Theory of light-induced Floquet topological states

Nature Comm. 6, 7047 (2015)

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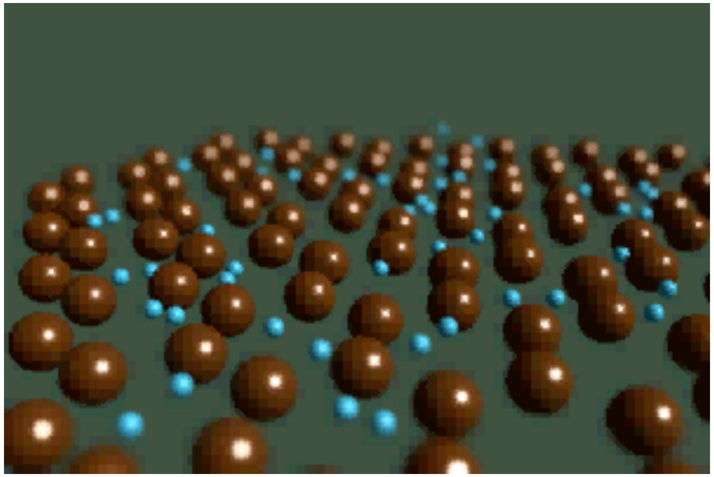
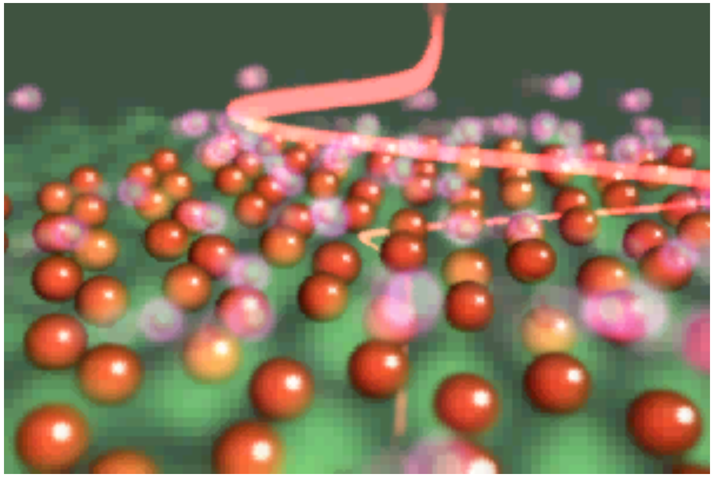
Max Planck Institute for the Structure and Dynamics of Matter

Artistic view of Floquet states

by Koichiro Tanaka (Kyoto university)



electrons in solids



Floquet state (photo-dressed state)

$$H$$

$$H_{\mathrm{eff}}$$

$$H_{\mathrm{eff}} = H_0 + \frac{[H_{-1}, H_1]}{\Omega} + \mathcal{O}(\Omega^{-2})$$

Outline

- Floquet topological states

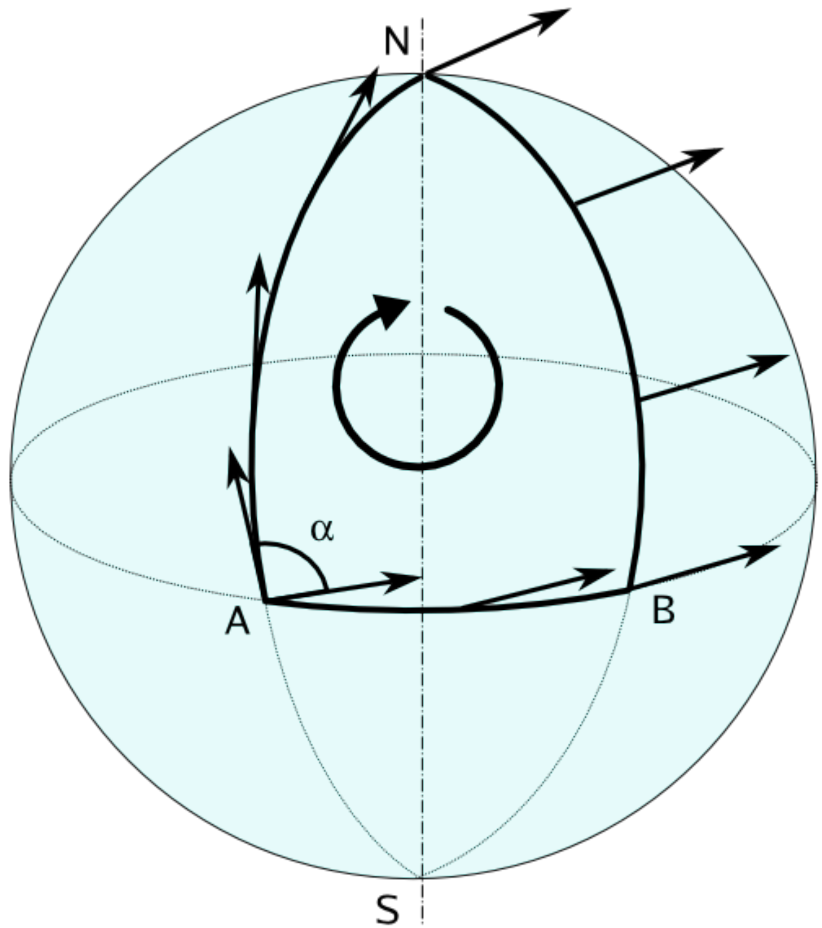
Topological band theory

+

Floquet theory of driven systems

Topological states of matter

Global Change without Local Change *illustrates Berry's Phase*



Topological states of matter

$$H(R(t))|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$$

M. V. Berry, Proc. R. Soc. A 392, 45 (1984)

$$H(R(t))|n(R(t))\rangle = E_n(R(t))|n(R(t))\rangle$$

$$|\psi(0)\rangle = |n(R(0))\rangle$$

Start system in the n^{th} eigenstate

$$|\psi(t)\rangle = e^{i\phi_n}|n(R(t))\rangle$$

Adiabatic theorem tells us that we stay in the n^{th} eigenstate, but we can pick up a phase that does not affect the physical state.

$$\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')dt'$$

$$\phi_n(t) = \theta_n(t) + \gamma_n(t)$$

Dynamical phase, but an additional phase is also allowed (this is called the Berry phase γ).

Topological states of matter

$$|\psi(t)\rangle = e^{i\phi_n}|n(R(t))\rangle$$

$$\phi_n(t) = \theta_n(t) + \gamma_n(t)$$

$$H(R(t))|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$$

$$\frac{\partial}{\partial t}|n(R)\rangle + i\frac{d}{dt}\gamma_n(t)|n(R)\rangle = 0$$

Equation for Berry's phase

$$\frac{d}{dt}\gamma_n(t) = i\langle n(R)|\frac{\partial}{\partial t}|n(R)\rangle$$

Operate with bra on l.h.s.

$$\frac{d}{dt}\gamma_n(t) = i\langle n(R)|\nabla_R|n(R)\rangle\frac{dR}{dt}$$

$$\gamma_n(t) = i\int_{R_i}^{R_f}\langle n(R)|\nabla_R|n(R)\rangle dR$$

Dynamical phase, but an additional phase is also allowed (this is called the **Berry phase** γ).

Topological states of matter

$$\gamma_n(t) = i \int_{R_i}^{R_f} \langle n(R)|\nabla_R|n(R)\rangle dR$$

If we now consider cyclic evolutions around a closed circuit C in a time T such that $R(0) = R(T)$ then the Berry phase looks like the following

$$\gamma_n(C) = i \oint_C \langle n(R)|\nabla_R|n(R)\rangle dR$$

Berry phase, related to changes of the eigenstate when moved along path in parameter space.

$$\nabla_R \langle n|n\rangle = 0$$

$$\langle \nabla_R n|n\rangle + \langle n|\nabla_R n\rangle = \langle n|\nabla_R n\rangle^* + \langle n|\nabla_R n\rangle = 0$$

$$2 \cdot \Re e \langle n|\nabla_R n\rangle = 0$$

Berry phase is real.

Topological states of matter

Berry connection as a gauge potential.

$$\gamma_n(C) = \oint_C A_n dR \qquad A_n(R) = i\langle n(R)|\nabla_R|n(R)\rangle$$

$$|n(R)\rangle \rightarrow |n(R)\rangle' = e^{i\xi_n(R)}|n(R)\rangle$$

Under gauge transformation.

$$A_n(R) \rightarrow A'_n(R) = A_n(R) - \nabla_R \xi_n(R)$$

$$\gamma_n(R) \rightarrow \gamma'_n(R) = \gamma_n(R)$$

Gives no change to the Berry phase.

Berry phase is gauge invariant and can be measured, e.g. Aharonov-Bohm effect.

Topological states of matter

C. Kane, "Topological band theory and the Z2 invariant", Chapter 1 in "Topological Insulators", Elsevier (2013)

mpsd

Topological band theory of solids

$$H(\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{r}} H e^{-i\mathbf{k}\cdot\mathbf{r}}$$

eigenvalues $E_n(\mathbf{k})$ and eigenvectors $|u_n(\mathbf{k})\rangle$

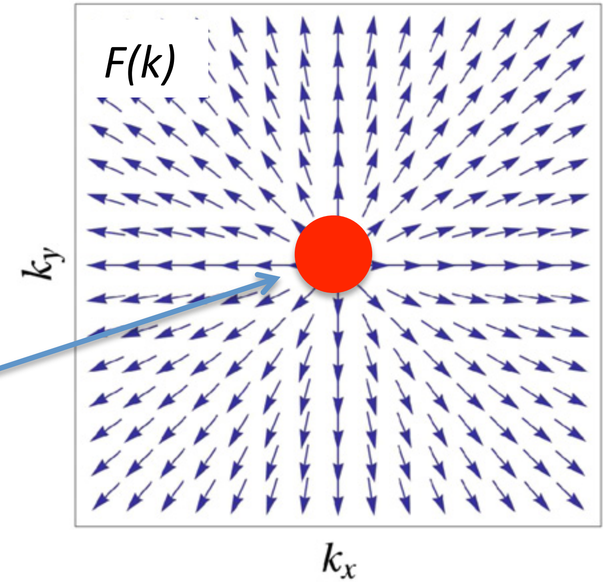
Bloch state under gauge transformation $\quad |u(\mathbf{k})\rangle \rightarrow e^{i\phi(\mathbf{k})}|u(\mathbf{k})\rangle$

Berry connection $\quad \mathbf{A} = -i\langle u(\mathbf{k})|\nabla_{\mathbf{k}}|u(\mathbf{k})\rangle \longrightarrow \mathbf{A} \rightarrow \mathbf{A} + \nabla_{\mathbf{k}}\phi(\mathbf{k})$

Berry phase $\quad \gamma_C = \oint_C \mathbf{A}\cdot d\mathbf{k} = \int_S \mathcal{F} d^2\mathbf{k}$

$\mathcal{F} = \nabla \times \mathbf{A}$ defines the Berry curvature

closed surface S $\quad n = \dfrac{1}{2\pi}\int_S \mathcal{F} d^2\mathbf{k}$

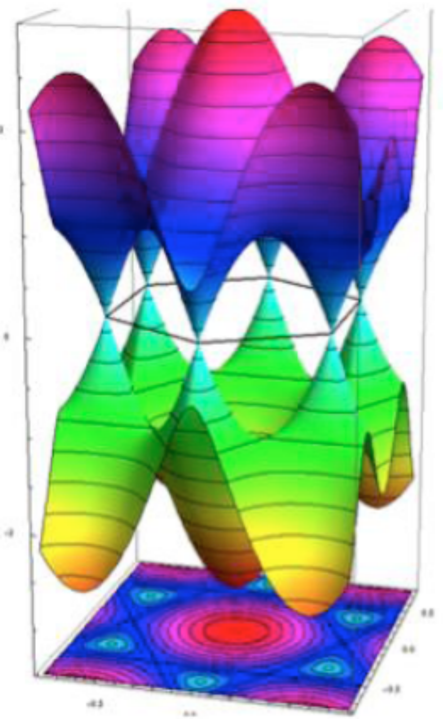


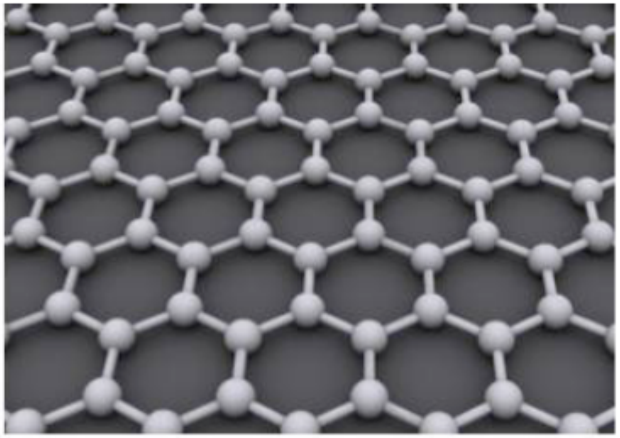
Chern number = topological invariant
= number of Dirac monopoles inside the surface

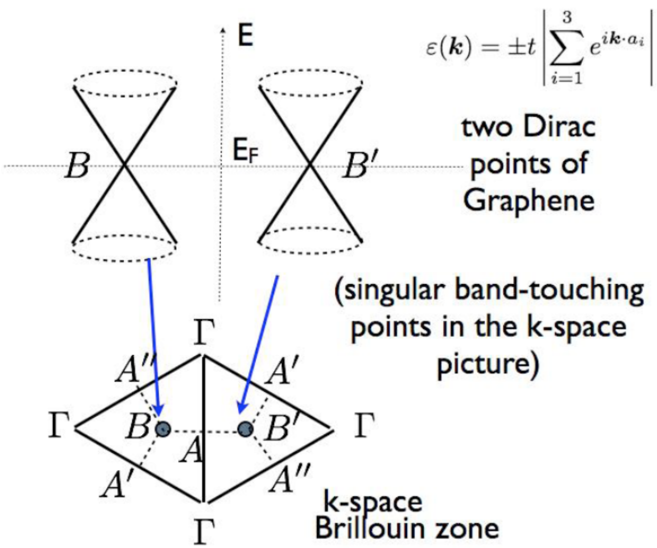
Topological states of matter

2D Graphene:

- Dirac points (2 valleys)







Topological states of matter

Dirac fermions in pseudospin representation: Decompose into Pauli matrices

$$H(K+q) = \begin{pmatrix} m_K & q_x + iq_y \\ q_x - iq_y & -m_K \end{pmatrix}$$

$$= p_x\sigma_x + p_y\sigma_y + p_z\sigma_z$$

$$\boxed{\begin{aligned} p_x &= q_x \\ p_y &= q_y \\ p_z &= m_K \end{aligned}}$$

Pseudospin winding <-> Berry phase

Berry phase on a closed loop around Dirac point is quantized = +/- π

+/- sign depends on sign of mass term m_K

+/- ½ Dirac monopole

Chern number C = sum of Dirac monopoles in the Brillouin zone

Distinguishes trivial from nontrivial (topological) insulators

C=0 C≠0

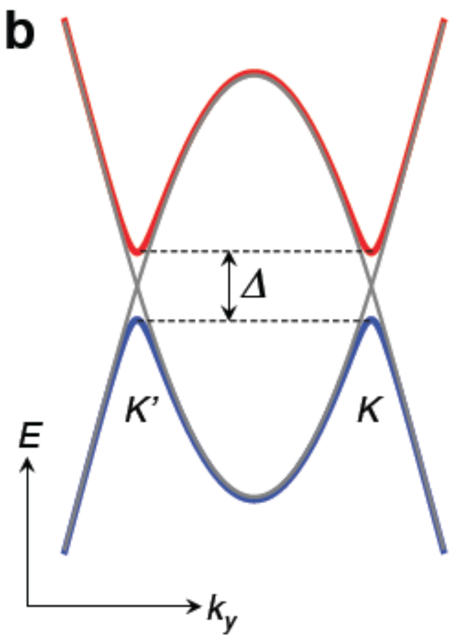
Topological states of matter

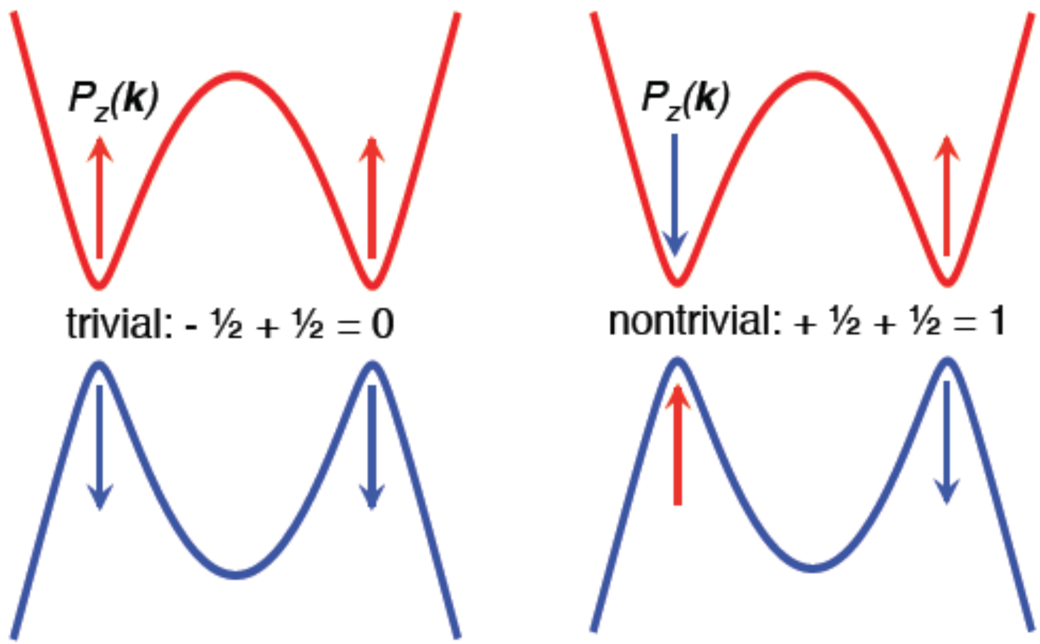
$$H(K'+q) = \begin{pmatrix} \boxed{m_{K'}} & q_x \boxed{-} iq_y \\ q_x + iq_y & -m_{K'} \end{pmatrix} \qquad H(K+q) = \begin{pmatrix} \boxed{m_K} & q_x \boxed{+} iq_y \\ q_x - iq_y & -m_K \end{pmatrix}$$

***K* vs. *K'*: opposite winding of in-plane pseudospin**

$m_K = m_{K'}$
trivial insulator

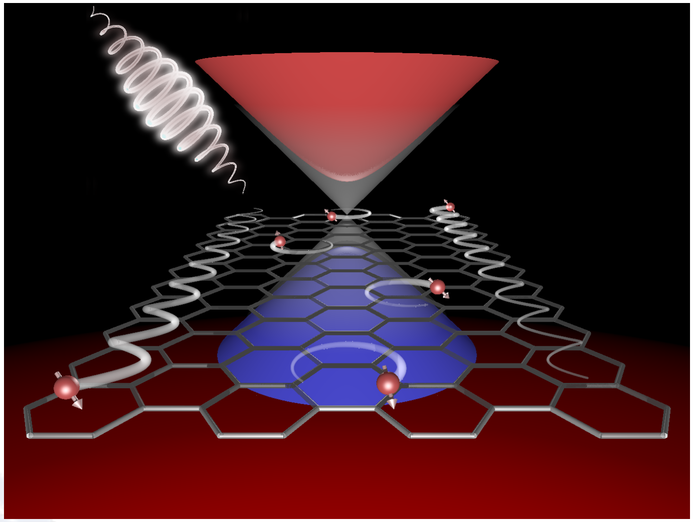
$m_K = - m_{K'}$
nontrivial insulator



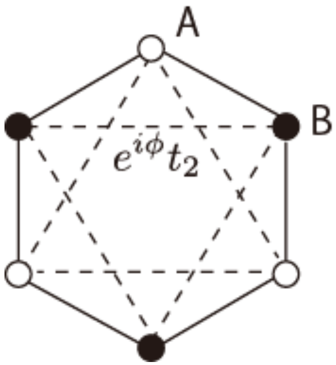


Floquet topological states

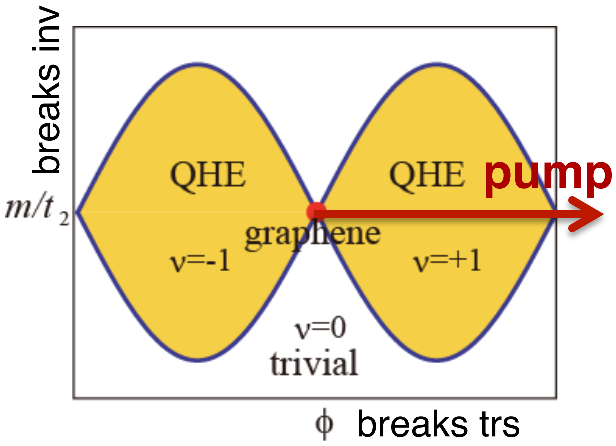
Graphene + circularly polarized light (breaks trs)



Haldane model (PRL 61, 2015 (1988))



Local flux ϕ
Staggered field m
Fictitious fields!



Floquet states of matter

time periodic system

$$i\partial_t \psi = H(t)\psi \qquad H(t) = H(t+T) \qquad \Omega = 2\pi/T$$

"Floquet mapping"

=discrete Fourier trans.

$$\Psi(t) = e^{-i\varepsilon t} \sum_m \phi^m e^{-im\Omega t}$$

Floquet Hamiltonian (static eigenvalue problem)

$$\sum_{m=-\infty}^{\infty} \mathcal{H}^{mn} \phi_\alpha^m = \varepsilon_\alpha \phi_\alpha^n$$

ε: Floquet quasi-energy

$$(\mathcal{H})^{mn} = \frac{1}{T} \int_0^T dt H(t) e^{i(m-n)\Omega t} \boxed{+ m\delta_{mn}\Omega I}$$

comes from the $i\partial_t$ term

$$H_m = \mathcal{H}^{m0}$$

~ absorption of m "photons"

Floquet states of matter

Time-periodic quantum system = Floquet theory (exact) ~ effective theory

$$i\partial_t\psi = H(t)\psi$$

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

$$\mathcal{H}\phi = \varepsilon\phi$$

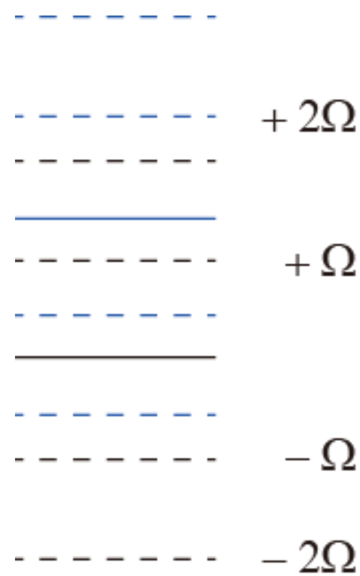
$$H_{\text{eff}} = H_0 + \frac{[H_{-1}, H_1]}{\Omega} + \mathcal{O}(\Omega^{-2})$$

Fictitious fields!

Floquet theory

projection to the original Hilbert space

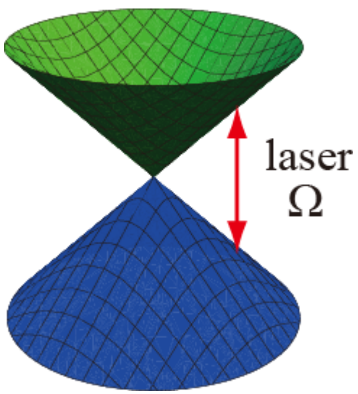
two states + periodic driving



Hilbert sp. size
= original system

n-photon dressed state
Floquet side bands

Dirac fermion + circularly polarized laser



coupling to AC field

$$\boldsymbol{k} \to \boldsymbol{k} + \boldsymbol{A}(t)$$

$$k = k_x + ik_y$$
$$\boldsymbol{A}(t) = (F/\Omega \cos \Omega t,\, F/\Omega \sin \Omega t)$$
$$A = F/\Omega$$

time dependent Schrodinger equation

$$i\partial_t \psi_k = \begin{pmatrix} 0 & k + Ae^{i\Omega t} \\ \bar{k} + Ae^{-i\Omega t} & 0 \end{pmatrix} \psi_k$$

Floquet theory

$$(\mathcal{H})^{mn} = \frac{1}{T}\int_0^T dt H(t) e^{i(m-n)\Omega t} + m\delta_{mn}\Omega I$$

$$H^{\mathrm{Floquet}} = \begin{pmatrix} \Omega & k & 0 & A & 0 & 0 \\ \bar{k} & \Omega & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & k & 0 & A \\ A & 0 & \bar{k} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\Omega & k \\ 0 & 0 & A & 0 & \bar{k} & -\Omega \end{pmatrix}$$

truncated at m=0,+1, -1 for display

Dirac fermion + circularly polarized laser

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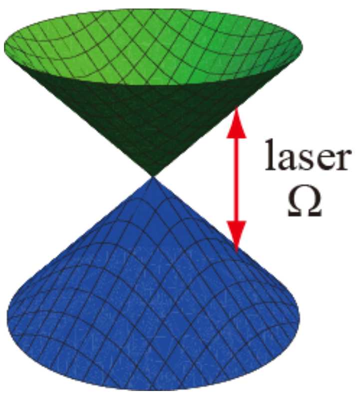
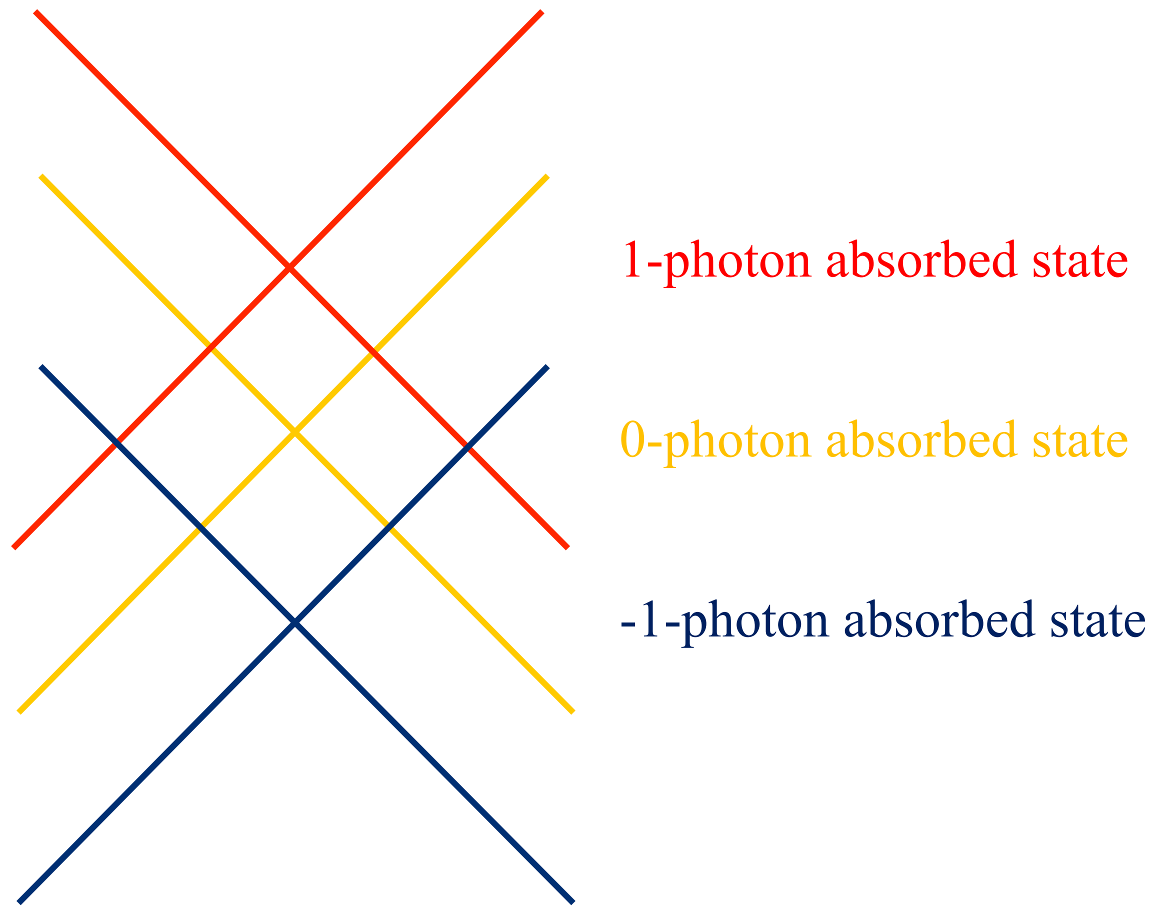


$$H^{\mathrm{Floquet}} = \begin{pmatrix} \Omega & k & 0 & A & 0 & 0 \\ \bar{k} & \Omega & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & k & 0 & A \\ A & 0 & \bar{k} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\Omega & k \\ 0 & 0 & A & 0 & \bar{k} & -\Omega \end{pmatrix}$$

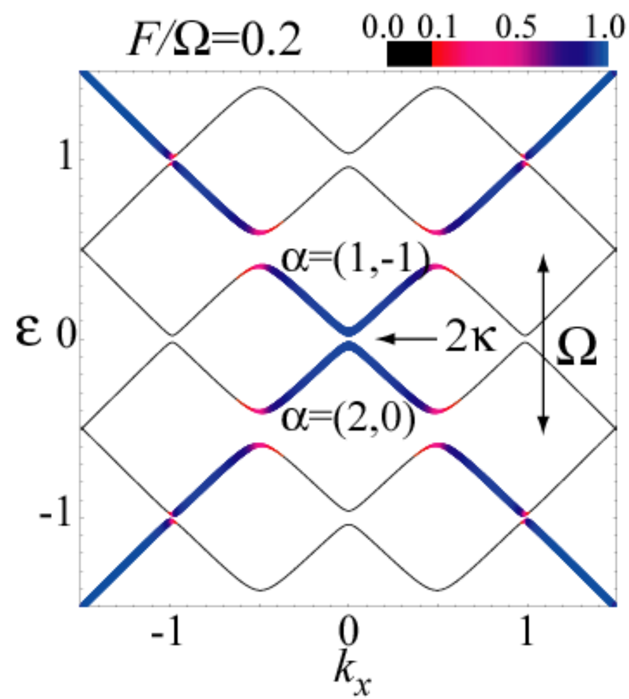


Dirac fermion + circularly polarized laser

Mass term =
synthetic field stemming from a real time-dependent field A(t)

$$\kappa = \frac{\sqrt{4A^2+\Omega^2}-\Omega}{2} \sim A^2/\Omega$$

$$H^{\mathrm{Floquet}} = \begin{pmatrix} \Omega & k & 0 & A & 0 & 0 \\ \bar{k} & \Omega & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & k & 0 & A \\ A & 0 & \bar{k} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\Omega & k \\ 0 & 0 & A & 0 & \bar{k} & -\Omega \end{pmatrix}$$



1-photon absorbed state

0-photon absorbed state

-1-photon absorbed state

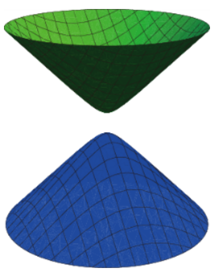
Oka and Aoki, PRB 79, 081406 (2009)

Dirac fermion + circularly polarized laser

Projection to the original Hilbert space

$$H^{\text{Floquet}} = \begin{pmatrix} \Omega & k & 0 & A & 0 & 0 \\ \bar{k} & \Omega & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & k & 0 & A \\ A & 0 & \bar{k} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\Omega & k \\ 0 & 0 & A & 0 & \bar{k} & -\Omega \end{pmatrix}$$

near Dirac point



2κ

2nd order perturbation

$$H_{\text{eff}} = H_0 + \boxed{\frac{[\underbrace{\boxed{H_{-1}}}_{}^{\sim A\sigma_-}, \overbrace{\boxed{H_1}}^{\sim A\sigma_+}]}{\Omega}} + \mathcal{O}(A^4)$$

Dynamical gap

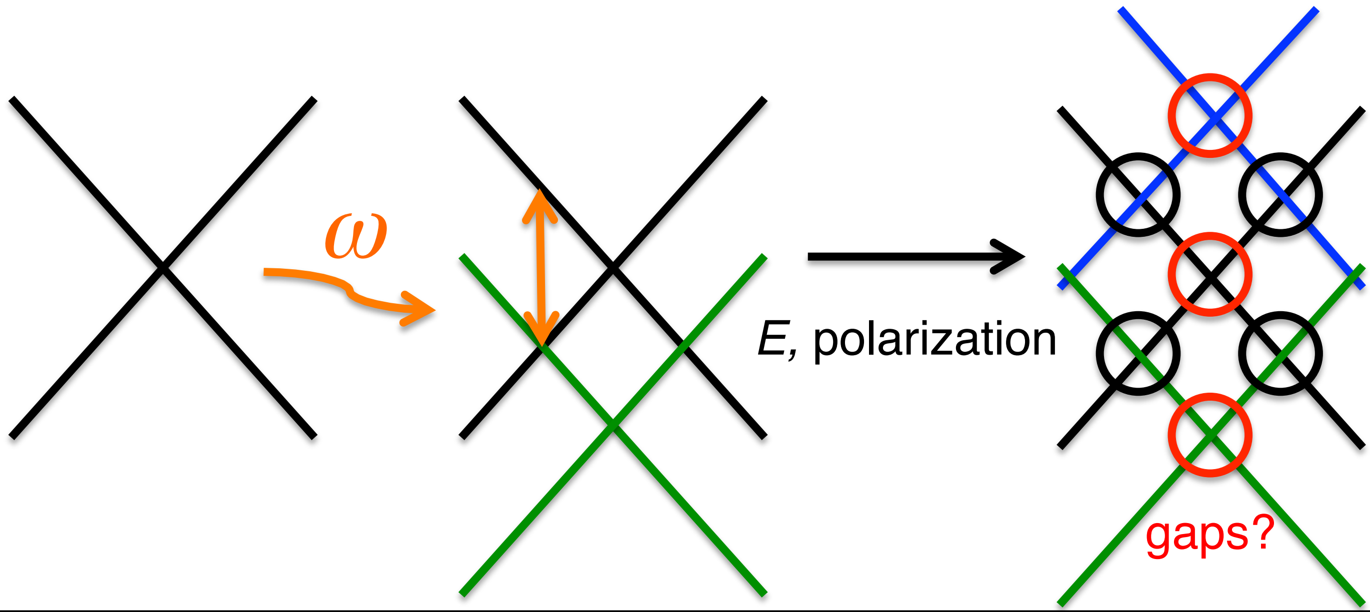
$$\kappa = \frac{\sqrt{4A^2 + \Omega^2} - \Omega}{2} \sim A^2/\Omega$$

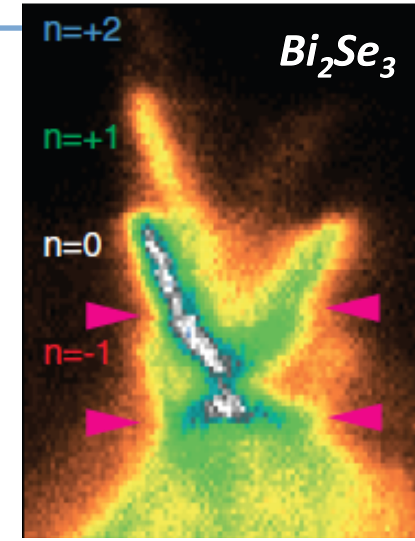
Mass term =
synthetic field stemming from a
real time-dependent field A(t)

$$\sim v(k_x\sigma_y - \tau_z k_y \sigma_x) \boxed{\pm \tau_z \frac{v^2 A^2}{\Omega}\sigma_z}$$

$$A = F/\Omega$$

Floquet topological states in graphene





Wang et al., Science 342, 453 (2013)

<u>Floquet + topology in ac driven systems:</u>

Oka&Aoki PRB 79, 081406 (09), Kitagawa et al PRB 82, 235114 (10), Kitagawa et al PRB 84, 235108 (11), Lindner et al Nature Phys 7, 490 (11), Gu et al PRL 107, 216601 (11), Calvo et al APL 98, 232103 (11), Dora et al PRL 108, 056602 (12), Suarez Morell et al PRB 86, 125449 (12), Rudner et al PRX 3, 031005 (13), Iadecola et al, PRL 110, 176603 (13), Gomez-Leon&Platero PRL 110, 200403 (13), Fregoso et al PRB 88, 155129 (13), Perez-Piskunow et al, arXiv:1308.4362, Grushin et al, arXiv:1309.3571 … INCOMPLETE

Our work:

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- continuous field ⟶ pulsed field?
- exact time evolution, realistic parameters
- Floquet states evolving in real time?

Floquet topological states in graphene

2x2 model for honeycomb tight-binding electrons:

$$\mathcal{H}(t) = \sum_{\mathbf{k}} \begin{pmatrix} a_{\mathbf{k}}^\dagger & b_{\mathbf{k}}^\dagger \end{pmatrix} \begin{pmatrix} 0 & g(\mathbf{k}-\mathbf{A}(t)) \\ g^*(\mathbf{k}-\mathbf{A}(t)) & 0 \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ b_{\mathbf{k}} \end{pmatrix}$$

$$g(\mathbf{k}) = V\left[2\cos\left(\frac{\sqrt{3}k_x}{2}\right)\cos\left(\frac{k_y}{2}\right) + \cos(k_y) + i\left(-2\cos\left(\frac{\sqrt{3}k_x}{2}\right)\sin\left(\frac{k_y}{2}\right) + \sin(k_y)\right)\right]$$

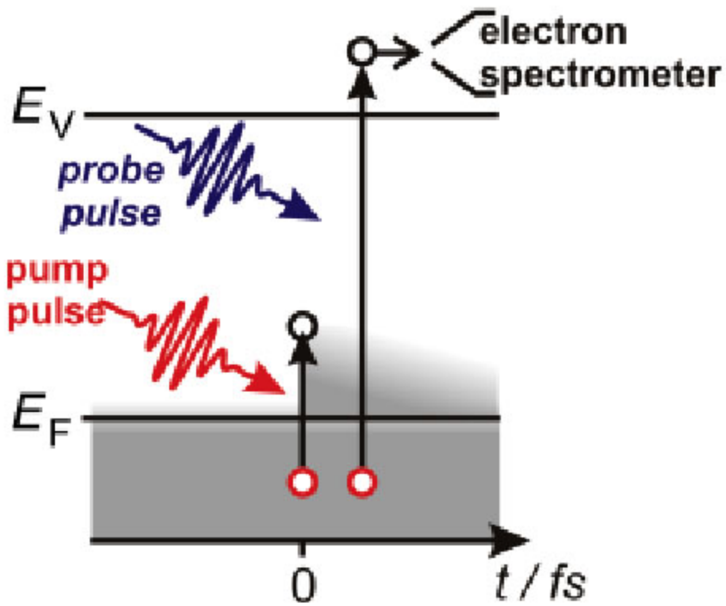
Compute Green functions using exact time evolution:

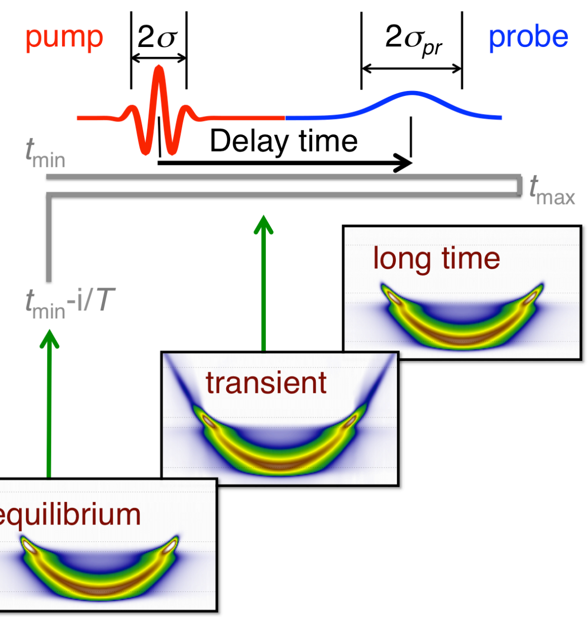
$$G^<_{\alpha\beta}(\mathbf{k},t,t') \equiv i\langle \alpha_{\mathbf{k}}^\dagger(t)\beta_{\mathbf{k}}(t')\rangle$$

Floquet topological states in graphene

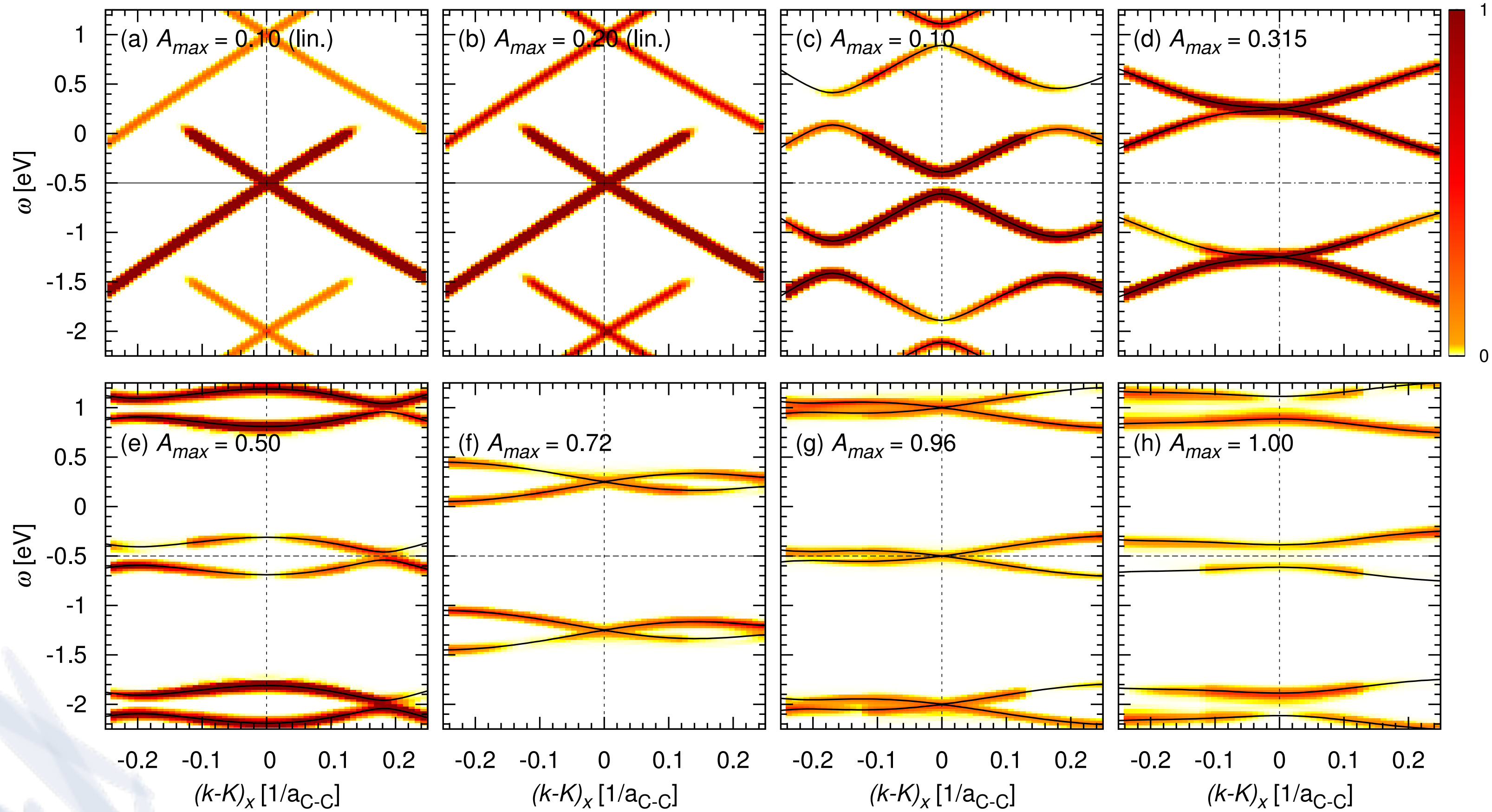
Obtain photocurrent from lesser Green function:

$$I(\mathbf{k},\omega,\Delta t) = \mathrm{Im}\sum_a \int \mathrm{d}t_1 \int \mathrm{d}t_2 s_{\sigma_{\mathrm{probe}}}(t_{\mathrm{pr}}-t_1)s_{\sigma_{\mathrm{probe}}}(t_{\mathrm{pr}}-t_2)e^{i\omega(t_1-t_2)}G^{<}_{aa}(\mathbf{k},t_1,t_2)$$



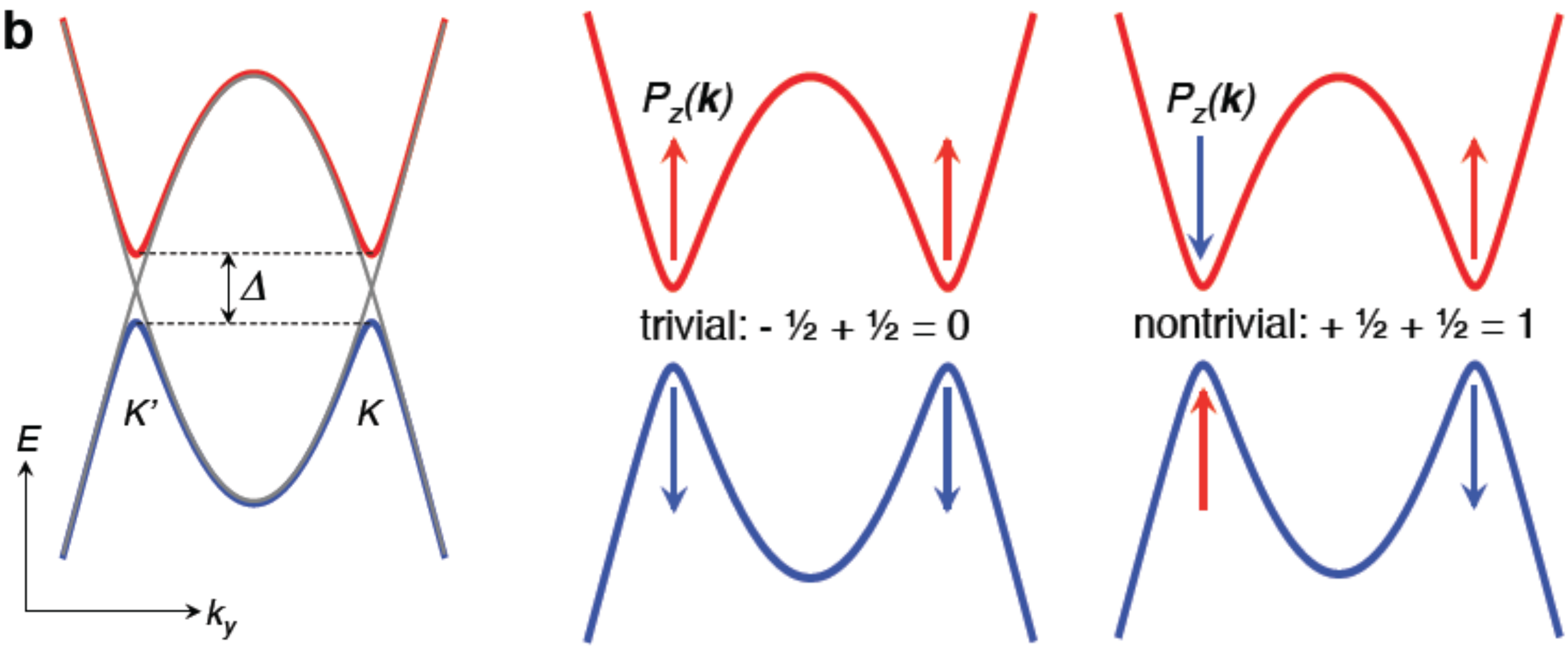


Floquet topological states in graphene



- Circularly polarized laser induces energy gap
- Good agreement with Floquet band structure

Floquet topological states in graphene



- pseudospin <-> orbital content
- determines Berry phase (topology)

Floquet topological states in graphene

Pseudospin components:

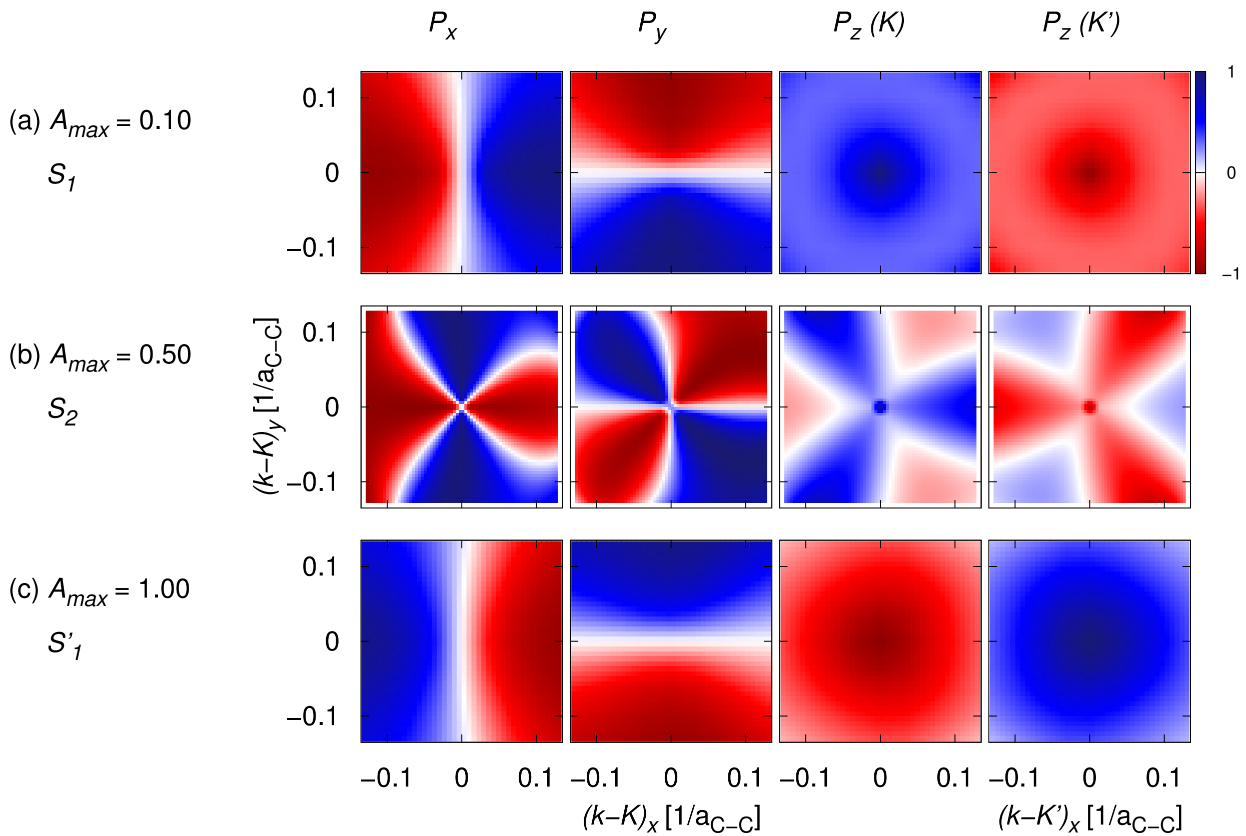
$$G_x(\mathbf{k},t,t') \equiv G_{AB}(\mathbf{k},t,t') + G_{BA}(\mathbf{k},t,t'),$$

$$G_y(\mathbf{k},t,t') \equiv -i(G_{AB}(\mathbf{k},t,t') - G_{BA}(\mathbf{k},t,t')),$$

$$G_z(\mathbf{k},t,t') \equiv G_{AA}(\mathbf{k},t,t') - G_{BB}(\mathbf{k},t,t').$$

Pseudospin measures orbital configuration in bands

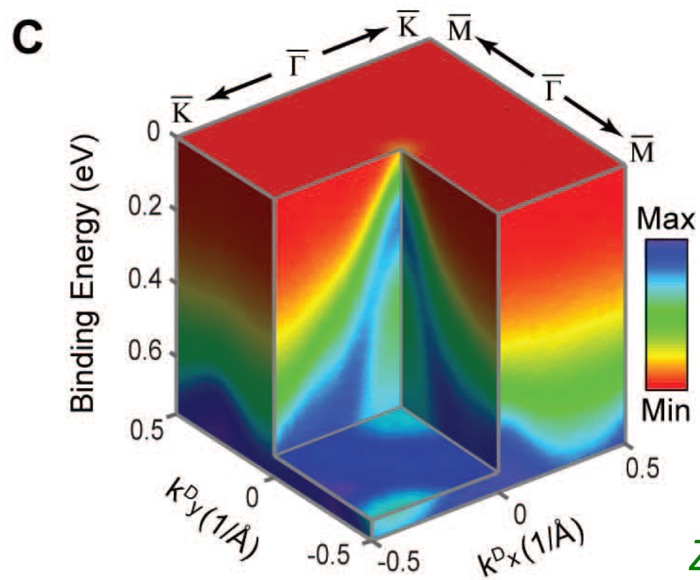
Floquet topological states in graphene



- Pseudospin changes sign between *K* and *K'*
- Light-controlled Berry phase

Beyond graphene: 3D NaBi

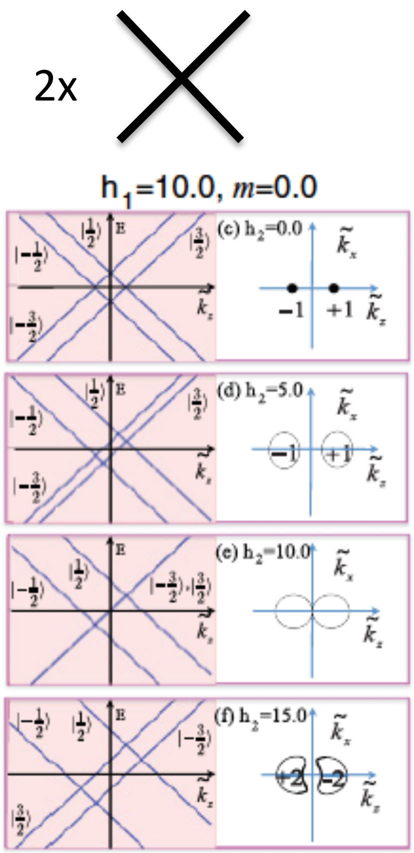
- 3D Dirac semimetal NaBi
- Dirac point with spin-orbit = 2 degenerate Weyl points of opposite chirality



Z. K. Liu et al., Science 343, 864 (2014)

Beyond graphene: 3D NaBi

- Proposed engineering of topological states via fictitious fields h_1, h_2 (analogue of Haldane model)

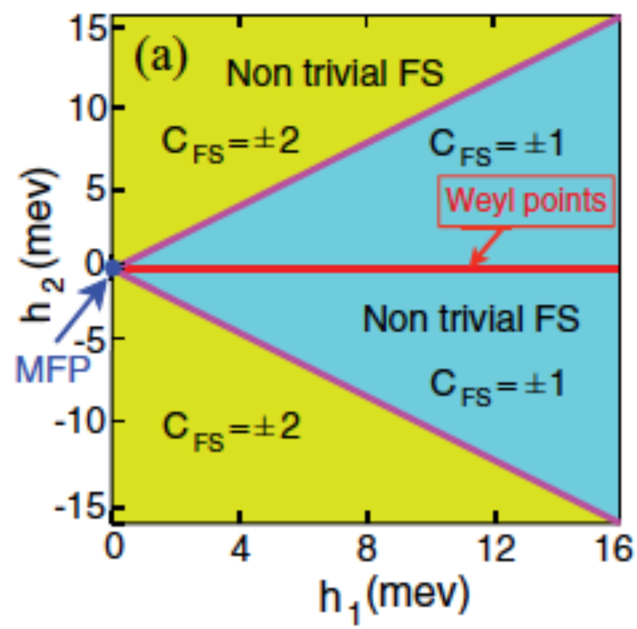
2x 

$$\mathcal{H} = \epsilon_0(\mathbf{k}) + \begin{pmatrix} M(\mathbf{k}) & Dk_+ & 0 & B^*(\mathbf{k}) \\ Dk_- & -M(\mathbf{k}) & B^*(\mathbf{k}) & 0 \\ 0 & B(\mathbf{k}) & M(\mathbf{k}) & -Dk_- \\ B(\mathbf{k}) & 0 & -Dk_+ & -M(\mathbf{k}) \end{pmatrix}$$

Fictitious fields:

$$M_1 = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}$$

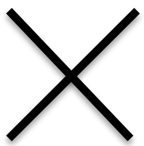
$$M_2 = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}$$



Z. Wang et al., PRB 85, 195320 (2012)

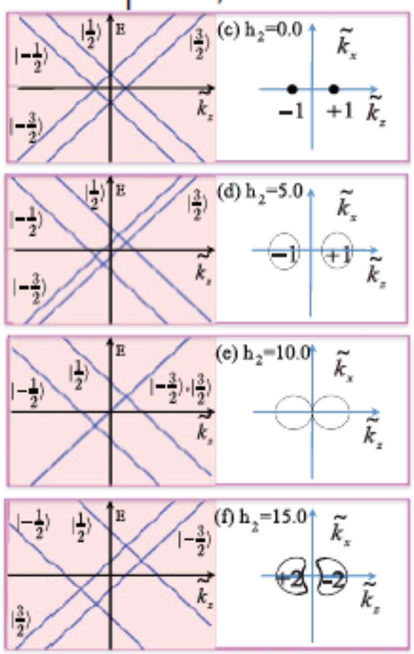
Beyond graphene: 3D NaBi

- Question: Can these fictitious fields be generated with lasers via Floquet engineering?

2x 

$$\mathcal{H} = \epsilon_0(\mathbf{k}) + \begin{pmatrix} M(\mathbf{k}) & Dk_+ & 0 & B^*(\mathbf{k}) \\ Dk_- & -M(\mathbf{k}) & B^*(\mathbf{k}) & 0 \\ 0 & B(\mathbf{k}) & M(\mathbf{k}) & -Dk_- \\ B(\mathbf{k}) & 0 & -Dk_+ & -M(\mathbf{k}) \end{pmatrix}$$

h$_1$=10.0, m=0.0



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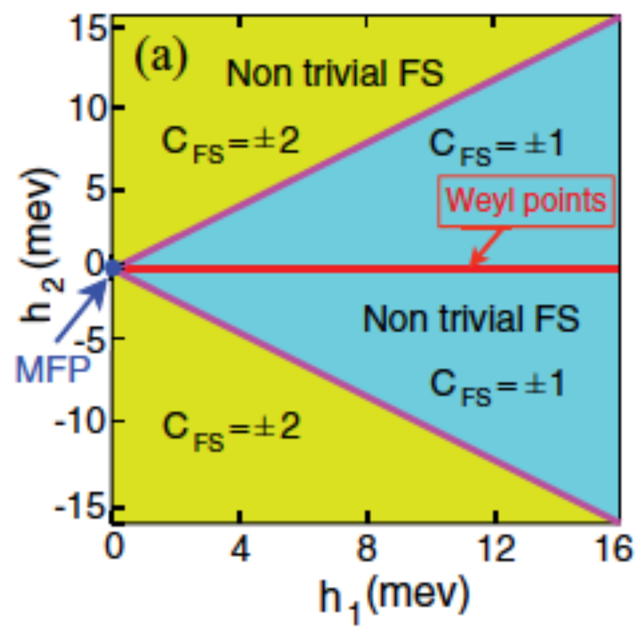
$$M_1 = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}$$

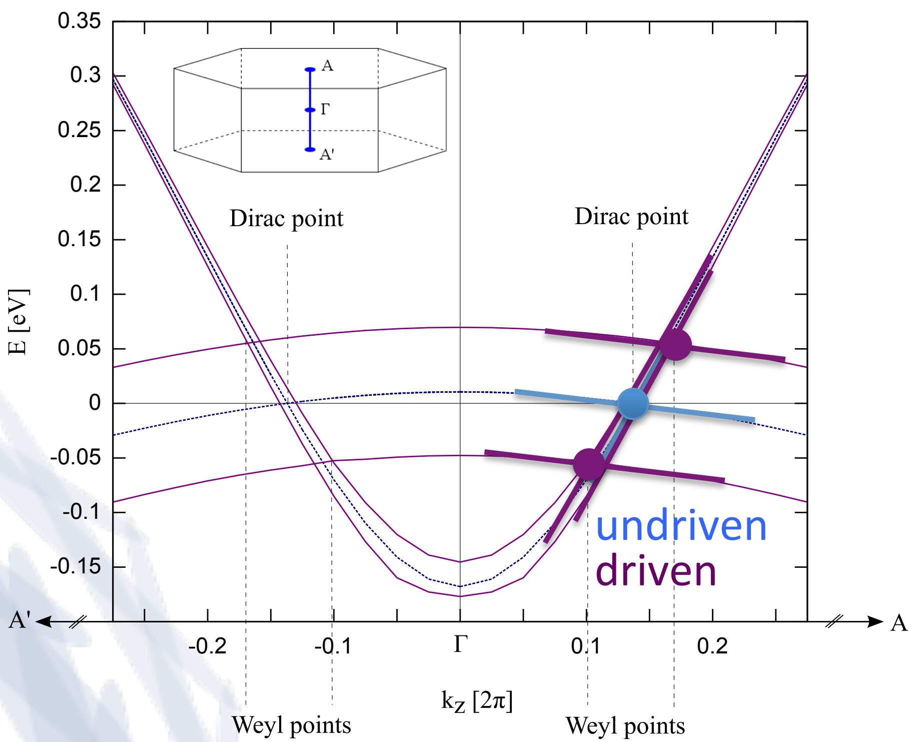
$$M_2 = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}$$



Project with H. Hübener, A. F. Kemper, U. de Giovannini, A. Rubio

Beyond graphene: 3D NaBi

- Question: Can these fictitious fields be generated with lasers via Floquet engineering?
- Preliminary result using ab initio TDDFT + Floquet downfolding: yes (to some extent)



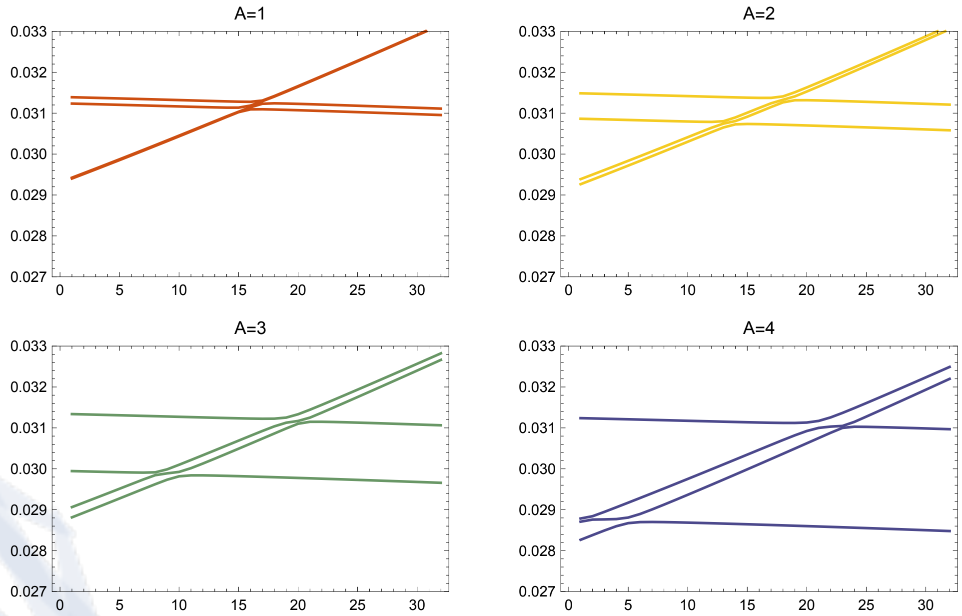
Splitting of two 3D Dirac point into two pairs of Weyl points

Project with H. Hübener, A. F. Kemper, U. de Giovannini, A. Rubio

Beyond graphene: 3D NaBi

mpsd

- Question: Can these fictitious fields be generated with lasers via Floquet engineering?
- Preliminary result using ab initio TDDFT + Floquet downfolding: yes (to some extent)



Splitting of 3D Dirac into 2 Weyl points

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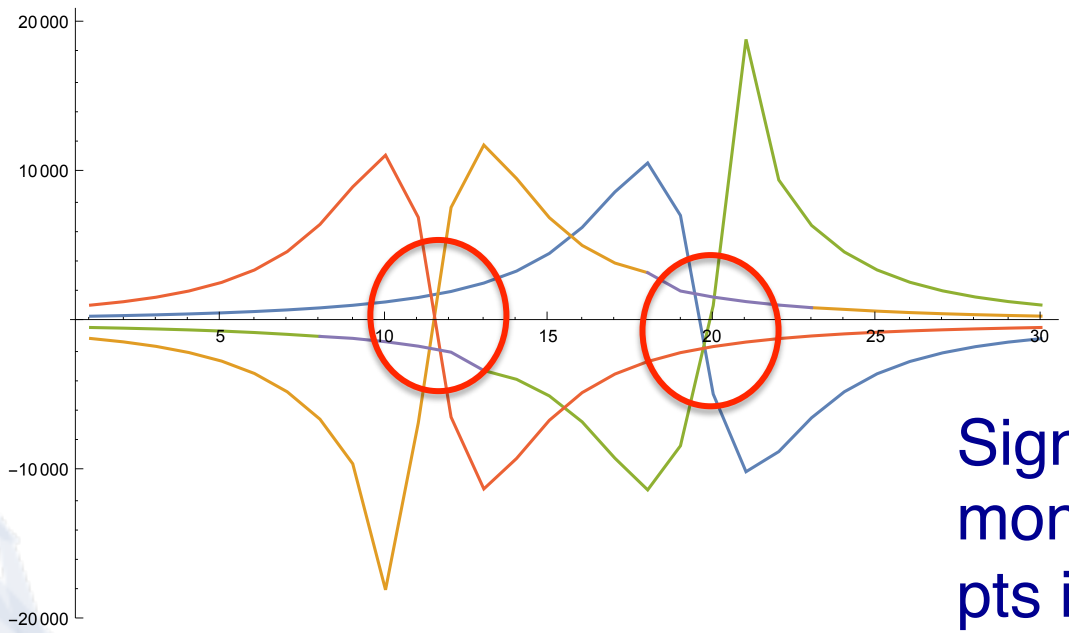
Beyond graphene: 3D NaBi

- Question: Can these fictitious fields be generated with lasers via Floquet engineering?
- Preliminary result using ab initio TDDFT + Floquet downfolding: yes (to some extent)



Signature of Dirac monopoles at Weyl pts in Berry curvature

Project with H. Hübener, A. F. Kemper, U. de Giovannini, A. Rubio

Summary

- Floquet states: engineering of fictitious gauge fields with real laser fields
- laser control of topological states of matter
- examples: 2D graphene, 3D Dirac semimetal

THANK YOU!