Quantum geometry and topological order in solids

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CVD Graphene PET/Glass Base Film

Outline

- ❑ Topological order in momentum space
- ❑ Topological marker in real space
- ❑ Quantum metric in momentum space
- ❑ Optical sum rules for the spread of Wannier functions

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Topology in our daily life

Topology from curvature: Gauss-Bonnet theorem

$$\int d^2\boldsymbol{r}\ \underbrace{\Omega(\boldsymbol{r})}_{\text{Gaussian curvature}} = 4\pi(1-\underbrace{g}_{\text{Number of holes}})$$

Example: a perfect sphere

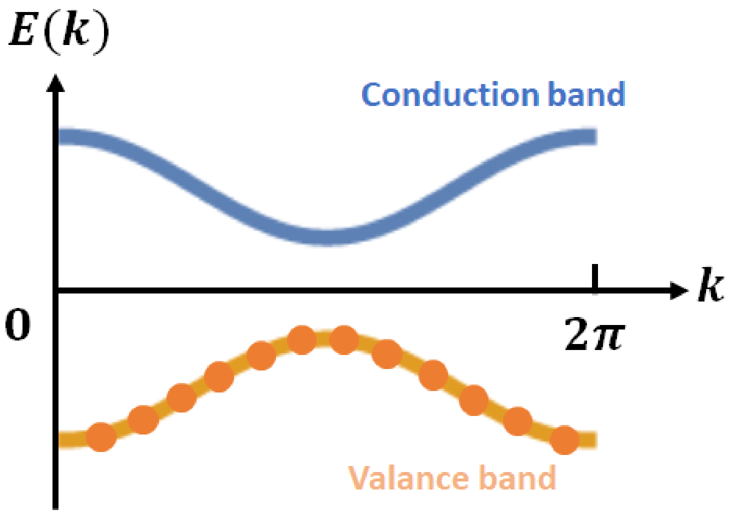
$$4\pi R^2 \times \frac{1}{R^2} = 4\pi(1-0)$$

Topology from surface normal: Gauss map

$$\hat{n} = \sin\theta\cos\varphi\,\hat{x} + \sin\theta\sin\varphi\,\hat{y} + \cos\theta\,\hat{z}$$

$$\int d\varphi \int d\theta\ \underbrace{\hat{n}\cdot(\partial_\theta\hat{n}\times\partial_\varphi\hat{n})}_{\text{Cyclic derivative of surface normal}} = \int d\varphi \int d\theta \sin\theta = 4\pi(1-\underbrace{0}_{\text{Number of holes}})$$

Topological insulators and superconductors described by Dirac models



Class	T	C	S	0	1	2	3	4	5	6	7
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	$+$	0	0	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
BDI	$+$	$+$	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
D	0	$+$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
DIII	$-$	$+$	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
AII	$-$	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
CII	$-$	$-$	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
C	0	$-$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
CI	$+$	$-$	1	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$

Schnyder et al. PRB 2008, Kitaev, AIP 2009, Ryu et al, NJP 2010

Dirac Hamiltonian $H(\mathbf{k}) = \boldsymbol{d}(\mathbf{k}) \cdot \boldsymbol{\Gamma}$

$\{\Gamma_i, \Gamma_j\} = 2\delta_{ij}$ $E(\mathbf{k}) = \pm|d(\mathbf{k})|$

TR, PH, and Chiral symmetries

$$TH^*(\mathbf{k})T^{-1} = H(-\mathbf{k}) \,,$$
$$CH^*(\mathbf{k})C^{-1} = -H(-\mathbf{k})$$
$$SH(\mathbf{k})S^{-1} = -H(\mathbf{k}) \,.$$

Examples: 2×2 Pauli matrices

$$H(\mathbf{k}) = d_1\sigma_1 + d_2\sigma_2 + d_3\sigma_3 = \begin{pmatrix} d_3 & d_1 - id_2 \\ d_1 + id_2 & d_3 \end{pmatrix}$$

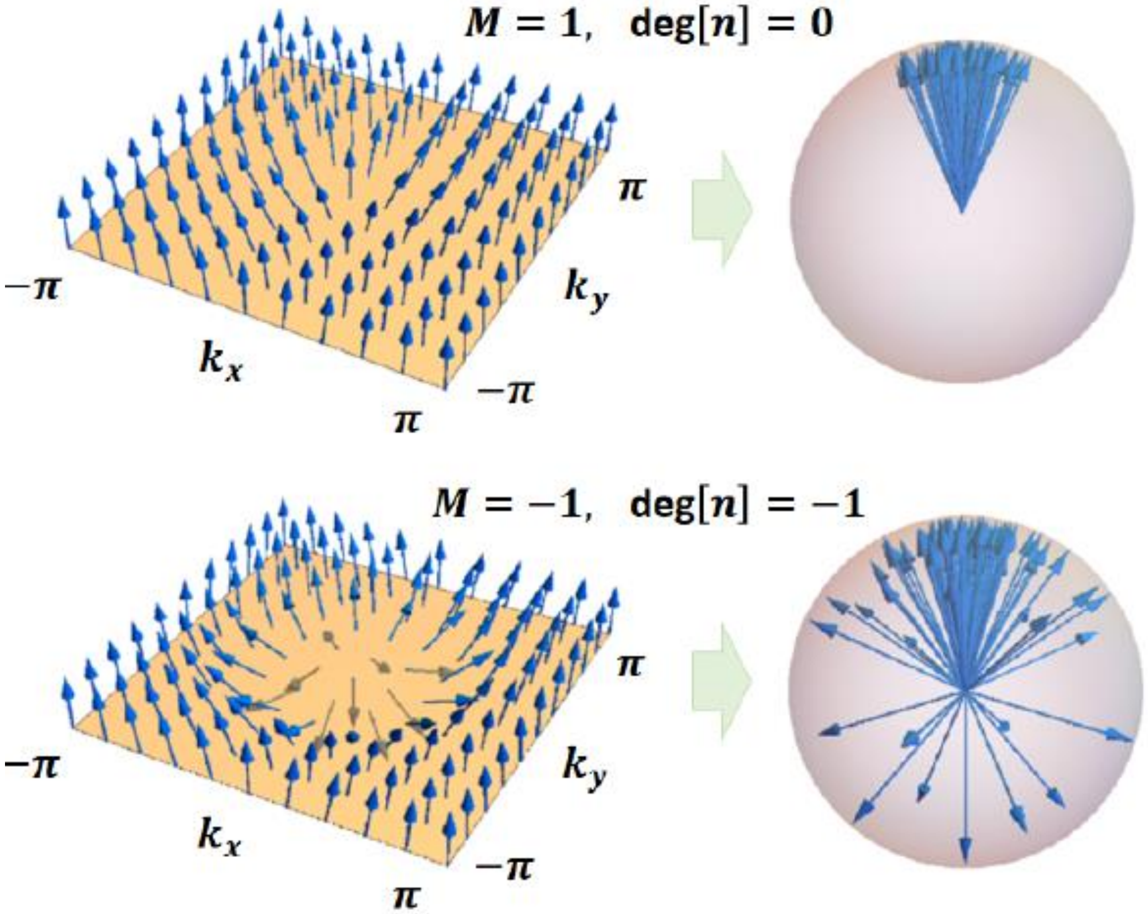
Introducing the wrapping number (a.k.a. degree of the map)

Dirac Hamiltonian $H(\mathbf{k}) = \boldsymbol{d}(\mathbf{k}) \cdot \boldsymbol{\Gamma}$ Unit vector $\boldsymbol{n}(\mathbf{k}) = \boldsymbol{d}(\mathbf{k})/|\boldsymbol{d}(\mathbf{k})|$

Degree of the map between T^D Brillouin zone and the “Dirac sphere” where $\boldsymbol{n}(\mathbf{k})$ forms

$$\deg[\boldsymbol{n}] = \frac{1}{V_D} \int d^D k \; \underbrace{\epsilon_{i_0 \ldots i_D} n^{i_0} \partial_1 n^{i_1} \ldots \partial_D n^{i_D}}_{\text{Cyclic derivative of } \boldsymbol{n}(\mathbf{k})}$$

$\boldsymbol{n}(\mathbf{k})$ in Brillouin Zone $\boldsymbol{n}(\mathbf{k})$ on Dirac sphere



Example: Lattice model of 2D Chern insulator

$$H(\mathbf{k}) = d_1\sigma_1 + d_2\sigma_2 + d_3\sigma_3$$

$$d_1 = \sin k_x \qquad d_2 = \sin k_y$$

$$d_3 = M + \cos k_x + \cos k_y$$

Universal topological markers

Universal topological invariant for any dimension and symmetry class

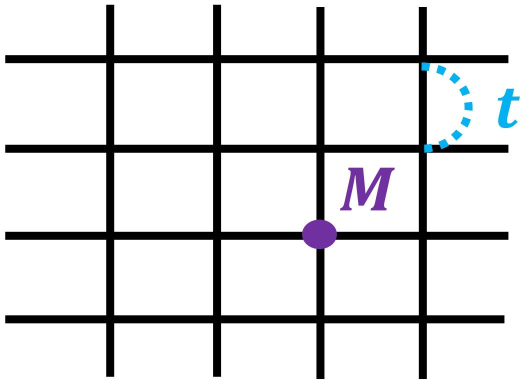
$$\deg[\boldsymbol{n}] = \frac{1}{V_D}\int d^D k\ \epsilon_{i_0 \ldots i_D} n^{i_0}\partial_1 n^{i_1} \ldots \partial_D n^{i_D}$$

Bianco and Resta,
PRB 84, 241106 (2011)

Momentum space $H(\mathbf{k}) = \boldsymbol{d}(\mathbf{k}) \cdot \boldsymbol{\Gamma}$

Fourier transform

Real space



WC, PRB 107, 045111 (2023)

Universal topological operator

$$\hat{\mathcal{C}} = N_D W \left[Q\,\hat{i}_1 P\,\hat{i}_2 \ldots \hat{i}_D \mathcal{O} + (-1)^{D+1} P\,\hat{i}_1 Q\,\hat{i}_2 \ldots \hat{i}_D \overline{\mathcal{O}}\right]$$

Unused Γ matrices

Alternating Q and P

Insert position operators

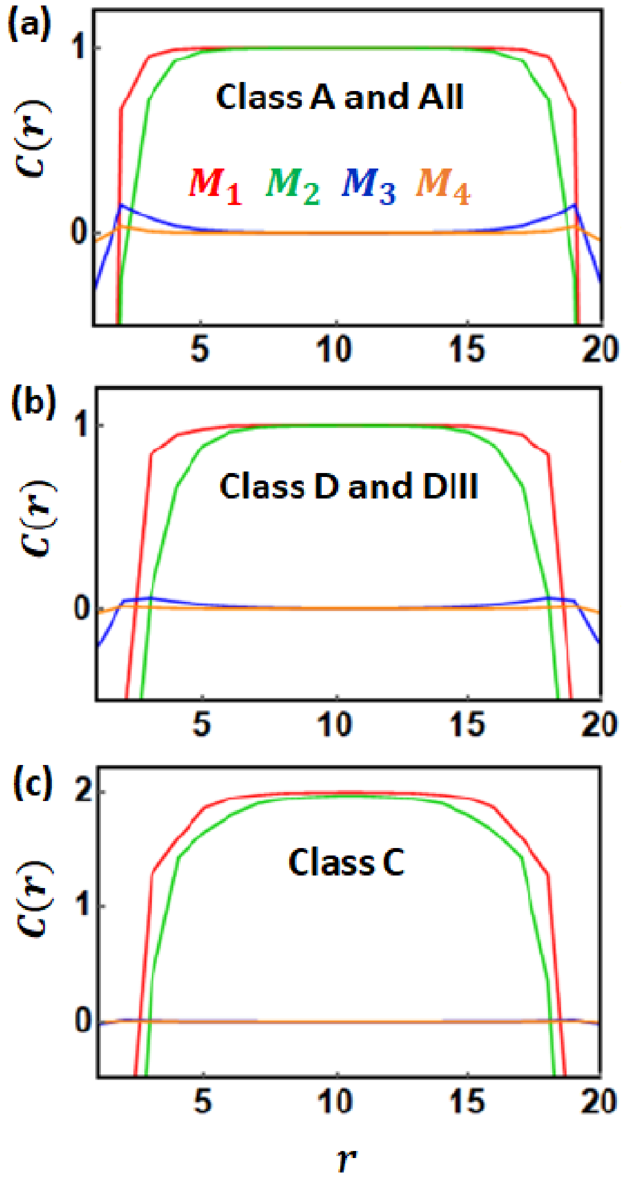
$$Q \equiv \sum_{E_m>0} |E_m\rangle\langle E_m| \qquad P \equiv \sum_{E_n<0} |E_n\rangle\langle E_n|$$

Local marker
quantized to integer

$$\mathcal{C}(\mathbf{r}) = \langle \mathbf{r}|\hat{\mathcal{C}}|\mathbf{r}\rangle = \sum_{\sigma} \langle \mathbf{r}\sigma|\hat{\mathcal{C}}|\mathbf{r}\sigma\rangle$$

Applications to 2D classes

Local marker



Topological operator in 2D

$$\hat{C}_{2D} = N_D W \left[Q\hat{x}P\hat{y}Q - P\hat{x}Q\hat{y}P \right]$$

Chern insulator, BHZ model

Chiral and Helical p-wave SC

Impurities as local variation of lattice Hamiltonian

If a impurity corresponds to varying nonzero matrix element λ in Hamiltonian

$$H = H_0 + \delta\lambda\,\partial_\lambda H_0$$

Expanding eigenstates by perturbation

$$|\ell'\rangle = |\ell\rangle + \delta\lambda \sum_{k\neq\ell} \frac{|k\rangle\langle k|\partial_\lambda H_0|\ell\rangle}{E_\ell - E_k}$$

Expanding projectors by perturbation

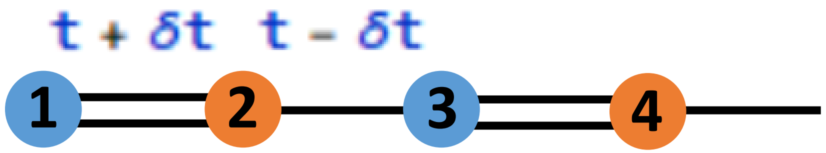
$$P' = P + \delta\lambda\partial_\lambda P, \qquad Q' = Q + \delta\lambda\partial_\lambda Q$$

The average marker will be changed by

$$\mathcal{C}' = \mathcal{C} + \delta\lambda\partial_\lambda\mathcal{C}$$

Question: Is the correction $\delta\lambda\partial_\lambda C$ zero?

Example: 1D SSH model in class BDI



$$H_0 = \begin{pmatrix} 0 & t+\delta t & 0 & t-\delta t \\ t+\delta t & 0 & t-\delta t & 0 \\ 0 & t-\delta t & 0 & t+\delta t \\ t-\delta t & 0 & t+\delta t & 0 \end{pmatrix}$$

Hopping impurity: varying nonzero element

$$H_{imp} = \begin{pmatrix} 0 & t+\delta t_{imp} & 0 & t-\delta t \\ t+\delta t_{imp} & 0 & t-\delta t & 0 \\ 0 & t-\delta t & U_{imp} & t+\delta t \\ t-\delta t & 0 & t+\delta t & 0 \end{pmatrix}$$

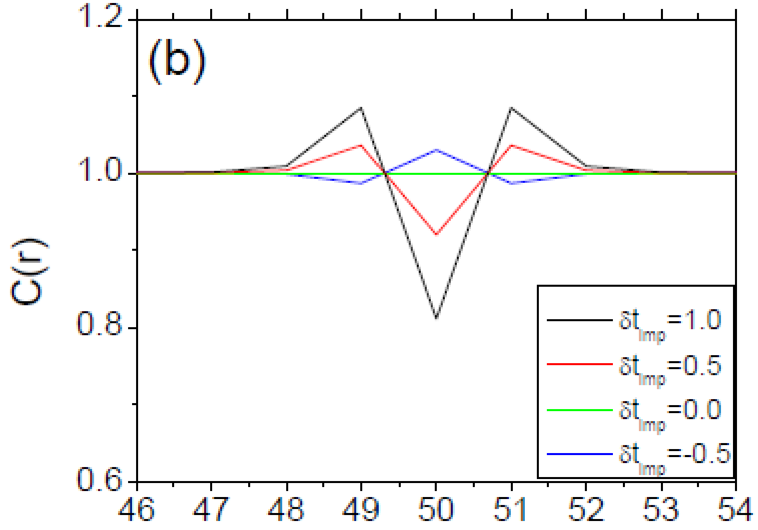
Potential impurity: varying zero element

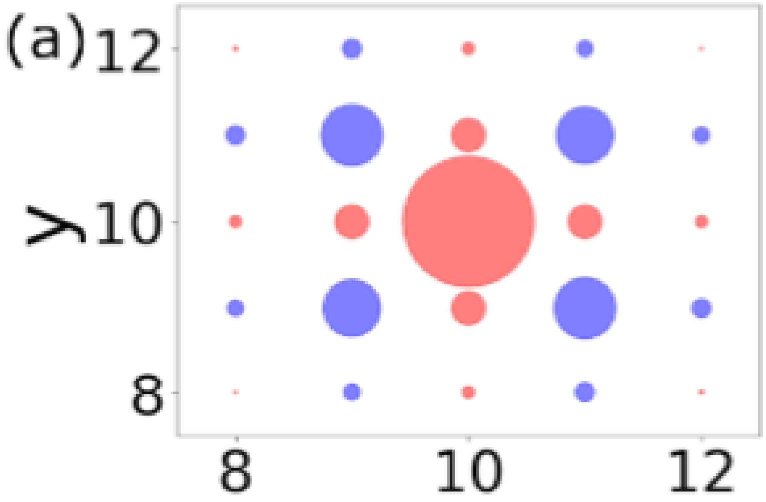
Numerical verification of the analytical proof

1D SSH model

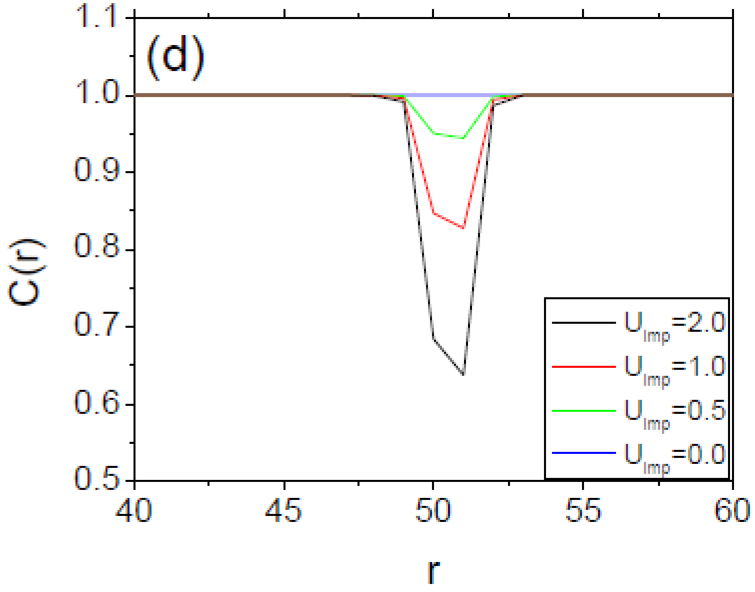
2D Chern inulator

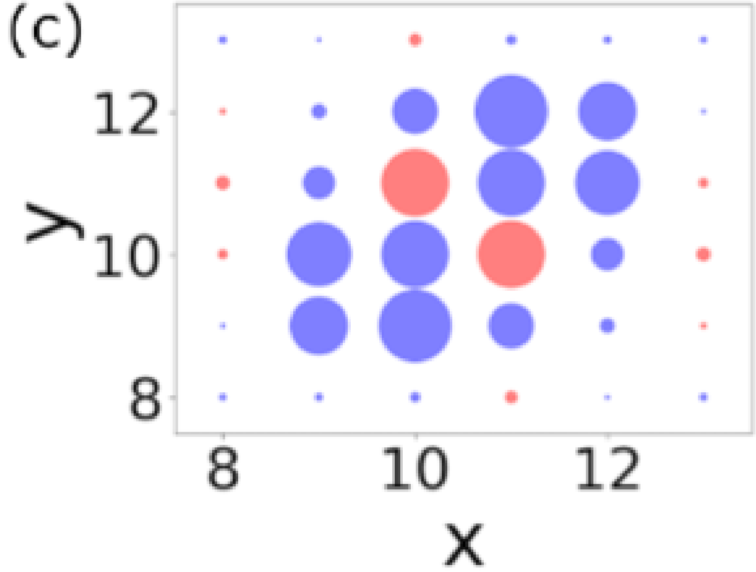
Varying nonzero element





Varying zero element





Investigating interacting SSH model by topological marker

Topological operator in 1D

$$\hat{\mathcal{C}}_{1D} = N_D W \left[Q\hat{x}P + P\hat{x}Q \right]$$

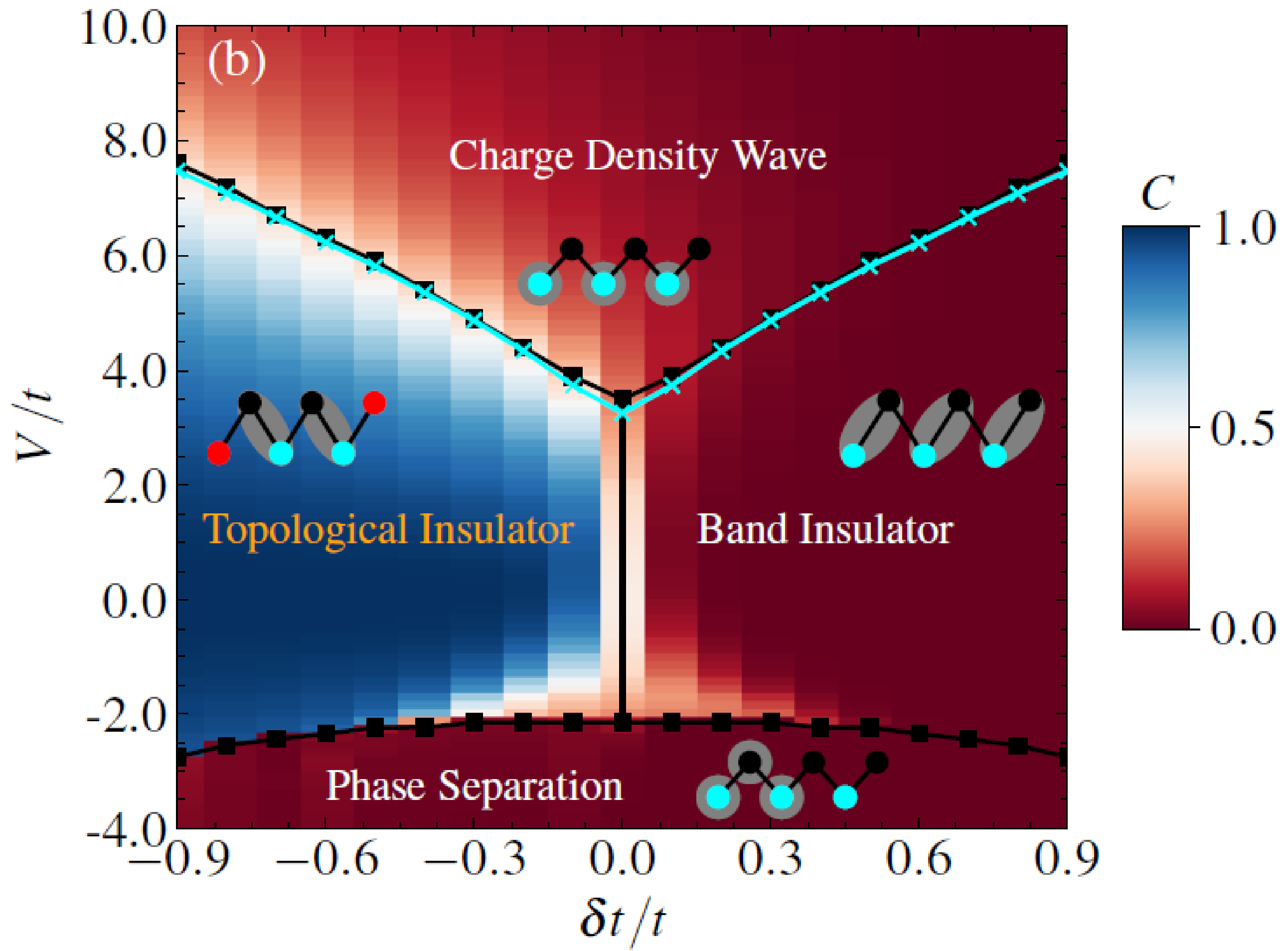
Generalizing the projectors to interacting systems using Green's fn

$$G_{i,j} = \langle \hat{c}_i \hat{c}_j^\dagger \rangle$$

$$\hat{P} \rightarrow \hat{G}$$

$$\hat{Q} \rightarrow \hat{\tilde{I}} - \hat{G}$$

Example: Interacting SSH model



$$\hat{\mathcal{H}} = \sum_{\langle i,j \rangle} \left(-t + \delta t (-1)^i \right) \left(\hat{c}_j^\dagger \hat{c}_i + \mathrm{H.c.} \right) + V \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j$$

Melo, Junior, WC, Mondaini, Paiva, PRB 108, 195151 (2023)

Quantum metric of (degenerate) filled band states

The N_--particle filled band state of Dirac models

$$|\psi(\mathbf{k})\rangle = \frac{1}{\sqrt{N_-!}}\varepsilon^{a_1 \dots a_{N_-}}|u^-_{a_1}\rangle|u^-_{a_2}\rangle \dots \left|u^-_{a_{N_-}}\right\rangle$$

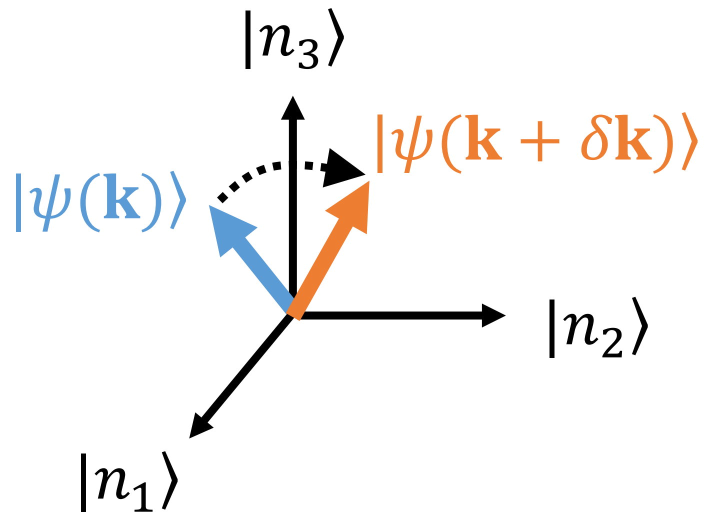
Quantum metric (aka fidelity susceptibility) on the BZ manifold

$$|\langle\psi(\mathbf{k})|\psi(\mathbf{k}+\delta\mathbf{k})\rangle| = 1 - \frac{1}{2}g_{\mu\nu}\delta k^\mu \delta k^\nu$$

$$g_{\mu\nu} = \frac{1}{2}\langle\partial_\mu\psi|\partial_\nu\psi\rangle + \frac{1}{2}\langle\partial_\nu\psi|\partial_\mu\psi\rangle - \langle\partial_\mu\psi|\psi\rangle\langle\psi|\partial_\nu\psi\rangle$$

For Dirac models

$$g_{\mu\nu} = \frac{N}{8}\partial_\mu \boldsymbol{n}\cdot\underbrace{\partial_\nu \boldsymbol{n}}_{\text{Vielbein}}$$



Provost and Vallee, Comm. Math. Phys. 76, 289 (1980)
Ma et al, EPL 103, 10008 (2013)

Metric-curvature correspondence

The wrapping number can be written as the integration of a Jacobian

$$\deg[\boldsymbol{n}] = \frac{1}{V_D}\int d^D k \; J_{\boldsymbol{n}}(\mathbf{k}) \qquad\qquad J_{\boldsymbol{n}}(\mathbf{k}) = \det(\boldsymbol{n}, \partial_1\boldsymbol{n}, \partial_2\boldsymbol{n} \ldots \partial_D\boldsymbol{n}) = \det(\boldsymbol{n}, \partial_\mu\boldsymbol{n})$$

The square of the Jacobian is also given by the vielbein form

$$J_{\boldsymbol{n}}^2 = \det\begin{pmatrix} \boldsymbol{n}\cdot\boldsymbol{n} & \boldsymbol{n}\cdot\partial_\nu\boldsymbol{n} \\ \partial_\mu\boldsymbol{n}\cdot\boldsymbol{n} & \partial_\mu\boldsymbol{n}\cdot\partial_\nu\boldsymbol{n} \end{pmatrix} = \det \partial_\mu\boldsymbol{n}\cdot\partial_\nu\boldsymbol{n}$$

Thus the module of the Jacobian is equal to the square of $\det g_{\mu\nu}$

$$|J_{\boldsymbol{n}}| = \left(\frac{8}{N}\right)^{\frac{D}{2}} \sqrt{\det g_{\mu\nu}}$$

“Metric-curvature correspondence”

von Gersdorff and WC, PRB 104, 095113 (2021)

This means topological order can be measured via measuring the quantum metric!!!

Time-dependent perturbation theory of measuring quantum metric

Applying a pulse electric field of profile $g(t)$ and polarization $\hat{\boldsymbol{\mu}}$

$$\boldsymbol{E}(t) = \hat{\boldsymbol{\mu}}\, E^0 h(t) = \ i\, E^0 h(t) \partial_\mu$$

Causes a transition of electrons from filled bands a to empty bands b, which is equal to quantum metric

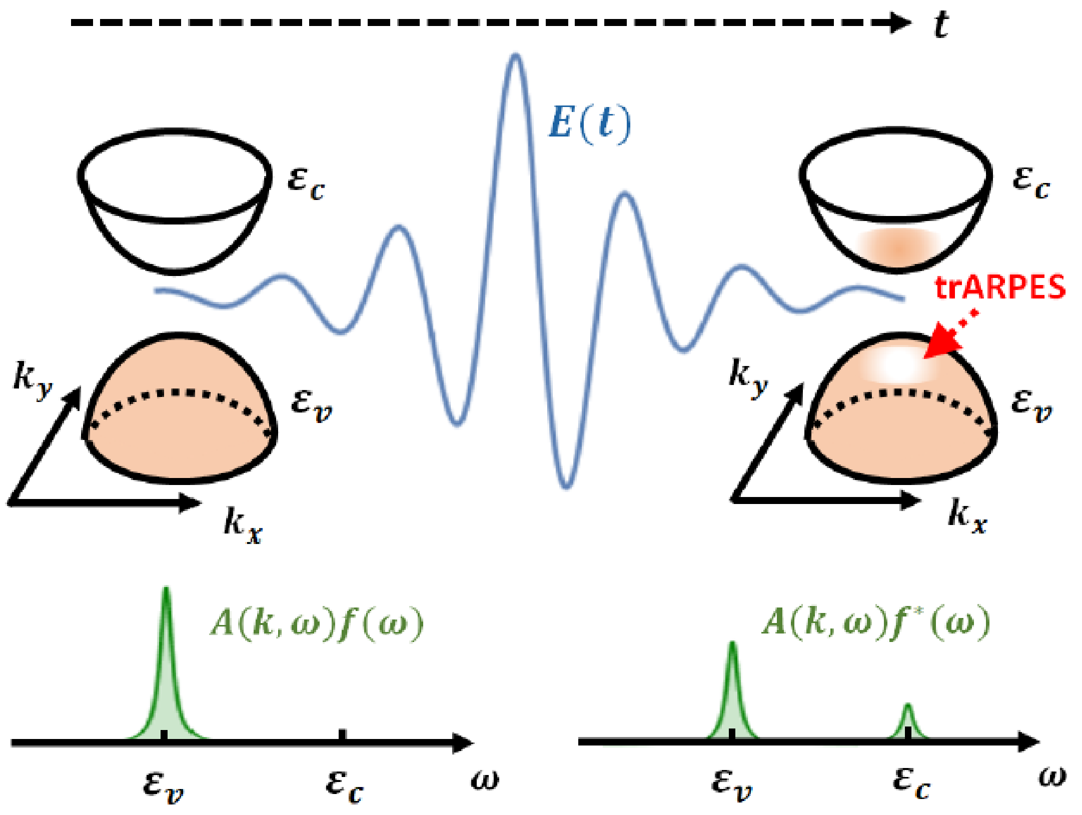
$$\nu(\mathbf{k}) = \left(\frac{eE^0}{\hbar}\right)^2 |\tilde{h}(\omega(\mathbf{k}))|^2 \sum_{a,b} |\langle u_b(\boldsymbol{k})|\partial_\mu u_a(\mathbf{k})\rangle|^2$$

$$= \left(\frac{eE^0}{\hbar}\right)^2 |\tilde{h}(\omega(\mathbf{k}))|^2\, g_{\mu\mu}(\mathbf{k})$$

Which is equal to the loss of spectral weight in ARPES

$$\nu(\mathbf{k}) = \frac{N}{2} - \int_{-\infty}^{\infty} d\omega \ A(\mathbf{k}, \omega) f^*(\omega)$$

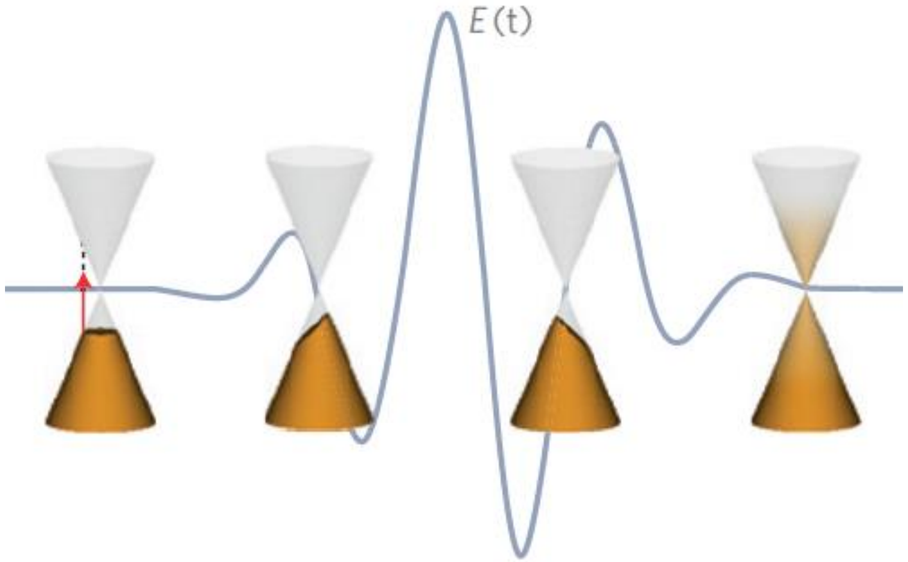
Ozawa and Goldman, PRB 97, 201117 (2018)

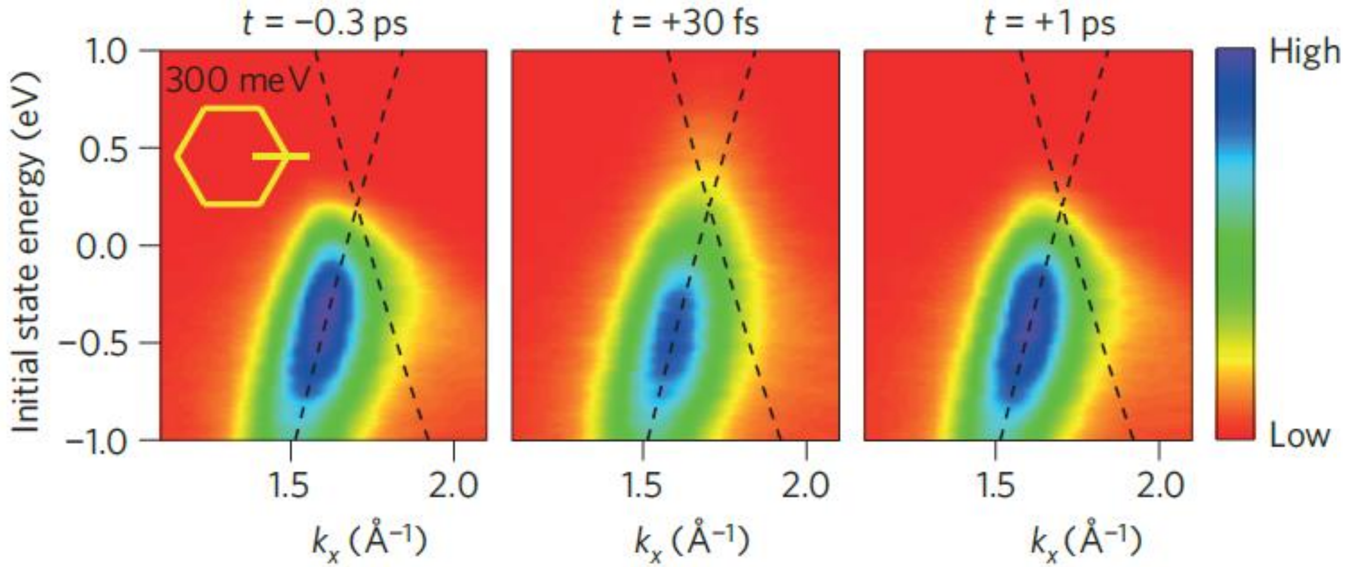


"Loss-fluence spectroscopy"

von Gersdorff and WC, PRB 104, 095113 (2021)

Pump-probe on graphene





Gierz et al, Mat. Mater. 12, 1119 (2013)

Message to experimentalists: Use polarized light!!

Relating spread of valence band Wannier functions to fidelity number

$$\mathcal{G}_{\mu\nu} = \int \frac{d^D k}{(2\pi)^D}\, g_{\mu\nu}$$

“Fidelity number”

Marzari and Vanderbilt, PRB 56, 12847 (1997).

de Sousa, Cruz, Chen, PRB 107, 205133 (2023).

Wannier function localized at $\mathbf{R}$ $\quad |\mathbf{R}\ell\rangle = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\hat{\mathbf{r}}-\mathbf{R})/\hbar}|\ell^{\mathbf{k}}\rangle$

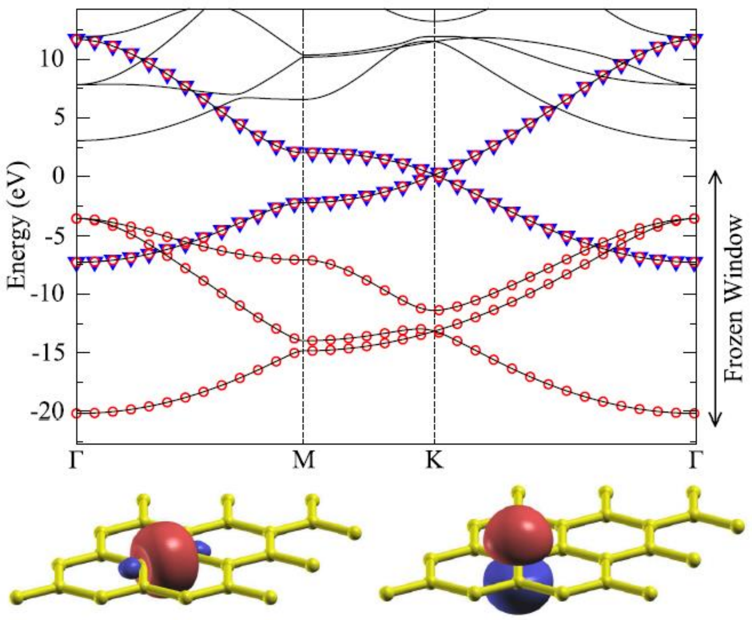
Spread of valence band Wannier function

$$\Omega = \sum_n \left[\langle 0n|r^2|0n\rangle - \langle 0n|\mathbf{r}|0n\rangle^2\right] = \Omega_I + \tilde{\Omega}$$

Gauge-invariant part of the spread is given by the trace of the fidelity number

$$\Omega_I = \sum_n \left[\langle 0n|r^2|0n\rangle - \sum_{\mathbf{R}n'} |\langle \mathbf{R}n'|\mathbf{r}|0n\rangle|^2\right] = \frac{V_{\text{cell}}}{\hbar^{D-2}}\, \mathrm{Tr}\, \mathcal{G}_{\mu\nu}$$

Souza, Wilkens, Martin, PRB 62, 1666 (2000).



Maximally localized Wannier functions

Marzari and Vanderbilt, PRB 56, 12847 (1997).

Marzari et al, RMB 2012

How to detect this gauge-invariant part of the spread experimentally?

Detecting the fidelity number by optical conductivity

$\boldsymbol{k}$-space optical conductivity = Quantum metric spectral function × frequency

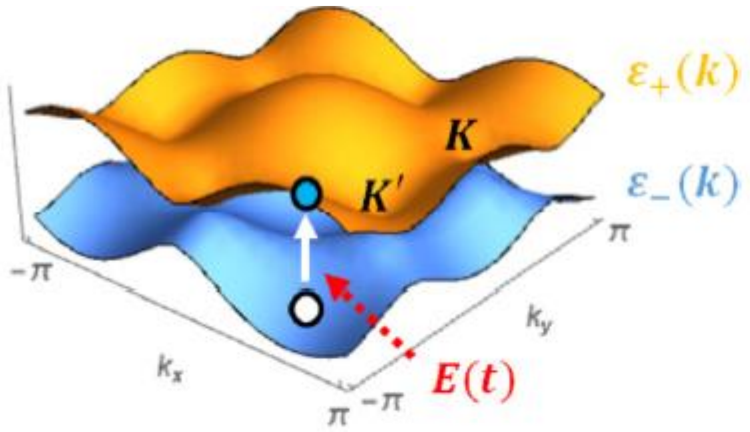
$$\sigma_{\mu\mu}(\mathbf{k},\omega)=\sum_{\ell<\ell'}\frac{\pi}{V_{\rm cell}\,\hbar\omega}\underbrace{\langle\ell|\hat{j}_\mu|\ell'\rangle\langle\ell'|\hat{j}_\mu|\ell\rangle}_{\text{Quantum metric}}\left[f(\varepsilon_\ell^{\mathbf{k}})-f(\varepsilon_{\ell'}^{\mathbf{k}})\right]\delta\left(\omega+\frac{\varepsilon_\ell^{\mathbf{k}}}{\hbar}-\frac{\varepsilon_{\ell'}^{\mathbf{k}}}{\hbar}\right)=\frac{\pi e^2}{V_{\rm cell}}\hbar\omega\, g_{\mu\mu}^d(\mathbf{k},\omega)$$

Real space optical conductivity = fidelity number spectral function × frequency

$$\sigma_{\mu\mu}(\omega)=\int\frac{d^D\mathbf{k}}{\hbar^D V_{BZ}}\sigma_{\mu\mu}(\mathbf{k},\omega)\;=\frac{\pi e^2}{\hbar^{D-1}}\omega\int\frac{d^D\mathbf{k}}{(2\pi)^D}g_{\mu\mu}^d(\mathbf{k},\omega)\equiv\frac{\pi e^2}{\hbar^{D-1}}\omega\,\mathcal{G}_{\mu\mu}^d(\omega)$$

$$\mathcal{G}_{\mu\mu}^d=\int_0^\infty d\omega\,\mathcal{G}_{\mu\mu}^d(\omega)\;\propto\;\Omega_I$$

Real space optical conductivity divided by frequency and then integrate over frequency gives the spread!



3D semiconductors: imaginary part of dielectric function

Complex Dielectric function given by optical conductivity

$$\varepsilon_{\mu\nu}(\omega) = 1 + i\frac{\tilde{\sigma}_{\mu\nu}(\omega)}{\varepsilon_0\omega}$$

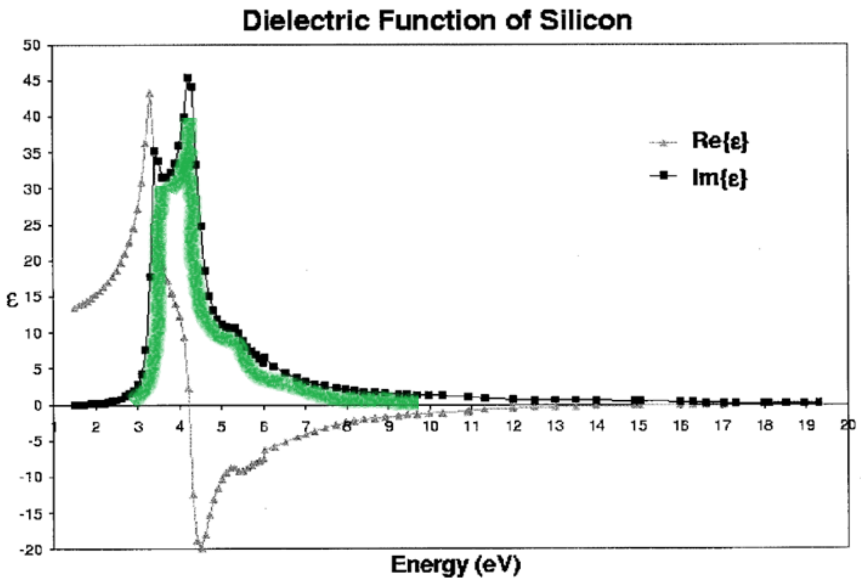
Imaginary part of dielectric function integrated over ω

$$\frac{1}{3}\sum_{\mu}\mathcal{G}^{d}_{\mu\mu} = \frac{\varepsilon_0\hbar}{\pi e^2}\int_0^\infty d(\hbar\omega)\,\mathrm{Im}[\varepsilon(\omega)]$$

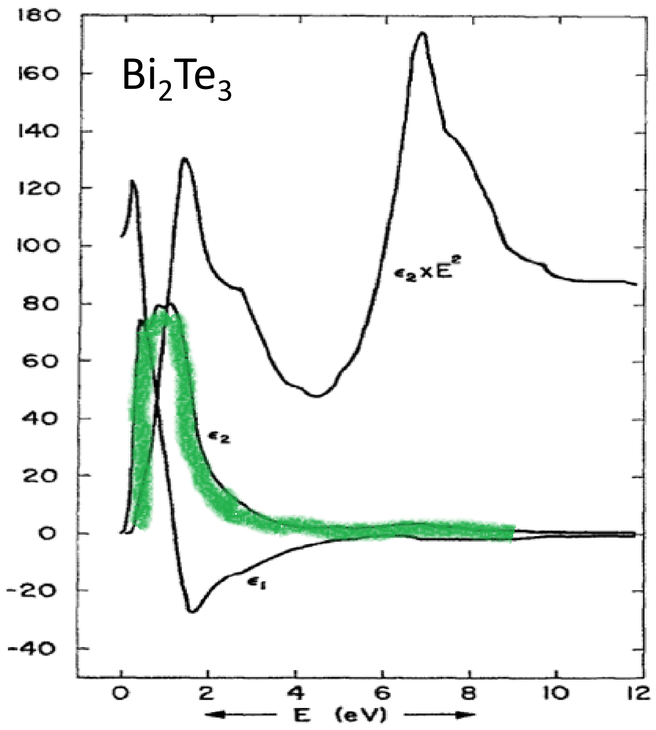
Experimental proposal

$$\Omega_I = \lim_{T\to 0}\frac{V_{\mathrm{cell}}}{\mathring{A}} \times 1.7591 \times 10^{-3} \times 3\nu$$

Area under the curve!!



Reed et al, PRB 1999



Greenaway and Harbeke 1965

Mat.	$V_{\mathrm{cell}}(\mathring{A}^3)$	ν	$\mathrm{Tr}\mathcal{G}_{\mu\nu}(\hbar/\mathring{A})$	$\Omega_I(\mathring{A}^2)$	$\Omega_I^{3/2}/V_{\mathrm{cell}}$
Si	160.1	80.6	0.425	68.1	3.51
Ge	181.3	87.0	0.459	83.24	4.19
Bi_2Te_3	545.3	141.6	0.747	407.48	15.08

Cardenas-Castillo et al, arXiv:2405.06146

Seeing topological charge of graphene by naked eyes

Opacity of 2D materials $\mathcal{O}(\omega) = 4\pi^2\alpha\omega \times \mathcal{G}_{\mu\mu}(\omega)$

Opacity of graphene at visible light $\lim_{T\to 0} \mathcal{O}(\omega) = \pi\alpha \times 4\mathcal{C}^2 = \pi\alpha \approx 2.3\%$

CVD Graphene PET/Glass Base Film

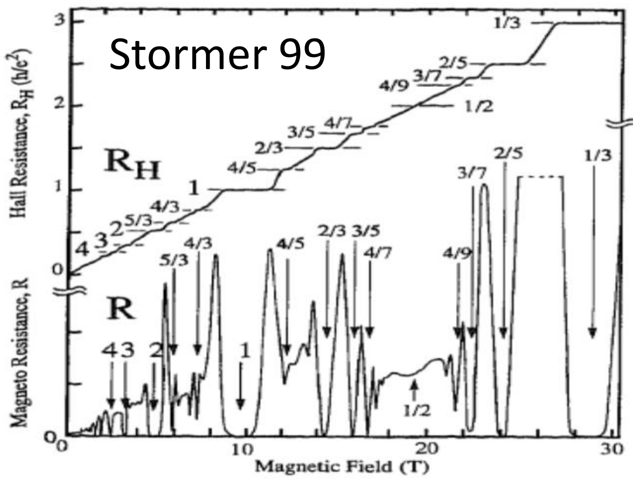
This implies:

de Sousa and Chen, PRB 108, 165201 (2023)

(1) One can literally see the topological charge by naked eyes

(2) All 2D Dirac semimetals have the same opacity at infrared

(3) The fine-structure constant is topologically protected

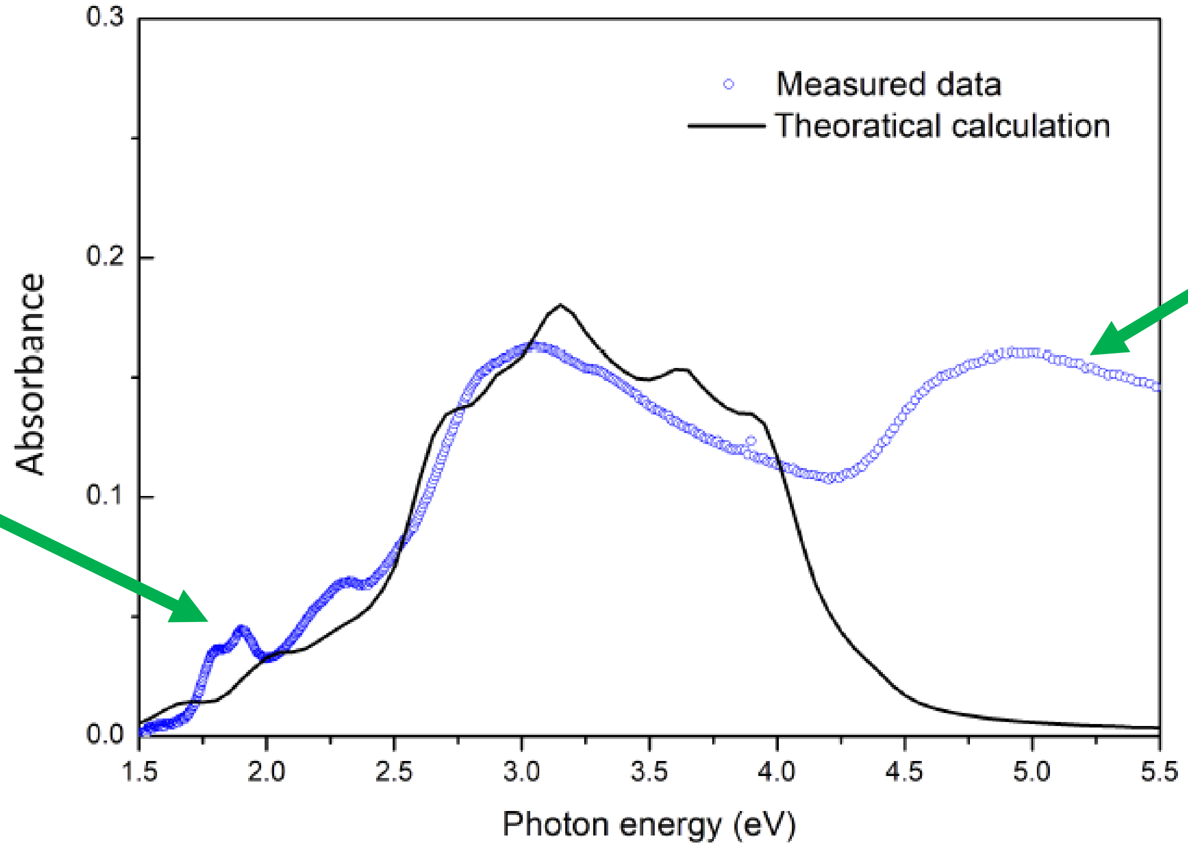


The only other topologically protected constant is the von Klitzing constant h/e^2 in QHE. Our paper thus plays the same role as the TKNN paper that links the quantized Hall conductance to a topological invariant.

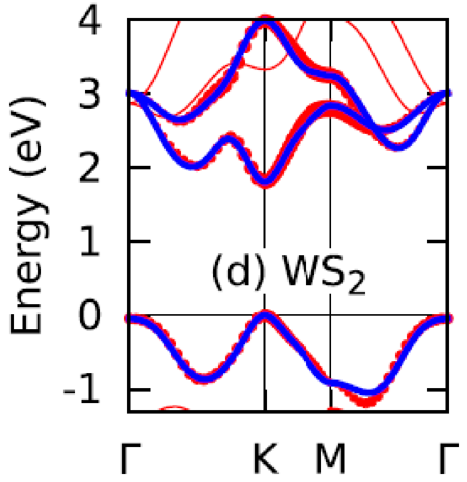
Thouless, Kohmoto, Nightingale, and den Nijs, PRL 49, 405 (1982).

Experimental absorbance of WS_2 on fused silica

Don't count excitons because they are bosons



Sulfur orbitals absorb light at higher frequencies



Liu et al, PRB 88, 085433 (2013)

Cardenas-Castillo et al, arXiv:2405.06146

Quantum metric of singlet superconductors

$\mathbf{n} \equiv \mathbf{d}/|\mathbf{d}|$

Singlet superconductors are also Dirac models

$$H(\boldsymbol{k}) = \begin{pmatrix} \varepsilon_k & \Delta_k \\ \Delta_k & -\varepsilon_k \end{pmatrix} = d_1\sigma_1 + d_3\sigma_3$$

Quantum metric of filled quasihole state

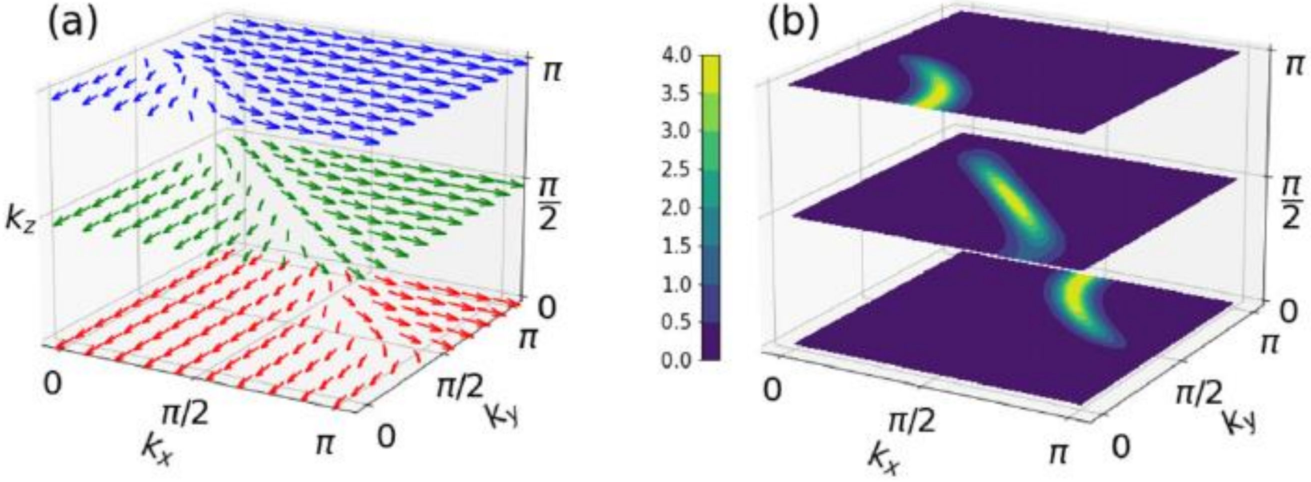
$$g_{\mu\nu} = \frac{1}{4}\partial_\mu \mathbf{n} \cdot \partial_\nu \mathbf{n} = (u_\mathbf{k}\partial_\mu v_\mathbf{k} - v_\mathbf{k}\partial_\mu u_\mathbf{k})(u_\mathbf{k}\partial_\nu v_\mathbf{k} - v_\mathbf{k}\partial_\nu u_\mathbf{k})$$

It is just the “twisting” of the field $\mathbf{w}_\mathbf{k} = (v_\mathbf{k}, -u_\mathbf{k})$

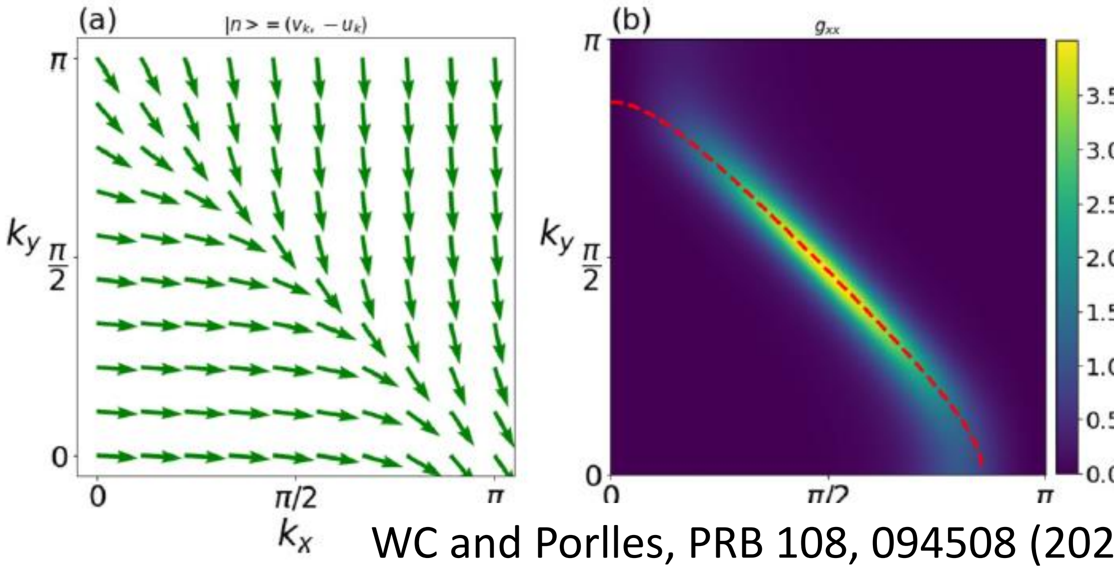
s-wave SC:

$$g_{\mu\nu} = \frac{\Delta^2 v_\mu v_\nu}{4E_\mathbf{k}^4}$$

3D s-wave



2D s-wave



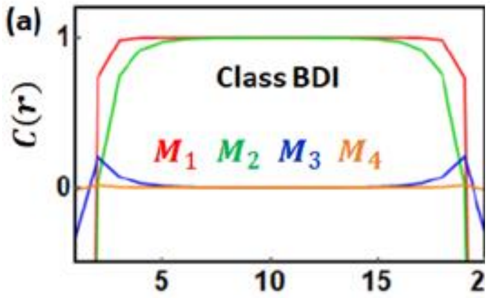
WC and Porlles, PRB 108, 094508 (2023)

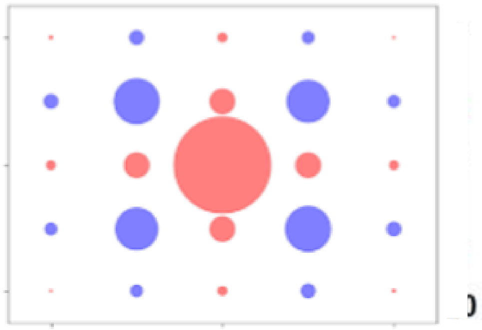
Summary

- Unification of topological invariants in Dirac models

von Gersdorff, Panahiyan, WC, PRB 103, 245146 (2021)

$$\deg[\boldsymbol{n}] = \frac{1}{V_D}\int d^D k \;\; \epsilon_{i_0 \dots i_D} n^{i_0} \partial_1 n^{i_1} \dots \partial_D n^{i_D}$$





- Universal topological marker

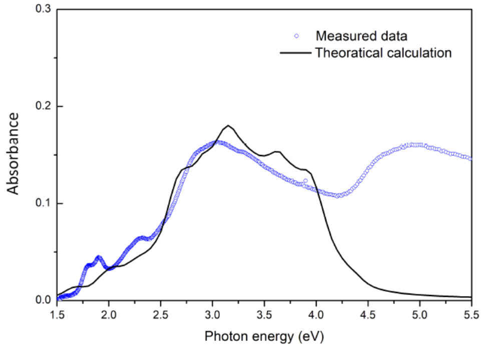
$$\hat{\mathcal{C}} = N_D W\left[Q\,\hat{i}_1 P\,\hat{i}_2 \dots \hat{i}_D \mathcal{O} + (-1)^{D+1} P\,\hat{i}_1 Q\,\hat{i}_2 \dots \hat{i}_D \overline{\mathcal{O}}\right]$$

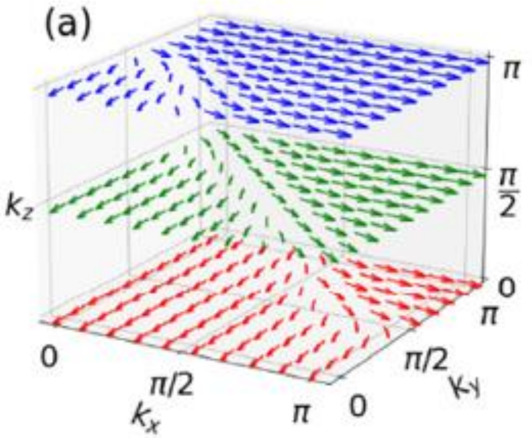
WC, PRB 107, 045111 (2023)

Melo, Junior, WC, Mondaini, Paiva, PRB 108, 195151 (2023)

- Robustness of topological order $\mathcal{C}' = \mathcal{C} + \delta\lambda\partial_\lambda \mathcal{C}$

L. A. Oliveira and WC, PRB 109, 094202 (2024)





- Quantum metric and optical effects

$$|\langle\psi(\mathbf{k})|\psi(\mathbf{k}+\delta\mathbf{k})\rangle| = 1 - g_{\mu\nu}\delta k^\mu \delta k^\nu/2$$

von Gersdorff and WC, PRB 104, 095113 (2021)

de Sousa, Cruz, Chen, PRB 107, 205133 (2023).

Cardenas-Castillo et al, arXiv:2405.06146

WC and Porlles, PRB 108, 094508 (2023)