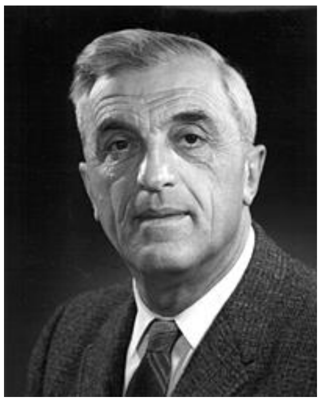
Non-Hermitian Quantum Mechanics & Topology of Finite-Lifetime Quasiparticles

Liang Fu

Kyoto workshop, 11/09/2017

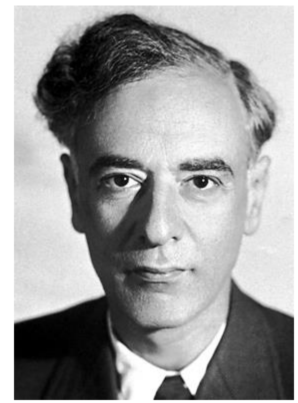
Quantum Theory of Solids: Two Foundations

Band Theory



- Bloch waves
- Energy bands in k-space

Quasiparticle



- Landau quasiparticles
- mass & lifetime

particle-wave duality

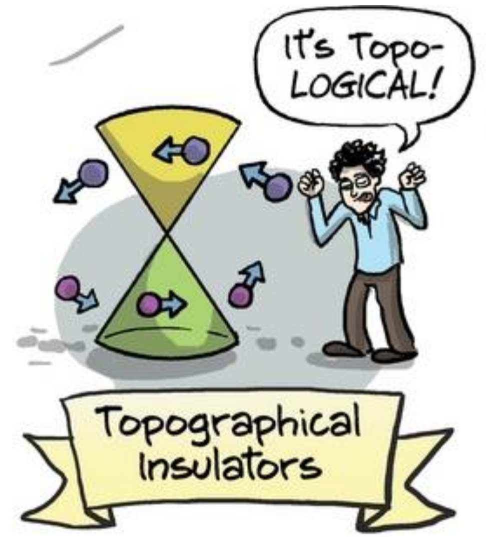
Modern Developments

Band Theory

Topological Band Theory

- global property of Bloch eigenstates $\psi(k)$ in k-space

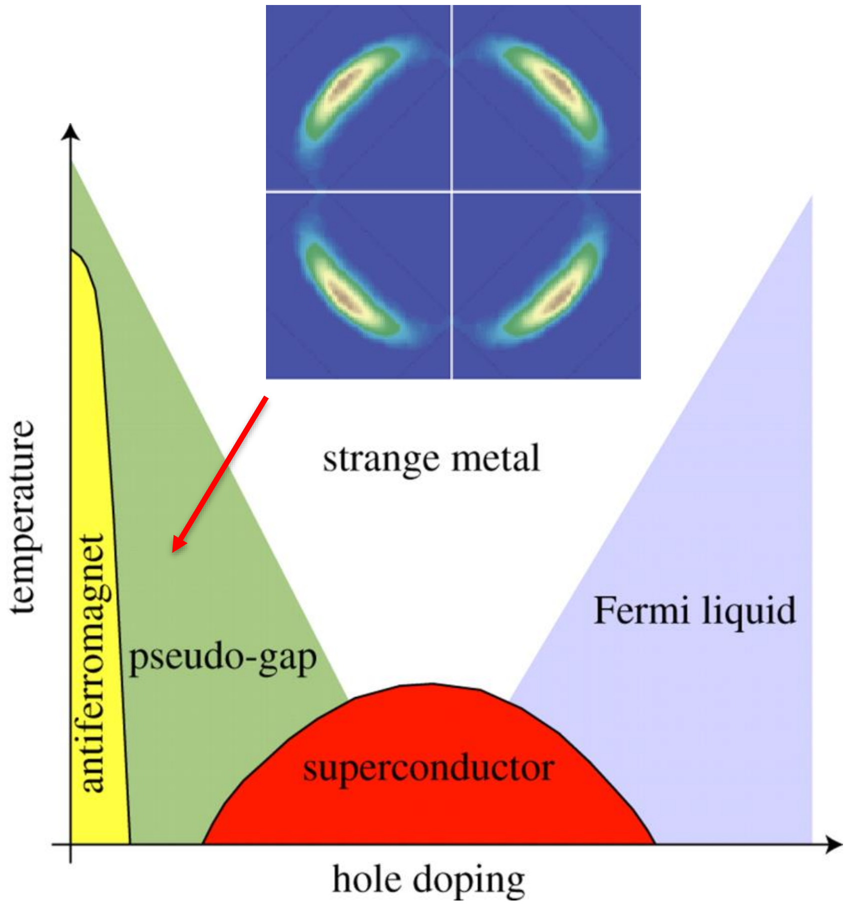
Thouless et al (1982), Haldane (1988)…



- Top. crystalline insulator
- Top. Kondo insulator
- Weyl/Dirac semimetals

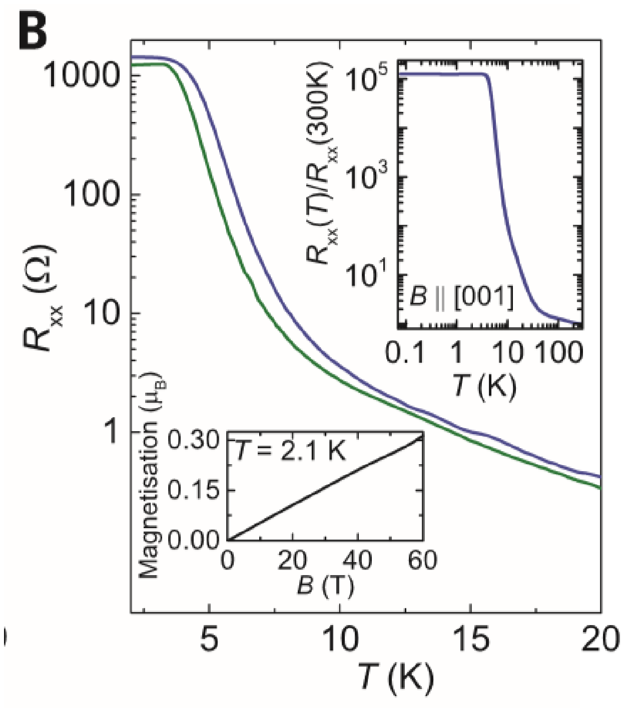
diverse phenomena, unified framework

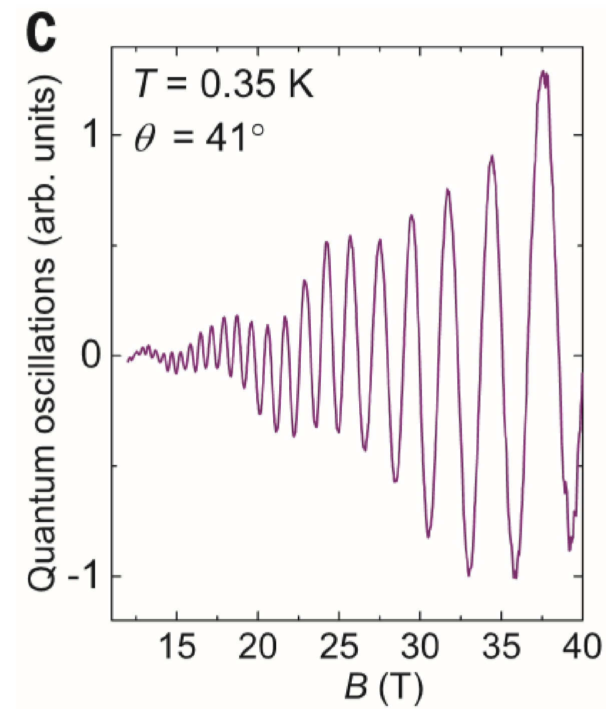
Bewildering Behaviors of Correlated Electron Systems



- Fermi arc: topological integrity of Fermi surface violated

Bewildering Behaviors of Correlated Electron Systems





Sebastian et al, Science (2015); Li et al, Science (2014)

- SmB_6 & YbB_{12}: quantum oscillation in heavy fermion insulators

Bulk Fermi arc & Insulator’s Fermi surface

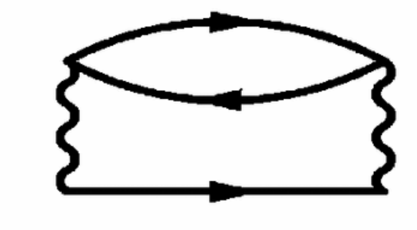
- shaking the fundamental of solid-state theory?
- special or generic phenomena?
- theoretical framework?

Quasiparticles vs. Noninteracting Electrons

Fundamental distinction:

- Quasiparticles have finite lifetime resulting from e-e and e-phonon interaction at $T \neq 0$, and impurity scattering at all T.
- Non-interacting electrons last forever.

Fermi liquid:



$$\mathrm{Im}\Sigma(k_F, \omega = 0) \propto T^2 < k_B T$$

Electron-phonon, quantum critical & chaotic systems:

$$\mathrm{Im}\Sigma(\omega \sim 0) \sim k_B T$$

Damping + Dispersion

Green's function: $G^R(\boldsymbol{k},\omega) = \quad (\omega - H(\boldsymbol{k},\omega)\,)^{-1}$

Quasiparticle Hamiltonian: $H(\boldsymbol{k},\omega) \;\equiv\; H_0(\boldsymbol{k}) + \Sigma(\boldsymbol{k},\omega)$

(non-Hermitian)

Bloch Hamiltonian self-energy

Finite lifetime means Σ is non-Hermitian: $\Sigma = \Sigma' + i\Sigma''$

Complex spectrum of $H(\boldsymbol{k},\omega\sim 0)$ determines quasiparticle properties

Re(E_k) : quasiparticle dispersion

Im(E_k) : inverse lifetime

single-band system: $E_k = \epsilon_{\mathrm{k}} - i\gamma_{\mathrm{k}}$

Damping Reshapes Dispersion

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multi-orbital systems: H_0 & Σ are matrices and generally do not commute

- imaginary part of self-energy resulting from qp decay can have dramatic **feedback effect** on qp dispersion in zero/small-gap systems.

Kozii & LF, arXiv:1708.05841

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yin and yang of quasiparticles

multi-orbital systems: H_0 & Σ are matrices and generally do not commute

- imaginary part of self-energy Σ'' resulting from qp decay can have dramatic feedback effect on qp dispersion in zero/small-gap systems.

The whole is more than the sum of its parts !

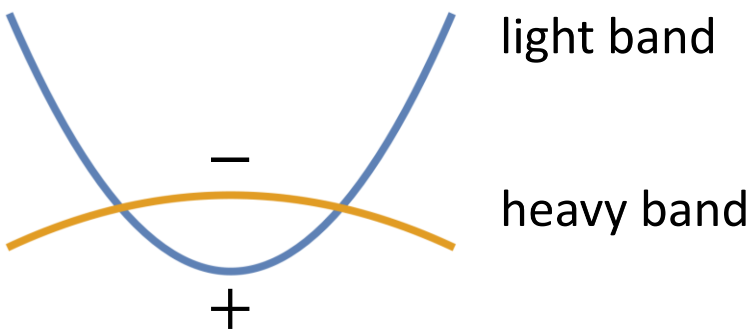
Quasiparticles in Zero/Small Gap Systems

Bloch Hamiltonian + self-energy with two lifetimes

$$H_0(\mathbf{k}) = \begin{pmatrix} \epsilon_{1\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta^*_{\mathbf{k}} & \epsilon_{2\mathbf{k}} \end{pmatrix} \sim \begin{pmatrix} v_1 k_x & v_y k_y \\ v_y k_y & -v_2 k_x \end{pmatrix}$$

near hybridization nodes

$$\Sigma = \begin{pmatrix} i\Gamma_1 & 0 \\ 0 & i\Gamma_2 \end{pmatrix}$$



Two orbitals unrelated by symmetry generally have different lifetimes.

Example: d- and f-orbitals in heavy fermion systems.

Kozii & LF, arXiv:1708.05841

Microscopic Origins of Two Lifetimes

Electron-phonon interaction: Kozii & LF, 1708.05841

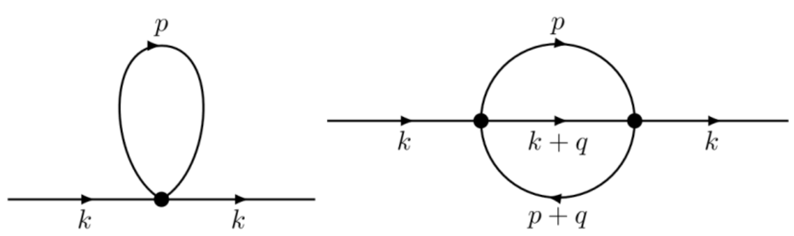
- two orbitals with different e-ph coupling constants $\lambda_{1,2}$.

Electron-electron interaction:

- periodic Anderson model Yang Qi, Kozii & LF, to appear

$$H = \sum_k \epsilon_d(k) d_k^+ d_k + \epsilon_f(k) f_k^+ f_k + \left(V_k d_k^+ f_k + h.c.\right) + \sum_i U n_{f\uparrow,i} n_{f\downarrow,i}$$

interaction on f-orbital only



(a) (b)

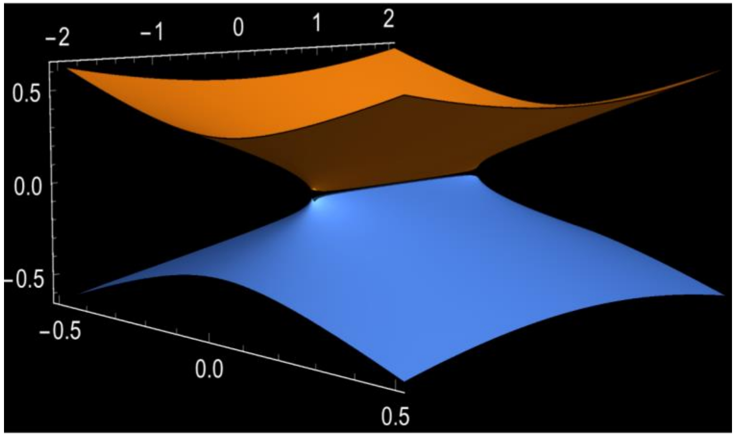
$$\Sigma = \begin{pmatrix} 0 & 0 \\ 0 & \Sigma_f \end{pmatrix}$$

Asymmetric Damping Reshapes Dispersion

Quasiparticle Hamiltonian $H(\mathbf{k}) = \begin{pmatrix} v_x k_x - i\Gamma_1 & v_y k_y \\ v_y k_y & -v_x k_x - i\Gamma_2 \end{pmatrix}$

Quasiparticle dispersion Re(E_k):

$\Gamma_1 \neq \Gamma_2$



- $\Gamma_1 - \Gamma_2 \equiv 2\gamma \neq 0$: two bands stick together to form a bulk Fermi arc, terminating at $k_x = 0,\ k_y = \pm\gamma/v_y$
- new fermiology: constant dos, strong anisotropy

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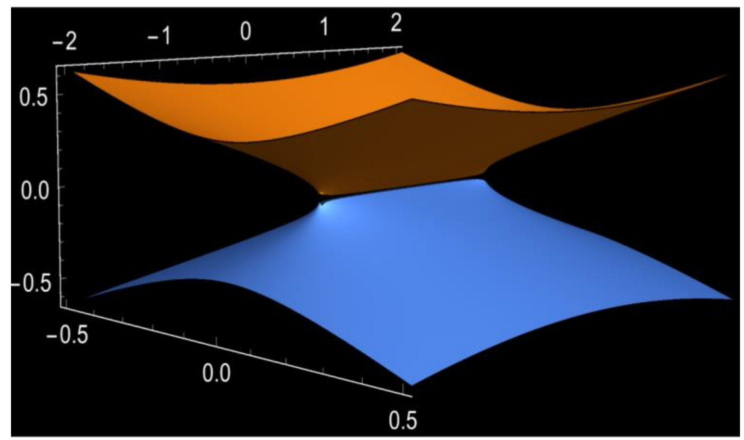
Quasiparticle dispersion Re(E_k):

Prediction: bulk Fermi arc in heavy fermion systems



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Interplay of Damping and Coherence

Non-Hermitian quasiparticle Hamiltonian:

$$H(\mathbf{k}) = \begin{pmatrix} \epsilon_{1\mathbf{k}} - i\Gamma_1 & \Delta_{\mathbf{k}} \\ \Delta^*_{\mathbf{k}} & \epsilon_{2\mathbf{k}} - i\Gamma_2 \end{pmatrix}$$

$$\gamma \equiv (\Gamma_1 - \Gamma_2)/2, \quad \Gamma \equiv (\Gamma_1 + \Gamma_2)/2.$$

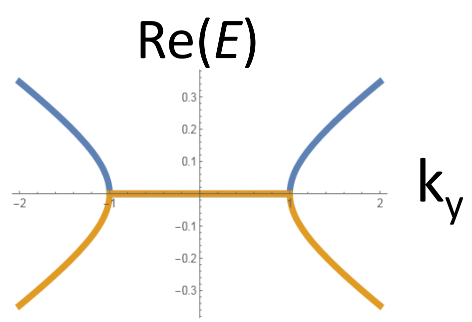
Complex-energy spectrum:

$$E_\pm(\boldsymbol{k}) = \overline{\epsilon_{\boldsymbol{k}}} \pm \sqrt{(\epsilon_{1\boldsymbol{k}} - \epsilon_{2\boldsymbol{k}} - i\gamma)^2 + |\Delta^2_{\boldsymbol{k}}|} - i\Gamma$$

without hybridization, Fermi surface at band crossing $\epsilon_{1\boldsymbol{k}} = \epsilon_{2\boldsymbol{k}}$

with hybridization and asymmetric damping,

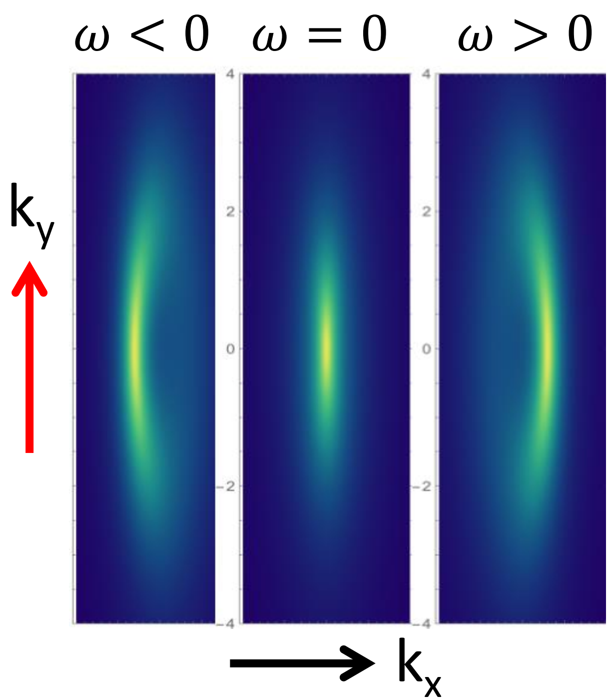
- for $|\Delta_{\boldsymbol{k}}| > \gamma$: $\mathrm{Re}(E_+) \neq - \mathrm{Re}(E_-)$ (gap opens)
- for $|\Delta_{\boldsymbol{k}}| < \gamma$: $\mathrm{Re}(E_+) = \mathrm{Re}(E_-) = 0$ (gap closes)



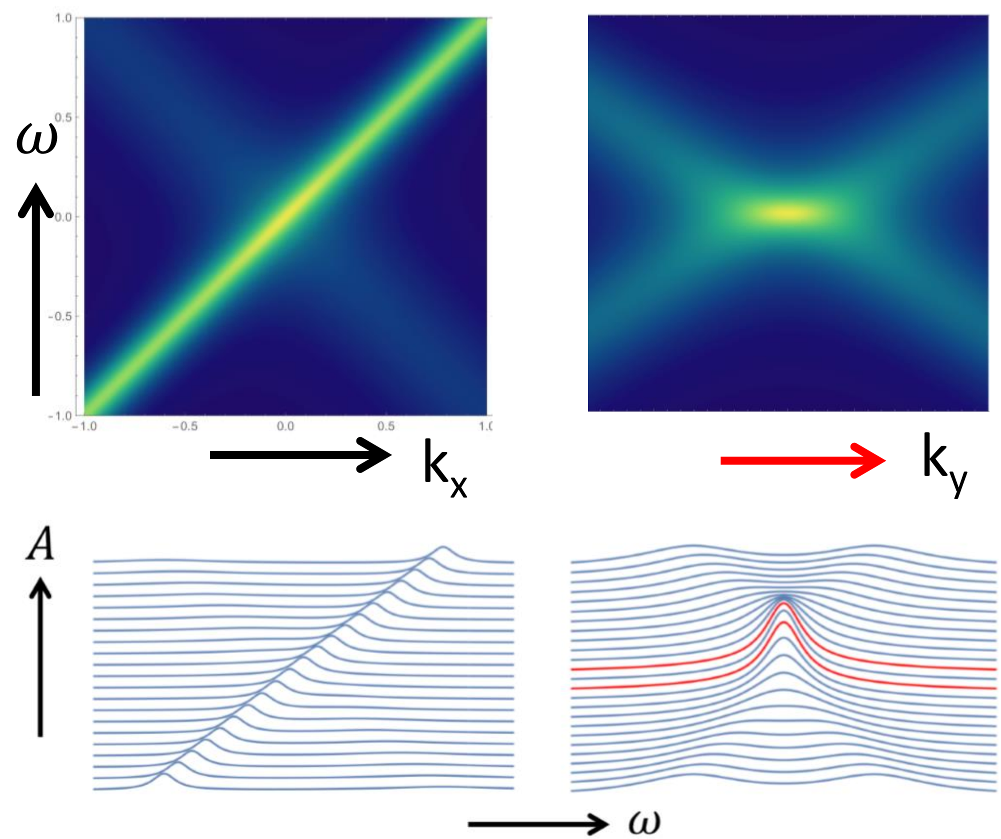
Spectral Function

$$A(\boldsymbol{k},\omega) = -\mathrm{Im}\big(\mathrm{Tr}G^{R}(\boldsymbol{k},\omega)\big) = -\mathrm{Im}\left(\frac{1}{\omega - E_{+}(\boldsymbol{k})} + \frac{1}{\omega - E_{-}(\boldsymbol{k})}\right)$$

constant-energy contour



linecuts

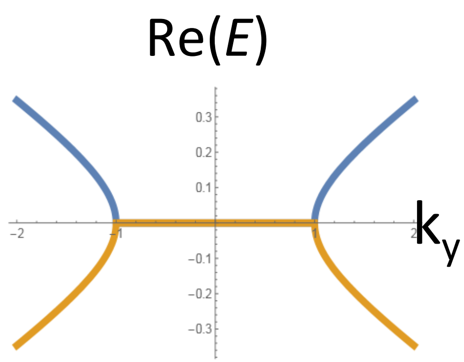


- Dirac point spreads into an arc
- Asymmetry due to two lifetimes

Topological Stability of Bulk Fermi Arc

$$H(\boldsymbol{k}) = (v_x k_x - i\,\gamma)\sigma_z + v_y k_y \sigma_x$$

$$\rightarrow \gamma(-i\,\sigma_z \pm \sigma_x) \quad \text{at } \pm\boldsymbol{k_0} \equiv (0, \pm\gamma/v_y)$$



$$E_\pm(k) = \pm\sqrt{(v_x k_x - i\gamma)^2 + v_y^2 k_y^2}$$

- at two ends of Fermi arc $\boldsymbol{k} = \pm\boldsymbol{k_0}$, matrix *H* is non-diagonalizable and has only one eigenstate!
- eigenvalue coalescence is unique to non-Hermitian operators.

Exceptional Points

DIE GRUNDLEHREN DER MATHEMATISCHEN WISSENSCHAFTEN IN EINZELDARSTELLUNGEN

VOLUME 132

Perturbation Theory for Linear Operators

T. Kato

1966

ON THE COMPLETENESS OF THE EIGENFUNCTIONS OF SOME CLASSES OF NON-SELFADJOINT LINEAR OPERATORS[1]

M. V. Keldysh 1971

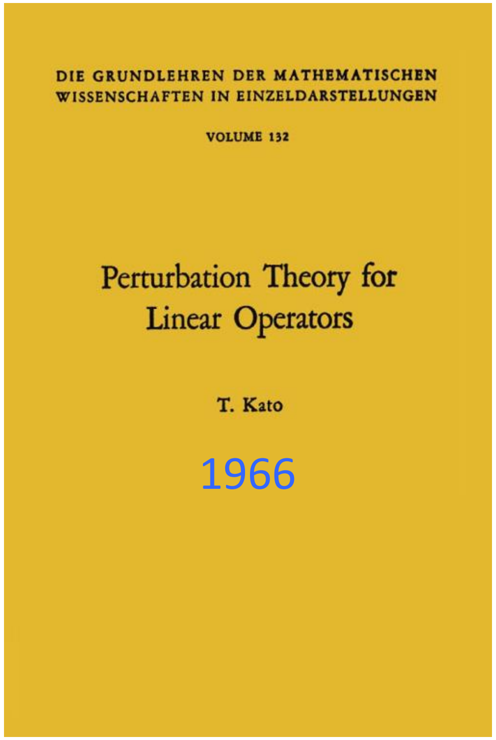
Physics of nonhermitian degeneracies

M.V. Berry **) 2004

Spawning rings of exceptional points out of Dirac cones 2015

Bo Zhen[1]*, Chia Wei Hsu[1,2]*, Yuichi Igarashi[1,3]*, Ling Lu[1], Ido Kaminer[1], Adi Pick[1,4], Song-Liang Chua[5], John D. Joannopoulos[1] & Marin Soljačić[1]

Exceptional Points



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- In open systems, non-Hermiticity results from coupling with external bath.
- In interacting many-body systems, microscopic Hamiltonian is Hermitian, while *one-body* quasiparticle Hamiltonian is *non-Hermitian* due to damping.

Kozii & LF, arXiv:1708.05841

Topology of Finite-Lifetime Quasiparticles

k-space:

Non-Hermitian Hamiltonian:

$$H(\boldsymbol{k},\omega) \equiv H_0(\boldsymbol{k}) + \Sigma(\boldsymbol{k},\omega)$$

Topology of non-Hermitian quasiparticle Hamiltonian:
the generalization of topological band theory
to interacting electron systems.

*quasiparticles can be electron, magnon, exciton...

Shen, Zhen & LF, arXiv:1706.07435

Topological Band Theory for Non-Hermitian Hamiltonians

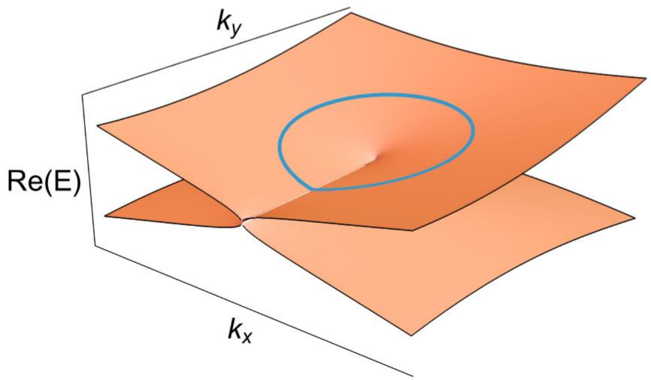
arXiv:1706.07435

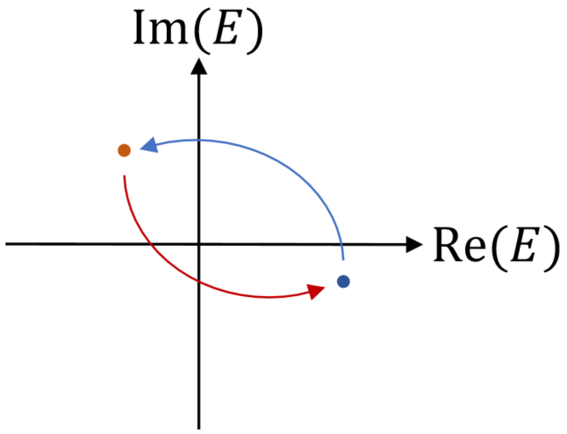
generic Hamiltonian $H(k_x, k_y)$ near exceptional point (EP):

$$H = \epsilon\sigma_+ + \lambda_{ij}k_i\sigma_j \quad \Rightarrow \quad E_\pm(k) = \pm\sqrt{\epsilon(v_x k_x + v_y k_y)}$$

($v_x,\ v_y,\ v_y/v_x$ are complex)

due to double-valuedness of square root, encircling an EP in k-space swaps the pair of complex eigenvalues: $E_+ \rightarrow E_-$, $E_- \rightarrow E_+$





Topological Band Theory for Non-Hermitian Hamiltonians

arXiv:1706.07435

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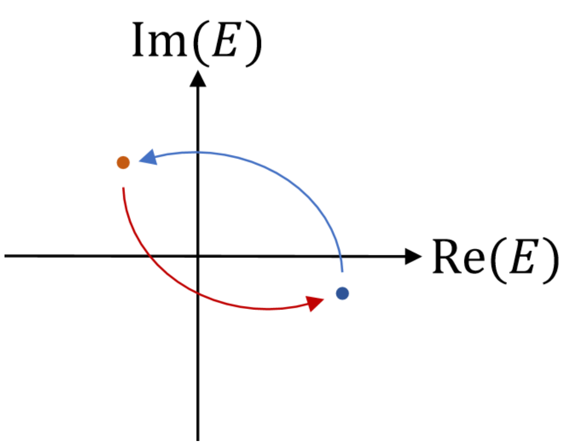
topological index: vorticity of complex energy “gap” in k-space

$$\nu_{mn}(\Gamma) = -\frac{1}{2\pi}\oint_\Gamma \nabla_{\mathbf{k}} \arg\left[E_m(\mathbf{k}) - E_n(\mathbf{k})\right] \cdot d\mathbf{k},$$

topological charge of exceptional point: $\nu = \pm\frac{1}{2}$

topology guarantees a line of real gap closing (= Fermi arc) emanates from EP.



Exceptional Points: *Ubiquitous* in $d \geq 2$

How many parameters must be tuned to hit a degeneracy?

- Hermitian: 3

  $\vec{a} \cdot \vec{\sigma}$ is degenerate when $\vec{a} = 0$ => topological <u>Weyl points</u> in 3D

- non-Hermitian: 2

  $(\vec{a} + i\vec{b}) \cdot \vec{\sigma}$ is defective when $\vec{a} \cdot \vec{b} = 0$ and $|\vec{a}| = |\vec{b}|$

=> topological <u>exceptional points</u> in 2D and <u>exceptional loops</u> in 3D.

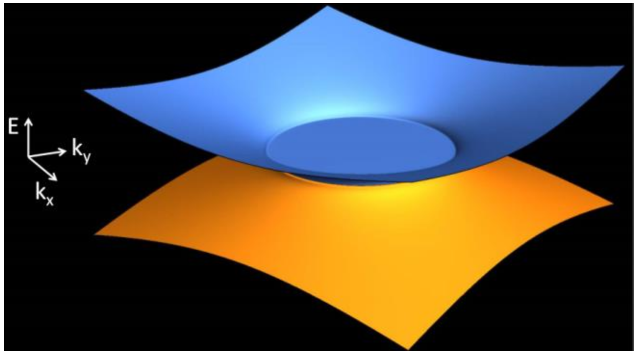
Exceptional Points in 2D

Introducing generic damping to 2D Dirac fermion: arXiv:1706.07435

$$H(\boldsymbol{k}) = (k_x - i\kappa_1)\sigma_z + (k_y - i\kappa_2)\sigma_x + (m - i\delta)\sigma_y$$

- imaginary vector potential:
  Dirac point turns into Fermi arc ending at a pair of EPs.

- imaginary Dirac mass
  Dirac point turns into “Fermi disk” ending at a **ring** of EPs



LETTER

Spawning rings of exceptional points out of Dirac cones

Bo Zhen[1]*, Chia Wei Hsu[1,2]*, Yuichi Igarashi[1,3]*, Ling Lu[1], Ido Kaminer[1], Adi Pick[1,4], Song-Liang Chua[5], John D. Joannopoulos[1] & Marin Soljačić[1]

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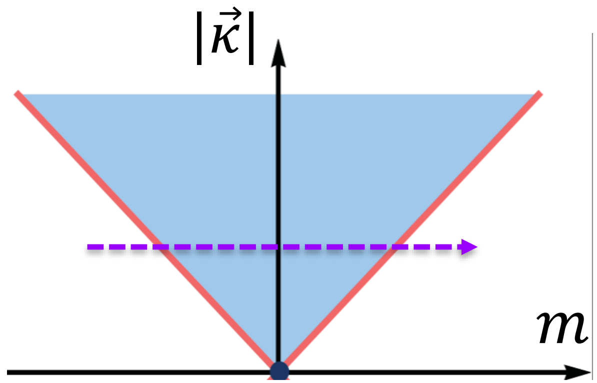
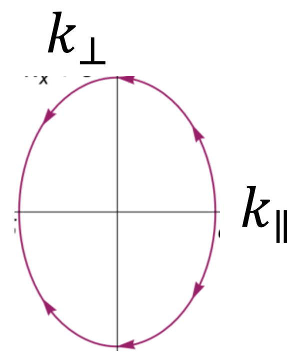




Direct quantum Hall transition is replaced by intermediate phase with a pair of exceptional points at momenta:

$$\mathbf{k}_\pm = -\frac{m\delta}{\kappa}\hat{\mathbf{n}} \pm \frac{\sqrt{(\kappa^2 - m^2)(\kappa^2 + \delta^2)}}{\kappa}\hat{\mathbf{z}} \times \hat{\mathbf{n}}.$$

Topological Band Theory for Non-Hermitian Hamiltonians

arXiv:1706.07435

Exceptional points cannot be created or removed alone.

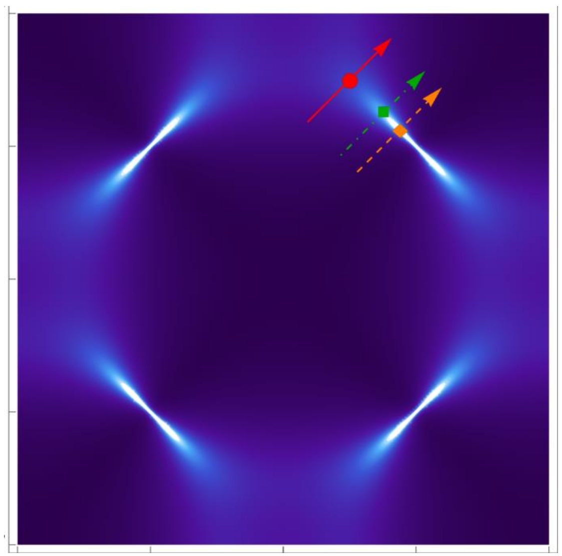
Merging a pair of exceptional points:

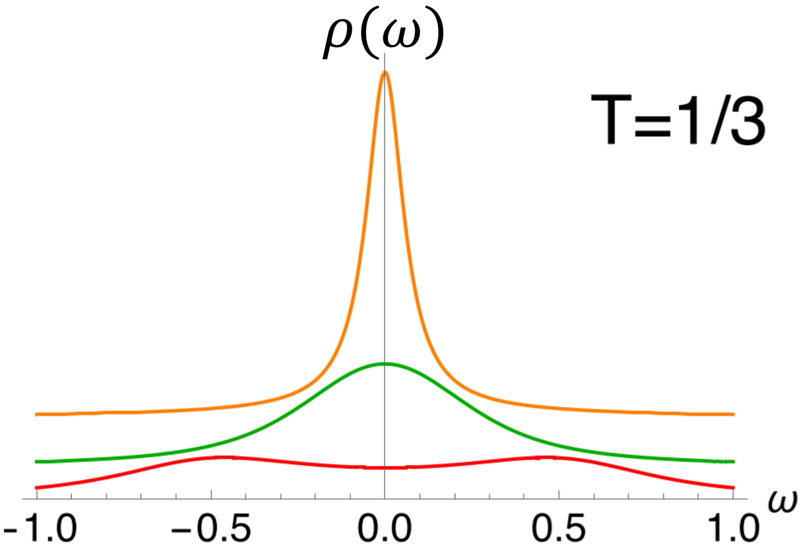
- $\frac{1}{2}+\frac{1}{2}=1$: results in a topological "vortex point".
- $\frac{1}{2}-\frac{1}{2}=0$: results in a "hybrid point", which can be gapped.

TABLE I. Four types of degeneracy in non-Hermitian Hamiltonians with their properties.

Degeneracy	Vorticity	Defectiveness
Exceptional point	Half-integer	Defective
Hybrid point	Zero	Defective
Dirac point	Zero	Non-defective
Vortex point	Nonzero integer	Non-defective

Fermi Arc in Heavy Fermion Systems





Yuki Nagai
(JAEA & MIT)

DMFT shows temperature-dependent bulk Fermi arc in periodic Anderson model with d-wave hybridization.

Topology of "Gapped" Non-Hermitian Band Structure

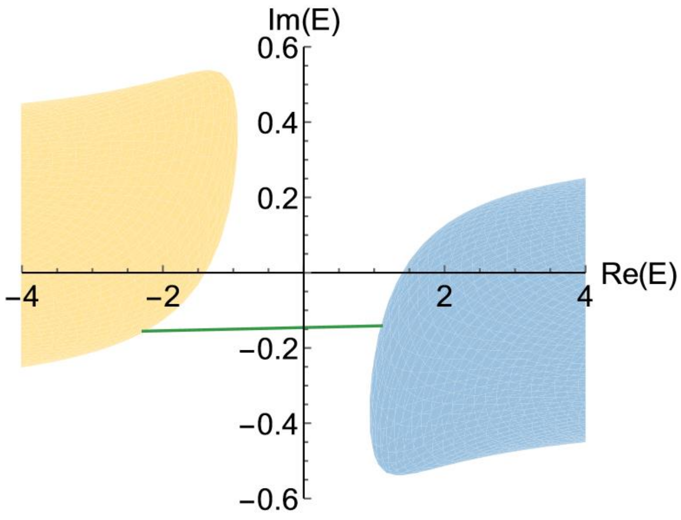
While $E_n(\mathbf{k})$ are generally complex, we define a band n to be "separable" if its energy $E_n(\mathbf{k}) \neq E_m(\mathbf{k})$ for all $m \neq n$ and all $\mathbf{k}$. We define a band n to be "isolated" if $E_n(\mathbf{k}) \neq E_m(\mathbf{k}')$ for all $m \neq n$ and all $\mathbf{k}, \mathbf{k}'$, i.e., the region of energies $\{E_n(\mathbf{k}), \mathbf{k} \in \mathrm{BZ}\}$ in the complex plane does not overlap with that of any other band. In this case, we say the band $E_n(\mathbf{k})$ is surrounded by a "gap" in the complex energy plane where no bulk states exist. A band is called "inseparable" if at some momentum the complex-energy is degenerate with another band. Our

Left and right eigenstates: $H\,|\psi_n^{\mathrm{R}}\rangle = E_n\,|\psi_n^{\mathrm{R}}\rangle\,,\; H^\dagger\,|\psi_n^{\mathrm{L}}\rangle = E_n^*\,|\psi_n^{\mathrm{L}}\rangle$

Shen, Zhen & LF, arXiv:1706.07435

Gapped Non-Hermitian Band Structures

Complex energy plane



LL, RR, LR, RL Berry curvature

$$B_{n,ij}^{\alpha\beta}(\mathbf{k}) \equiv i \langle \partial_i \psi_n^{\alpha}(\mathbf{k}) | \partial_j \psi_n^{\beta}(\mathbf{k}) \rangle ,$$

Chern numbers: all equal!

$$N_n^{\alpha\beta} = \frac{1}{2\pi} \int_{\mathrm{BZ}} \epsilon_{ij} B_{n,ij}^{\alpha\beta}(\mathbf{k}) d^2\mathbf{k},$$

Proof based on the fact

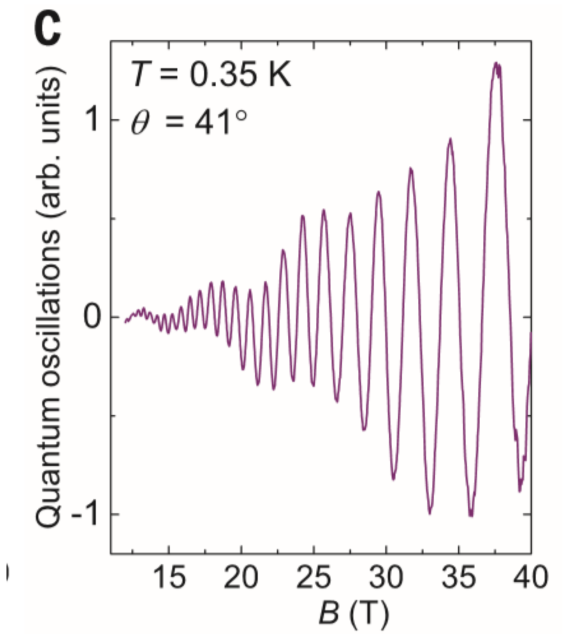
$$\langle \psi_n^{\mathrm{L}} | \psi_n^{\mathrm{R}} \rangle \neq 0$$

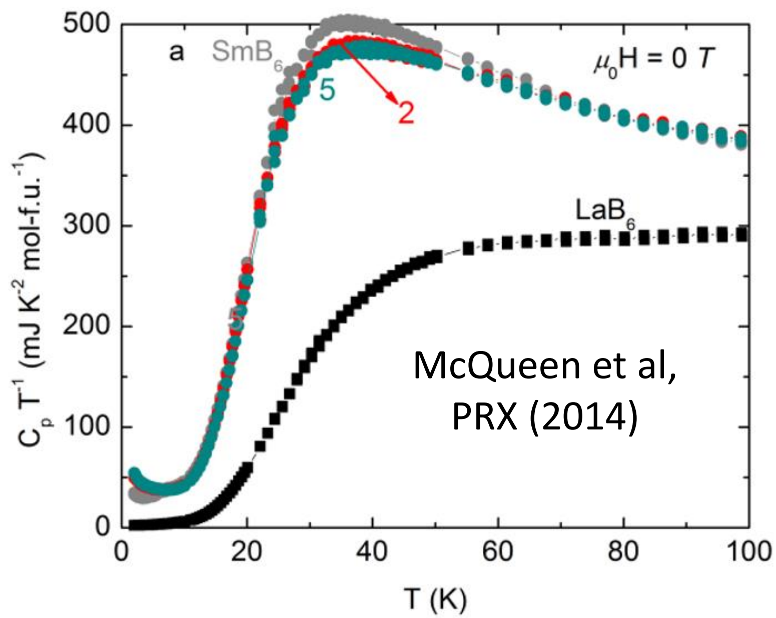
- topologically protected edge state of non-Hermitian Hamiltonians

Shen, Zhen & LF, arXiv:1706.07435

Fermi Surface & Quantum Oscillation of In-Gap Quasiparticles

Motivation: quantum oscillation in SmB_6 & YbB_{12}:





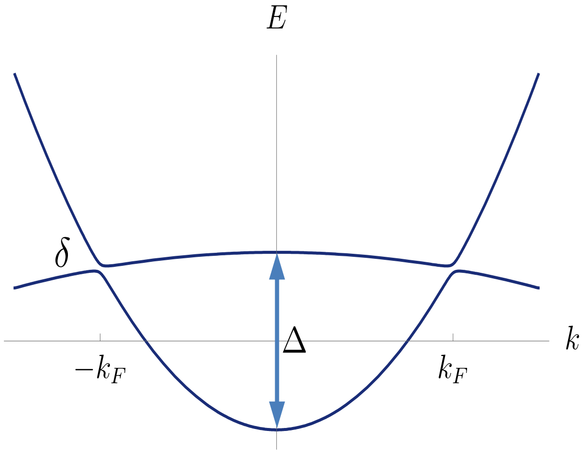
- Ground state of Kondo insulator in periodic Anderson model is adiabatically connected to band insulator
- In-gap states seen in specific heat, optical conductivity

Fermi Surface & Quantum Oscillation of In-Gap Quasiparticles

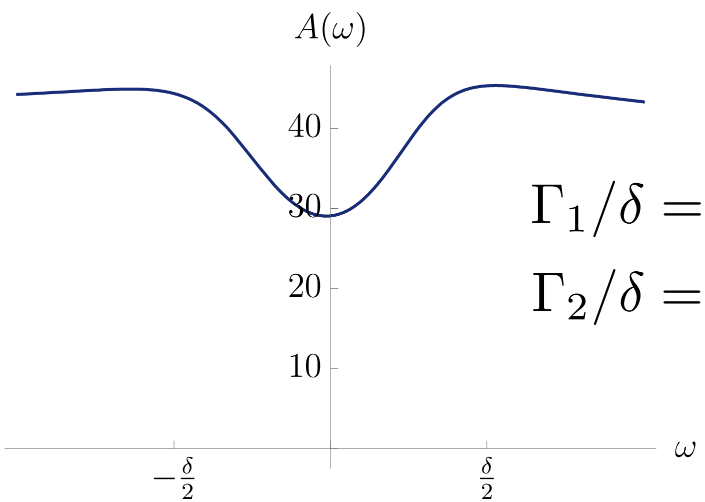
Our proposal: Huitao Shen & LF, to appear

In-gap states are due to quasiparticle damping (e.g., impurity scattering)

$$H_0(\mathbf{k}) = \begin{pmatrix} \epsilon_{1\mathbf{k}} - i\Gamma_1 & \delta \\ \delta & \epsilon_{2\mathbf{k}} - i\Gamma_2 \end{pmatrix}$$



Inverted gap



$\Gamma_1/\delta = 2$

$\Gamma_2/\delta = 0.1$

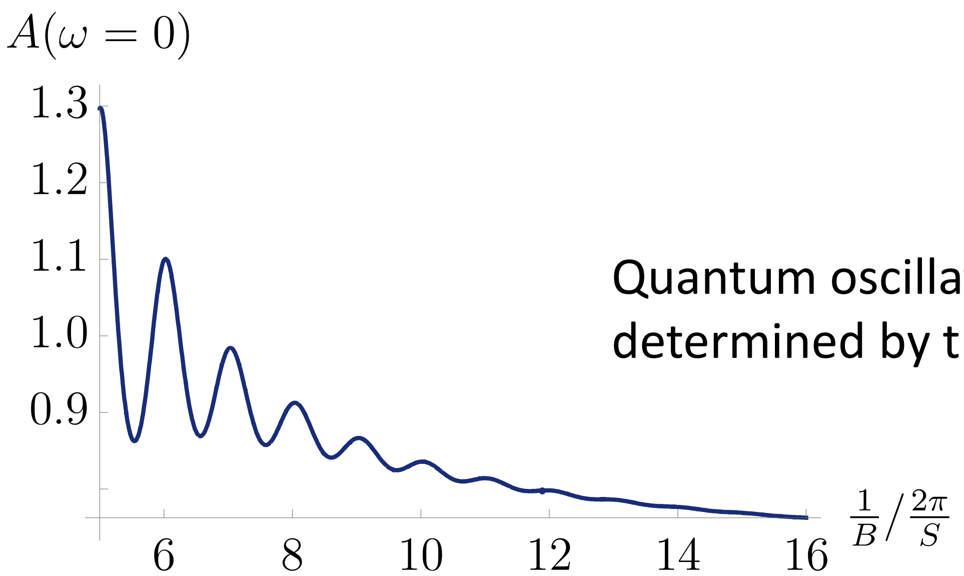
- f-electrons have much smaller damping rate due to localized nature

Fermi Surface & Quantum Oscillation of In-Gap Quasiparticles

Complex-energy spectrum: $E_{\pm}(\boldsymbol{k}) = \overline{\epsilon_{\boldsymbol{k}}} \pm \sqrt{(\epsilon_{1\boldsymbol{k}} - \epsilon_{2\boldsymbol{k}} - i\gamma)^2 + \delta^2} - i\Gamma$

$\Gamma_1 - \Gamma_2 > 2\delta$: Re($E_+$) = Re($E_-$) band gap closes & Fermi surface recovers!

Solution of non-Hermitian Landau level problem:



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Quantum oscillation amplitude is largely determined by the long lifetime of f-band

Quasiparticles in Correlated Electron Systems

Damping =non-Hermicity: reshapes dispersion
& leads to new topology.

Prediction:

- Bulk Fermi arc in heavy fermion systems
- Quantum oscillation in insulators with inverted gap

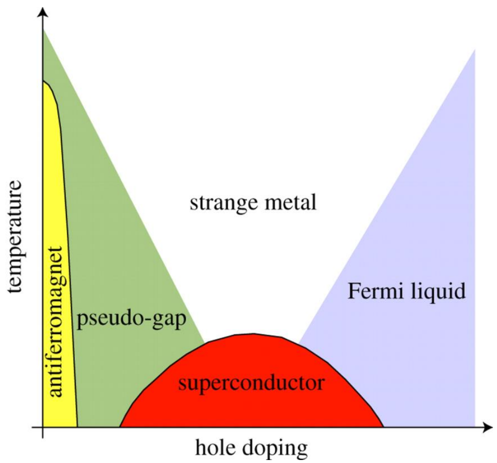
Outlook:

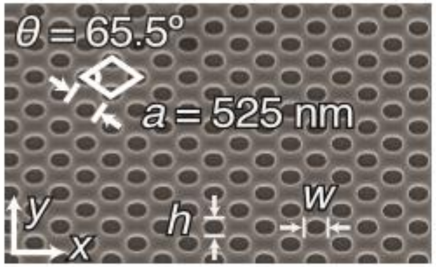
- non-Hermitian topology + DMFT => material calculation/prediction
- thermodynamics & transport of *exceptional quasiparticles*

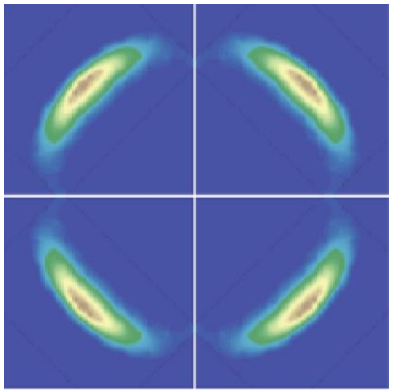
Damping Reshapes Dispersion

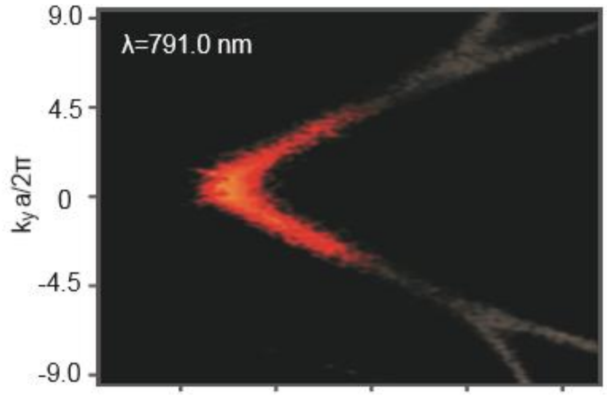
Postscript: **Observation of Bulk Fermi Arc and Polarization Half Charge from Paired Exceptional Points**

Hengyun Zhou,[1,2,*] Chao Peng,[1,3,*] Yoseob Yoon,[4] Chia Wei Hsu,[5] Keith A. Nelson,[4] Liang Fu,[1] John D. Joannopoulos,[1] Marin Soljačić,[1] and Bo Zhen[1,6,†]









Non-Hermitian Quantum Mechanics:

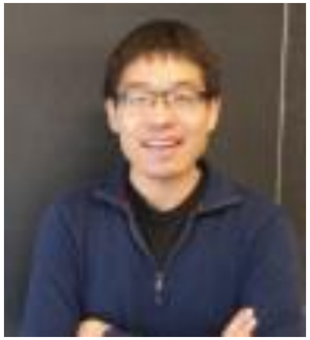
As an effective theory, it is natural and everywhere. Its many unusual consequences are waiting to be explored.

Non-Hermitian = dissipative, open system, subsystem…

Thanks to

Vlad Kozii

Huitao Shen

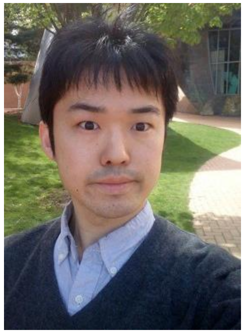


Bo Zhen

Yang Qi

Michal Papaj

Yuki Nagai



Hiroki Isobe