Flat bands and the geometry of Bloch wave functions

Jun-Won Rhim(임준원)
Physics Department, Ajou University

Era of Berry curvature

Berry connection $$\mathcal{A}_n(\boldsymbol{R}) = i\langle n(\boldsymbol{R})|\frac{\partial}{\partial \boldsymbol{R}}|n(\boldsymbol{R})\rangle$$

Berry curvature $$\boldsymbol{\Omega}_n(\boldsymbol{R}) = \boldsymbol{\nabla}_{\boldsymbol{R}} \times \mathcal{A}_n(\boldsymbol{R})$$

Di Xiao, Ming-Che Chang, and Qian Niu, Rev. Mod. Phys. **82**, 1959 (2010)

Era of Berry curvature

Semiclassical equations of motion

Anomalous velocity

$$\boldsymbol{v}_n(\boldsymbol{k}) = \frac{\partial \varepsilon_n(\boldsymbol{k})}{\hbar \partial \boldsymbol{k}} - \frac{e}{\hbar}\boldsymbol{E} \times \boldsymbol{\Omega}_n(\boldsymbol{k})$$

Di Xiao, Ming-Che Chang, and Qian Niu, Rev. Mod. Phys. **82**, 1959 (2010)

Era of Berry curvature

$$\boxed{\text{Semiclassical equations of motion}}$$

Anomalous velocity

$$\boldsymbol{v}_n(\boldsymbol{k}) = \frac{\partial \varepsilon_n(\boldsymbol{k})}{\hbar \partial \boldsymbol{k}} - \frac{e}{\hbar}\boldsymbol{E} \times \boldsymbol{\Omega}_n(\boldsymbol{k})$$

- Quantum Hall effect
- Anomalous Hall effect
- Valley Hall effect

⋮

Di Xiao, Ming-Che Chang, and Qian Niu, Rev. Mod. Phys. **82**, 1959 (2010)

Era of Berry curvature

$\boxed{\text{Semiclassical equations of motion}}$

Anomalous velocity
$$\boldsymbol{v}_n(\boldsymbol{k}) = \frac{\partial \varepsilon_n(\boldsymbol{k})}{\hbar \partial \boldsymbol{k}} - \frac{e}{\hbar}\boldsymbol{E} \times \boldsymbol{\Omega}_n(\boldsymbol{k})$$

- **<u>Quantum Hall effect</u>** ⟶ $$\boxed{\sigma_{xy} = \frac{e^2}{\hbar}\int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2}\Omega_{k_x k_y}}$$ Chern number
- Anomalous Hall effect
- Valley Hall effect

⋮

Di Xiao, Ming-Che Chang, and Qian Niu, Rev. Mod. Phys. **82**, 1959 (2010)

Era of Berry curvature

Semiclassical equations of motion

Anomalous velocity $$\boldsymbol{v}_n(\boldsymbol{k}) = \frac{\partial \varepsilon_n(\boldsymbol{k})}{\hbar \partial \boldsymbol{k}} - \frac{e}{\hbar}\boldsymbol{E} \times \boldsymbol{\Omega}_n(\boldsymbol{k})$$

- **<u>Quantum Hall effect</u>** → $$\sigma_{xy} = \frac{e^2}{\hbar}\int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2}\Omega_{k_x k_y}$$ Chern number
- Anomalous Hall effect
- Valley Hall effect

⋮

↓

Topological analysis of solid state systems

Di Xiao, Ming-Che Chang, and Qian Niu, Rev. Mod. Phys. **82**, 1959 (2010)

Era of Berry curvature

Electric polarization

Berry connection

$$P_{e,\perp} = \frac{-ie}{(2\pi)^3} \int_{\mathcal{A}} d\mathbf{k}_{\|} \sum_{n=1}^{M} \boxed{\int_0^{G_\perp} dk_\perp \left\langle u_{n\mathbf{k}} \middle| \frac{\partial}{\partial k_\perp} \middle| u_{n\mathbf{k}} \right\rangle}$$

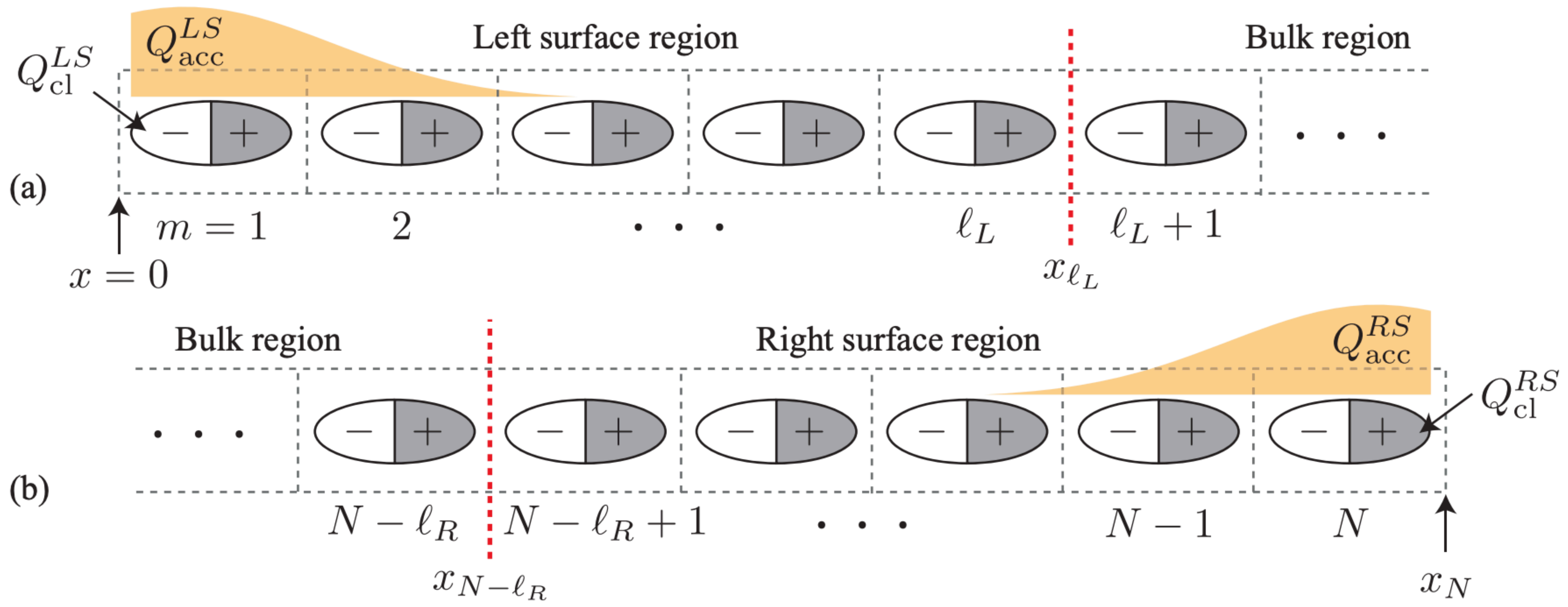
Zak phase

R. D. King-Smith and David Vanderbilt, Phys. Rev. B **47**, 1651(R) (1993)

Era of Berry curvature

Electric polarization

$$P_{e,\perp} = \frac{-ie}{(2\pi)^3} \int_{\mathcal{A}} d\mathbf{k}_{\|} \sum_{n=1}^{M} \int_0^{G_\perp} dk_\perp \left\langle u_{n\mathbf{k}} \left| \frac{\partial}{\partial k_\perp} \right| u_{n\mathbf{k}} \right\rangle$$

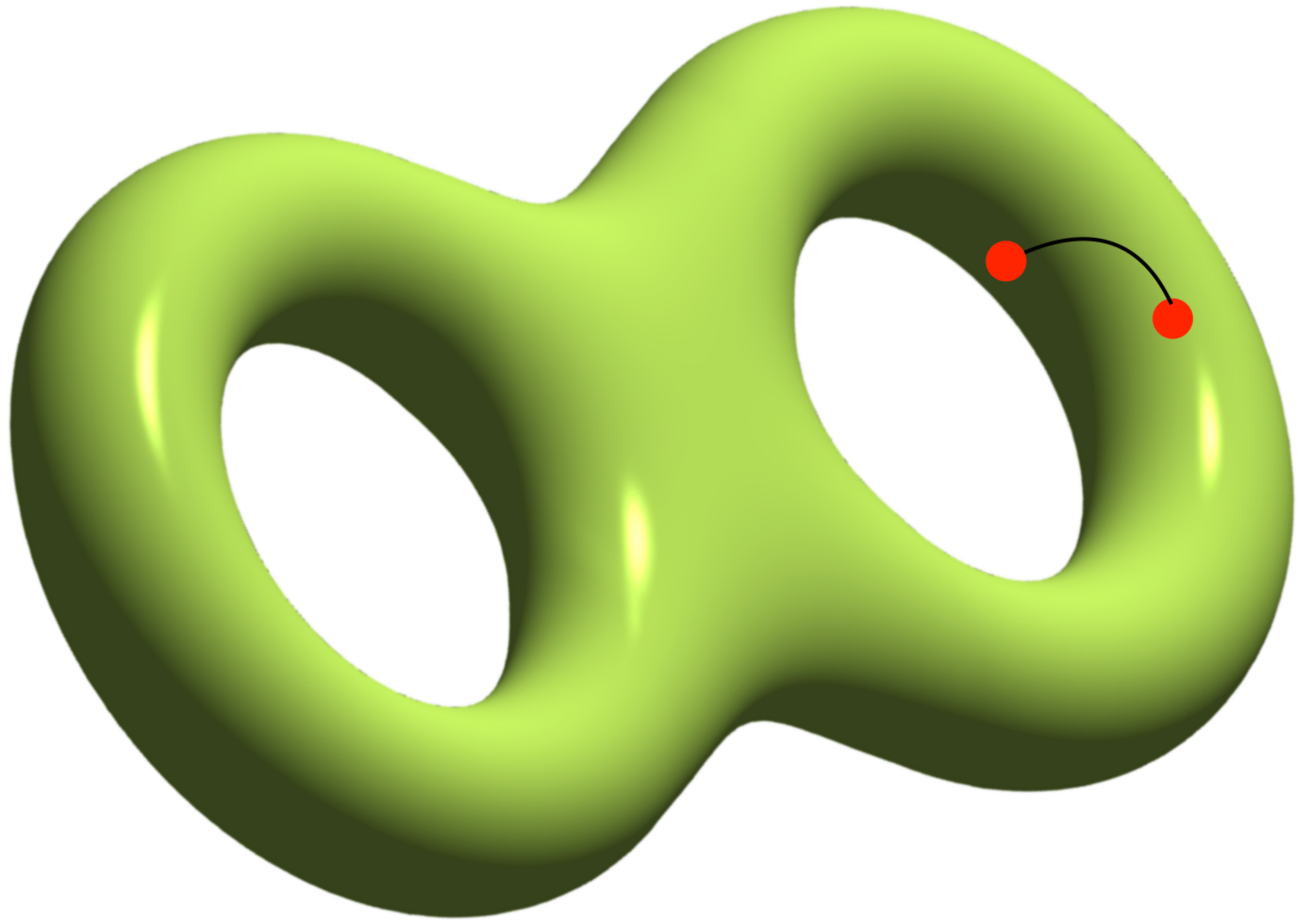


1-D bulk-boundary correspondence

Jun-Won Rhim, Jan Behrends, and Jens H. Bardarson, Phys. Rev. B **95**, 035421 (2017)

R. D. King-Smith and David Vanderbilt, Phys. Rev. B **47**, 1651(R) (1993)

Distance or metric?



Berry curvature $\quad \boldsymbol{\Omega}_n(\boldsymbol{R}) = \boldsymbol{\nabla}_{\boldsymbol{R}} \times \mathcal{A}_n(\boldsymbol{R})$

Distance or metric?

The Quantum Phase, Five Years After

M. V. Berry

H.H.Wills Physics Laboratory
Tyndall Avenue, Bristol BS8 1TL, U.K.

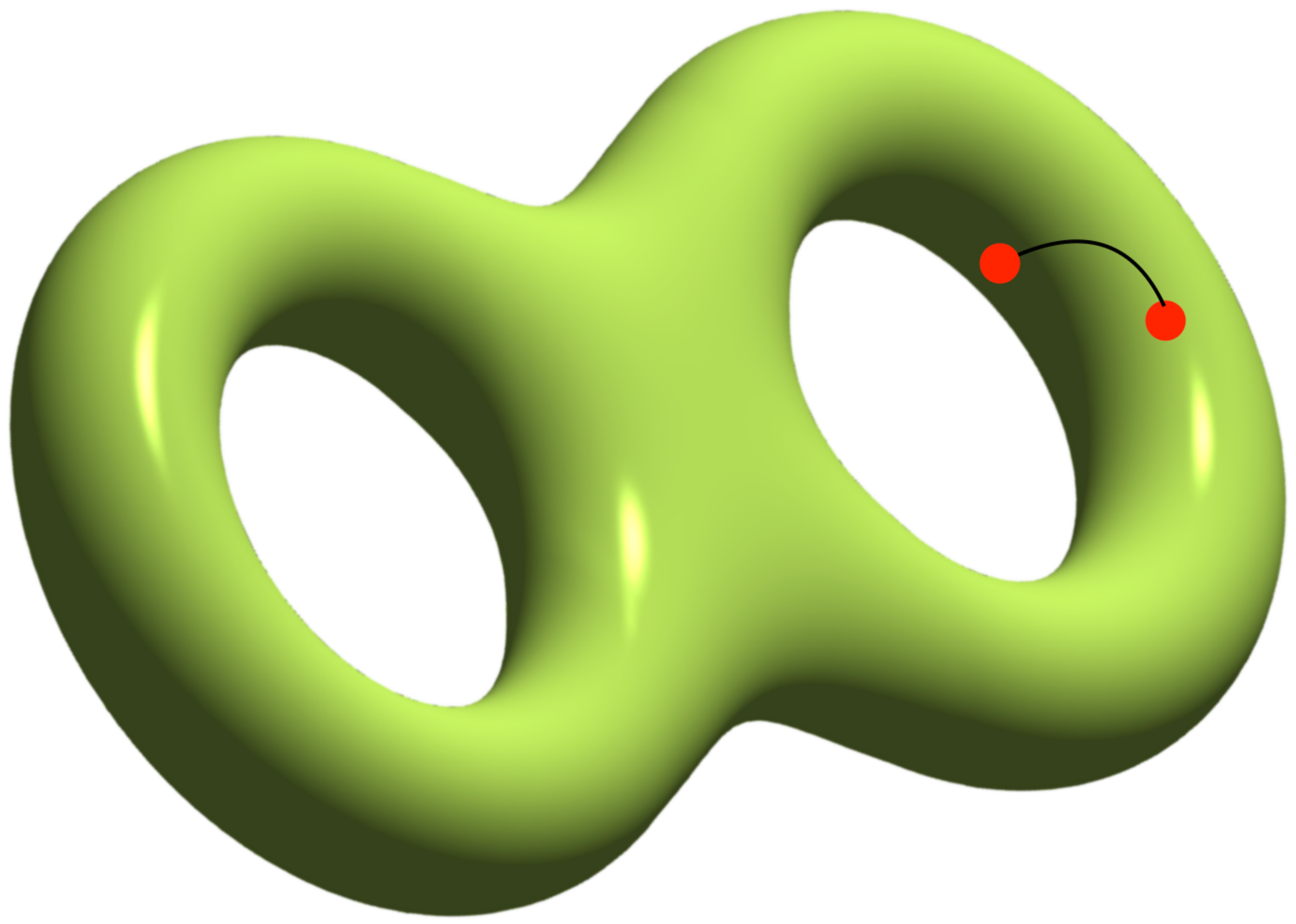
Commun. Math. Phys. 76, 289–301 (1980)

Communications in Mathematical Physics

Riemannian Structure on Manifolds of Quantum States

J. P. Provost and G. Vallee

Physique Théorique, Université de Nice*,**



Berry curvature $\boldsymbol{\Omega}_n(\boldsymbol{R}) = \boldsymbol{\nabla}_{\boldsymbol{R}} \times \mathcal{A}_n(\boldsymbol{R})$

Quantum distance $\boxed{s^2 = 1 - |\langle v_{\mathbf{k}} | v_{\mathbf{k}'} \rangle|^2}$

Distance or metric?

Quantum distance $$s^2 = 1 - |\langle v_{\mathbf{k}} | v_{\mathbf{k}'} \rangle|^2$$

$$\Downarrow$$

$$ds^2 = 1 - |\, \langle u_n(\mathbf{k}) | u_n(\mathbf{k} + d\mathbf{k}) \rangle \,|^2$$

$$= \left(\Re\left[\left\langle \partial_{k_i} u_n \middle| \partial_{k_j} u_n \right\rangle \right] - \left\langle \partial_{k_i} u_n \middle| u_n \right\rangle \left\langle u_n \middle| \partial_{k_j} u_n \right\rangle \right) dk_i dk_j$$

$$= g_{ij}^n dk_i dk_j$$

Distance or metric?

Quantum distance $$s^2 = 1 - \left|\left\langle v_{\mathbf{k}} \middle| v_{\mathbf{k}'} \right\rangle\right|^2$$

$$ds^2 = 1 - |\langle u_n(\mathbf{k}) | u_n(\mathbf{k} + d\mathbf{k})\rangle|^2$$

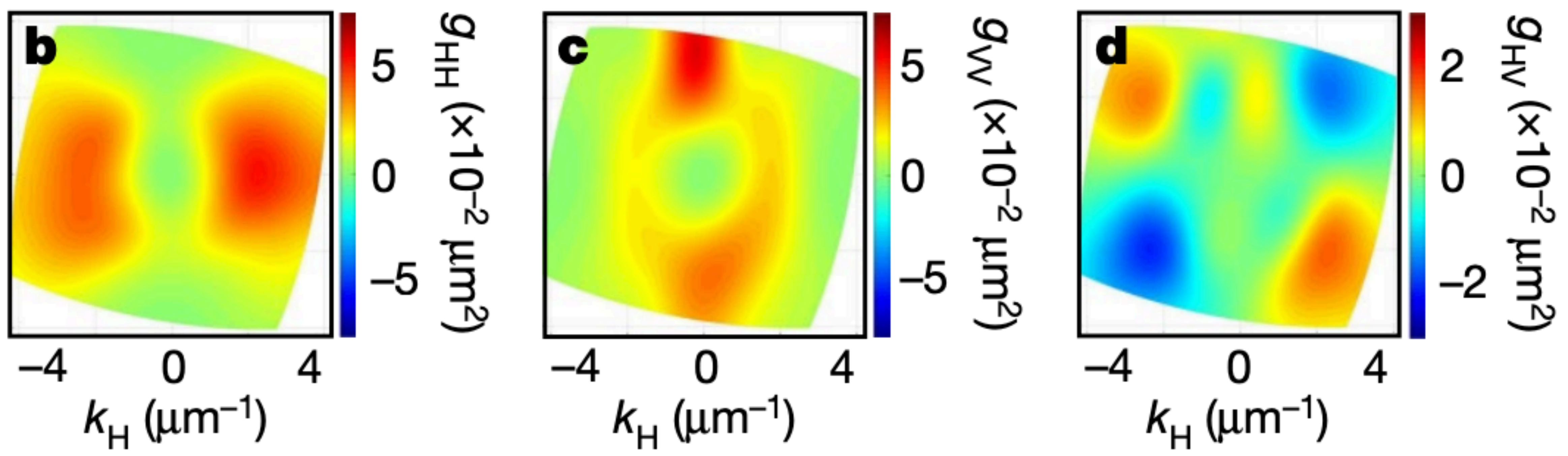
$$= \boxed{\left(\Re\left[\left\langle \partial_{k_i} u_n \middle| \partial_{k_j} u_n \right\rangle\right] - \left\langle \partial_{k_i} u_n \middle| u_n \right\rangle \left\langle u_n \middle| \partial_{k_j} u_n \right\rangle\right)} dk_i dk_j$$

$$= \boxed{g^n_{ij}} dk_i dk_j$$

Quantum metric

Research on quantum metric

- Measurement of quantum metric from photon modes in a planar micro cavity. Nature **578**, 381 (2020)



- Superfluidity and quantum metric Nature Communications **6**, 8944 (2015)

$$[D_s]_{i,j} = \frac{2Un_\phi}{\pi\hbar^2}\nu(1-\nu)\mathcal{M}^{R}_{ij}$$

Superfluid weight

An integral of quantum metric and Berry curvature over the BZ.

- Current noise and quantum metric Physical review B **87**, 245103 (2013)

$$S_{\mu\nu}(\omega) = -2\pi\omega^2 \int_{BZ} \frac{d^d\boldsymbol{k}}{\Omega_{BZ}} \delta[\omega - \varepsilon_2(\boldsymbol{k}) + \varepsilon_1(\boldsymbol{k})]\, Q^{11}_{\mu\nu}(\boldsymbol{k}),$$

Current noise

A combination of quantum metric and Berry curvature.

- Orbital magnetic susceptibility and quantum metric Physical review B **94**, 134423 (2016)

$$\chi_{inter} = \chi_\Omega + \boxed{\chi_g + \tilde{\chi}_g}$$

Interband contribution

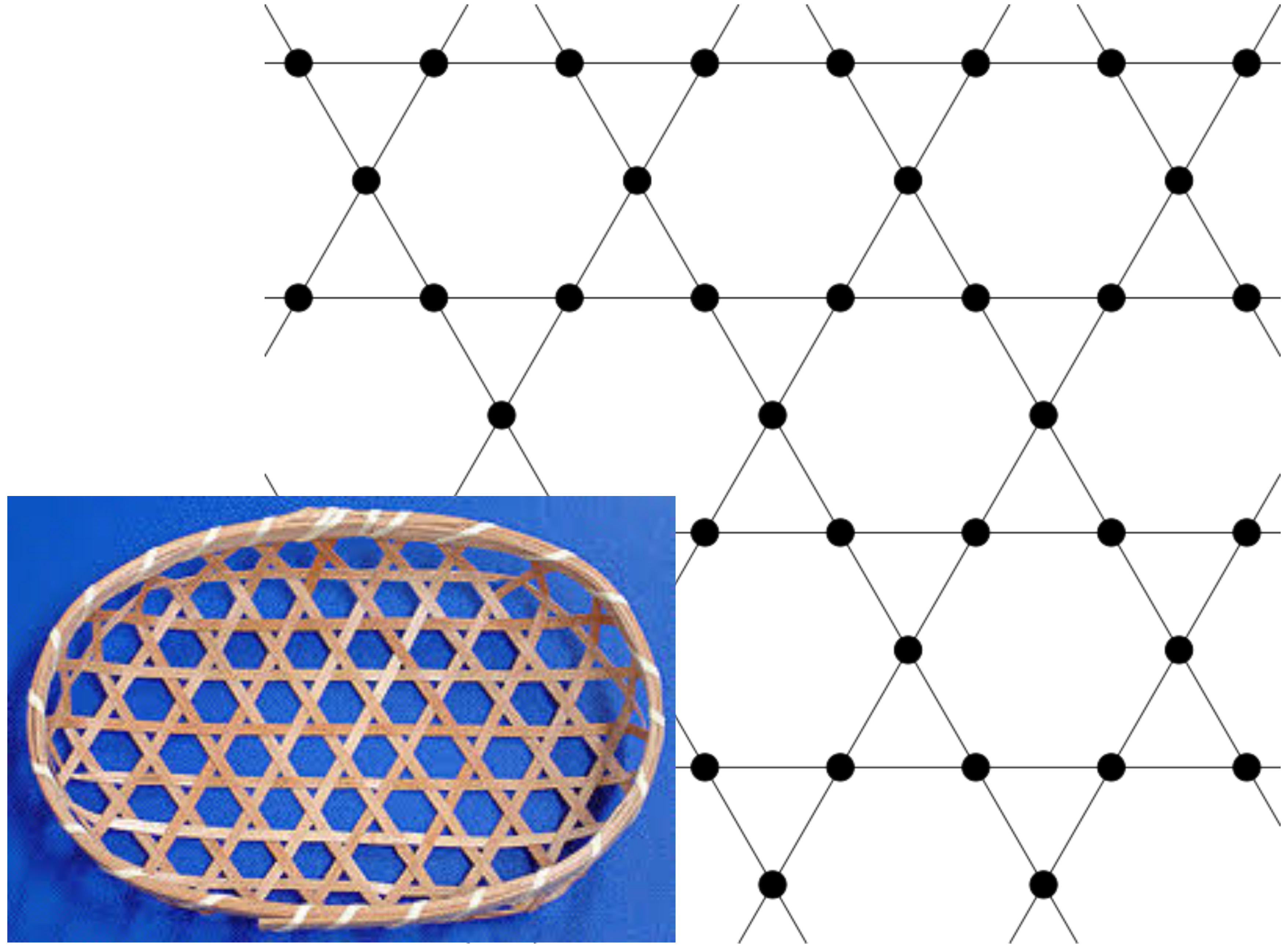
Depends on quantum metric

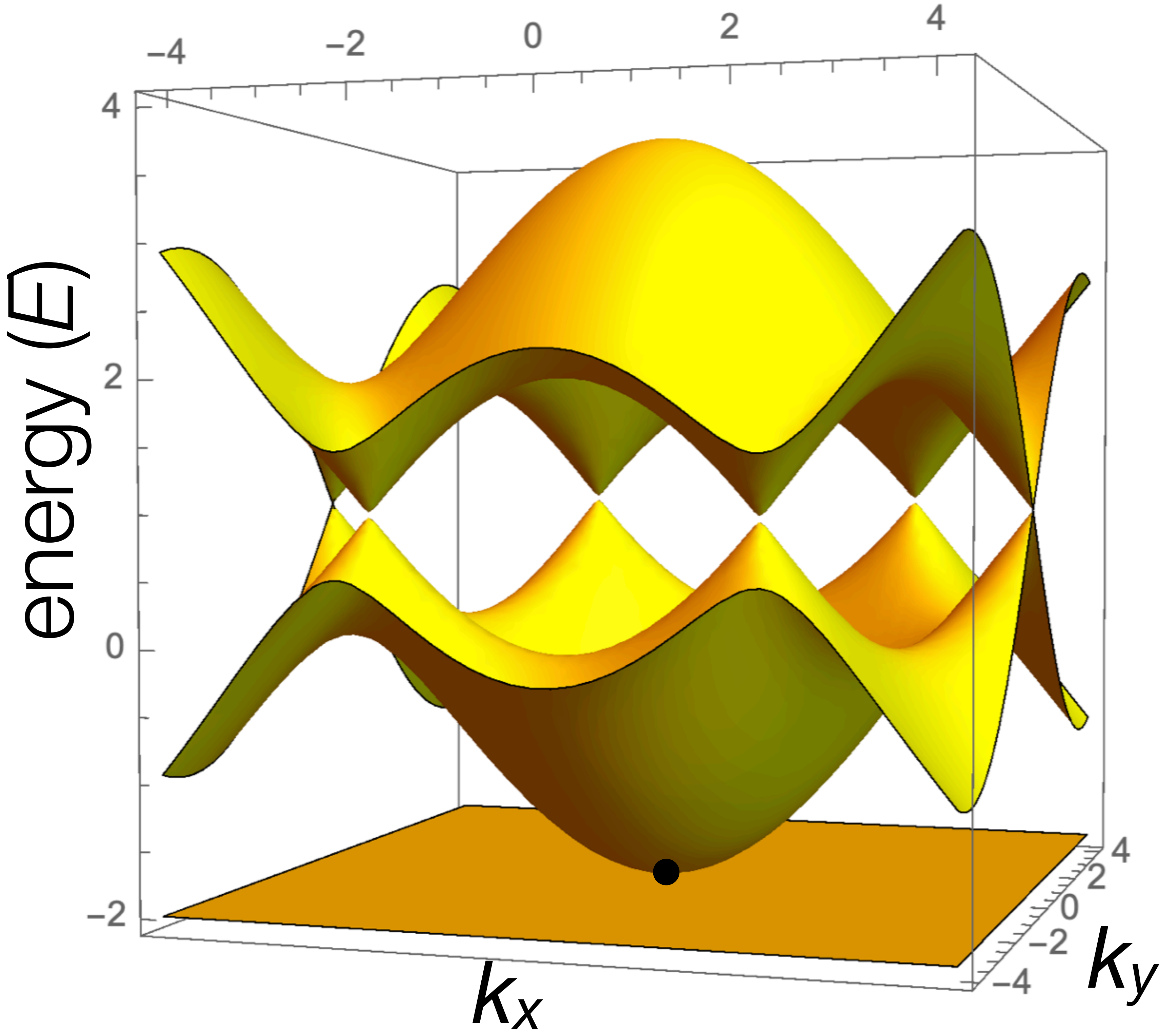
Flat band systems

Flat bands might be an ideal platform
to study the quantum metric and quantum distance.

Flat band systems

Kagome lattice





Group velocity ➡ 0

Effective mass ➡ ∞

$$v_k = \frac{1}{\hbar}\frac{\partial E_k}{\partial k}$$

Flat band systems

Group velocity ➡ 0
Effective mass ➡ ∞

⬇

Interactions become important. ($K \ll U$)

⬇

Many-body ground states can be induced easily.

Flat band systems

Group velocity ➡ 0

Effective mass ➡ ∞

- Ferromagnetism

(H. Tasaki, PRL **69** 1608)

- Superconductivity

(G. E. Volovik, Jetp Lett. **107** 516)

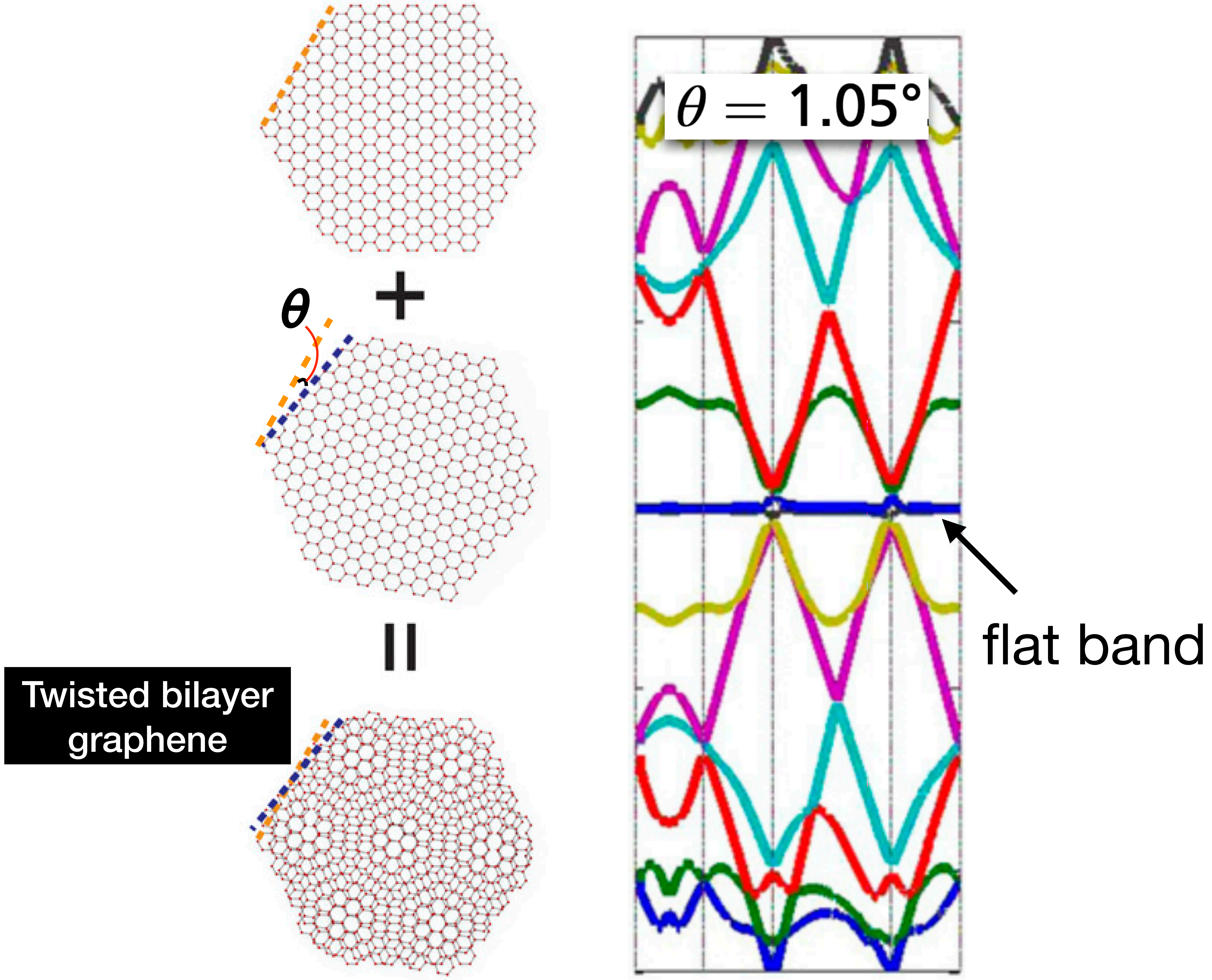
- Wigner crystal

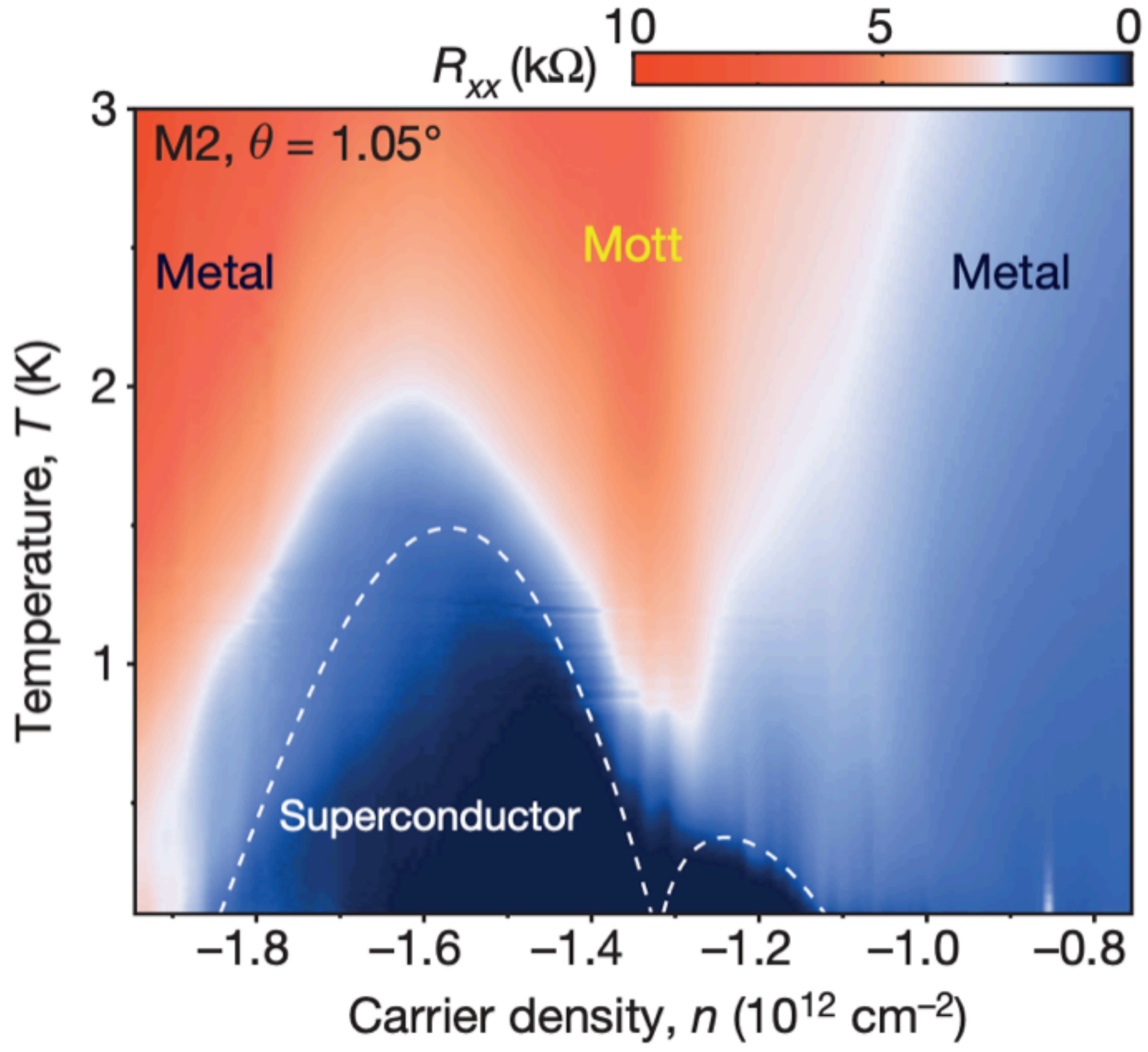
(C. Wu et al, PRL **99** 070401)

Int ≪U)

Many-body ground states can be induced easily.

Flat band systems





Y. Cao et al, Nature **556** 43 (2018)

R. Bistritzer and A. H. MacDonald, Proc. Natl Acad. Sci. USA **108**, 12233 (2011)

Flat band systems

Fast Track Communications

IOP Publishing — Journal of Physics A: Mathematical and Theoretical
J. Phys. A: Math. Theor. **47** (2014) 152001 (12pp) — doi:10.1088/1751-8113/47/15/152001

Fast Track Communications

The impossibility of exactly flat non-trivial Chern bands in strictly local periodic tight binding models

Li Chen[1], Tahereh Mazaheri[1], Alexander Seidel[1] and Xiang Tang[2]

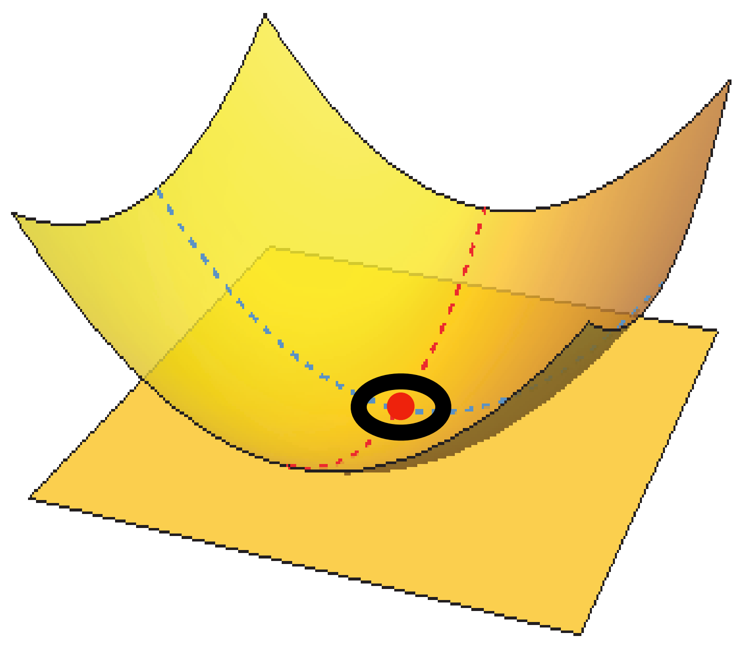
[1] Department of Physics, Washington University, St. Louis, MO 63130, USA
[2] Department of Mathematics, Washington University, St. Louis, MO 63130, USA

Article | Published: 05 August 2020

Quantum distance and anomalous Landau levels of flat bands

Jun-Won Rhim, Kyoo Kim & Bohm-Jung Yang

Nature **584**, 59–63(2020) | Cite this article

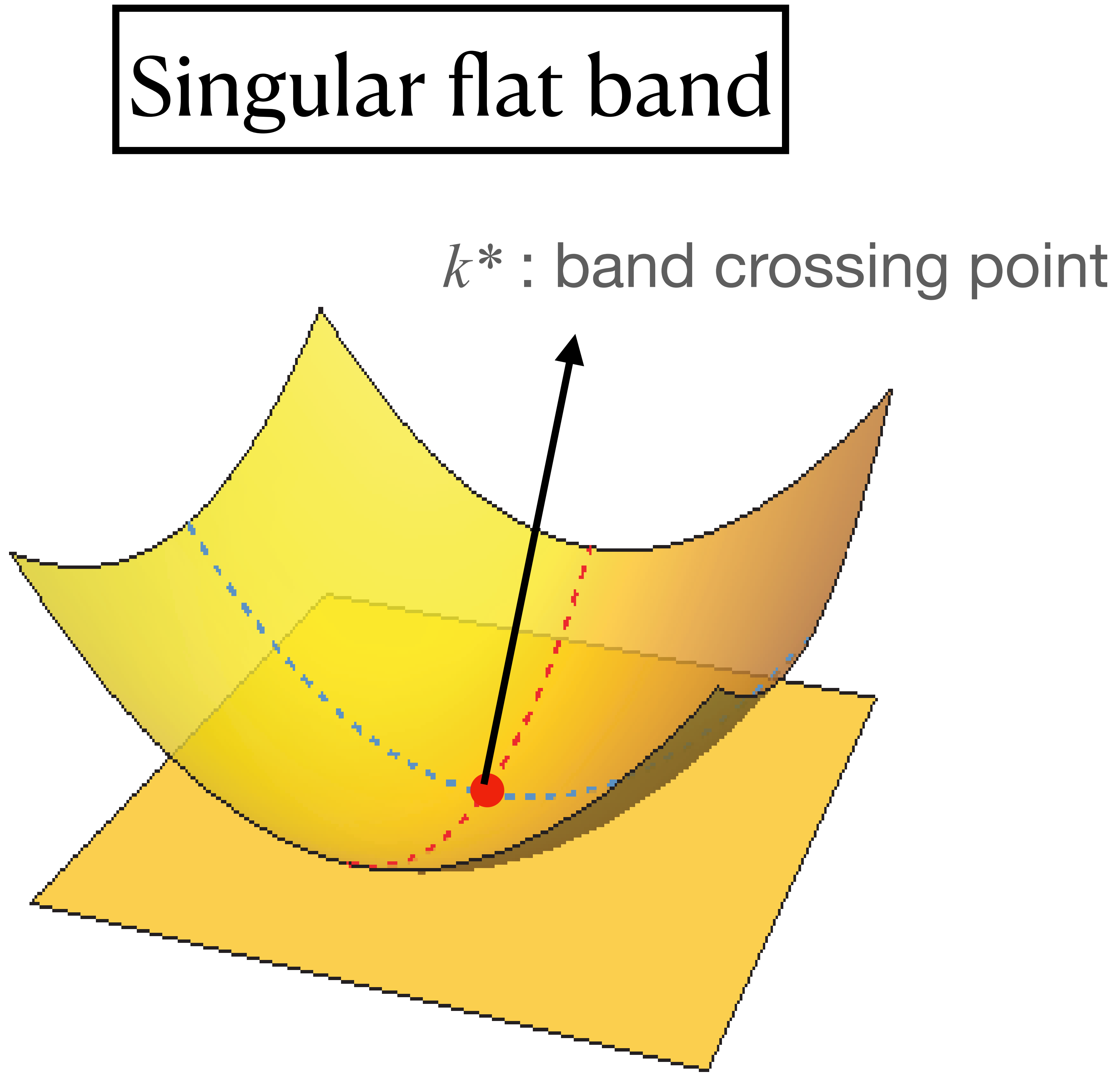


$$\gamma = i \oint_C \langle v_{\mathbf{k}} | \partial_{\mathbf{k}} | v_{\mathbf{k}} \rangle = \mp 2\pi$$

➡ In many cases, flat bands are topologically trivial

➡ Quantum distance or quantum metric could be crucial in flat bands

Singular flat band

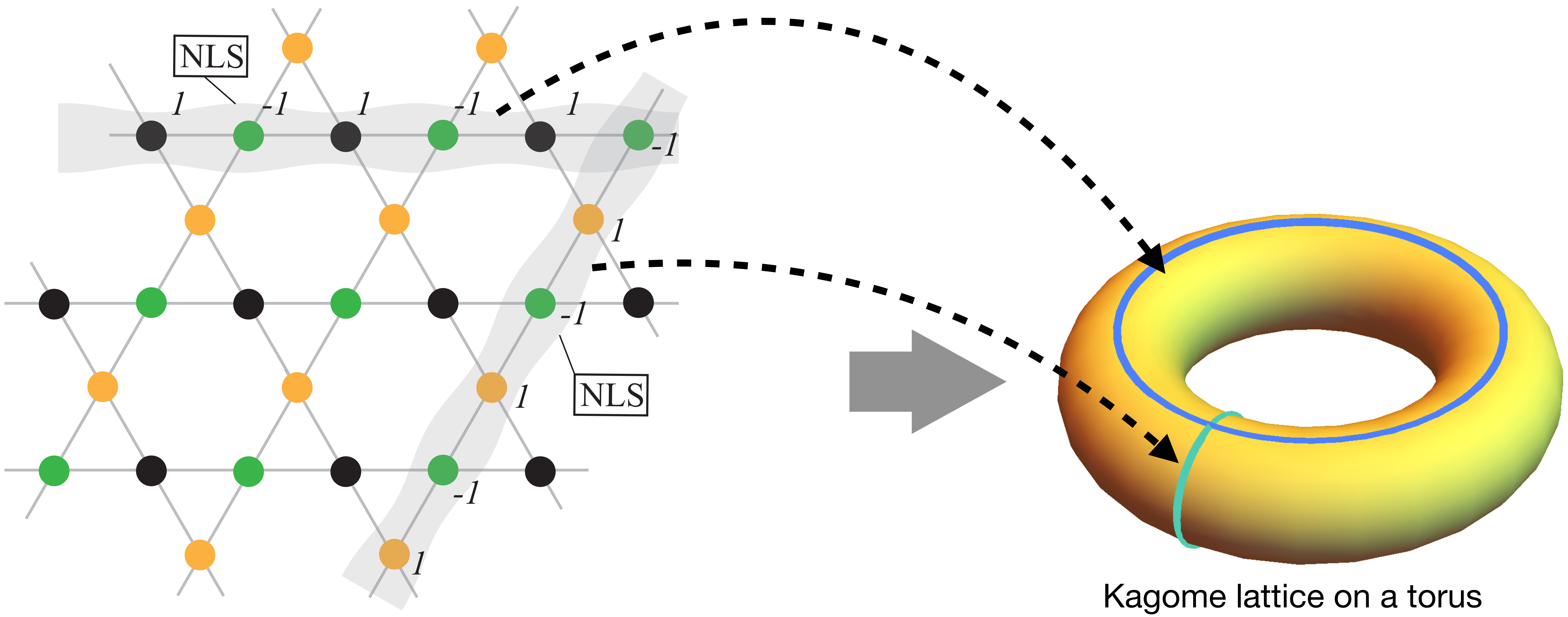


The unnormalized eigenvector of the flat band becomes zero at k*.

without any common factor between vector components

J.-W. Rhim and B.-J. Yang PRB 99 045107 (2019)

Singular flat band

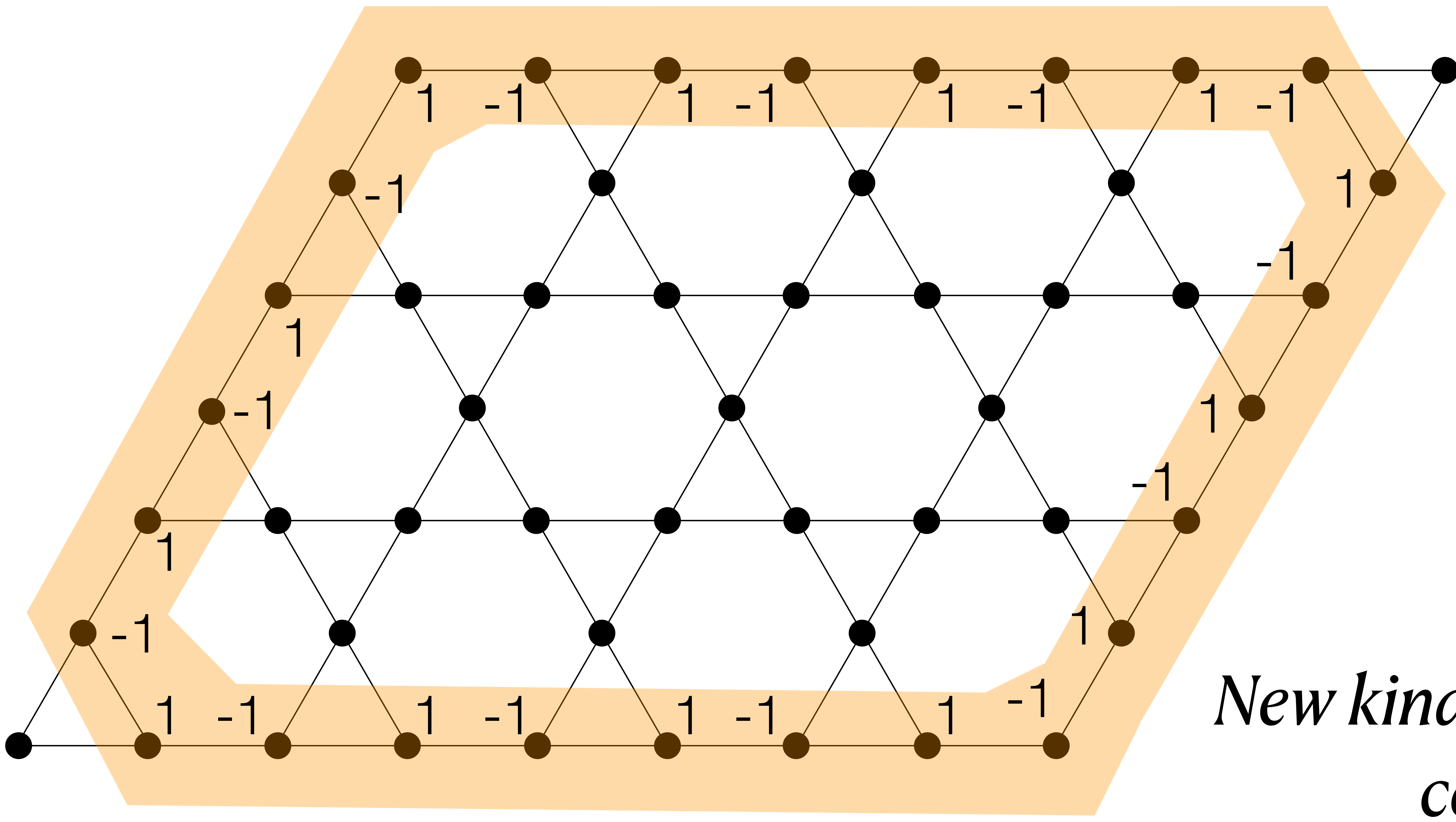


Kagome lattice on a torus
(periodic boundary condition)

Non-contractible loop states (NLSs)

J.-W. Rhim and B.-J. Yang PRB 99 045107 (2019)

Singular flat band



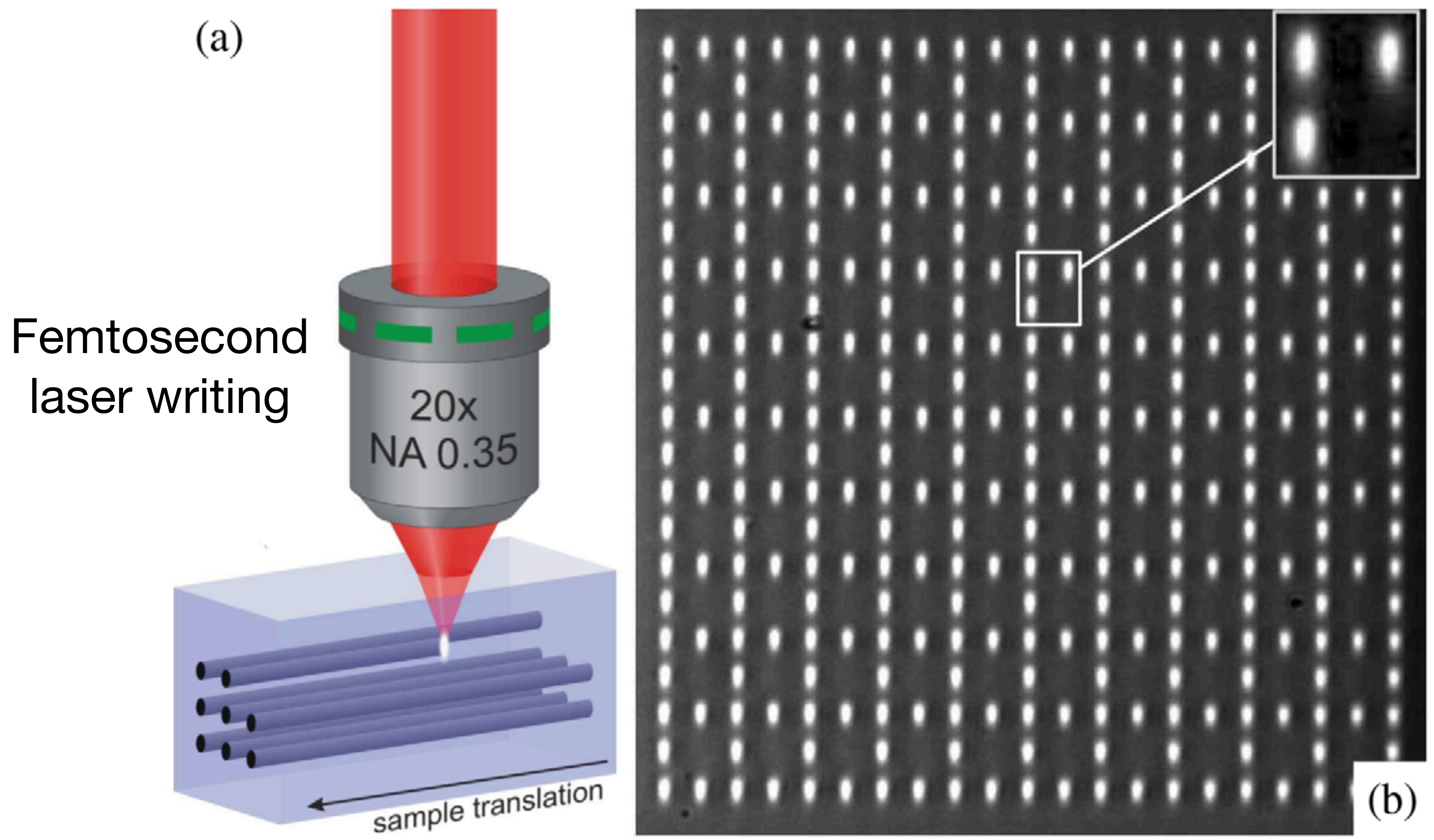
New kind of the bulk-boundary correspondence

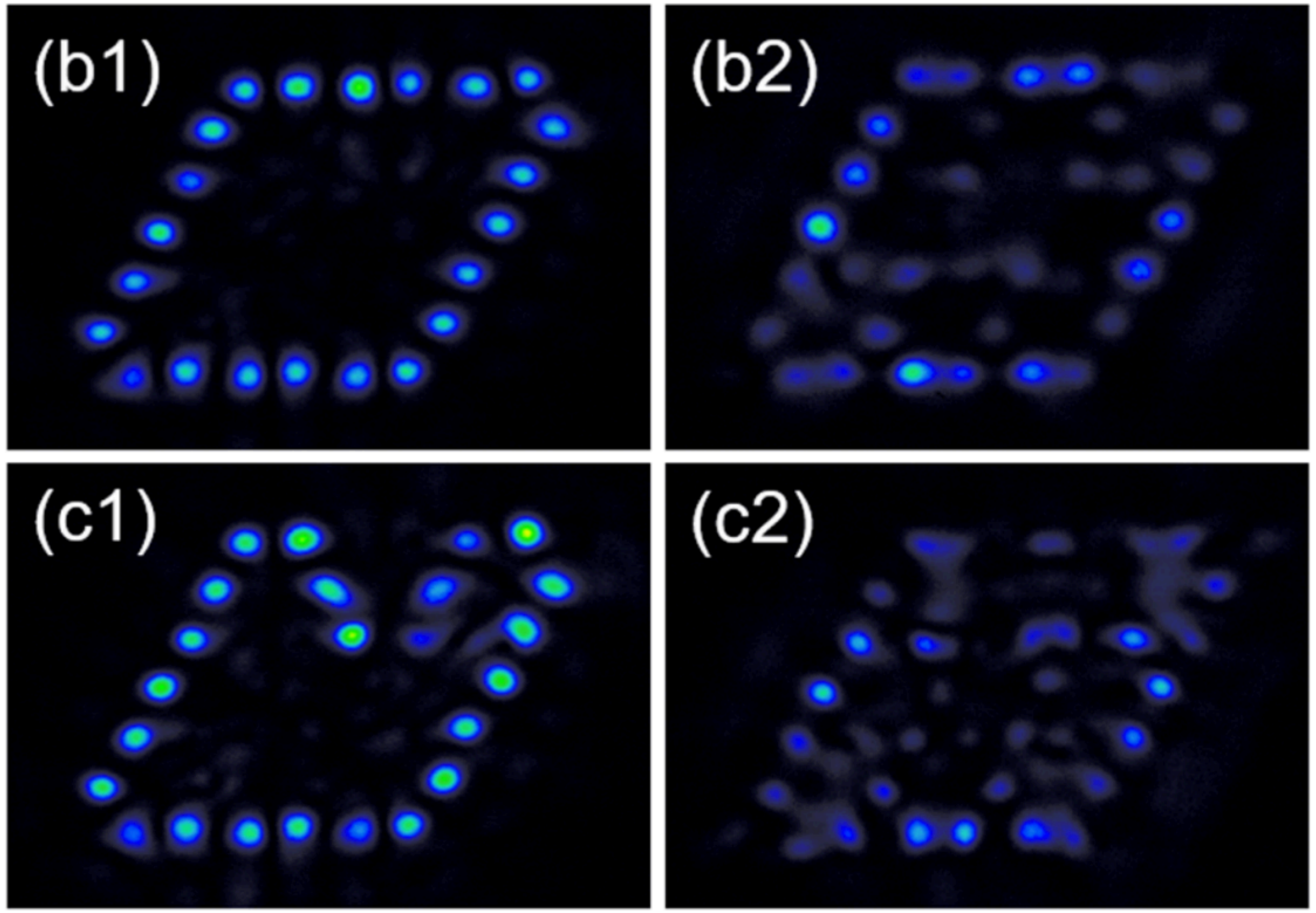
Robust boundary mode (RBM)

J.-W. Rhim and B.-J. Yang PRB 99 045107 (2019)

Singular flat band

Photonic lattice



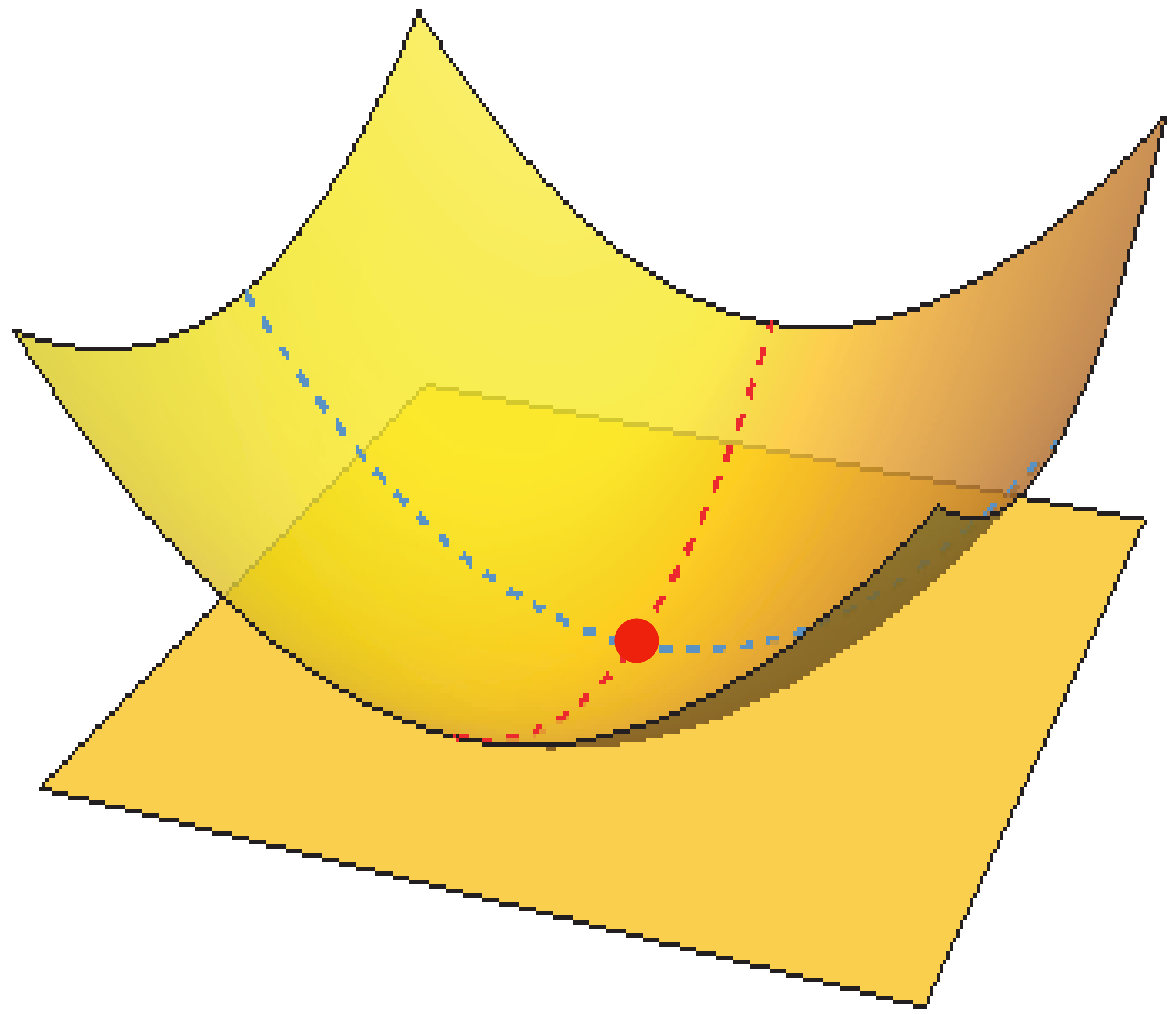


The first observation of the real-space topology in flat bands

J. Ma, **JWR**, et al, PRL **124** 183901 (2020)

Quantum distance and singular flat band

Singular flat band *with a discontinuity*

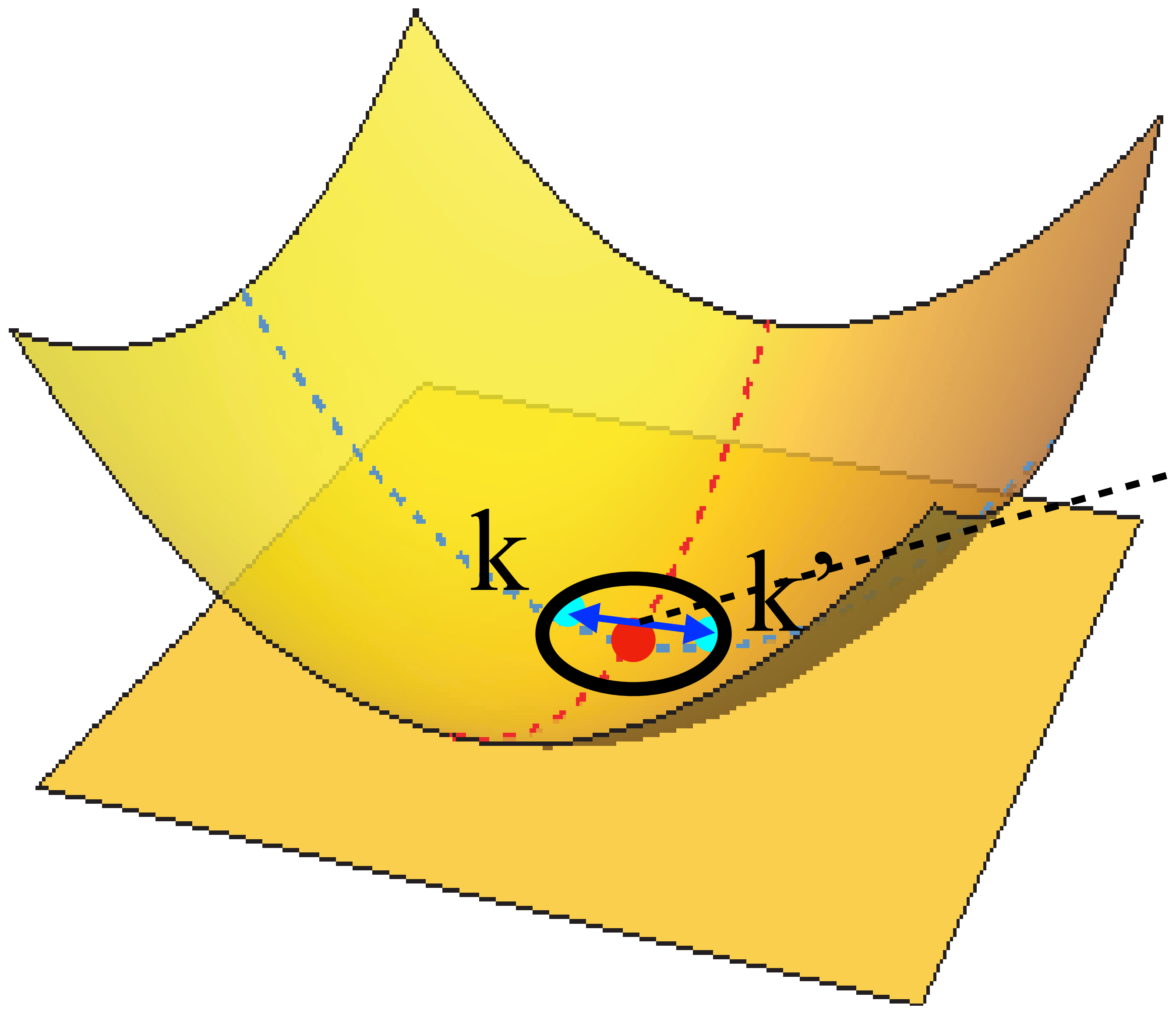


The normalized eigenvector of the flat band can be discontinuous at k*.

J.-W. Rhim and B.-J. Yang PRB 99 045107 (2019)

Quantum distance and singular flat band

$\boxed{\text{Singular flat band } \textit{with a discontinuity}}$



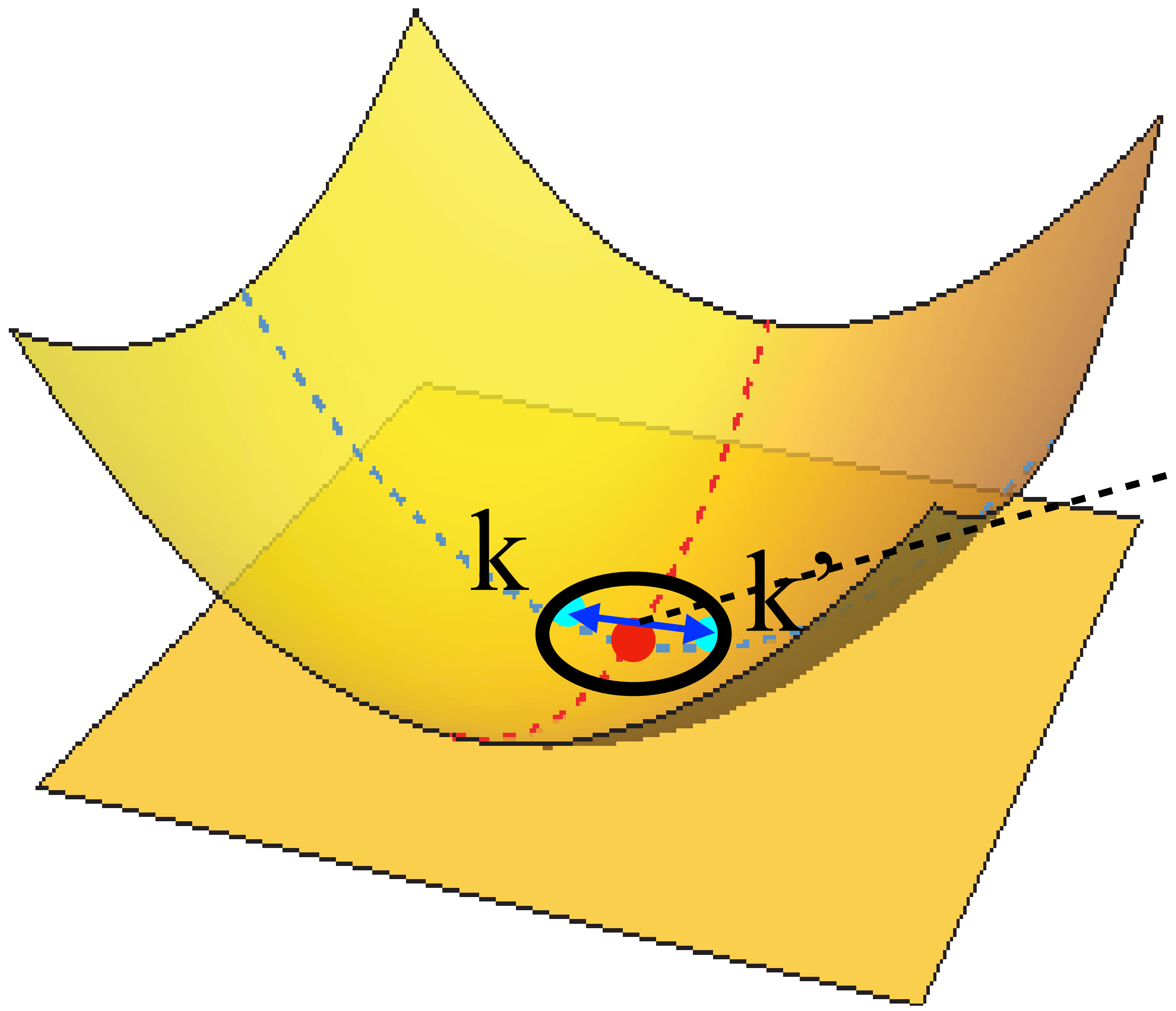
$$d^2 = 1 - |\langle v_{\mathbf{k}} | v_{\mathbf{k}'} \rangle|^2$$

$$\boxed{d_{\text{max}} \neq 0}$$

JWR, K. Kim, and B.-J. Yang, Nature **584** 59 (2020)

Quantum distance and singular flat band

Singular flat band *with a discontinuity*



$$d^2 = 1 - |\langle v_{\mathbf{k}} | v_{\mathbf{k}'} \rangle|^2$$

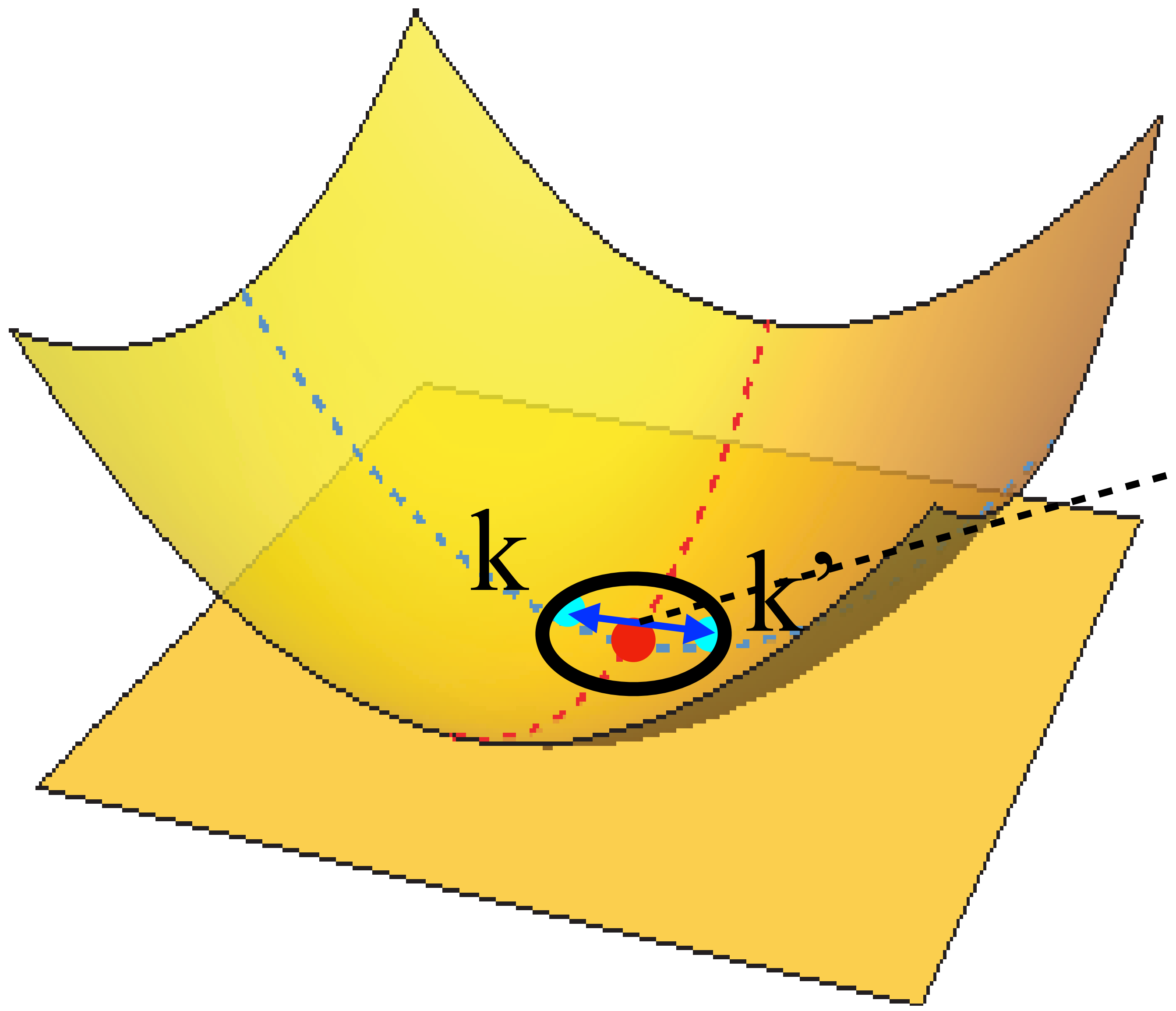
$$\boxed{d_{\max} \neq 0}$$

- Discontinuous singular flat band is characterized by the nonzero d_{max}.
- d_{max} represents the strength of the singularity.
- d_{max} quantifies the strength of the inter-band coupling.

JWR, K. Kim, and B.-J. Yang, Nature **584** 59 (2020)

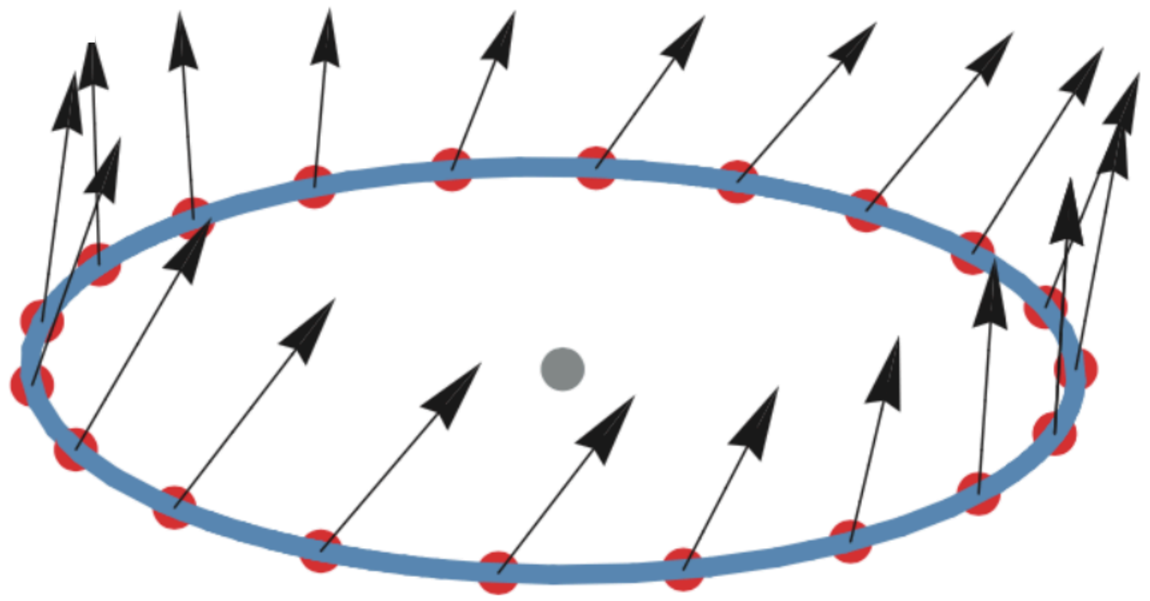
Quantum distance and singular flat band

Singular flat band *with a discontinuity*



$$d^2 = 1 - |\langle v_{\mathbf{k}} | v_{\mathbf{k}'} \rangle|^2$$

$$\Rightarrow \boxed{d_{\max} \neq 0}$$



- Discontinuous singular flat band is characterized by the nonzero d_{max}.
- d_{max} represents the strength of the singularity.
- d_{max} quantifies the strength of the inter-band coupling.
- d_{max} manifests itself as the pseudospin canting structure

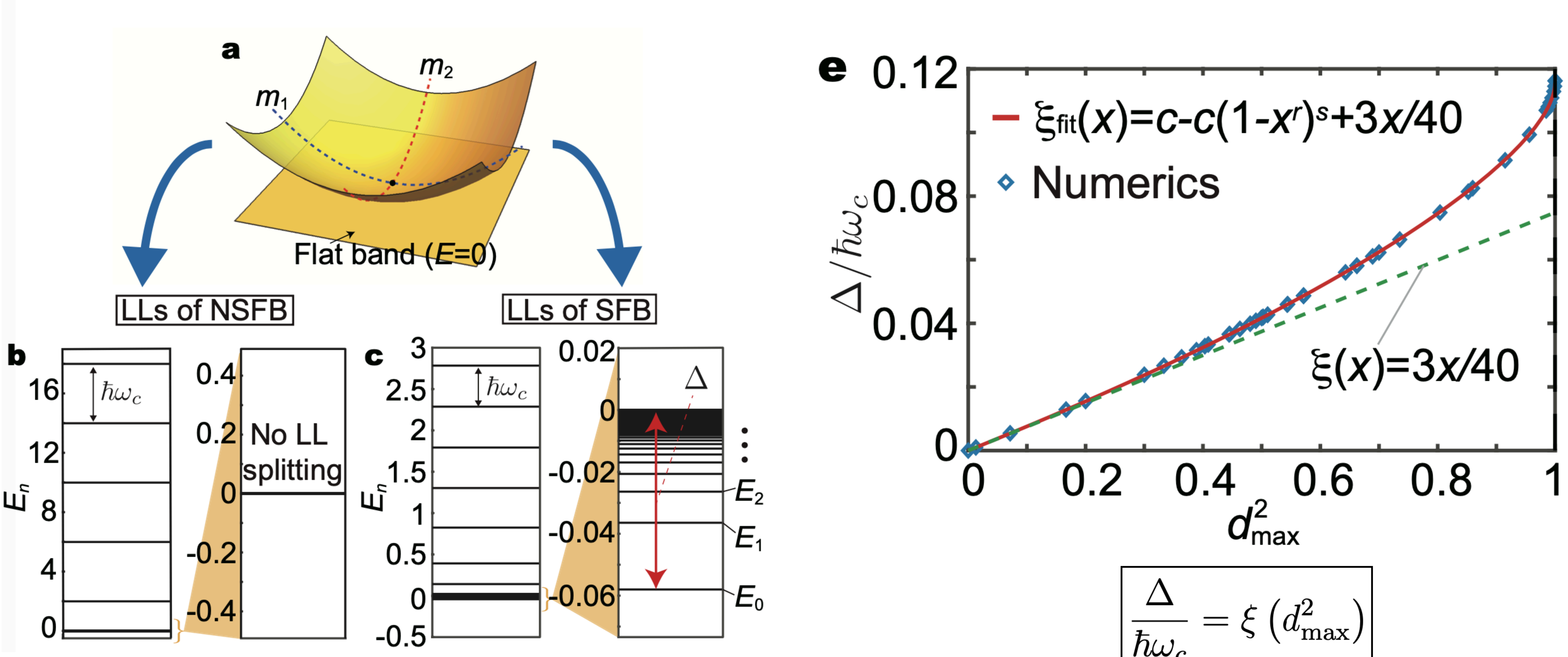
JWR, K. Kim, and B.-J. Yang, Nature **584** 59 (2020)

Quantum distance and singular flat band

How to measure d_{max}?

Quantum distance and singular flat band

Landau level spreading characterized by the quantum distance

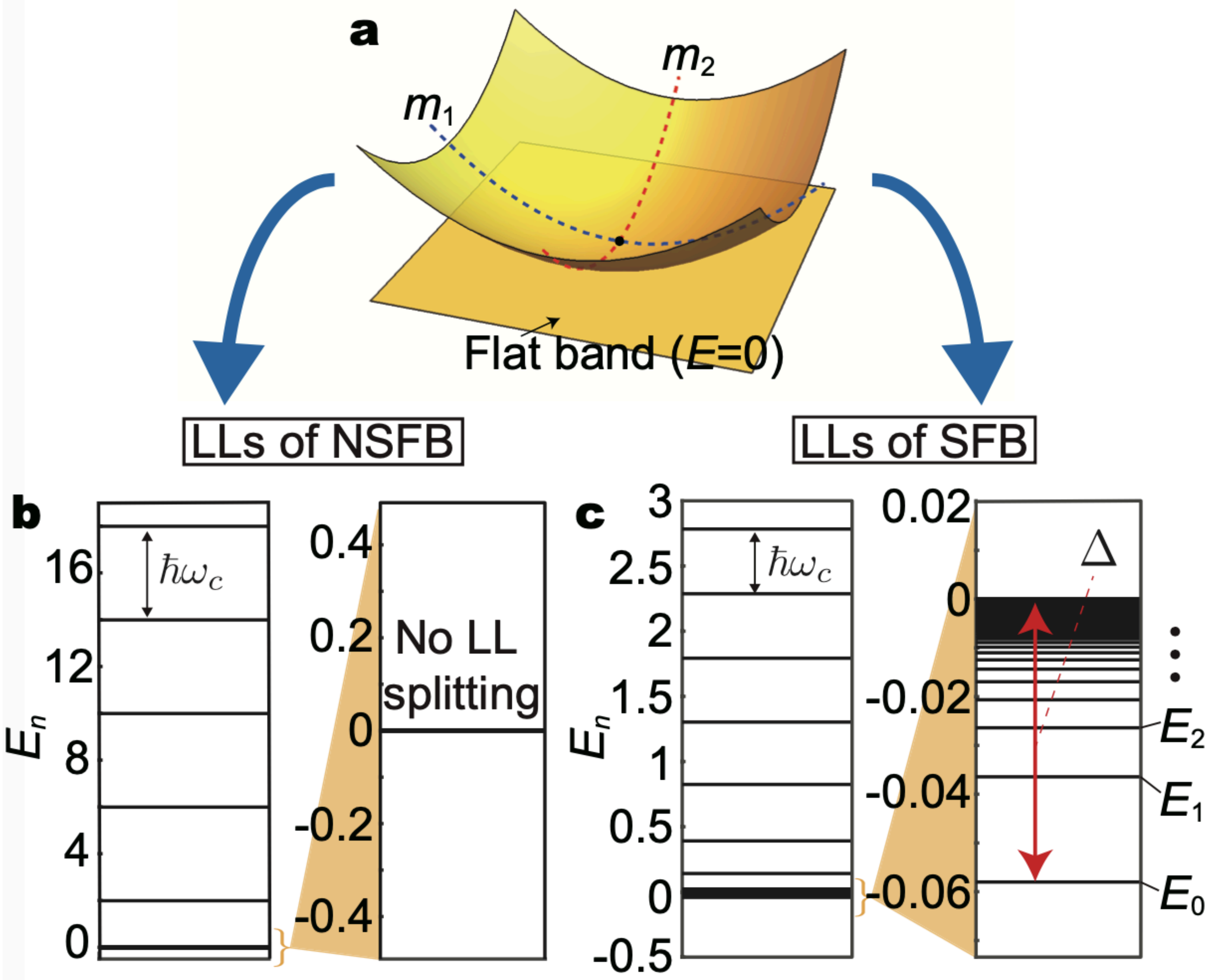


$$\frac{\Delta}{\hbar\omega_c} = \xi\left(d^2_{\max}\right)$$

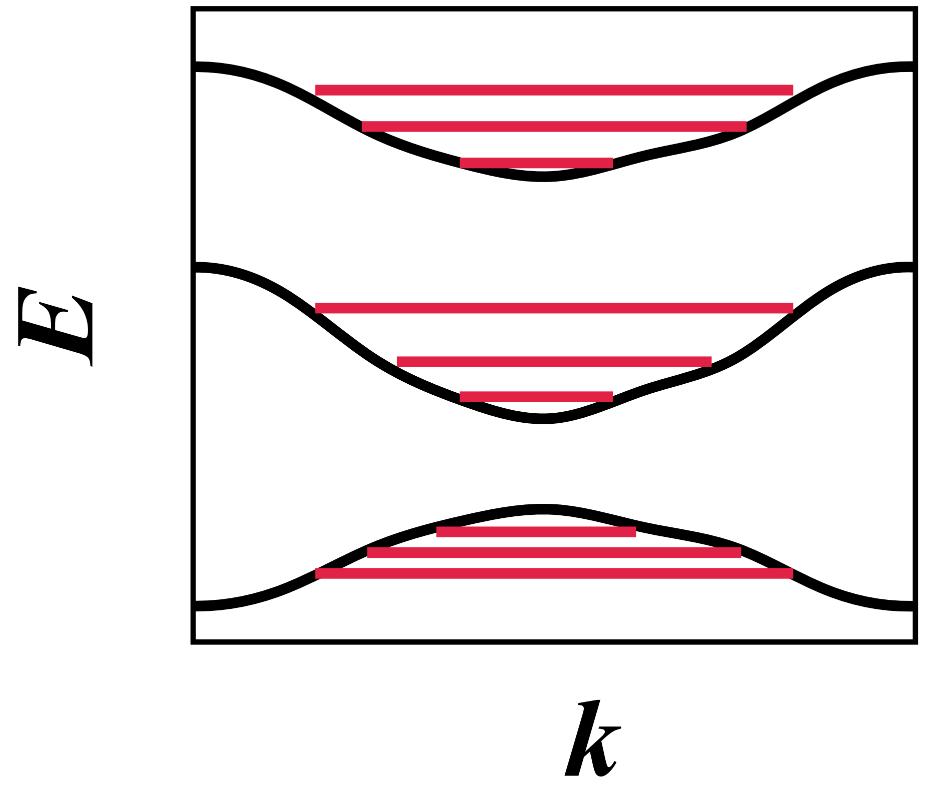
JWR, K. Kim, and B.-J. Yang, Nature **584** 59 (2020)

Quantum distance and singular flat band

Landau level spreading characterized by the quantum distance



$$S_0(\epsilon) = \frac{2\pi e B}{\hbar}\left(n + \frac{1}{2} - \frac{\gamma_{\epsilon,B}}{2\pi}\right)$$



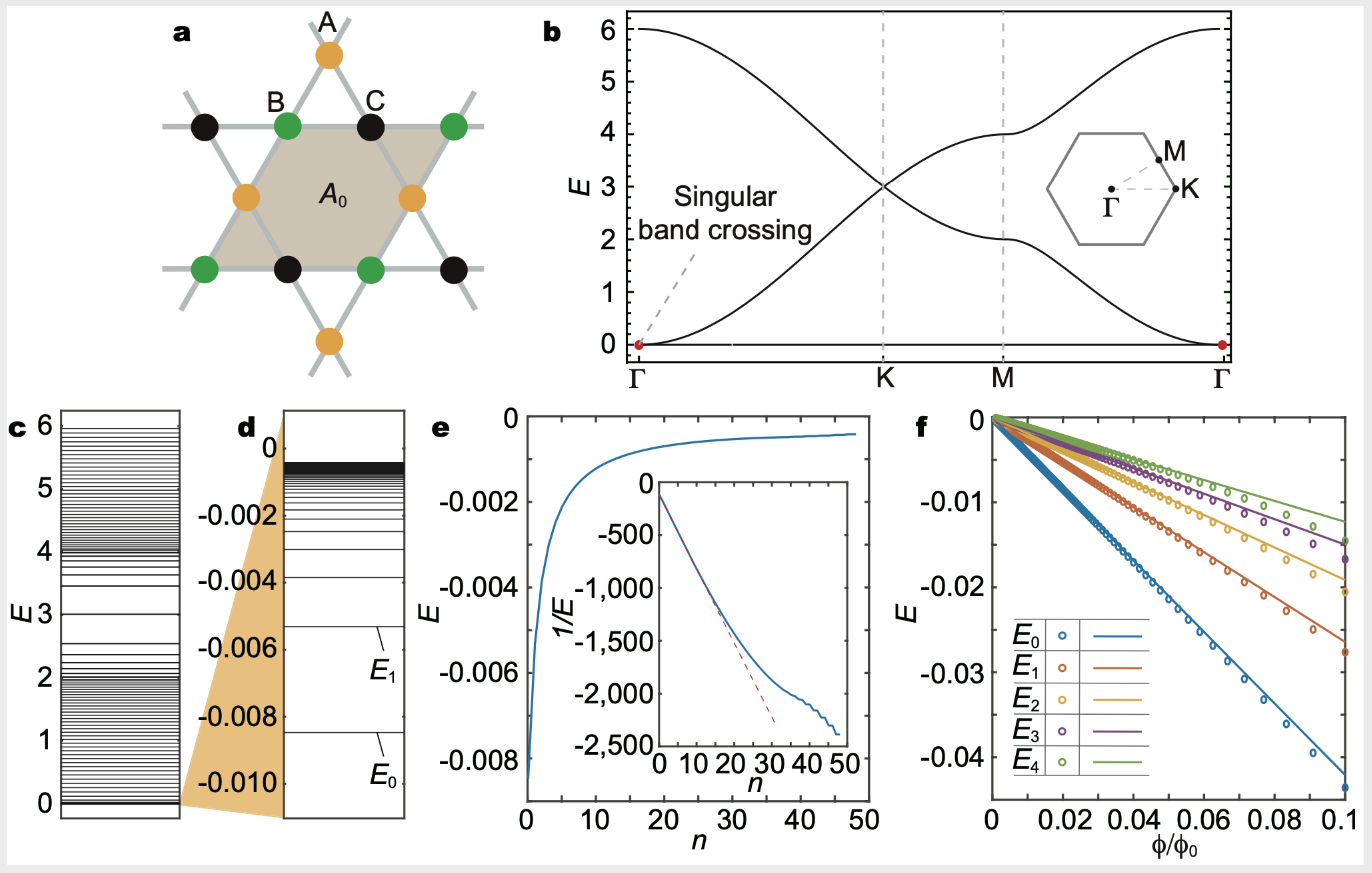
Contradicting to the conventional semiclassical idea

L. Onsager, Philos. Mag. **43**, 1006 (1952) J.-N. Fuchs et al SciPost Phys. **4**, 24 (2018) **JWR**, K. Kim, and B.-J. Yang, Nature **584** 59 (2020)

Quantum distance and singular flat band

Kagome lattice

$$\frac{\phi}{\phi_0} = \frac{1}{q}$$

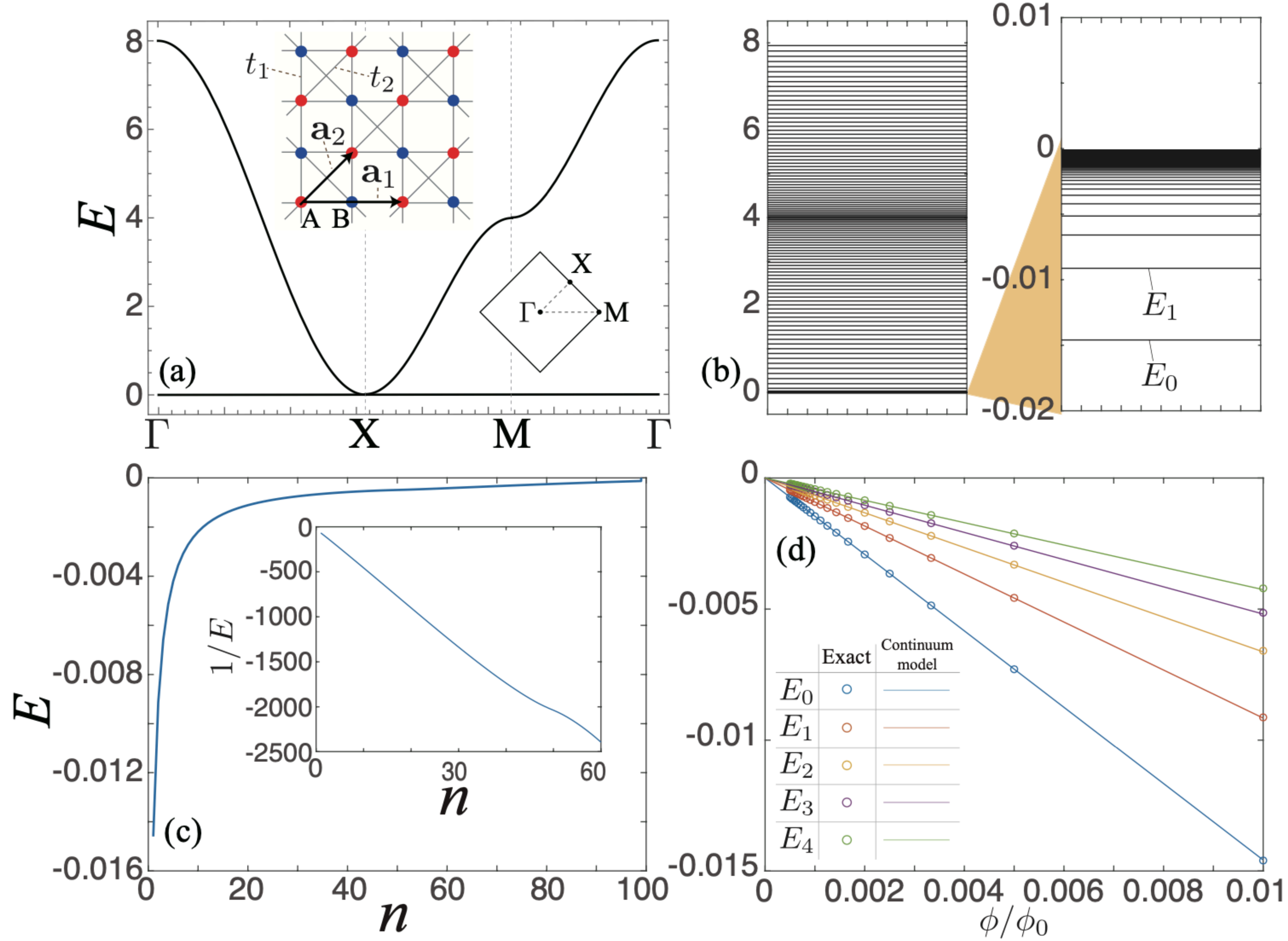


JWR, K. Kim, and B.-J. Yang, Nature **584** 59 (2020)

Quantum distance and singular flat band

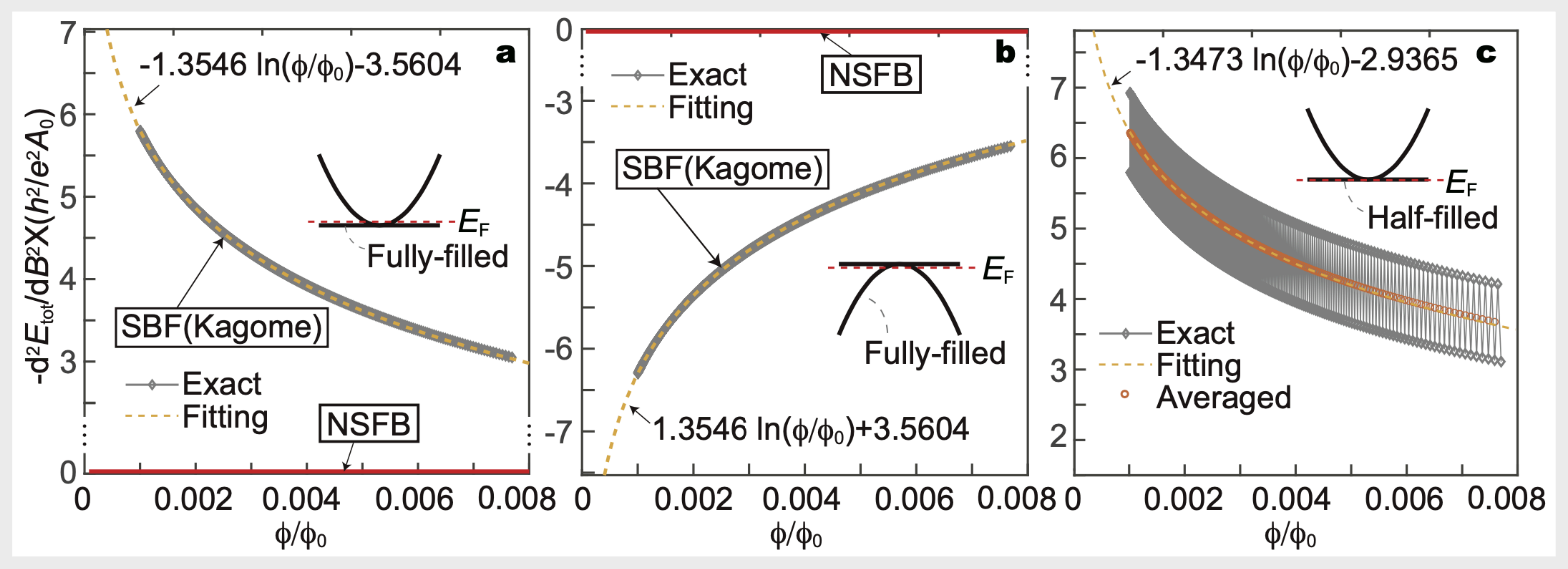
Checkerboard lattice

$$\frac{\phi}{\phi_0} = \frac{1}{q}$$



JWR, K. Kim, and B.-J. Yang, Nature **584** 59 (2020)

Quantum distance and singular flat band



$$E_{\text{tot}} \sim -B \sum_{n=1}^{q-1} \frac{B}{n} \longrightarrow \boxed{\chi \sim -\ln B}$$

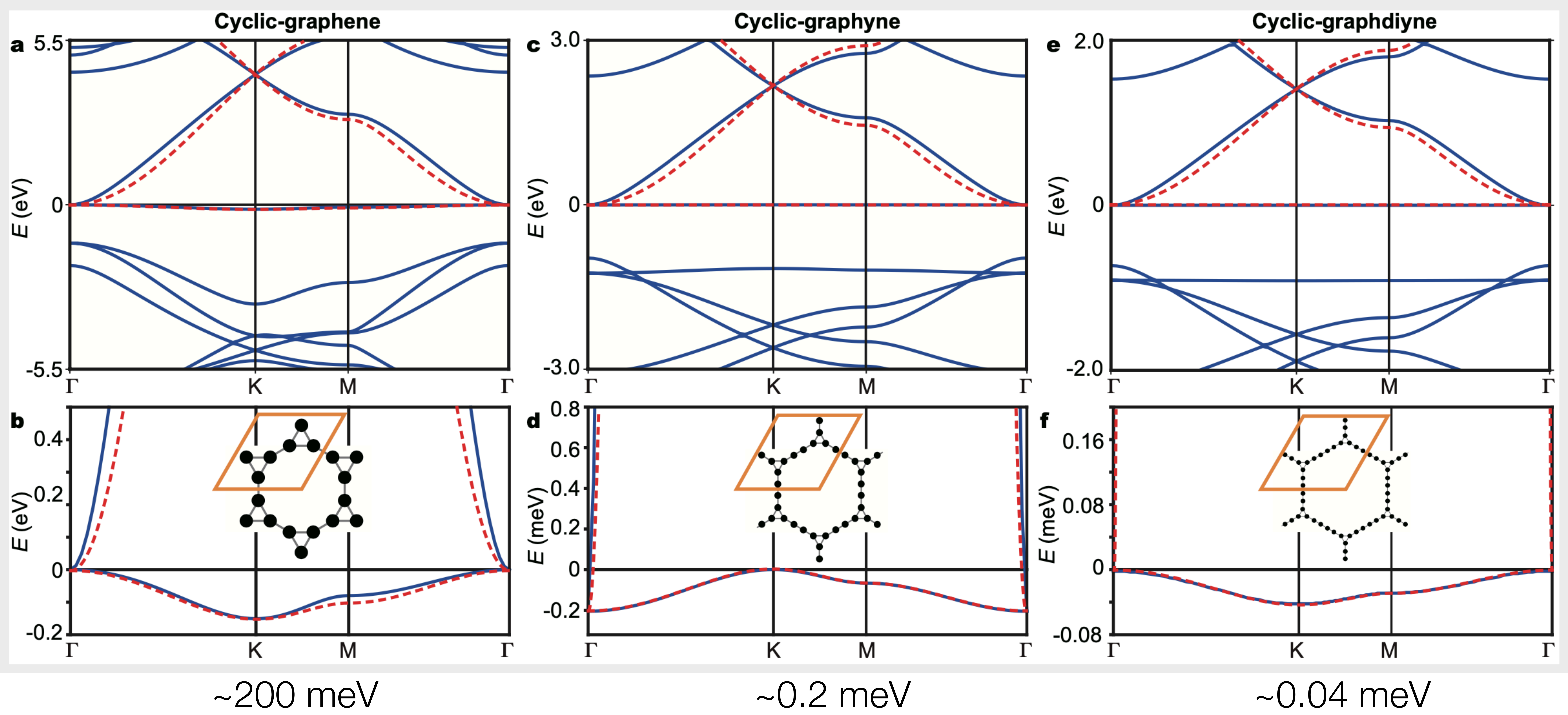
LL spacing

LL degeneracy

$$q \propto \frac{1}{B}$$

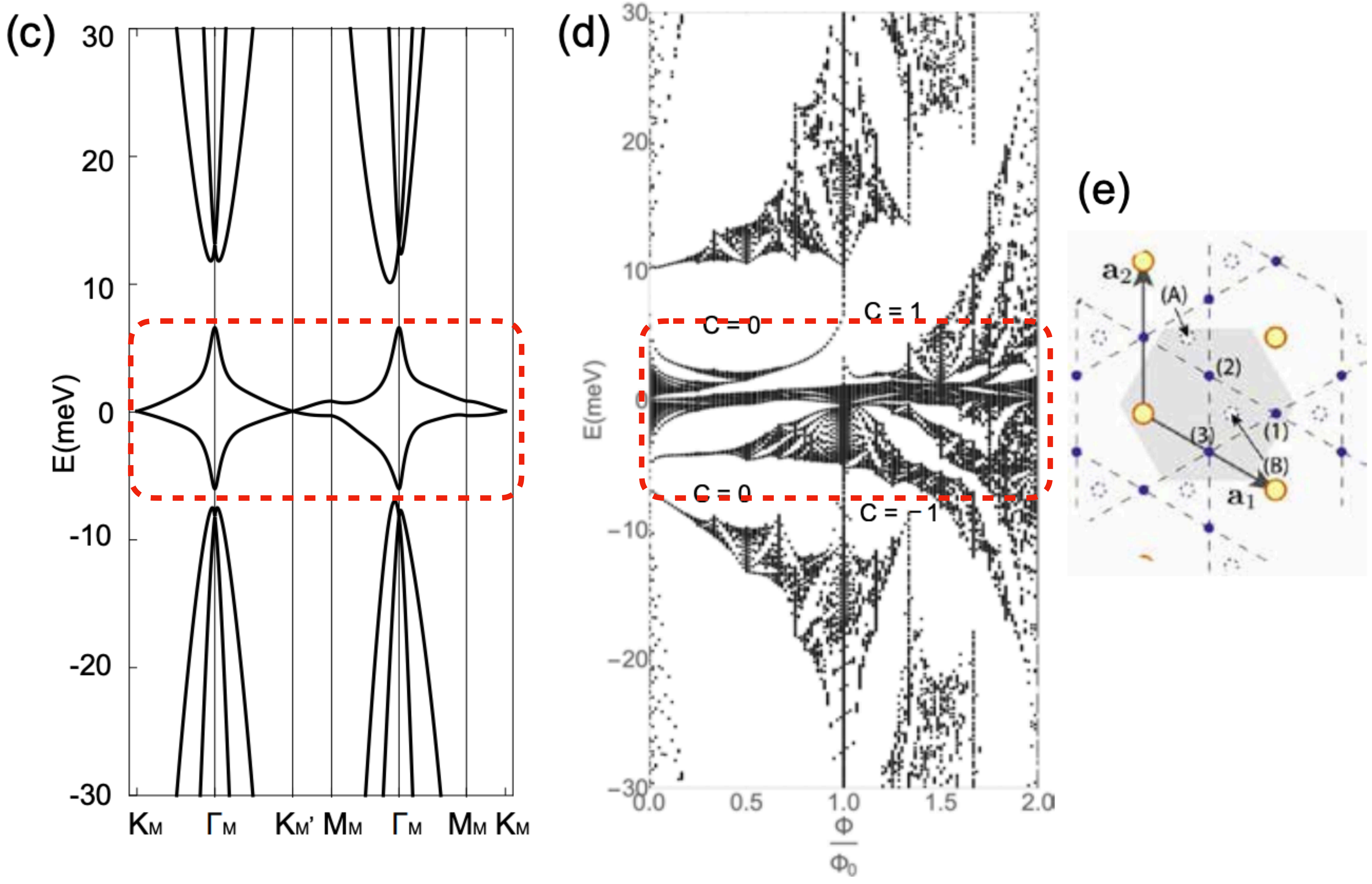
JWR, K. Kim, and B.-J. Yang, Nature **584** 59 (2020)

Quantum distance and singular flat band



JWR, K. Kim, and B.-J. Yang, Nature **584** 59 (2020)

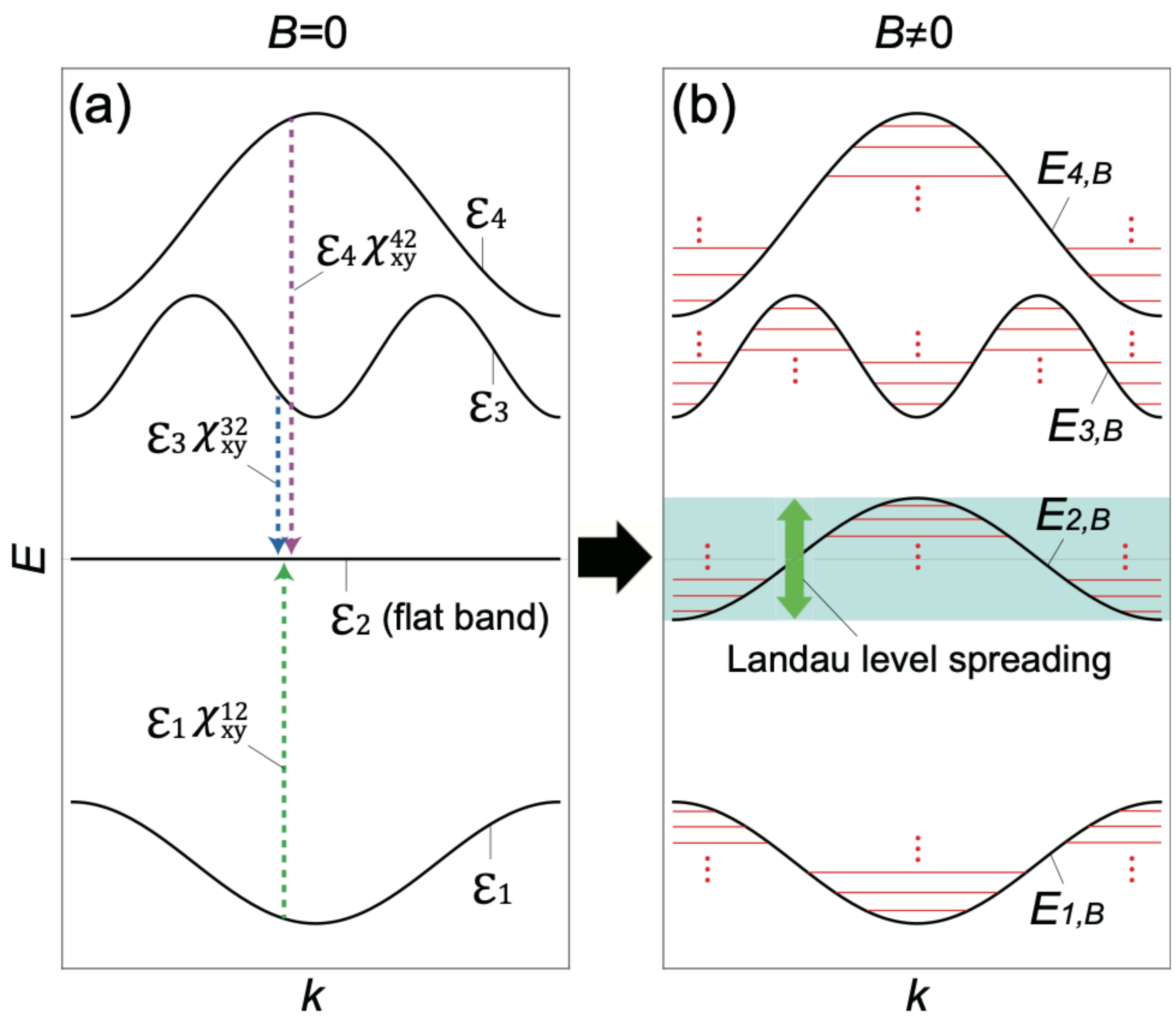
Cross-gap Berry connection and isolated flat band



Topological bands can develop in-gap Landau levels

Biao Lian, Fang Xie, and B. Andrei Bernevig, Phys. Rev. B **102**, 041402(R) (2020)

Cross-gap Berry connection and isolated flat band



$$E_{n,B}(\boldsymbol{k}) = -2\pi\frac{\phi}{\phi_0}\frac{1}{A_0}\mathrm{Im}\sum_{m\neq n}\varepsilon_m(\boldsymbol{k})\boxed{\chi^{nm}_{xy}(\boldsymbol{k})}$$

$$\chi^{nm}_{ij}(\boldsymbol{k}) = \langle\partial_i u_n(\boldsymbol{k})|u_m(\boldsymbol{k})\rangle\langle u_m(\boldsymbol{k})|\partial_j u_n(\boldsymbol{k})\rangle$$

$$= A^{nm}_i(\boldsymbol{k})^* A^{nm}_j(\boldsymbol{k})$$

Cross-gap Berry connection

Yoonseok Hwang, Jun-Won Rhim, and Bohm-Jung Yang, arXiv:2012.15132

Cross-gap Berry connection and isolated flat band

$$s^2 = 1 - |\langle v_{\mathbf{k}} | v_{\mathbf{k}'} \rangle|^2$$

$$ds^2 = g_{ij}^n dk_i dk_j$$

Quantum distance

$$F\left(u_n(\boldsymbol{k}), u_m(\boldsymbol{k}')\right) = |\langle u_n(\boldsymbol{k}) | u_m(\boldsymbol{k}')\rangle|^2,$$

$$F\left(u_n(\boldsymbol{k}), u_m(\boldsymbol{k}+d\boldsymbol{k})\right) = \chi_{ij}^{nm}(\boldsymbol{k}) dk_i dk_j.$$

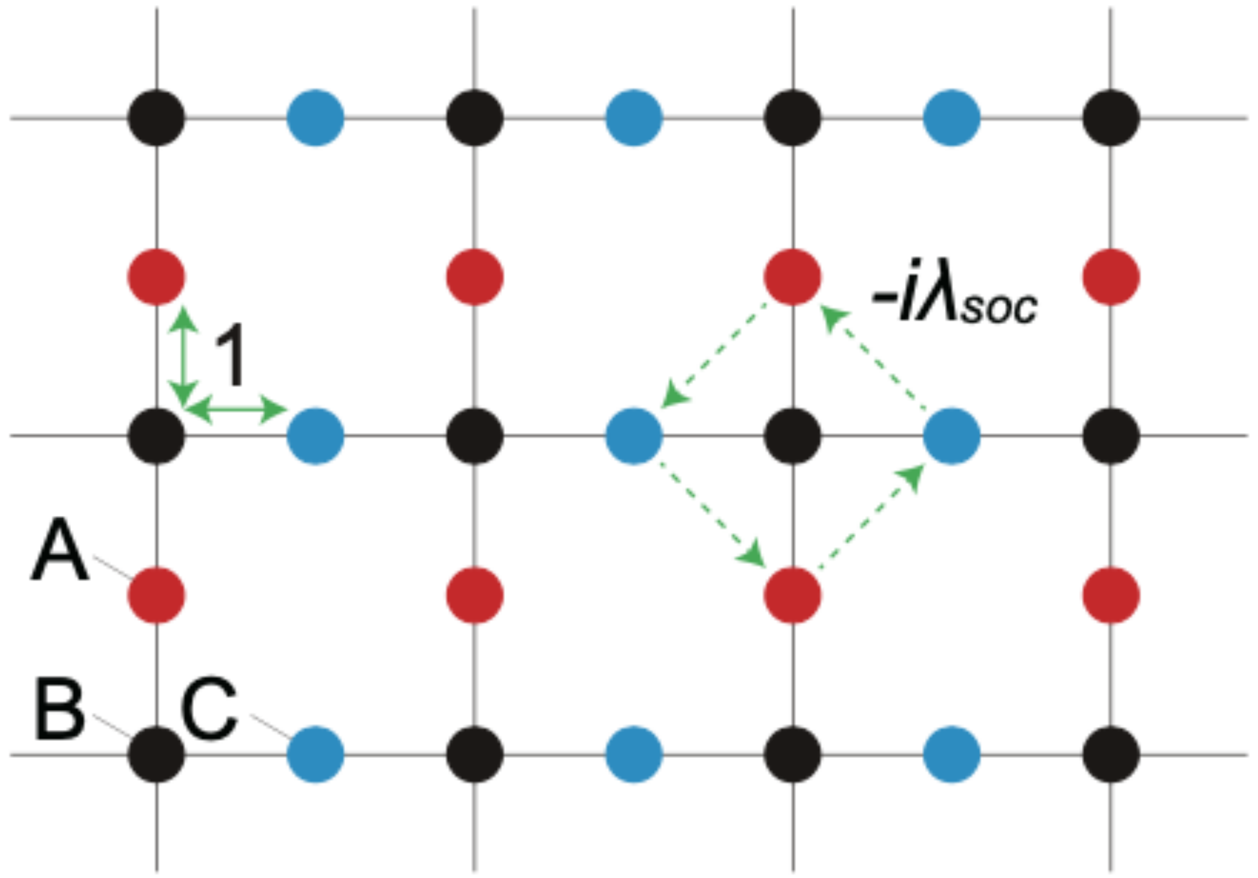
Fidelity

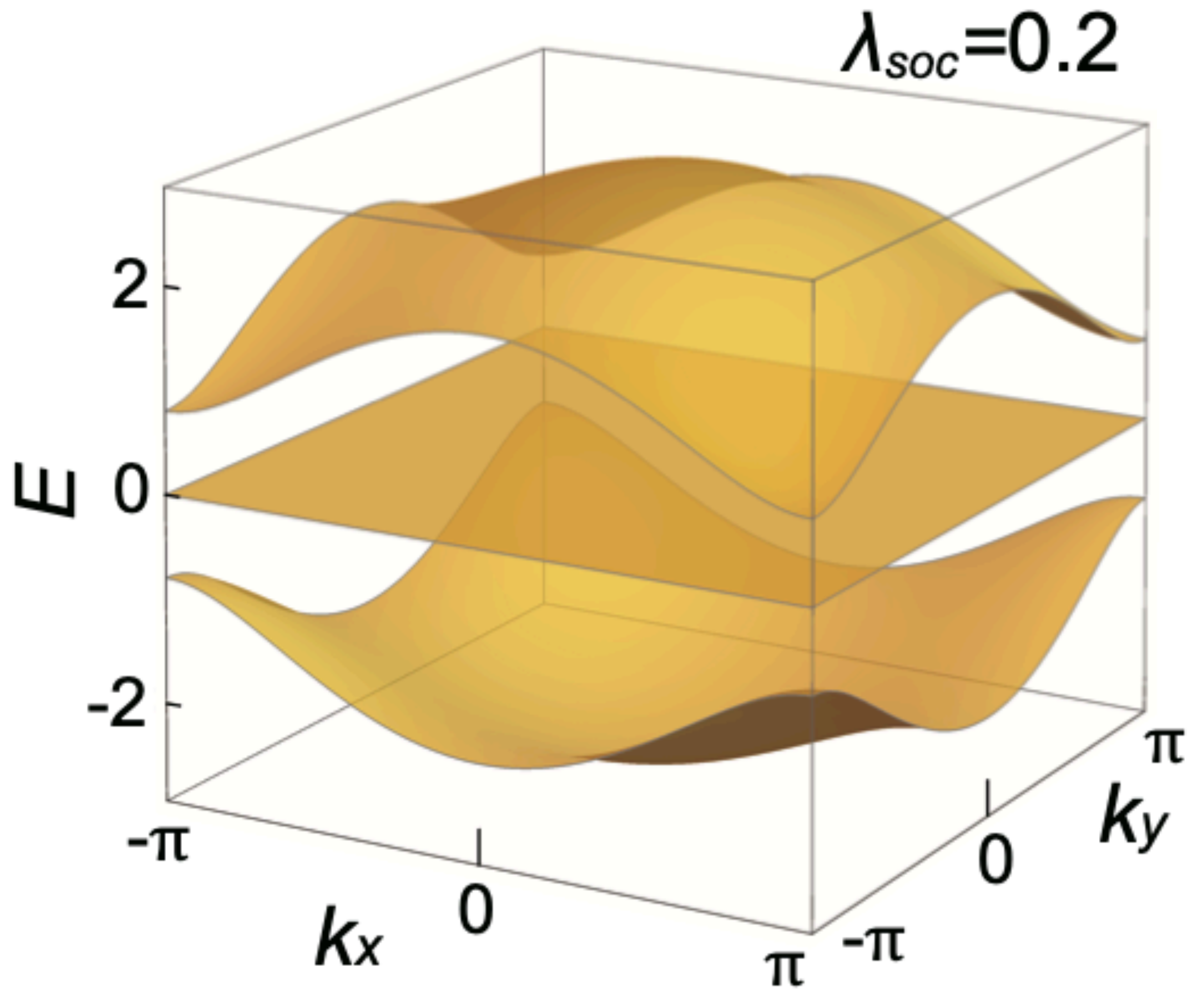
Fidelity tensor

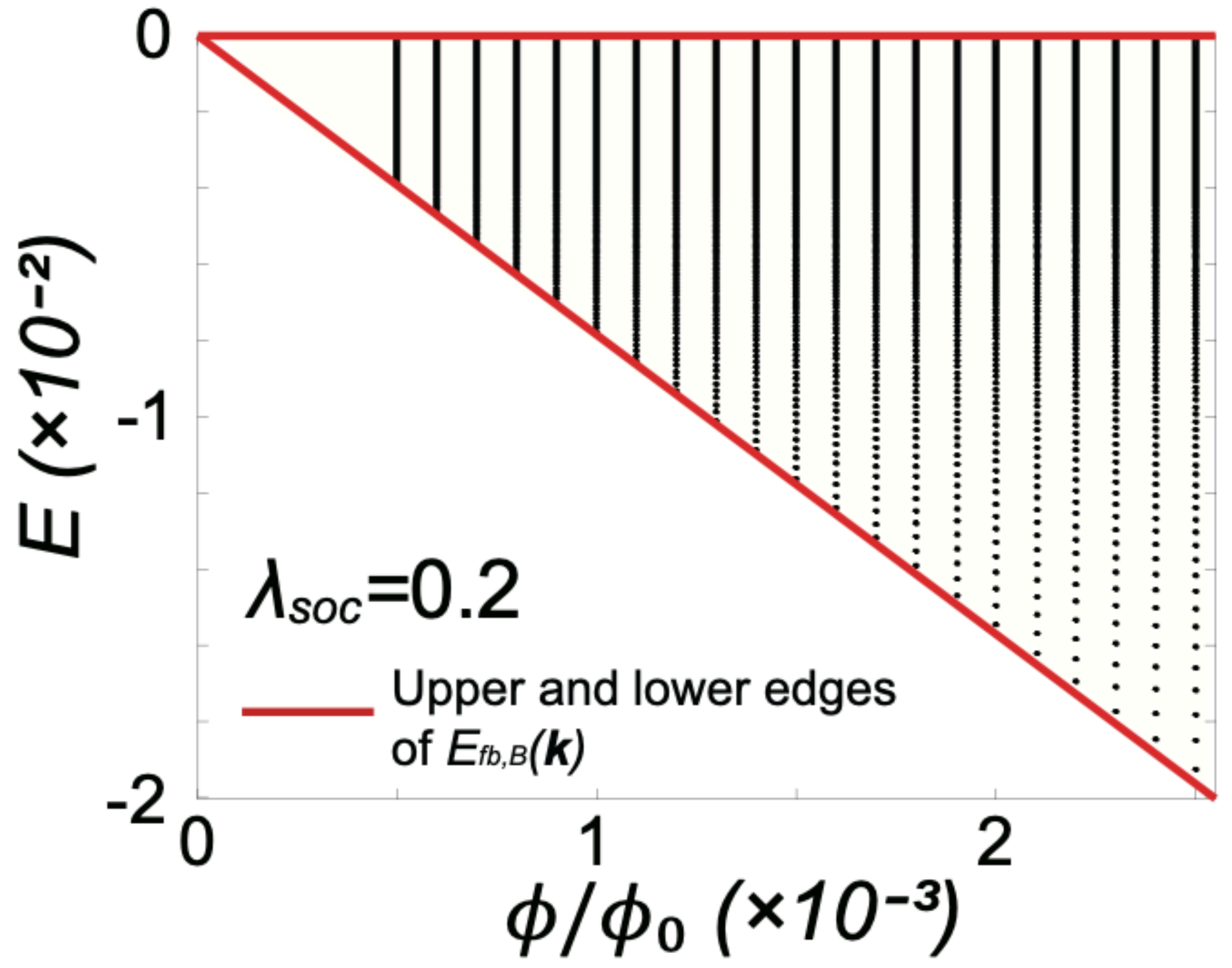
Yoonseok Hwang, Jun-Won Rhim, and Bohm-Jung Yang, arXiv:2012.15132

Cross-gap Berry connection and isolated flat band

Generic system



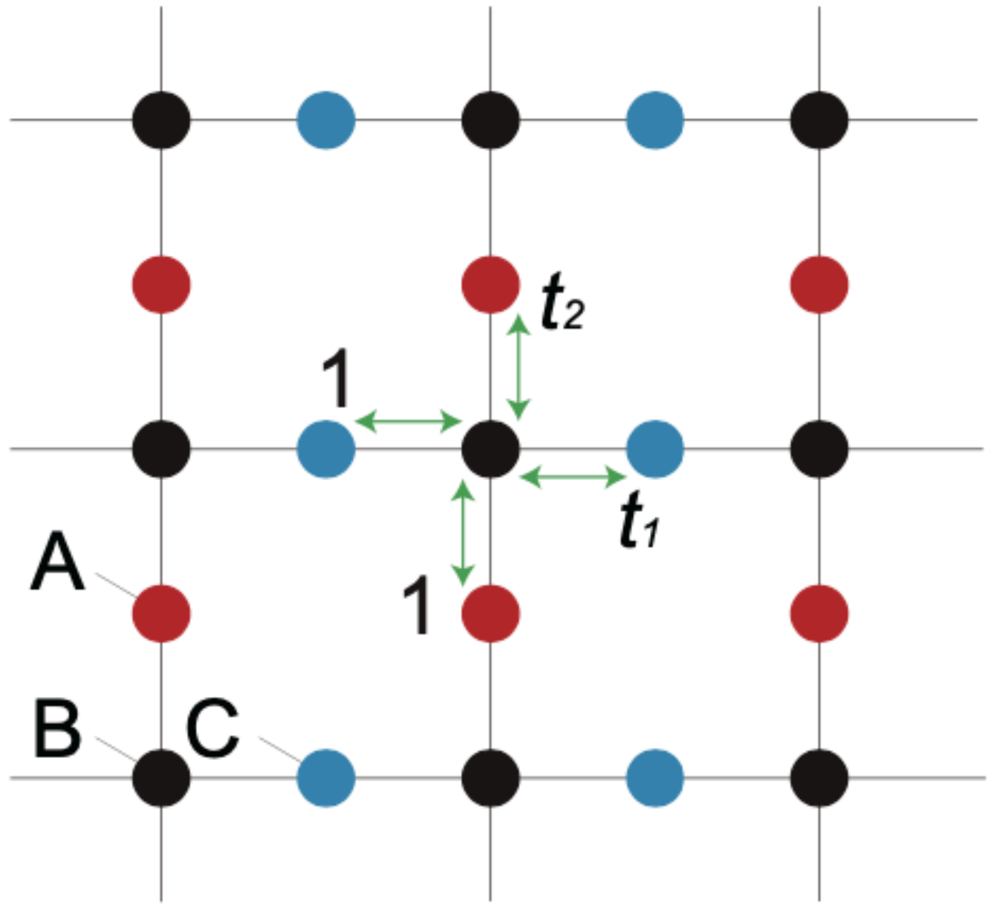


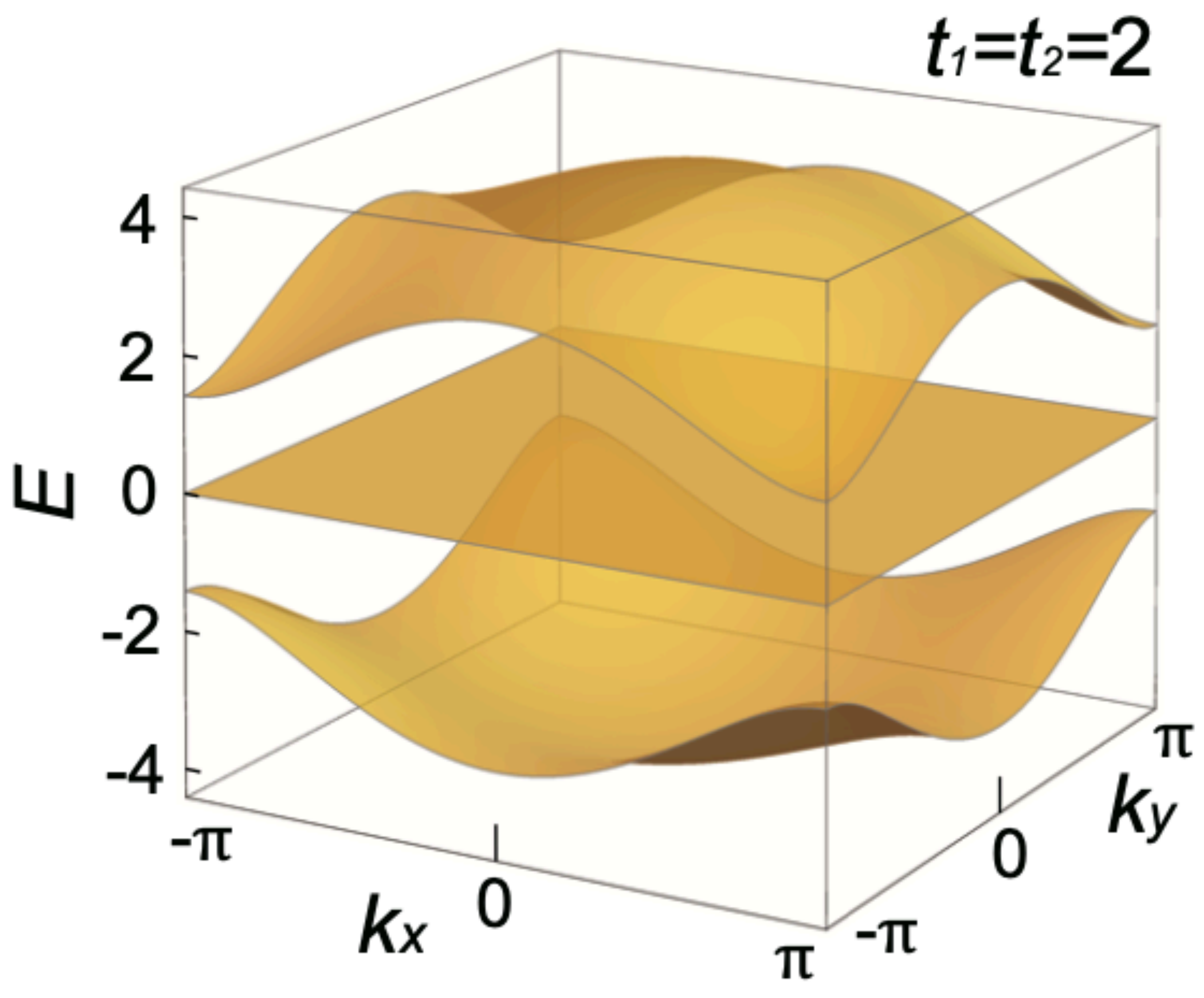


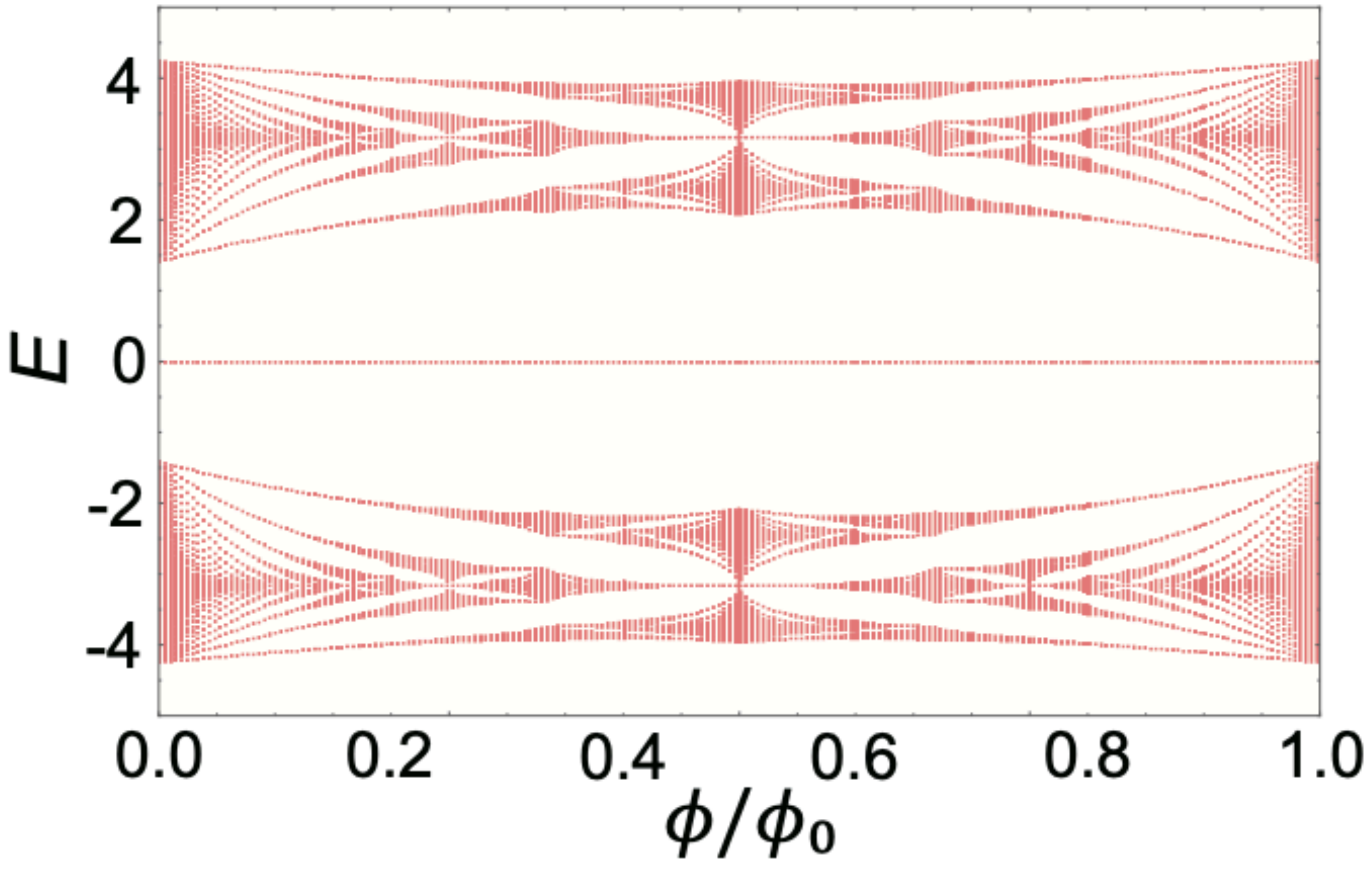
Yoonseok Hwang, Jun-Won Rhim, and Bohm-Jung Yang, arXiv:2012.15132

Cross-gap Berry connection and isolated flat band

System with chiral symmetry



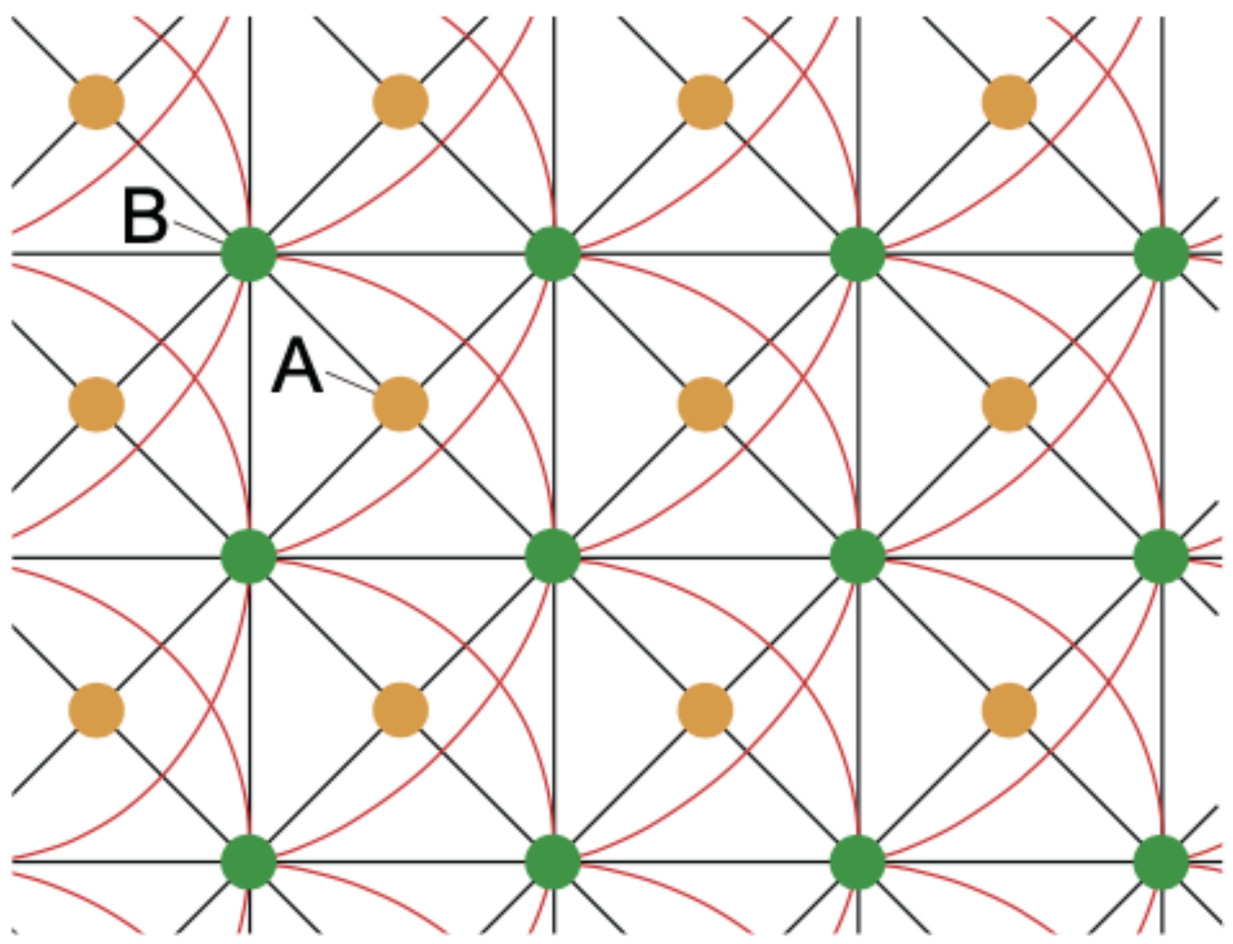


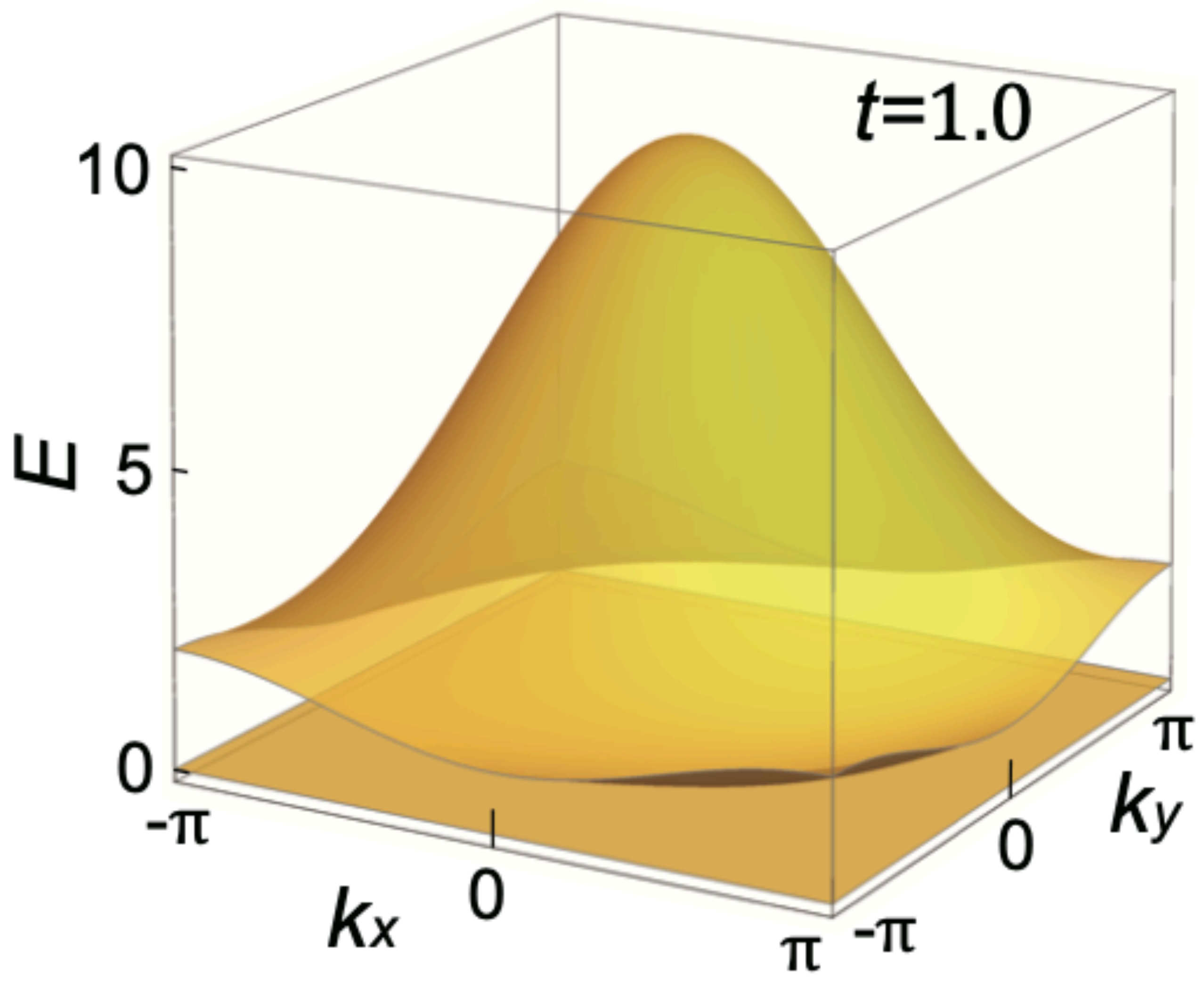


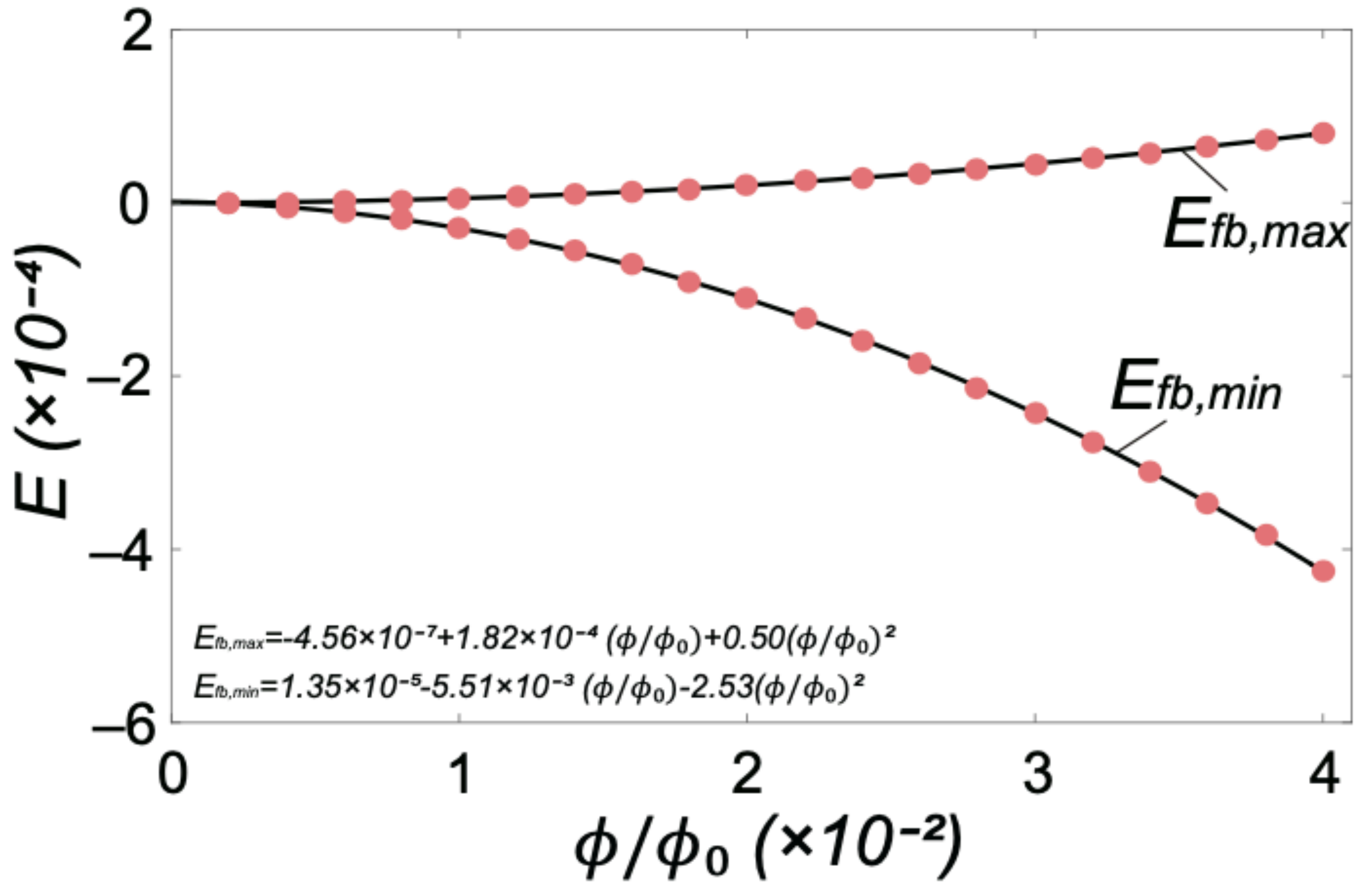
Yoonseok Hwang, Jun-Won Rhim, and Bohm-Jung Yang, arXiv:2012.15132

Cross-gap Berry connection and isolated flat band

System with space-time-inversion symmetry







Yoonseok Hwang, Jun-Won Rhim, and Bohm-Jung Yang, arXiv:2012.15132

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Summary

- Flat band systems are ideal platform to study various geometric properties of Bloch wavefunctions irrelevant to the topology.

- Band-crossing of a flat band, where the Bloch eigenvector is discontinuous, is characterized by d_{max}. (Graphene's band-crossing is characterized by the Berry phase.)

- Singular flat band's d_{max} manifests as the anomalous Landau level spreading.

- An isolated flat band can have Landau level spreading even though it is topologically trivial. This phenomenon is described by the cross-gap Berry connection.

[1] **JWR** and B.-J. Yang, ***PRB*** *99, 045107* (2019)

[2] J. Ma*, **JWR***, et al, ***PRL*** *124 183901* (2020)

[3] **JWR**, K. Kim, and B.-J. Yang, ***Nature*** *584 59* (2020)

[4] Y. Hwang, **JWR**, and B.-J. Yang, arXiv:2012.15132 (2020)