Soc. Jpn. 82, 102001 (2013)

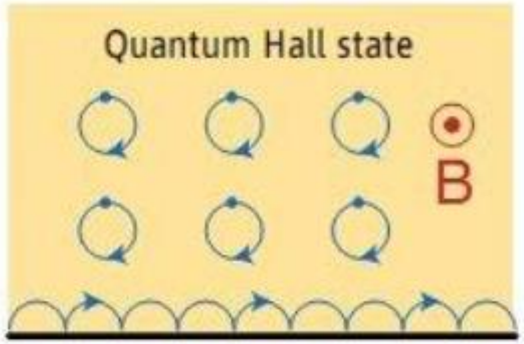
L. Fu and C. L. Kane, Phys. Rev. B 76, 045302 (2007).
M.Hasan and C. Kane, Rev. Mod. Phys. 82,3045 (2010).

In these systems the Spin-Orbit coupling is an essential ingredient !

2D electron gas QHE the first known Topological Insulator







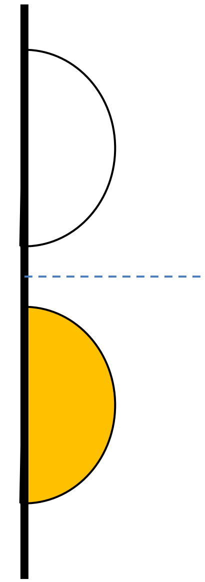
D. J. Thouless, M. Kohmoto, M. P. Nightingale,
M. den Nijs, Phys. Rev. Lett. 49, 405 (1982)

C. L. Kane, and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).
Graphene with SOC is a 2D TI
J. E. Moore and L. Balents: Phys. Rev. B 75 121306(R) (2007)
Extended the ideas to 3D systems
L. Fu and C. L. Kane: Phys. Rev. B 76 045302 (2007)
Proposed that BiSb alloys should be a TI

Experiments by Hsieh et al Nature (2008)

The Bulk – Boundary Correspondence Principle

Consider the Hall conductivity of a 2D system with full bands



$$\sigma_{xy} = \frac{e^2}{\hbar}\int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2}\underbrace{\Omega_{k_x k_y}}_{\text{Kubo} \rightarrow \text{Current –current correlation function}}\ ,$$

$$\psi(r) = e^{ik\cdot r}u_{n,k}(r)$$

For the n$^{\text{th}}$ band can be written as

$$\Omega_n(k) = i\langle \nabla_k u_n(k)| \times |\nabla_k u_n(k)\rangle$$ Berry curvature

Topological invariant: The Chern number

$$C_n = \frac{1}{2\pi}\int_{BZ} d^2k\,\Omega_n(k)$$

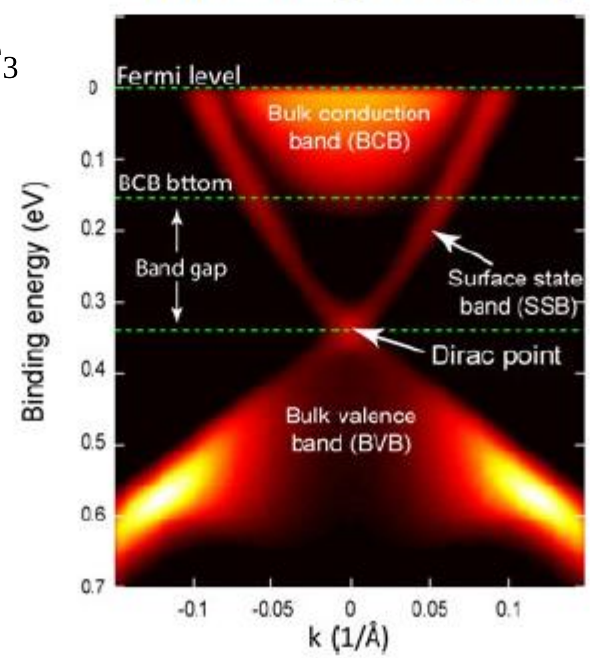
C_n is an integer number

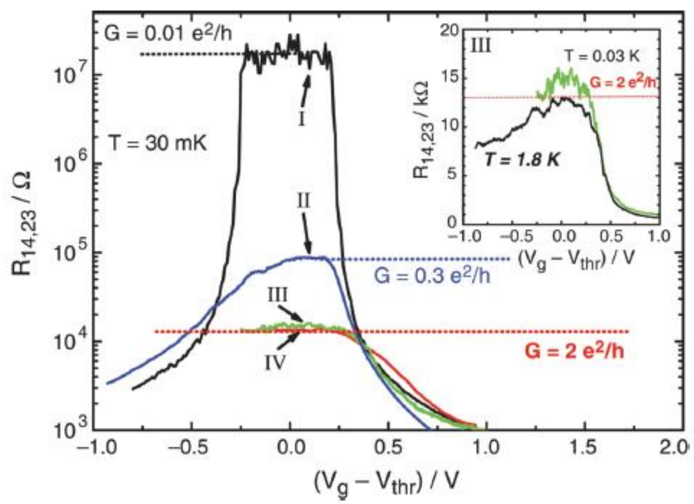
Since it is the Berry curvature Ω(k) what encodes all the topological properties of the wave functions, it would be important to find experimental techniques able to measure this quantity.

Experimentally it has easier to see the effects of a non-trivial Berry curvature (the existence of topologically protected edge states) than their origin (the structure of the Berry curvature)

Science **325**, 178 (2009)

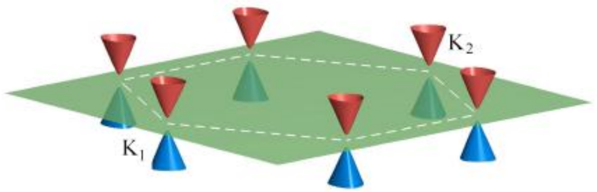
Bi_2Te_3





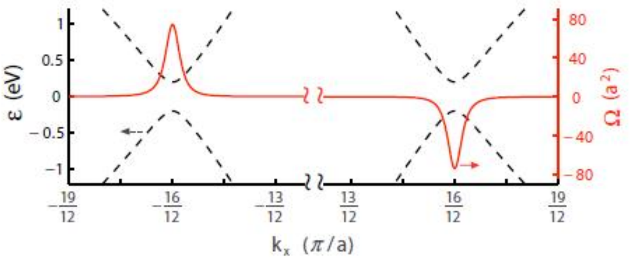
Transport in a HgTe quantum well
Science **318** 766 (2007)

In Graphene and Graphene-like systems, Pump and Probe ARPES with the appropriate x-Ray polarization and energy can unambiguously detect topological transitions, i.e. changes of the Chern numbers

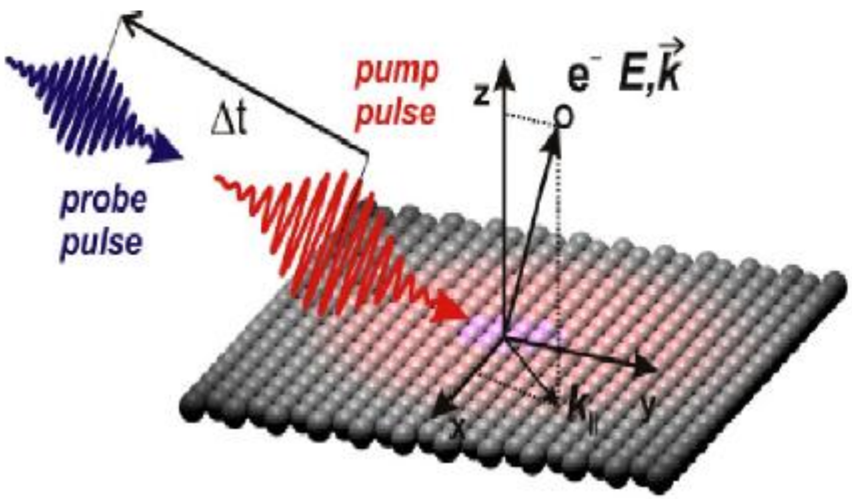


This is due to:

1.- Structure of the dipole matrix elements (photo-excitation process)
2.- The largest contribution to the Berry curvature comes fro two hot spots: the Dirac points



Xiao, Cheng and Niu Rev. Mod Phys (2009)



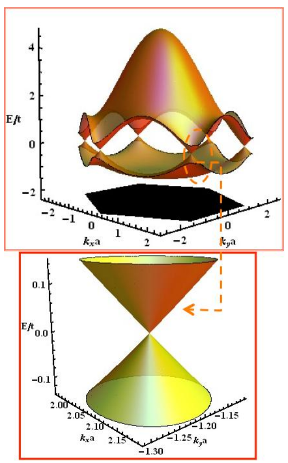
Floquet topological insulator in semiconductor quantum wells

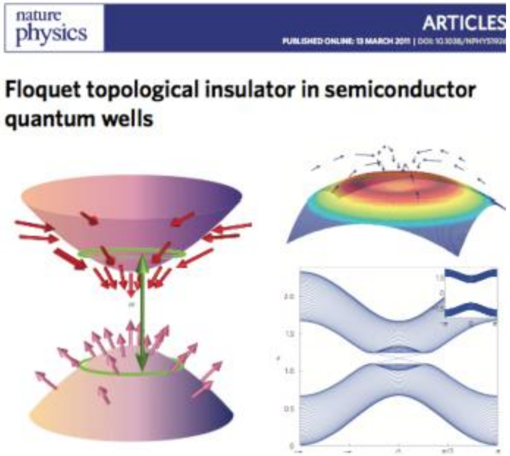
Netanel H. Lindner, Gil Refael and Victor Galitski.

NATURE PHYSICS JUNE 2011

In some (non-topological) semiconductors, the Chiral surface states can be induced by Irradiation with Microwave Frequencies

Floquet-Topological Insulators

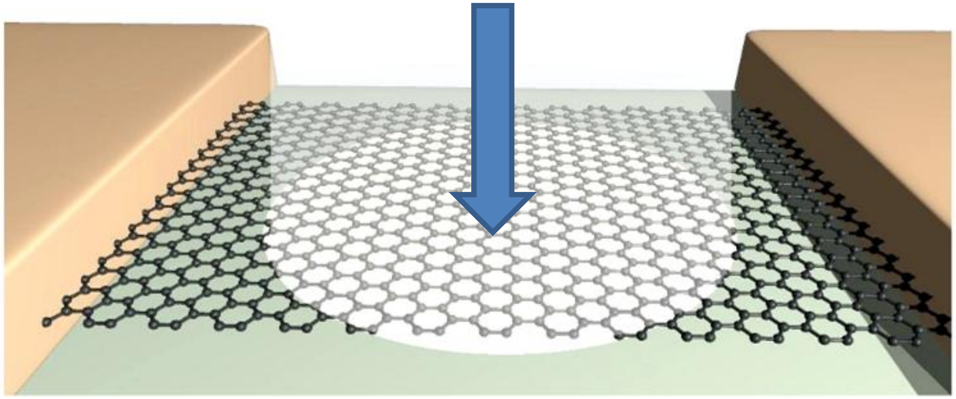




Lindner, Refael & Galitski (2010)

Graphene is not an Insulator , however ….

In periodically driven graphene, dynamical gaps may be generated and in special cases, these gaps are bridged by edge states like in a TI

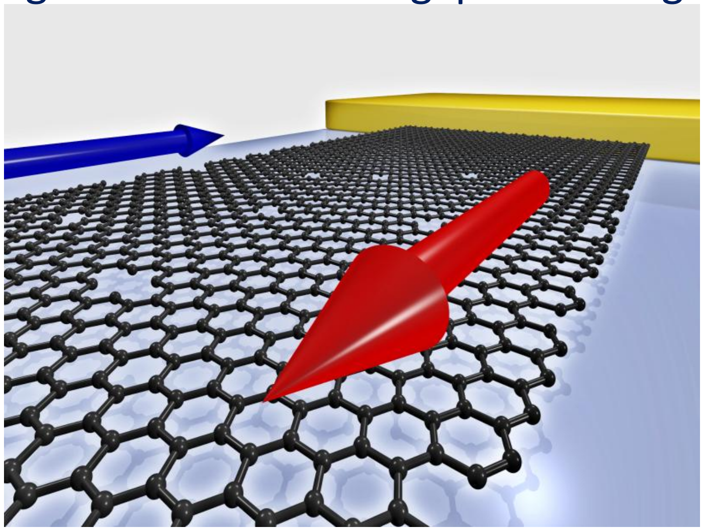


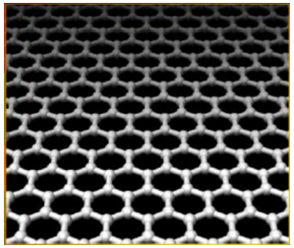
Radiation is described through a time dependent vector potential **A**(t)

$$\mathbf{A}(t) = A_0(\cos(\Omega t), \sin(\Omega t))$$

We have to deal with a time-dependent Hamiltonian H(t)

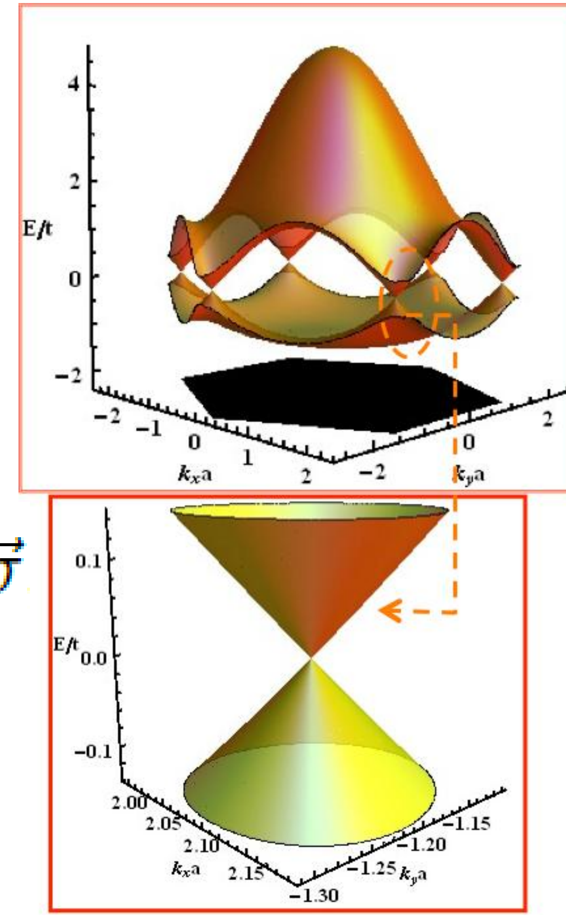
The idea is that radiation modifies the electronic structure opening (dynamical) gaps.
Radiation induces topological states and the gaps are bridged by edge-states like in TI



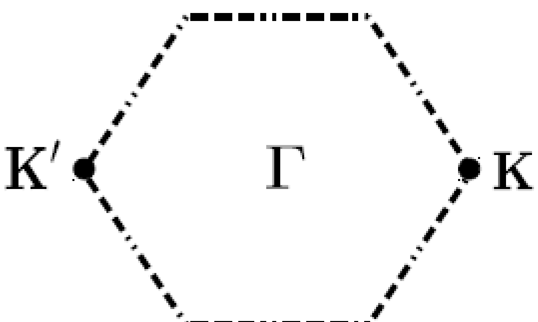


Graphene and Dirac Fermions

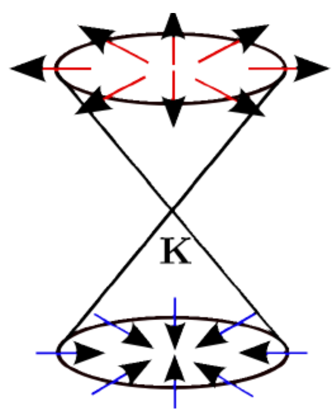
$$H = -t \sum_{\langle i,j \rangle} a_i^{\dagger} b_j + h.c$$



$$\hat{\mathcal{H}}_{\mathbf{k}\tau} = \hbar v_f (\tau k_x, k_y) \cdot \vec{\sigma} = v_f (\tau p_x, p_y) \cdot \vec{\sigma}$$



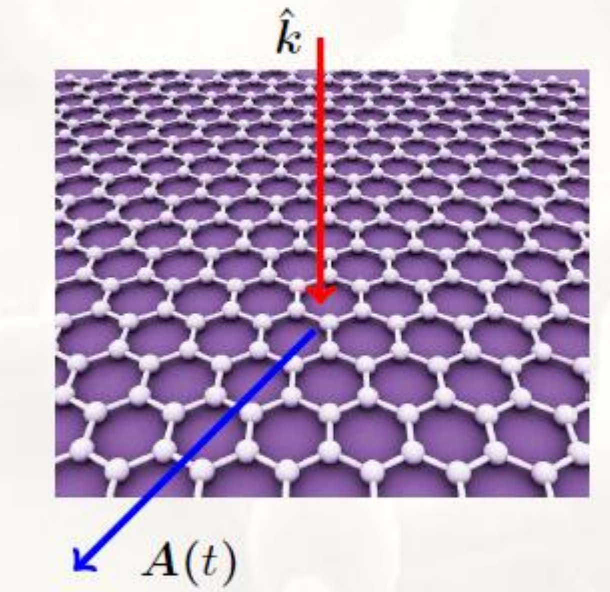
$$\mathbf{K}_{\tau} = \left(\tau \frac{4\pi}{3\sqrt{3}a}, 0\right)$$



Dynamically driven graphene

$$\hat{\mathcal{H}}(t) = v_F\, \boldsymbol{\sigma} \cdot \left[\boldsymbol{p} + \frac{e}{c} \boldsymbol{A}(t) \right]$$

$$\boldsymbol{\sigma} = (\sigma_x, \sigma_y),\ \boldsymbol{A}(t) = \mathrm{Re}\left\{ \boldsymbol{A}_0 e^{\mathrm{i}\Omega t} \right\}.$$



$$\boldsymbol{A}_0 = A_0(\hat{x} + \mathrm{i}\hat{y}).$$

Periodically driven systems - Floquet Theory

Space periodicity
Bloch Theorem

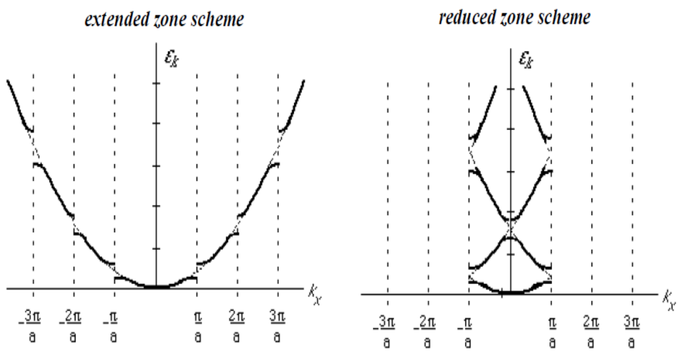
$$U(r) = U(r+R)$$

Wave Function

$$\psi(r) = e^{ik\cdot r} u_{n,k}(r)$$

k Quasi-momentum

$$u_{n,k}(r) = u_{n,k}(r+R)$$



Time periodicity
Floquet Theorem

$$H(r,t) = H(r,t+T)$$

Wave Function

$$\psi(r,t) = e^{-i\varepsilon_\alpha t/\hbar} u_\alpha(r,t)$$

ε_α Quasi-energy

$$u_\alpha(r,t) = u_\alpha(r,t+T)$$

Like in the Bloch case, here the quasi-energies can be taken in the reduced 1rst time-BZ

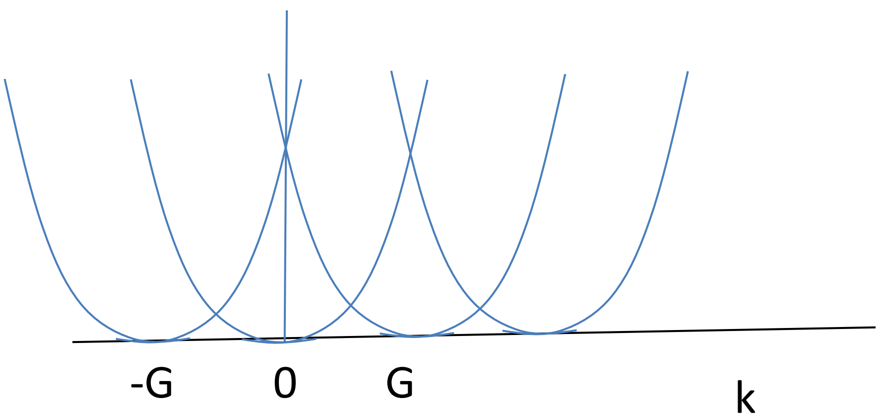
$$-\frac{\hbar\Omega}{2} \leq \varepsilon_\alpha \leq \frac{\hbar\Omega}{2}$$

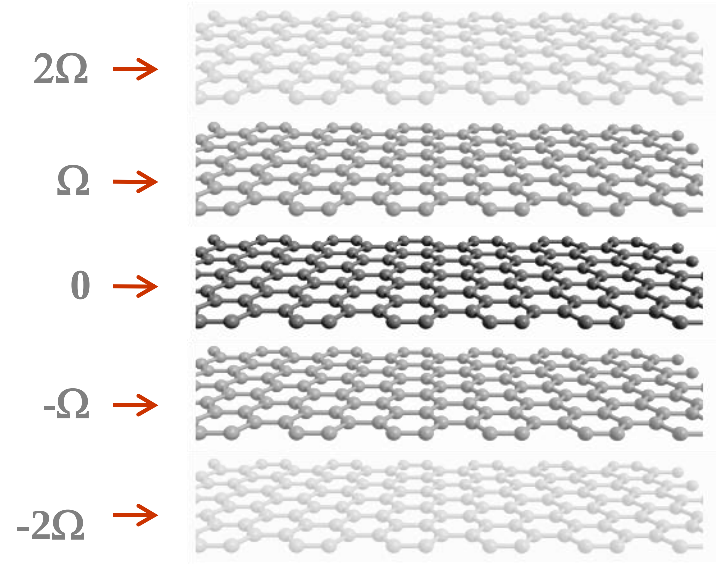
However, for clarity, I will show results in the extended zone

$$\psi(r,t) = e^{-i\varepsilon_\alpha t/\hbar} u_\alpha(r,t)$$

$$i\hbar \frac{\partial \psi(r,t)}{\partial t} = H\psi(r,t) \quad \Rightarrow \quad [H - i\hbar \frac{\partial}{\partial t}] u_\alpha(r,t) = \varepsilon_\alpha u_\alpha(r,t)$$

$$u_\alpha(r,t) = \sum_m u_{\alpha,m}(r)\, e^{im\Omega t}$$



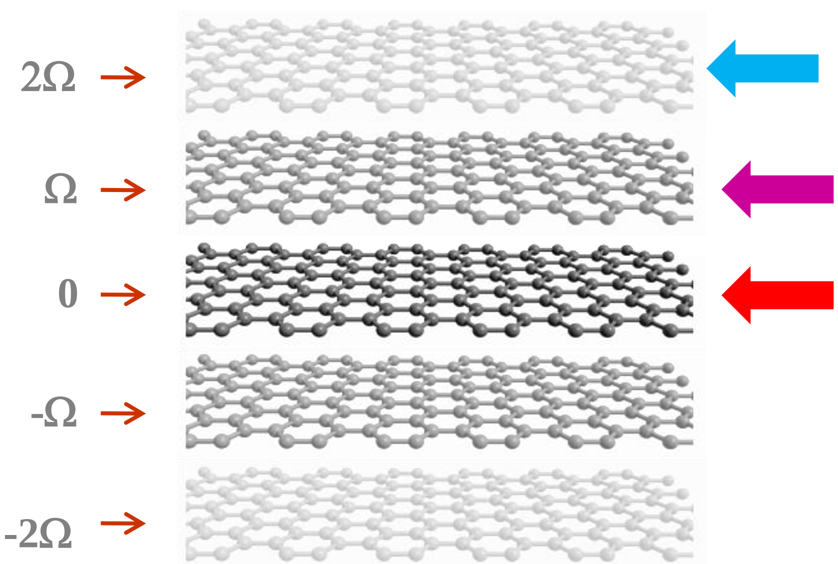


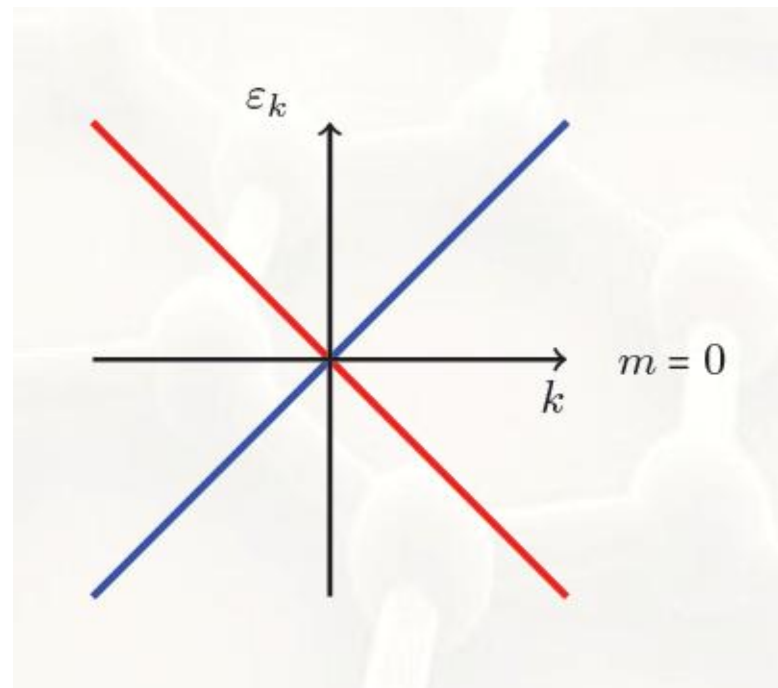
Bloch U(r)

Floquet U(t)

The Floquet Hamiltonian for graphene

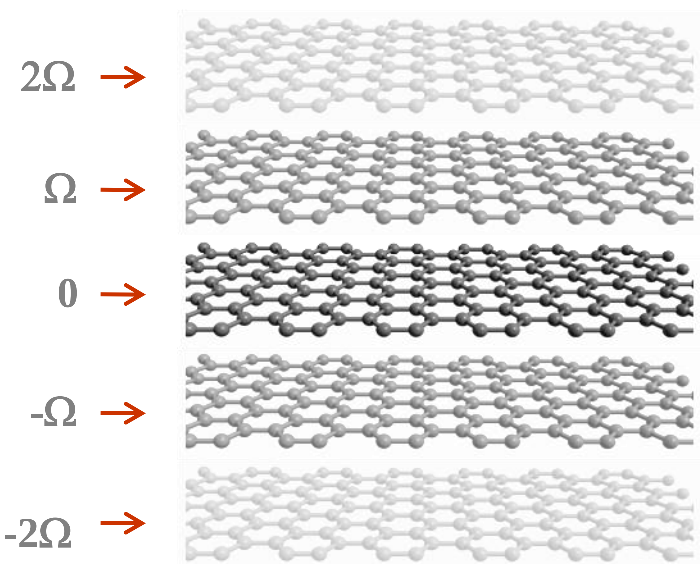
$$\tilde{\mathcal{H}}_F^\infty = \left(\begin{array}{c|c|c|c|c|c}
\ddots & \vdots & \vdots & \vdots & \vdots & \iddots \\ \hline
\cdots & \boxed{v_F \boldsymbol{p}\cdot\boldsymbol{\sigma} + 2\hbar\Omega I} & \frac{v_F e}{2c} A_0 \sigma_- & 0 & 0 & \cdots \\ \hline
\cdots & \frac{v_F e}{2c} A_0 \sigma_+ & \boxed{v_F \boldsymbol{p}\cdot\boldsymbol{\sigma} + \hbar\Omega I} & \frac{v_F e}{2c} A_0 \sigma_- & 0 & \cdots \\ \hline
\cdots & 0 & \frac{v_F e}{2c} A_0 \sigma_+ & \boxed{v_F \boldsymbol{p}\cdot\boldsymbol{\sigma}} & \frac{v_F e}{2c} A_0 \sigma_- & \cdots \\ \hline
\cdots & 0 & 0 & \frac{v_F e}{2c} A_0 \sigma_+ & v_F \boldsymbol{p}\cdot\boldsymbol{\sigma} - \hbar\Omega I & \cdots \\ \hline
\iddots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{array}\right)$$

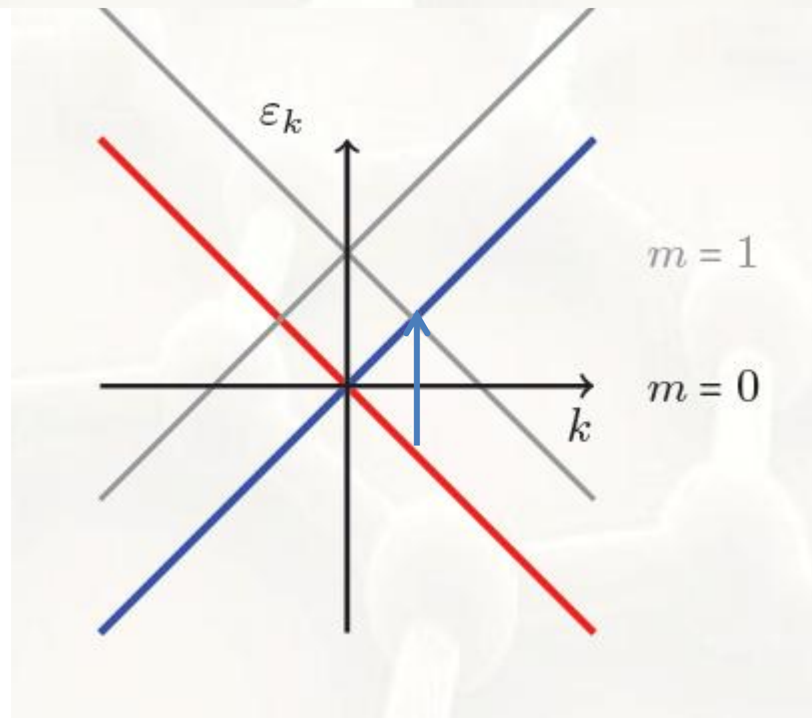


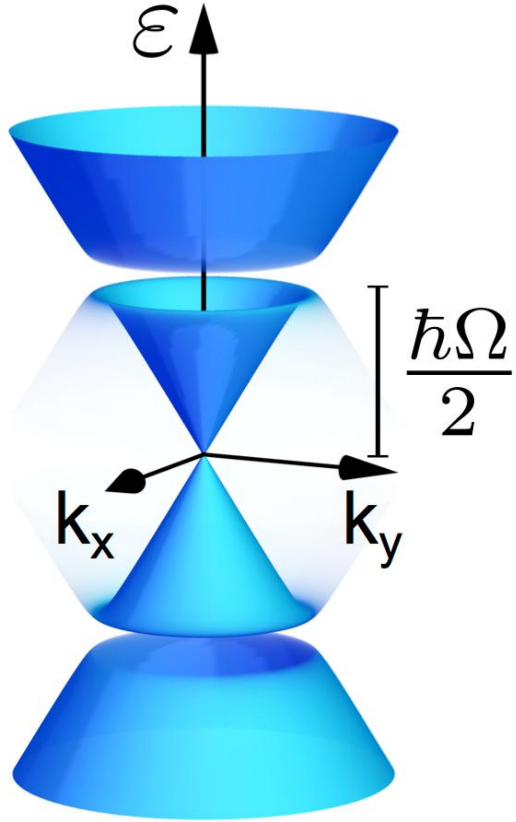


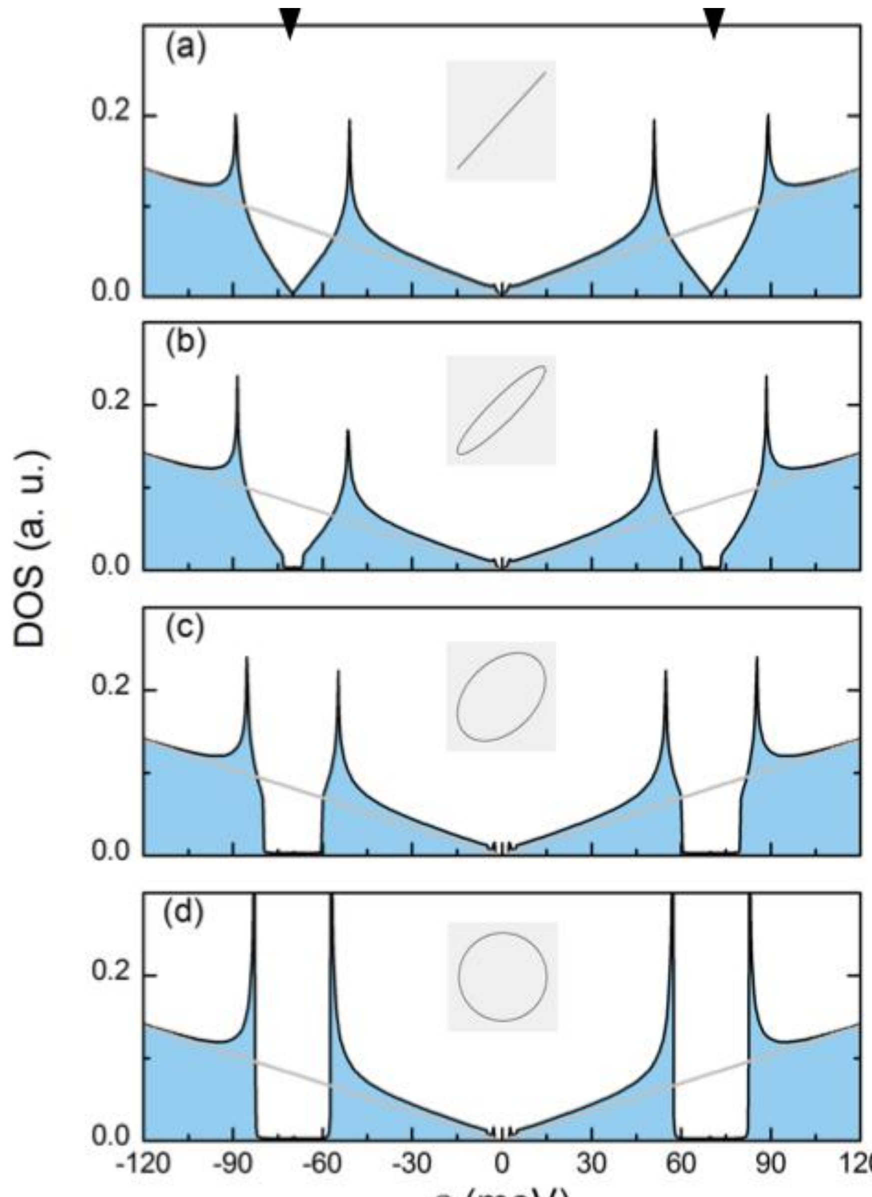
The Floquet Hamiltonian for graphene

$$\tilde{\mathcal{H}}_F^{\infty} = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & ⋰ \\ \cdots & v_F \boldsymbol{p}\cdot\boldsymbol{\sigma} + 2\hbar\Omega \boldsymbol{I} & \frac{v_F e}{2c} A_0 \sigma_- & 0 & 0 & \cdots \\ \cdots & \frac{v_F e}{2c} A_0 \sigma_+ & v_F \boldsymbol{p}\cdot\boldsymbol{\sigma} + \hbar\Omega \boldsymbol{I} & \frac{v_F e}{2c} A_0 \sigma_- & 0 & \cdots \\ \cdots & 0 & \frac{v_F e}{2c} A_0 \sigma_+ & v_F \boldsymbol{p}\cdot\boldsymbol{\sigma} & \frac{v_F e}{2c} A_0 \sigma_- & \cdots \\ \cdots & 0 & 0 & \frac{v_F e}{2c} A_0 \sigma_+ & v_F \boldsymbol{p}\cdot\boldsymbol{\sigma} - \hbar\Omega \boldsymbol{I} & \cdots \\ ⋰ & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$









T. Oka and H. Aoki, Phys. Rev. B 79, 081406 (2009).

H. L. Calvo, H. M. Pastawski, S. Roche, and L. Foa Torres, Appl. Phys. Lett. 98, 232103 (2011).

N. H. Lindner, G. Refael, and V. Galitski, Nat. Phys. 7, 490 (2011).

M. S. Rudner, N. H. Lindner, E. Berg, and M. Levin, Phys. Rev. X 3, 031005 (2013).

Physical reality of the (dynamical) gaps

Theory:

N. H. Lindner, G. Refael, and V. Galitski, Nat. Phys. 7, 490 (2011).
M. S. Rudner, N. H. Lindner, E. Berg, and M. Levin, Phys. Rev. X 3, 031005 (2013).

Observation of Floquet-Bloch states on the surface of a topological insulator

Y. H. Wang[†], H. Steinberg, P. Jarillo-Herrero & N. Gedik[*]

Science 342, 453 (2013)

Bi_2Se_3

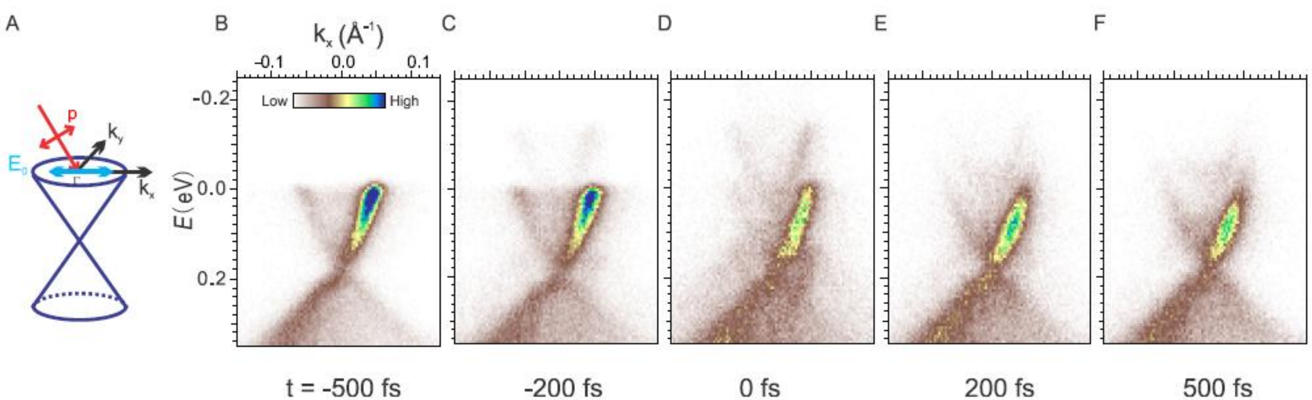
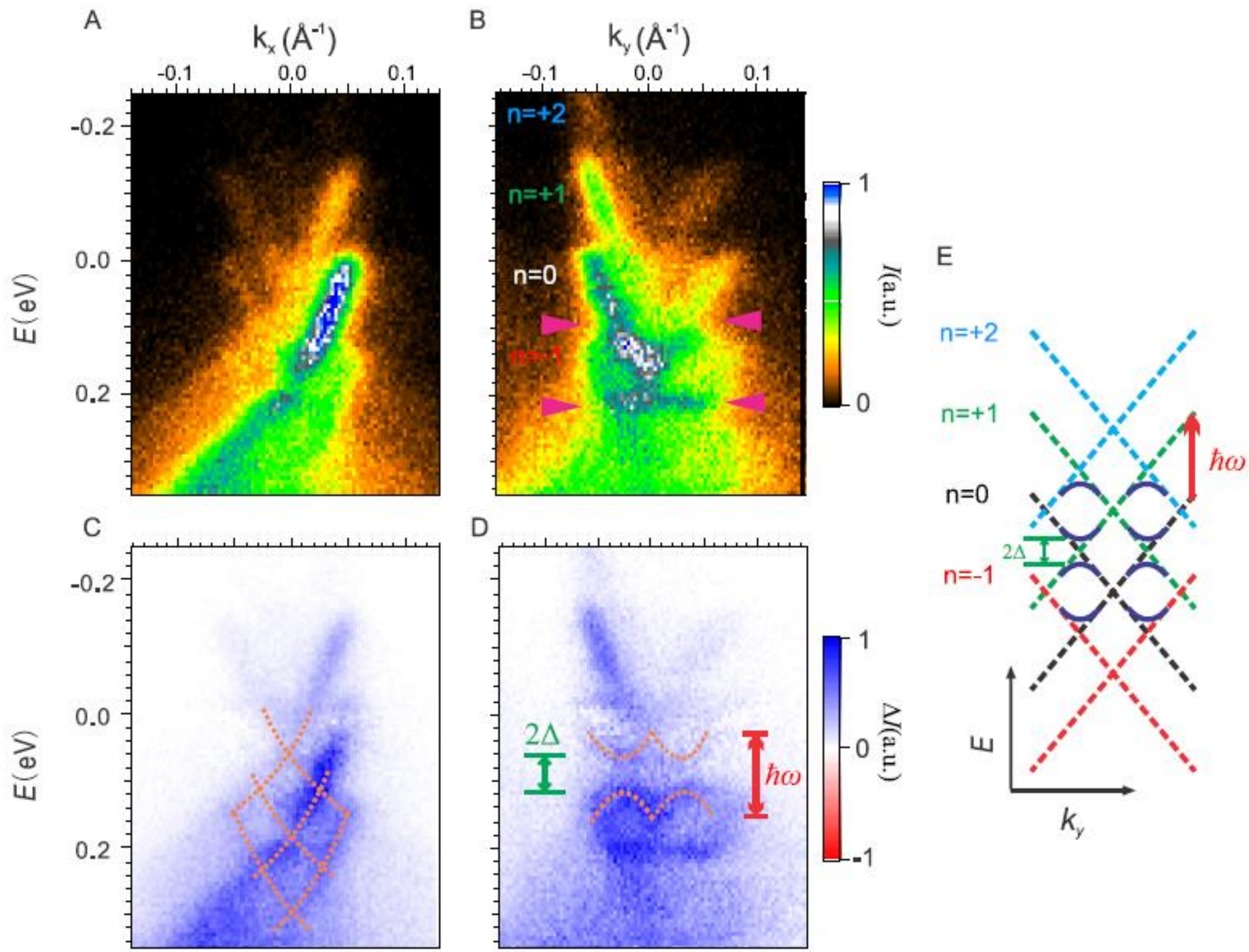
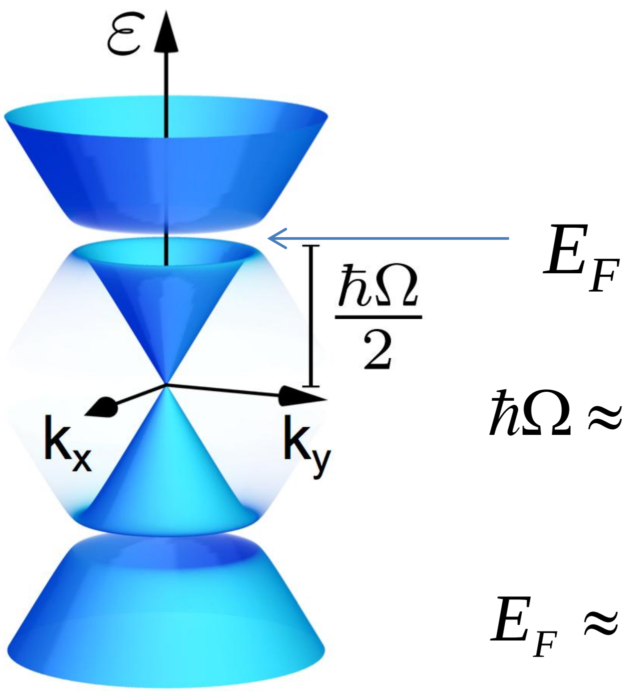


Fig. 1. Angle resolved photoemission spectra (APRES) of Bi_2Se_3. (**A**) A sketch of the experimental geometry for the p-polarized case. k_x is defined to be the in-plane electron momentum parallel to the pump scattering plane. (**B-F**) ARPES data for several pump-probe time delays t (values indicated in the figure) under strong linearly polarized mid-infrared (MIR) excitation of wavelength $\lambda = 10$ μm.



$$\hbar\Omega = 120 meV \quad 2\Delta = 62 meV$$

Physical accessibility of the gaps and chiral edge states in graphene



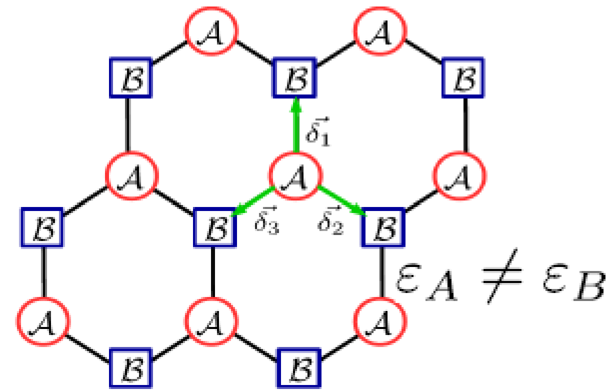
$$\hbar\Omega \approx 100\, meV \quad \rightarrow \quad \lambda \approx 10 \mu m$$

$$E_F \approx 50\, meV \;\rightarrow\; n \approx 2.5 \times 10^{11}\, cm^{-2}$$

MIR lasers (Titanium:Safire amplifier, Carbon monoxide and Carbon dioxide lasers are also in this range)

Graphene with a mass term

$$\mathcal{H}_{\mathrm{k}\tau} = \begin{pmatrix} \Delta & \hbar v_f |\vec{k}| e^{-i\tau\theta_{\vec{k}}} \\ \hbar v_f |\vec{k}| e^{i\tau\theta_{\vec{k}}} & -\Delta \end{pmatrix}$$



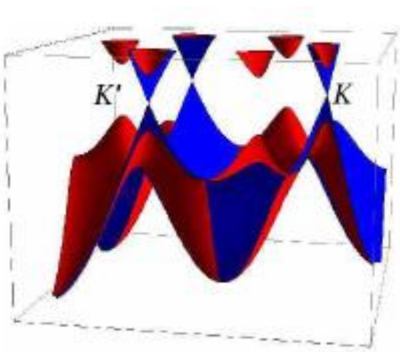
To lowest order in the amplitude of the radiation the Floquet Hamiltonian reduces to

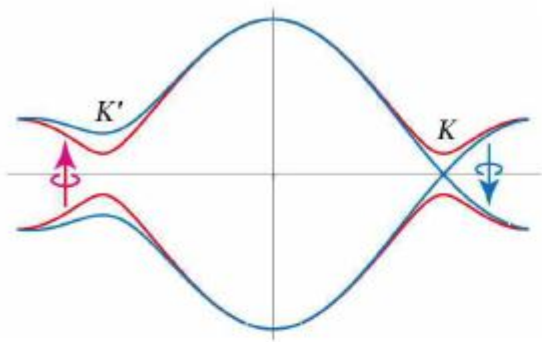
$$\widetilde{\mathcal{H}}_{\mathbf{F}\tau} = \begin{pmatrix} \tilde{\Delta}_\tau & \hbar v_f |\vec{k}| e^{-i\tau\theta_{\vec{k}}} \\ \hbar v_f |\vec{k}| e^{i\tau\theta_{\vec{k}}} & -\tilde{\Delta}_\tau \end{pmatrix}$$

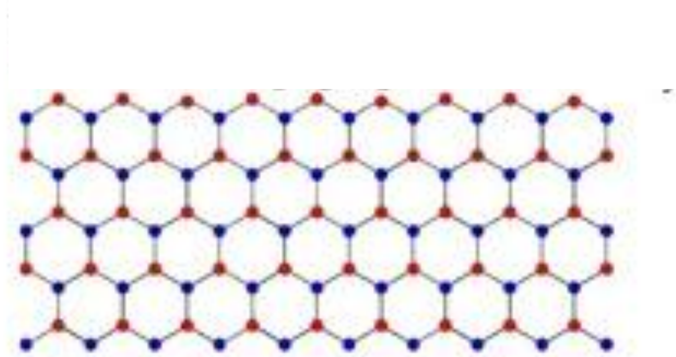
$$\boxed{\tilde{\Delta}_\tau = \Delta - \tau \frac{(e v_f A_0)^2}{\hbar\Omega - \tau\Delta}} \qquad \boxed{\mathcal{C}_\tau = \tau \frac{\mathrm{sg}(\tilde{\Delta}_\tau)}{2}}$$

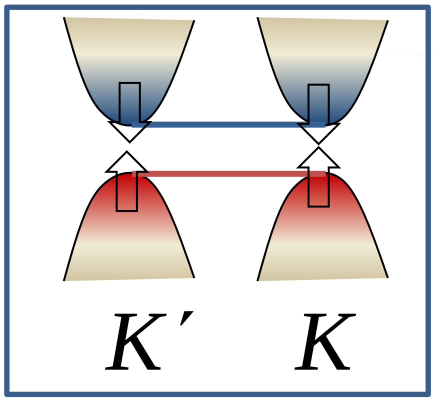
Closing gaps, changing topology and generating edge states that cross the gap

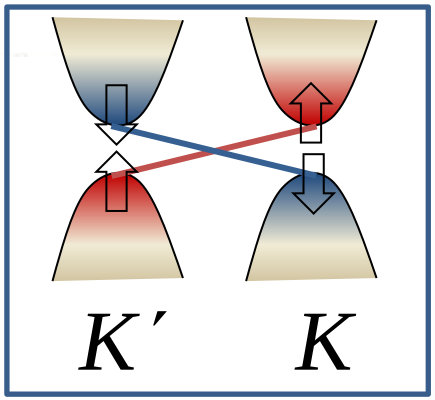
$$\tilde{\Delta}_\tau = \Delta - \tau \frac{(e v_f A_0)^2}{\hbar\Omega - \tau\Delta}$$







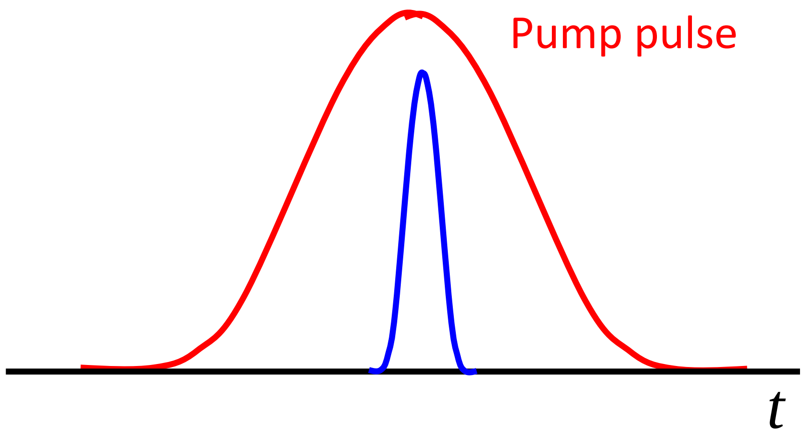




Theory of ARPES in dynamically driven Graphene

$$|\Psi_m(t)\rangle = \mathcal{U}(t,-\infty)\,|\Psi_m\rangle$$

$$\mathcal{U}(t,t') = \mathcal{T}exp\Big(-\frac{i}{\hbar}\int_{t'}^{t}\mathcal{H}(\tau)d\tau\Big)$$



PROBE

$$\mathcal{W}(t) = \mathcal{S}_{\mathcal{W}}(t)\sum_{\vec{k},\alpha} M_{\vec{k}\alpha}a^{\dagger}_{\vec{k}}c_{\alpha} + M^{*}_{\vec{k}\alpha}c^{\dagger}_{\alpha}a_{\vec{k}}.$$

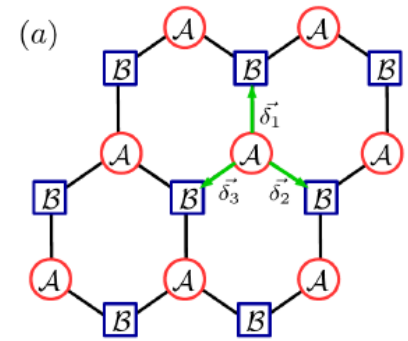
$$P_{\vec{k}}(t) = \sum_m f(E_m)\Big|\sum_{\alpha}\int_{t_0}^{t} M_{\vec{k}\alpha}e^{\frac{i}{\hbar}\varepsilon(\vec{k})t'}\mathcal{S}_{\mathcal{W}}(t')\,\langle 0|\,c_{\alpha}\mathcal{U}(t',-\infty)\,|\Psi_m\rangle\,dt'\Big|^2.$$

Phys. Rev. B **91, (2015)**

The Dipole Matrix Elements

$$\boxed{M^{\tau}_{\vec{k}\pm} = \langle f | \vec{A}(t) \cdot \vec{p} \, | \Psi^{\tau}_{\vec{k}\pm} \rangle}$$

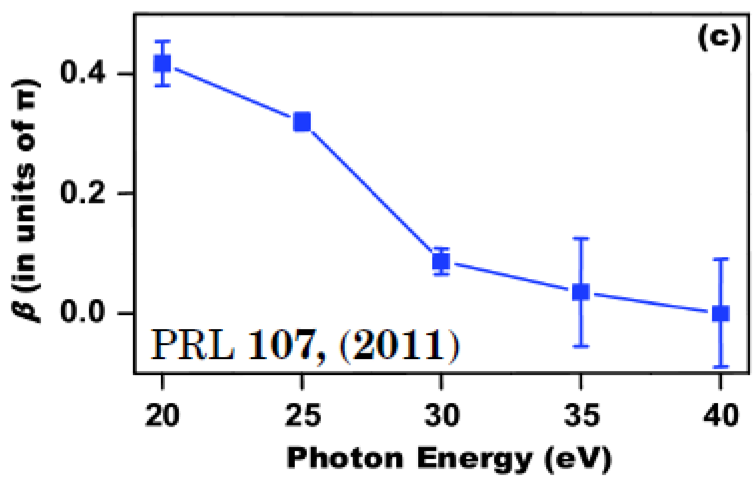
$$|\Psi^{\tau}_{\vec{k}\pm}\rangle = |\vec{k}A\rangle \pm \tau e^{i\tau\theta_{\vec{k}}} \, |\vec{k}B\rangle$$



$$\zeta_x = \langle f | \, p_x \, |\vec{k}A\rangle = \langle f | \, p_x \, |\vec{k}B\rangle$$

$$\zeta_y = \langle f | \, p_y \, |\vec{k}A\rangle = -\langle f | \, p_y \, |\vec{k}B\rangle$$

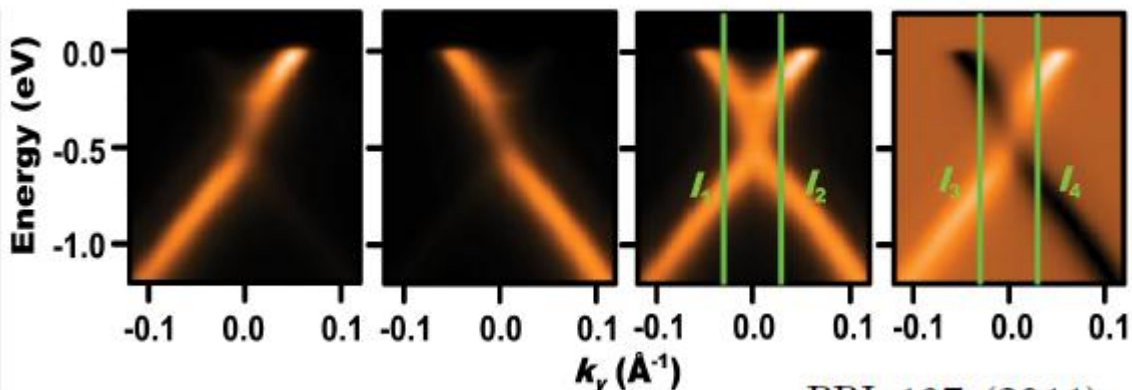
$$\frac{\zeta_y}{\zeta_x} = \lambda e^{i\beta}$$



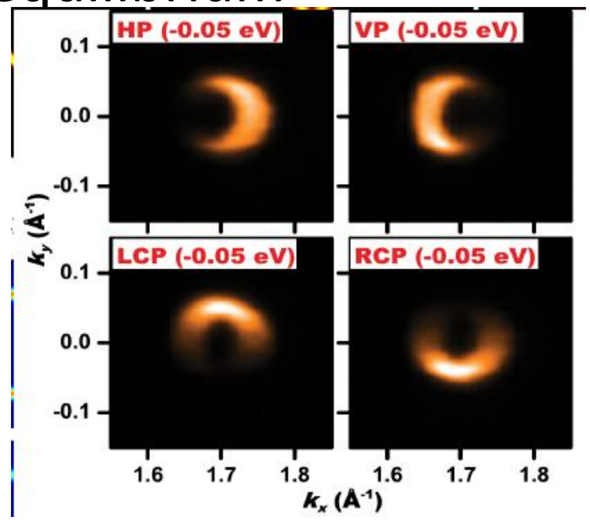
$$\vec{A} = A_0(t)[\cos(\chi)\hat{x} - i\sin(\chi)\hat{y}]$$

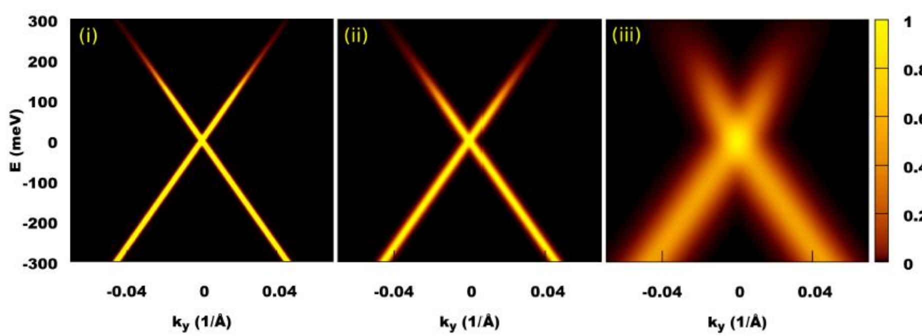
$$\boxed{M^{\tau}_{\vec{k}\pm} = A_0\left[\cos(\chi)\zeta_x(1 \mp \tau e^{i\tau\theta_{\vec{k}}}) - i\sin(\chi)\zeta_y(1 \pm \tau e^{i\tau\theta_{\vec{k}}})\right]}$$

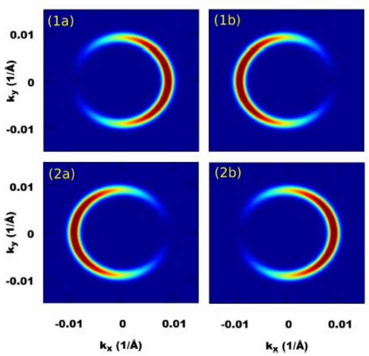
Time resolved ARPES for graphene in equilibrium



PRL **107**, (2011)

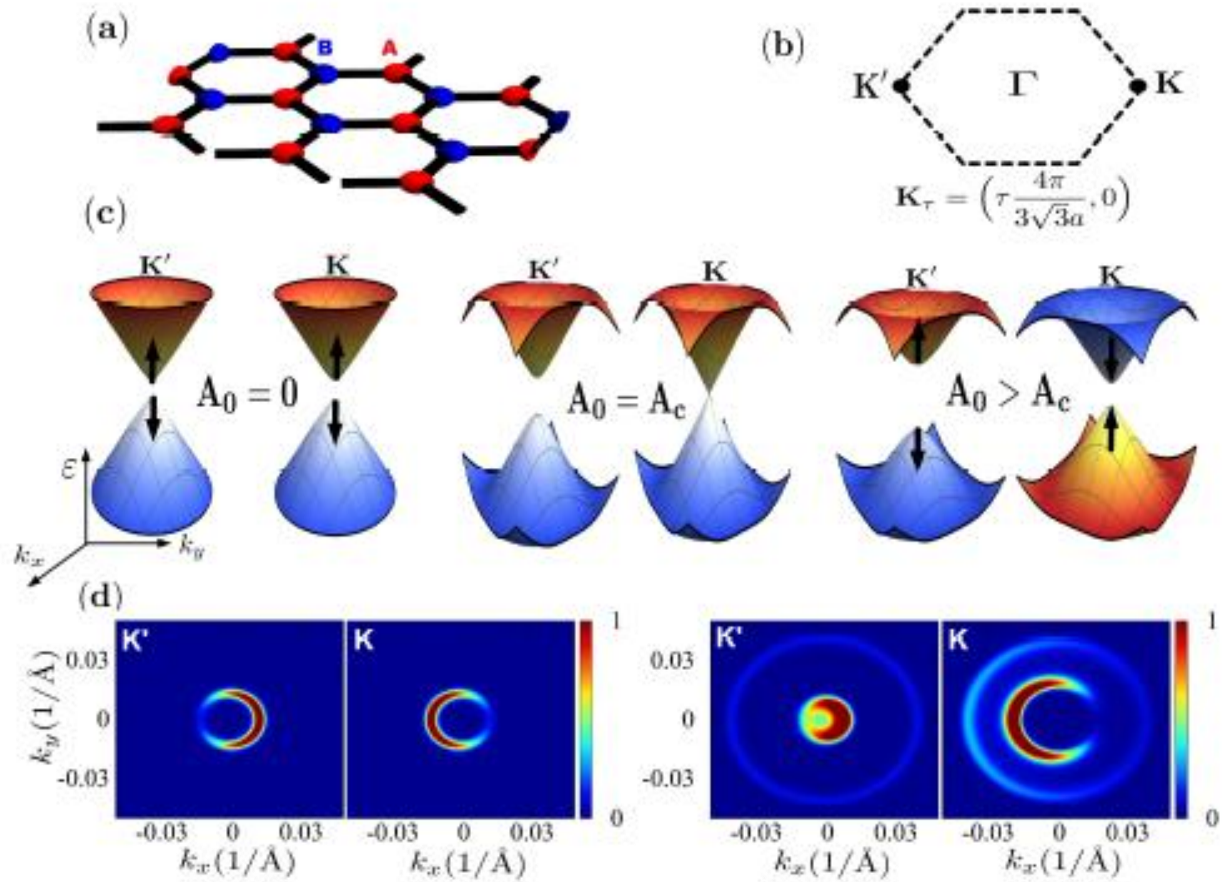




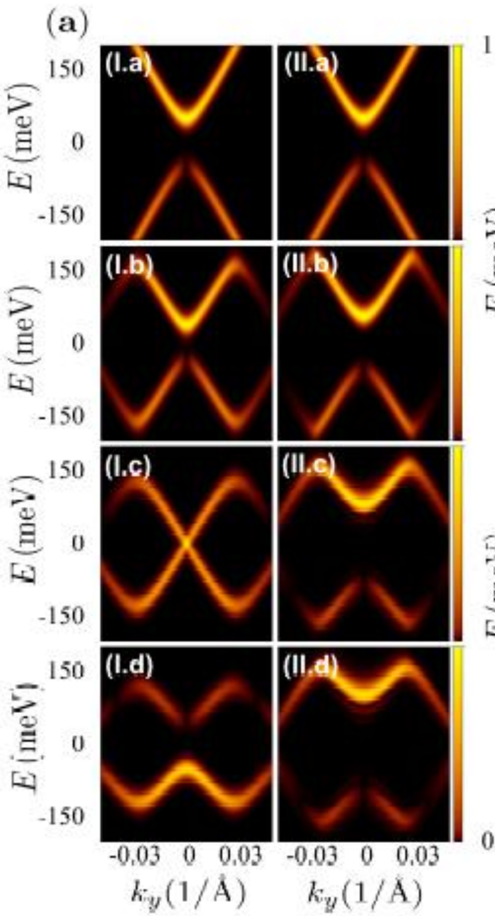


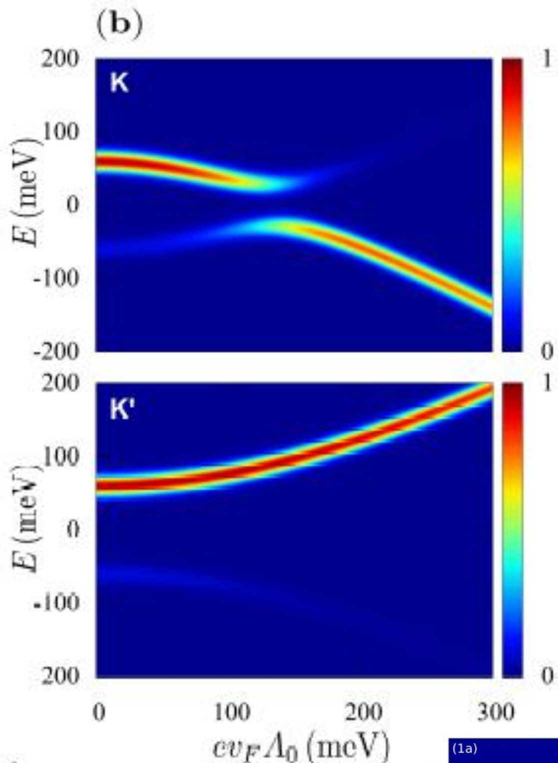
ARPES with a Pump pulse

Photoexcitation pulse with linear polarization and $\Delta \neq 0$



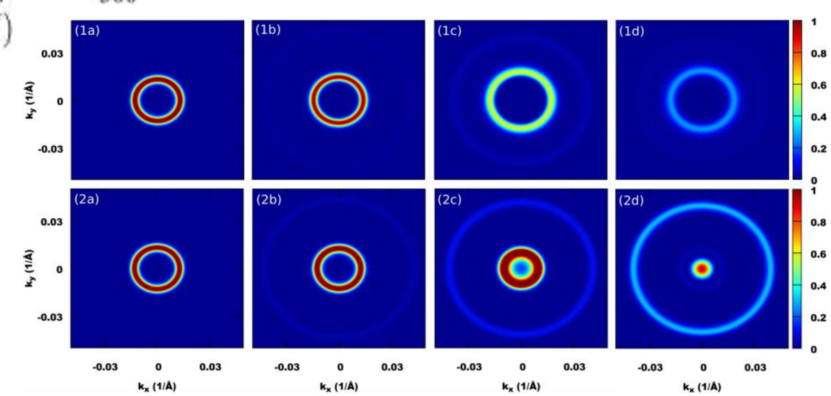
ARPES with a Pump pulse





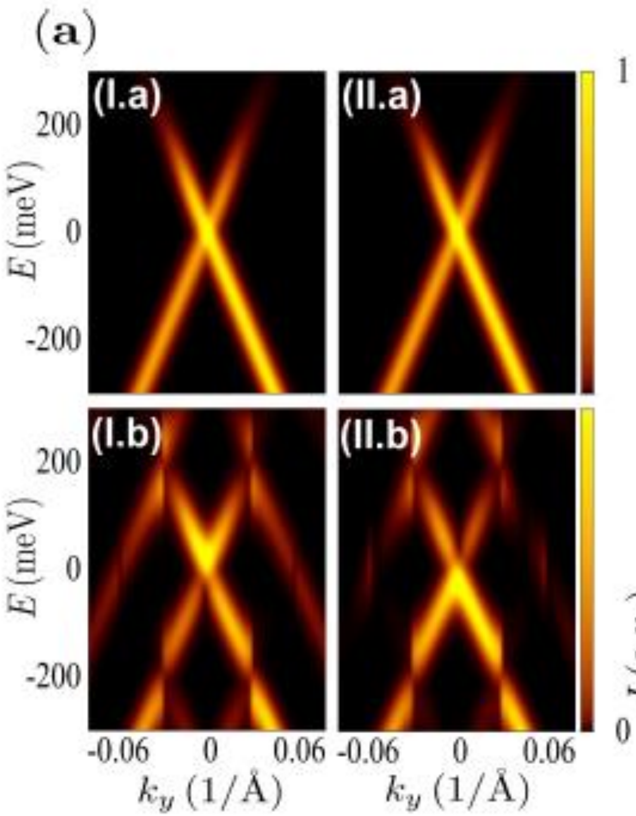
Same as before but with:

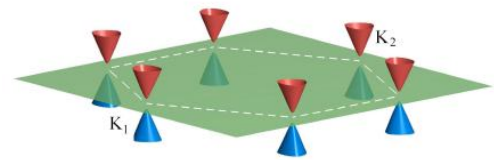
x-rays of 20eV and circularly polarized ($\beta = \pi/2$)

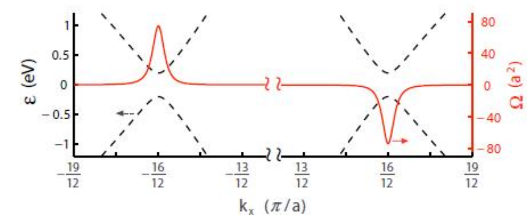


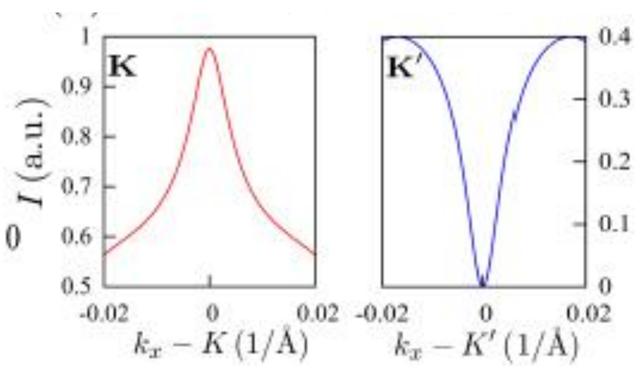
ARPES in Irradiated Graphene

X-Ray s of 20eV circularly polarized (β=0.4 π)

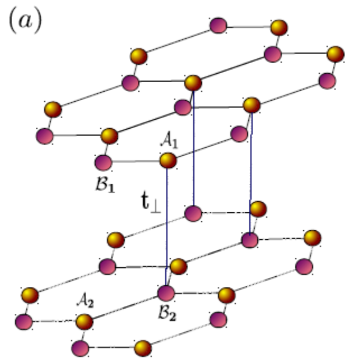


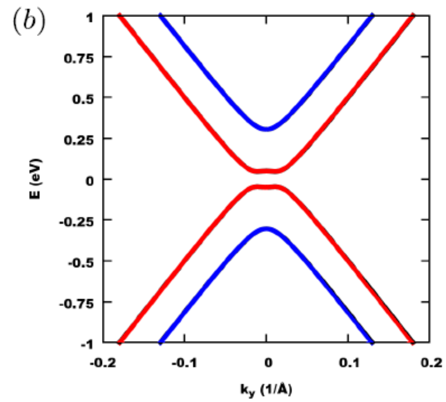


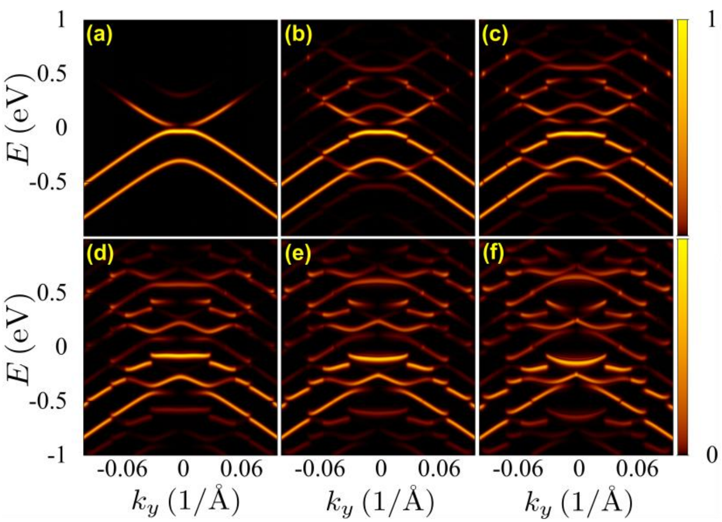


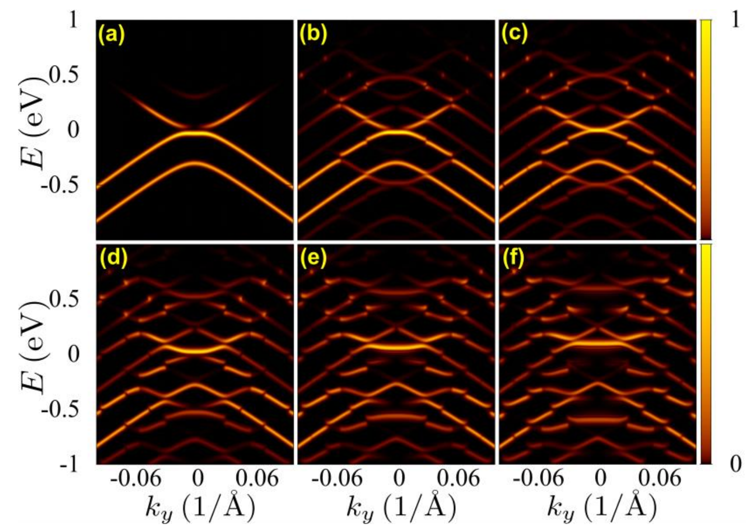


Tr-ARPES in Bilayer Graphene









K

K'

Conclusions

Time resolved ARPES can give clear information on the topology of the Floquet bands of Graphene and Graphene like systems.

The information is given by the intensity of the ARPES profiles close to de K and K´ points of the BZ.

To observe the effect the x-Ray energies have to e tuned to have a non-zero phase β.

This observation opens the road for a spectroscopic study of the topological properties of the bulk wave-functions of these 2D materials.

Thank you !