中国科学院物理研究所 INSTITUTE OF PHYSICS CHINESE ACADEMY OF SCIENCES | 北京凝聚态物理国家实验室 BEIJING NATIONAL LABORATORY FOR CONDENSED MATTER PHYSICS

Interaction effect on topological insulators

Studies based on interacting Green's functions

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Hao Shi & Shiwei Zhang, College of William & Mary

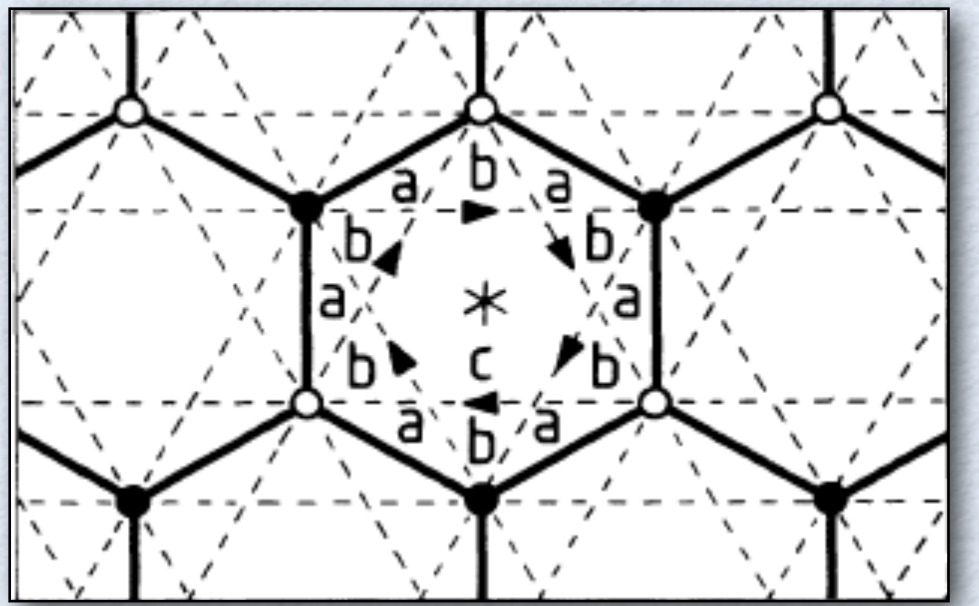
Shun-Li Yu, X. C. Xie and Jianxin Li, PRL, **107**, 010401 (2011)
Lei Wang, Hao Shi, Shiwei Zhang, Xiaoqun Wang, Xi Dai and X. C. Xie, arXiv:1012.5163
Lei Wang, Xi Dai and X. C. Xie, arXiv:1107.4403
Lei Wang, Hua Jiang, Xi Dai and X. C. Xie, in preparation

Outline

- Interaction effect on topological insulators
  - Solve interacting models
  - Characterize interacting topological phases
- Characterization based on interacting Green’s functions: Local self-energy approximation
  - Frequency domain winding number
  - (optional) Pole-expansion of self-energies
- Discussions

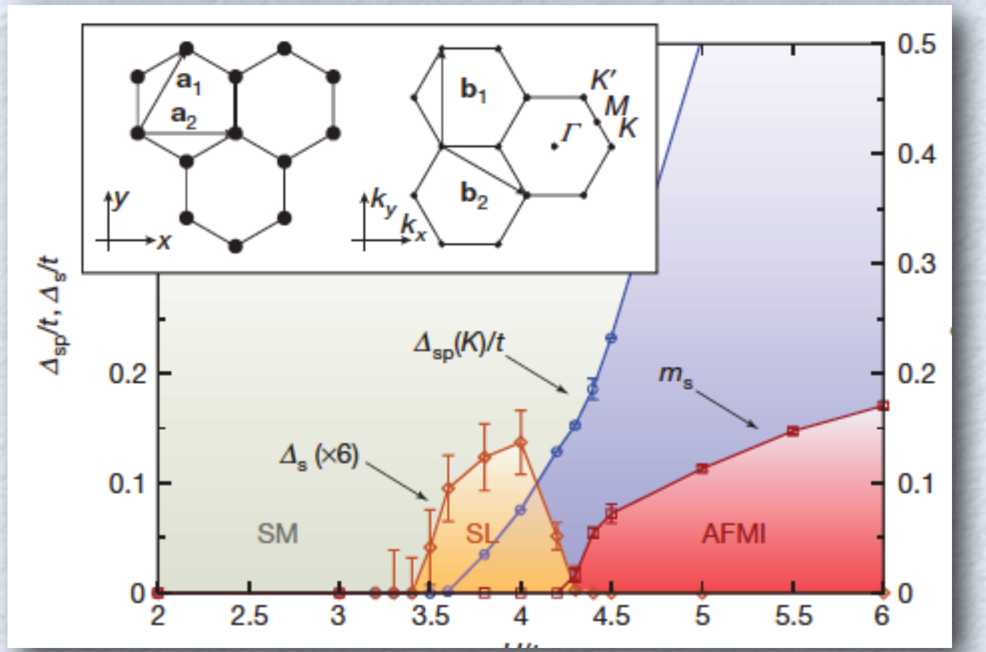
Kane-Mele-Hubbard model

$$H_0 = -t_1 \sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + it_2 \sum_{\langle\langle i,j\rangle\rangle,\sigma} \sigma \nu_{ij} c^{\dagger}_{i\sigma} c_{j\sigma}$$



$$H_1 = U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$$

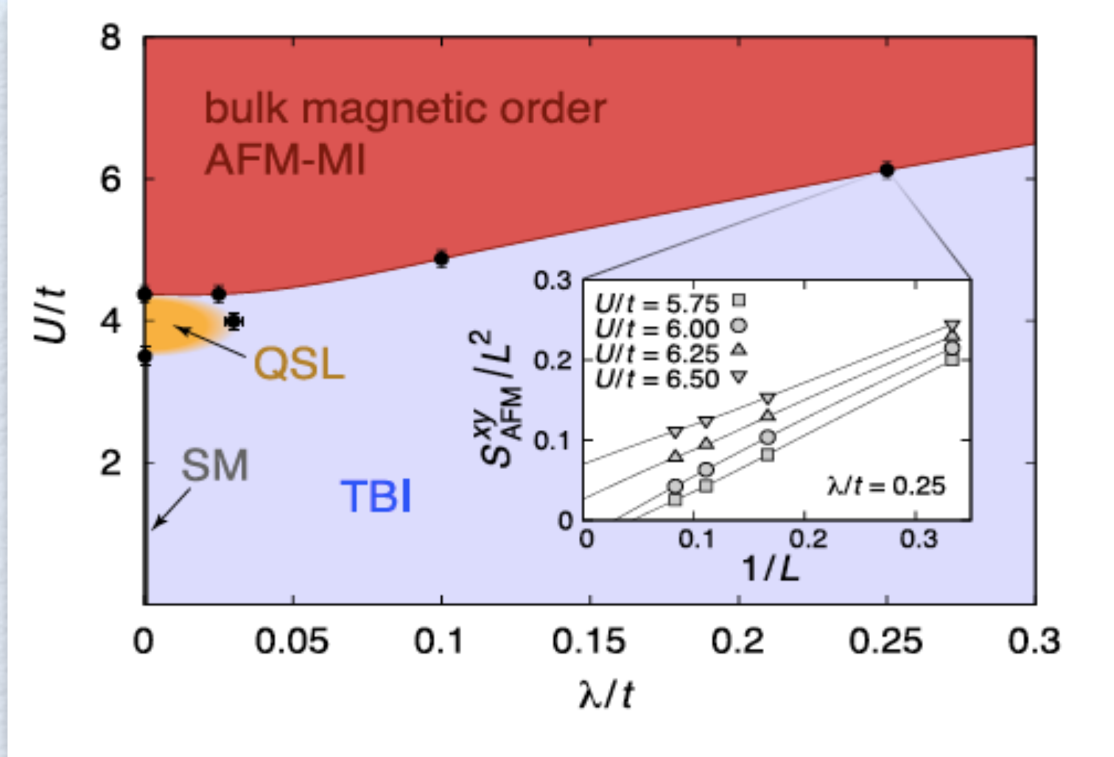
$$H = H_0 + H_1$$

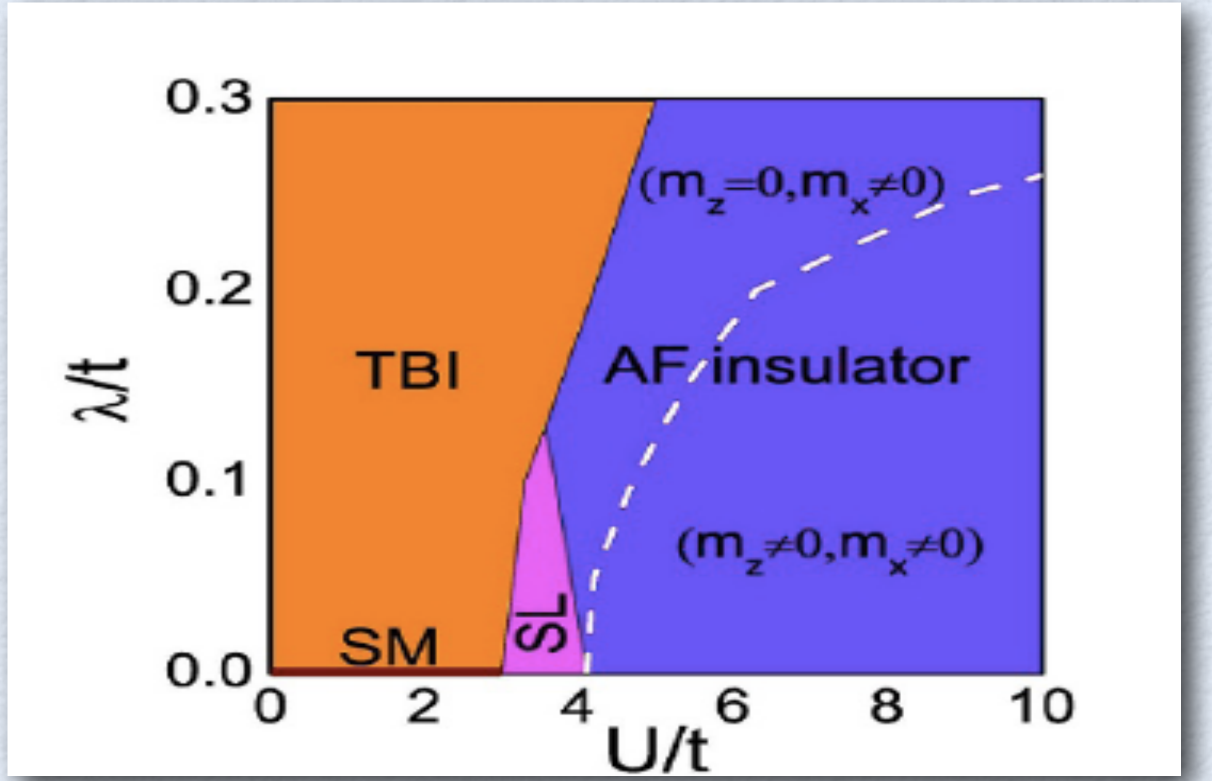


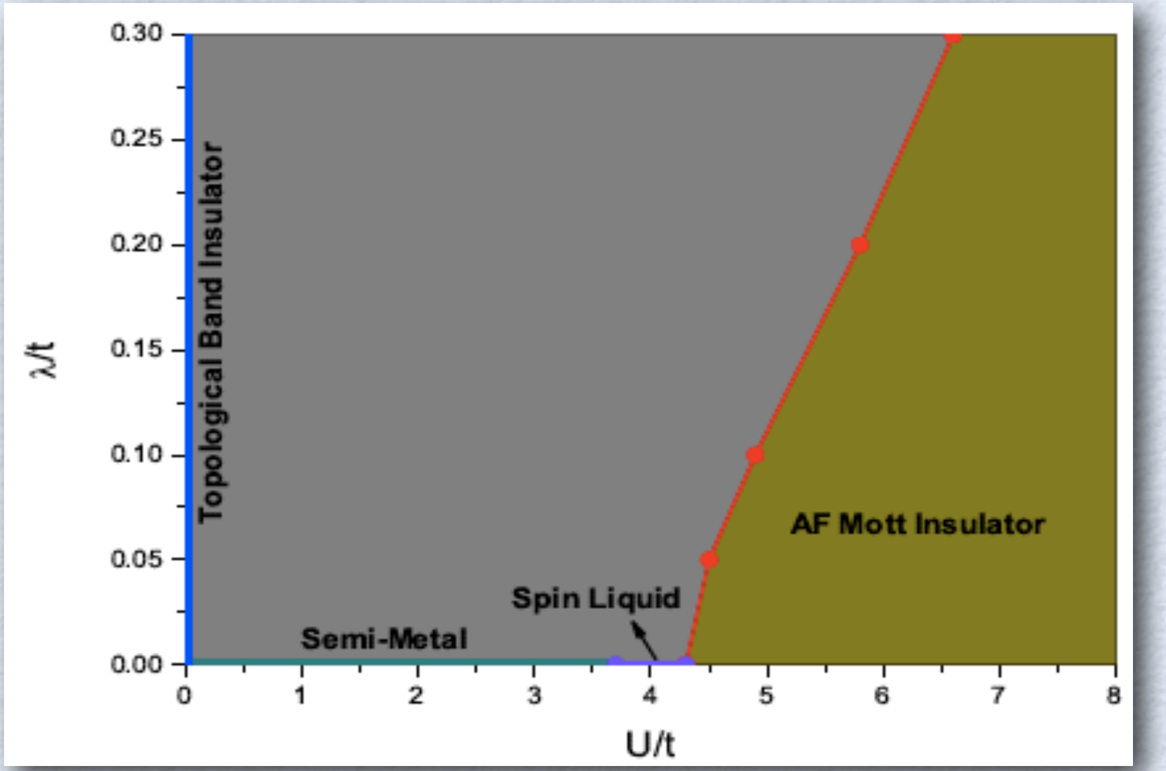
- Preserve PH & TR symmetry
- only t_1: Graphene model
- t_1 and t_2: Kane-Mele QSHE
- t_1 and U: Semimetal, spin liquid and AFI from small to large U

Phase diagrams

Hohenadler, Lang and Assaad, PRL, (2011)
Zheng,Wu and Zhang, Arxiv, (2010)
Yu, Xie and Li, PRL, (2011)





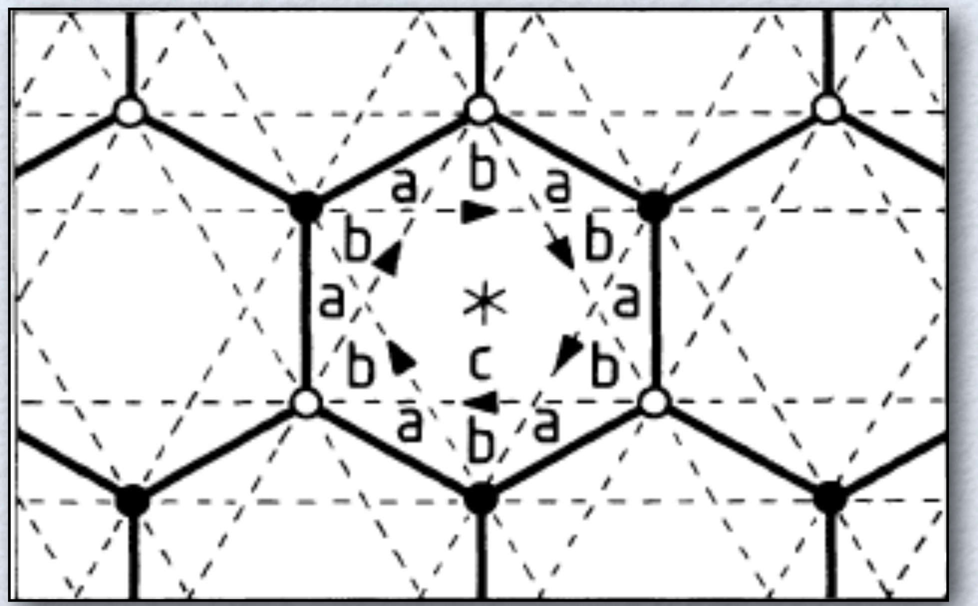


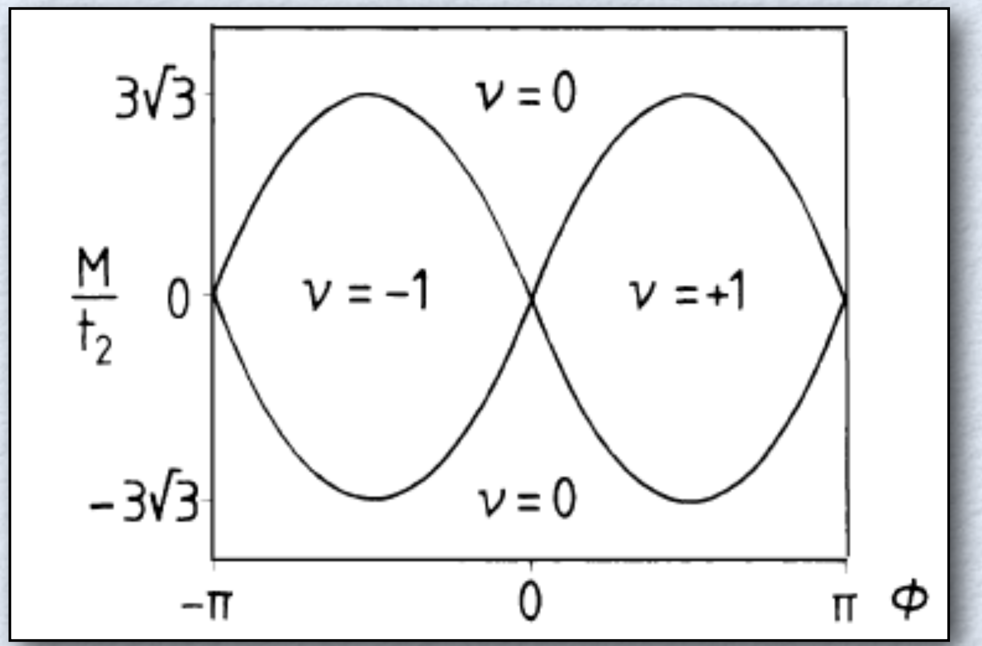
Interacting Haldane model

$$H_0 = -t_1 \sum_{\langle i,j \rangle} c_i^\dagger c_j + i t_2 \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} c_i^\dagger c_j$$

$$H_1 = V \sum_{\langle i,j \rangle} (n_i - \frac{1}{2})(n_j - \frac{1}{2})$$

$$H = H_0 + H_1$$





- Spinless: single copy of Kane-Mele model
- QHE without Landau levels
- Add staggered onsite energies: topological transition, Chern # changes, gap closes at phase boundary

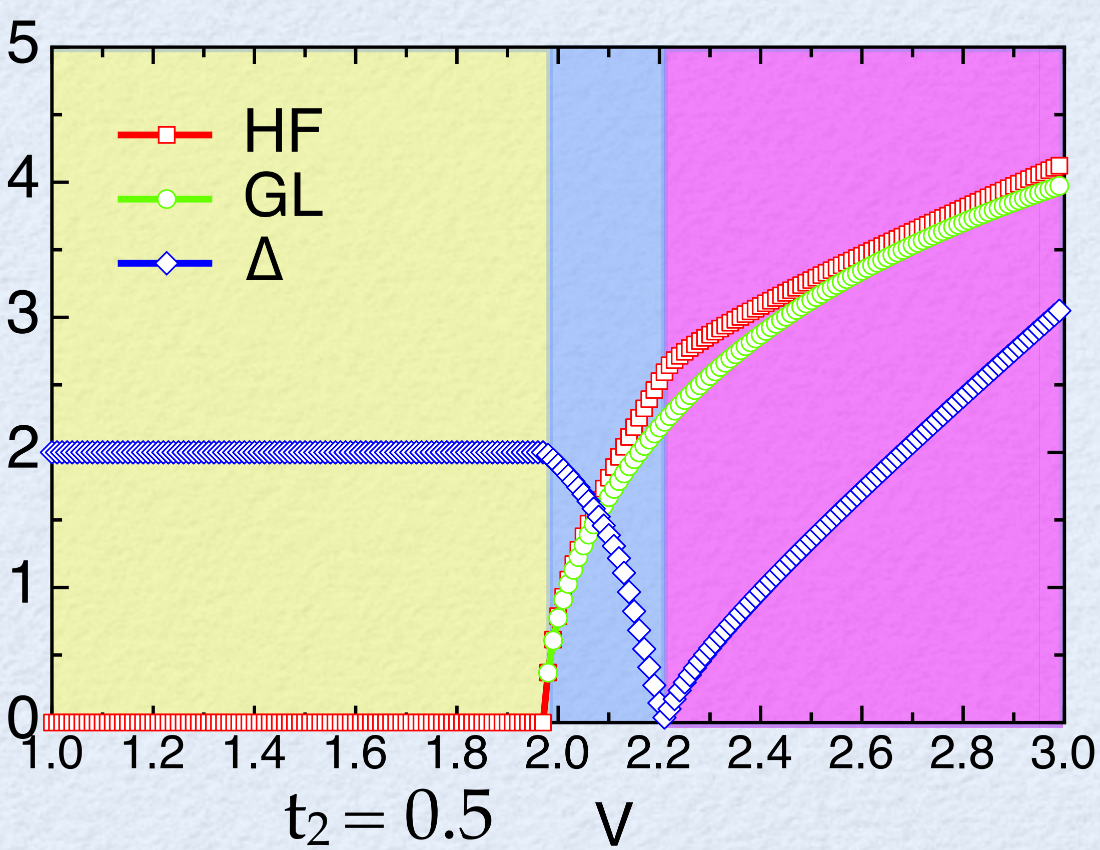
F. D. M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988)

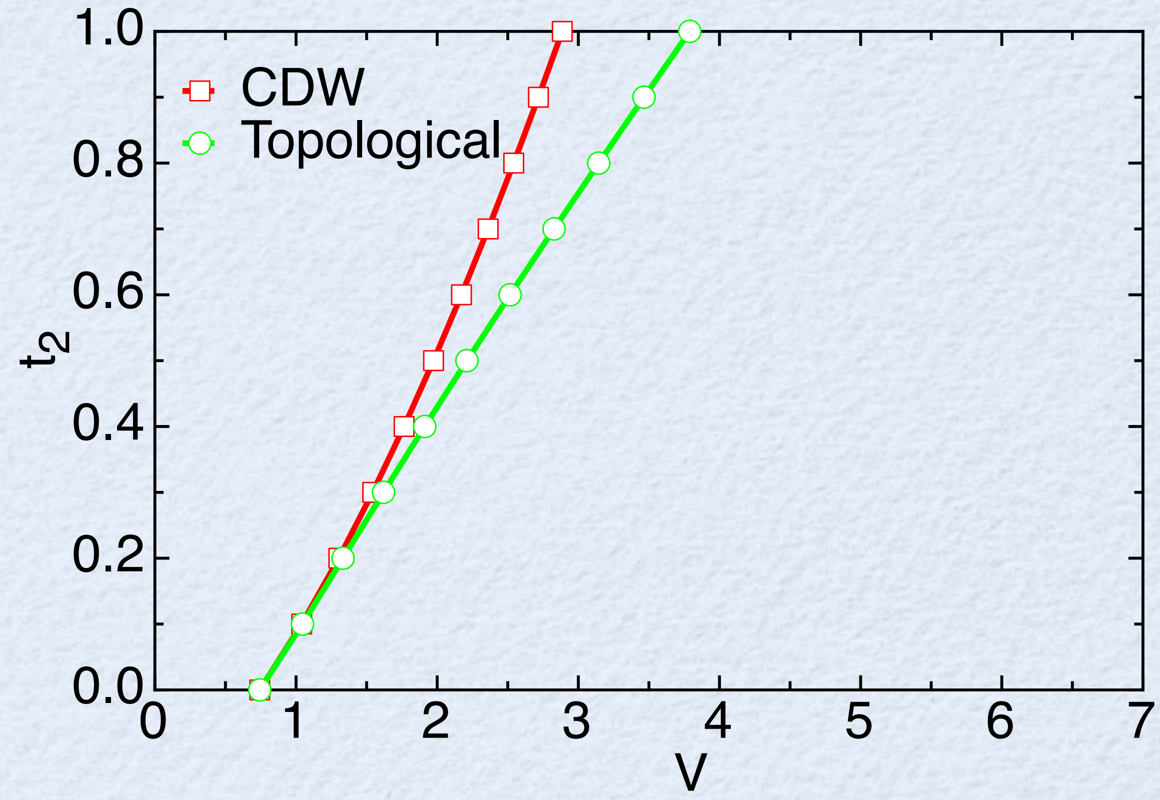
Mean-field phase diagram

$$V n_i n_j \to V\langle n_i\rangle n_j + V n_i \langle n_j\rangle \qquad \langle n_i\rangle = \frac{1}{2} + (-1)^{\eta_i}\phi$$

$$\to V\phi(n_i - n_j)$$

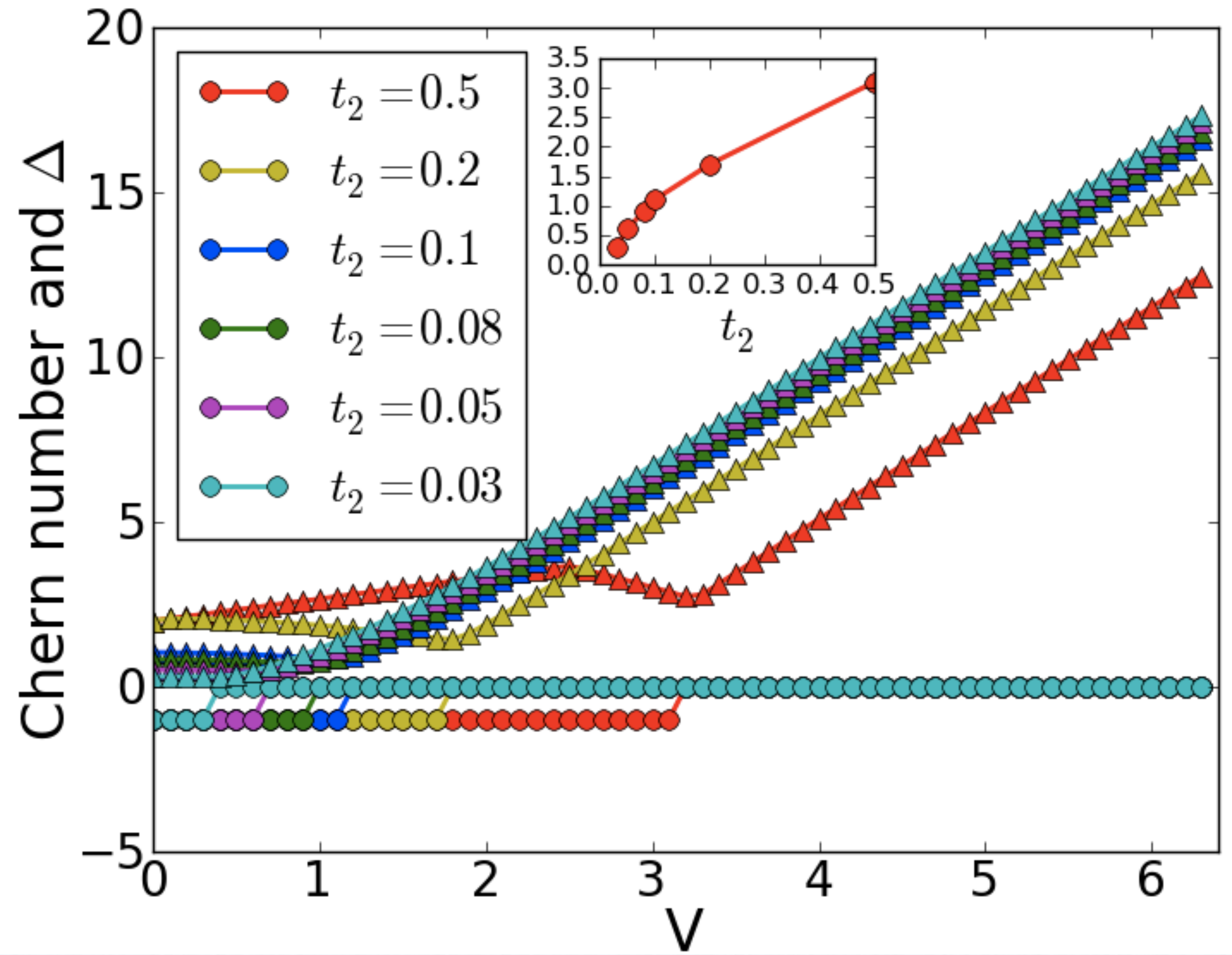
Interaction will generate the mass term and break the topological phase





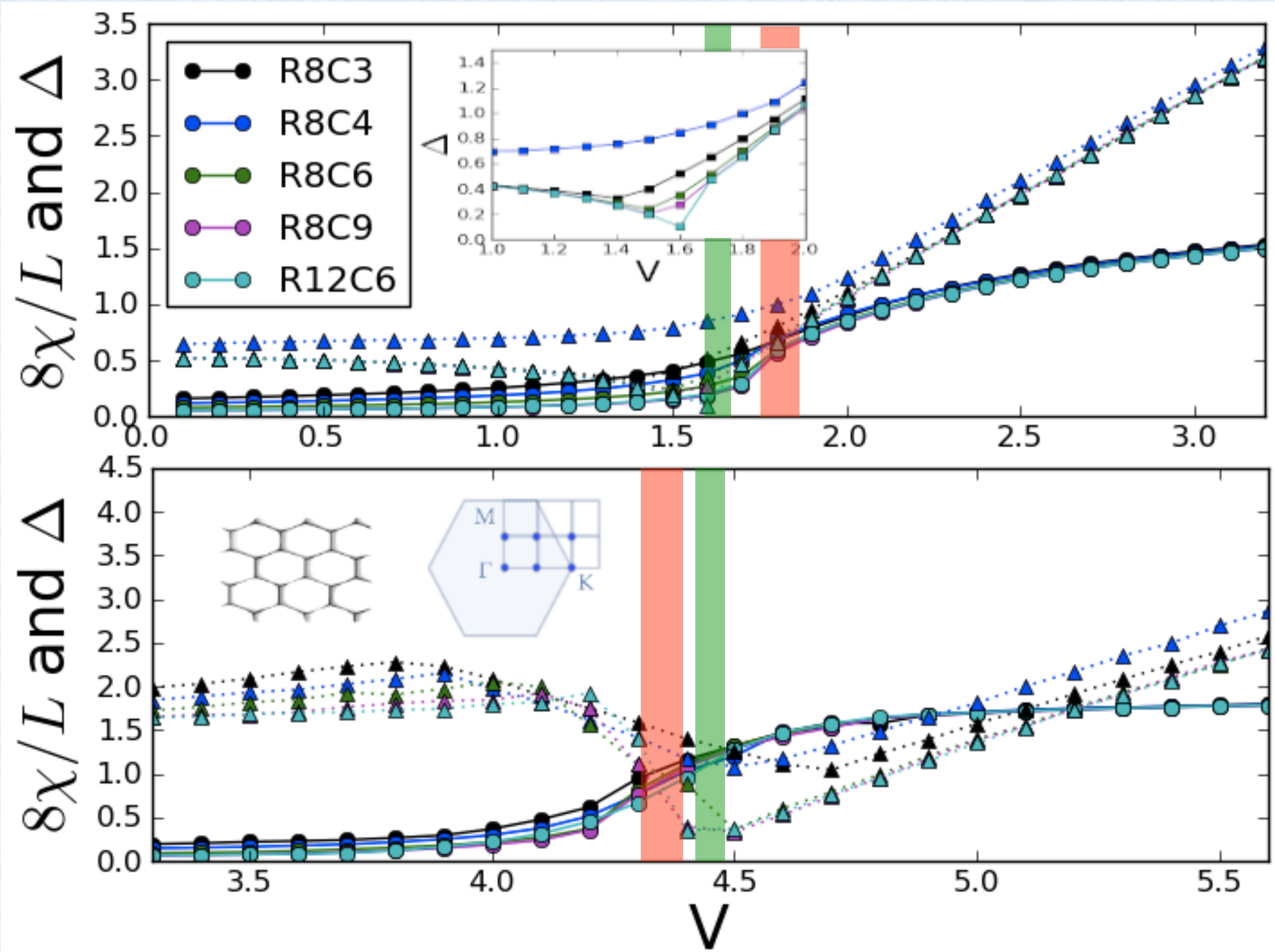
Chern number and Gap (ED)

$$C = \frac{i}{2\pi}\int\int d\theta_x d\theta_y [\langle\frac{\partial\Psi}{\partial\theta_x}|\frac{\partial\Psi}{\partial\theta_y}\rangle - \langle\frac{\partial\Psi}{\partial\theta_y}|\frac{\partial\Psi}{\partial\theta_x}\rangle]$$



- Topological transition point decreases with decreasing t_2
- CDW transition remains finite with vanishing t_2
- Topological transition occurs before CDW transition for small t_2
- Gap close links to the topological transition

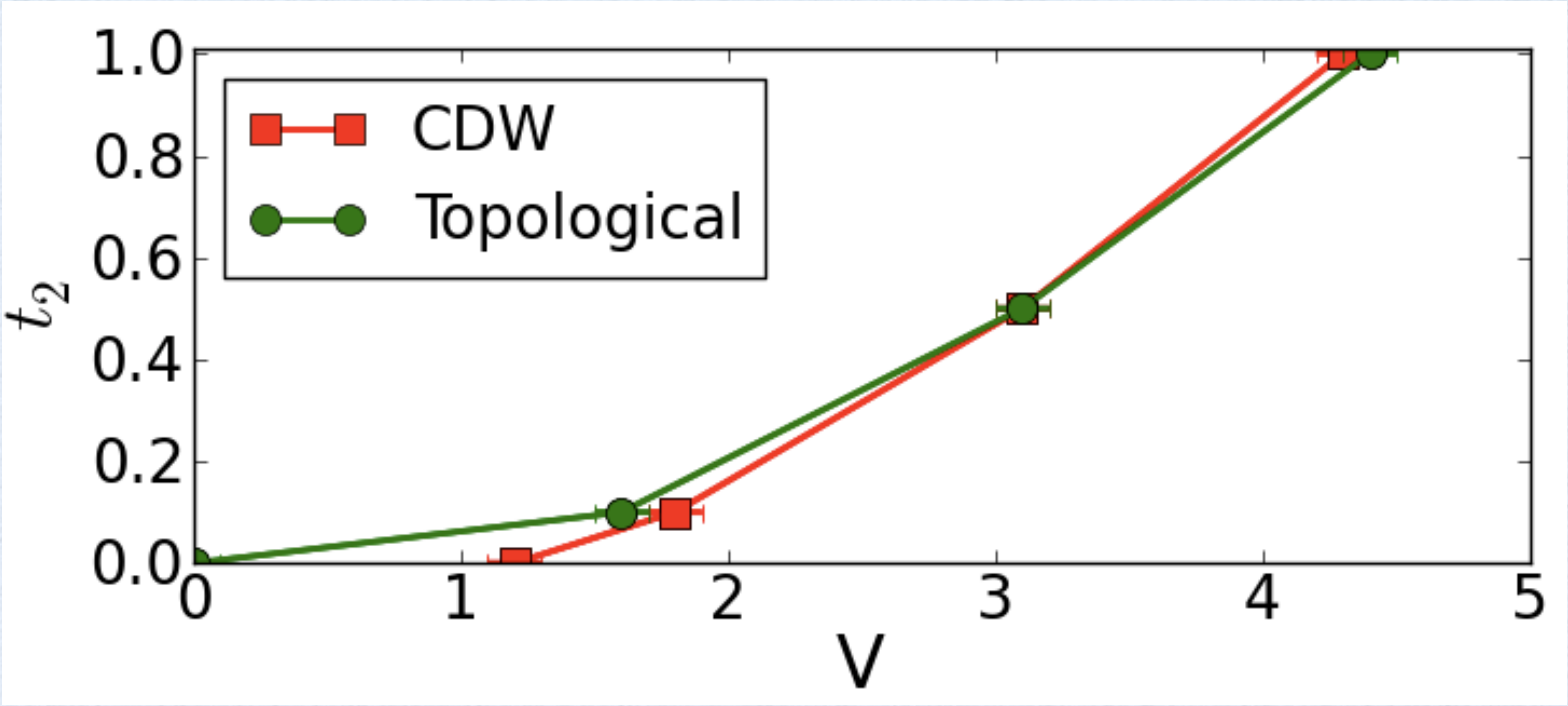
CDW structure factor and Gap (CPQMC)



$t_2 = 0.1$

$t_2 = 1.0$

Many-body phase diagram



- Studied the interplay of topological order and CDW long range order
- Mean-field picture: large CDW order destroys the topological phase
- Mean-body calculations: topological transition could occur before the CDW one

Summary on numerical findings

- Both uncover gapped featureless phase
- NO direct characterization: correlation functions, excitation gaps, edge currents, spectral functions ...
- Characterization beyond single particle basis:
  - Chern/Z_2 # with twisted boundary conditions
  - Entanglement entropy/spectrum
  - Topological indices expressed by Green's function

Ishikawa formula for 4D QHE

$$n = \frac{\varepsilon_{\mu\nu\rho\sigma\tau}}{15\pi^2} \mathrm{Tr} \int \frac{d^4k d\omega}{(2\pi)^5} G\partial_\mu G^{-1} G\partial_\nu G^{-1} G\partial_\rho G^{-1} G\partial_\sigma G^{-1} G\partial_\tau G^{-1}$$

- Appears as the coefficient of the Chern-Simons term. Describes Hall conductance physically.
- Mathematically: $\pi_5(GL(M, \mathbb{C})) = \mathbb{Z}$
- Single particle Green's function involved, taken into account the effect of interaction, disorder as well as finite temperature.

Ishikawa and Matsuyama, Z Phys C Part Fields, **33**, 41 (1986),
Ishikawa and Matsuyama, Nucl Phys B **280**, 523 (1987) ,
Qi, Hughes, and Zhang, PRB, **78**, 195424 (2008)

Noninteracting Case

$$H_{\mathbf{k}} = \sum_{a=1}^{5} h_{\mathbf{k}}^{a} \Gamma^{a} \qquad \hat{h}_{\mathbf{k}}^{a} \equiv h_{\mathbf{k}}^{a} / |h_{\mathbf{k}}|$$

$$G^{-1}(\omega, \mathbf{k}) = i\omega - H_{\mathbf{k}} \qquad \partial_{\omega} G^{-1} = i \qquad \partial_{k_i} G^{-1} = -\partial_{k_i} H_{\mathbf{k}}$$

$$n = \frac{\varepsilon_{\mu\nu\rho\sigma\tau}}{15\pi^2} \mathrm{Tr} \int \frac{d^4 k d\omega}{(2\pi)^5} G \partial_\mu G^{-1} G \partial_\nu G^{-1} G \partial_\rho G^{-1} G \partial_\sigma G^{-1} G \partial_\tau G^{-1}$$

$\Big\downarrow$ Integrated ω

$$n = \frac{3}{8\pi^2} \int_{\mathrm{BZ}} \mathrm{d}^4 k \, \varepsilon_{abcde} \hat{h}_{\mathbf{k}}^{a} \partial_{k_x} \hat{h}_{\mathbf{k}}^{b} \partial_{k_y} \hat{h}_{\mathbf{k}}^{c} \partial_{k_z} \hat{h}_{\mathbf{k}}^{d} \partial_{k_\lambda} \hat{h}_{\mathbf{k}}^{e}$$

4D TKNN formula

Interacting Case: Mean-field self-energy

$$G^{-1}(\omega, \mathbf{k}) = i\omega - H_{\mathbf{k}} - \Sigma(\omega, \mathbf{k})$$

Raghu, Qi, Honerkamp, and Zhang, PRL (2008) Li, Chu, Jain, and Shen, PRL (2009)
Dzero, Sun, Galitski, and Coleman, PRL (2010) Groth, Wimmer, Akhmerov, and Beenakker, PRL (2009)

Interacting Case: Mean-field self-energy

$$G^{-1}(\omega, \mathbf{k}) = i\omega - H_{\mathbf{k}} - \Sigma(\cancel{\omega}, \mathbf{k}) = i\omega - \tilde{H}_{\mathbf{k}}$$

Raghu, Qi, Honerkamp, and Zhang, PRL (2008)
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Groth, Wimmer, Akhmerov, and Beenakker, PRL (2009)

Interacting Case: Mean-field self-energy

$$G^{-1}(\omega, \mathbf{k}) = i\omega - H_{\mathbf{k}} - \Sigma(\cancel{\omega}, \mathbf{k}) = i\omega - \tilde{H}_{\mathbf{k}}$$

- Topological “Mott” insulator: mean-field bond-order wave states
- Topological “Kondo” insulator: renormalized-hybridization Hamiltonian
- Topological “Anderson” insulator: self-consistent Born approximation

Raghu, Qi, Honerkamp, and Zhang, PRL (2008)
Dzero, Sun, Galitski, and Coleman, PRL (2010)
Li, Chu, Jain, and Shen, PRL (2009)
Groth, Wimmer, Akhmerov, and Beenakker, PRL (2009)

Interacting Case: Local self-energy approximation

$$G^{-1}(\omega, \mathbf{k}) = i\omega - H_{\mathbf{k}} - \Sigma(\omega, \mathbf{k}) \approx i\omega - H_{\mathbf{k}} - \Sigma(\omega)$$

$$\boxed{\Sigma(\omega, \mathbf{k}) \approx \Sigma(\omega)}$$

Interacting Case: Local self-energy approximation

$$G^{-1}(\omega, \mathbf{k}) = i\omega - H_{\mathbf{k}} - \Sigma(\omega, \mathbf{k}) \approx i\omega - H_{\mathbf{k}} - \Sigma(\omega)$$

$$\equiv G^{-1}_{\mathrm{atom}}(\omega) - H_{\mathbf{k}}$$

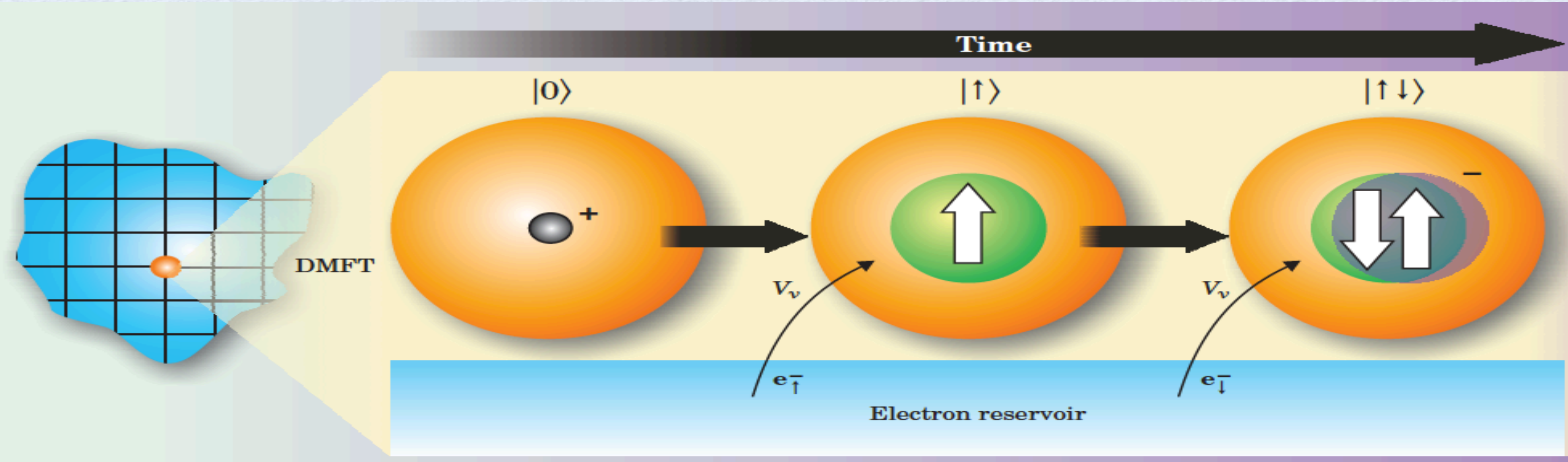
$$\boxed{\Sigma(\omega, \mathbf{k}) \approx \Sigma(\omega)}$$

Interacting Case: Local self-energy approximation

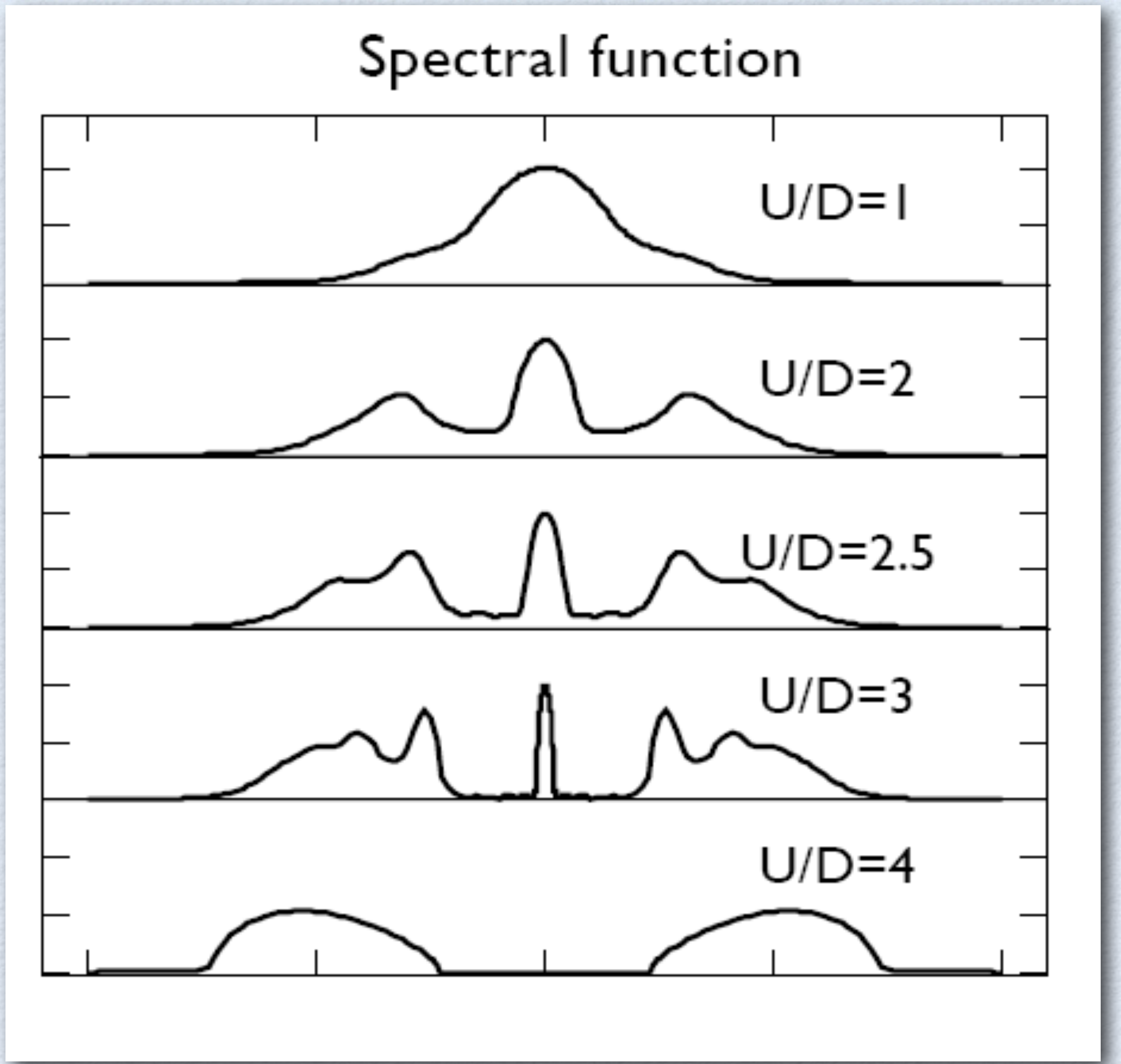
$$G^{-1}(\omega,\mathbf{k}) = i\omega - H_{\mathbf{k}} - \Sigma(\omega,\mathbf{k}) \approx \boxed{i\omega} - H_{\mathbf{k}} \boxed{-\Sigma(\omega)}$$

$$\equiv \boxed{G^{-1}_{\mathrm{atom}}(\omega)} - H_{\mathbf{k}}$$

$$\boxed{\Sigma(\omega,\mathbf{k}) \approx \Sigma(\omega)}$$



Metal-Insulator transition



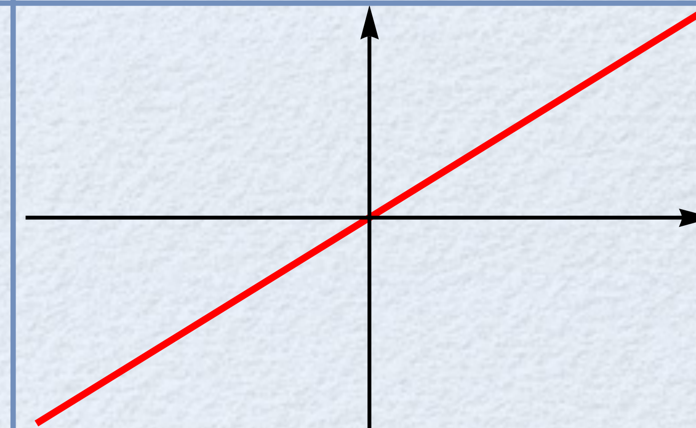
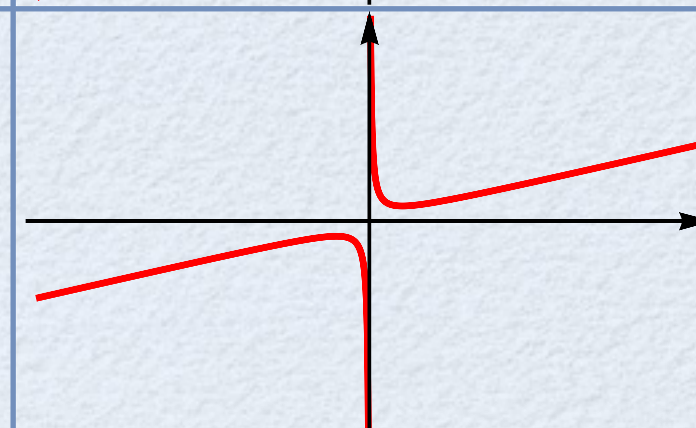
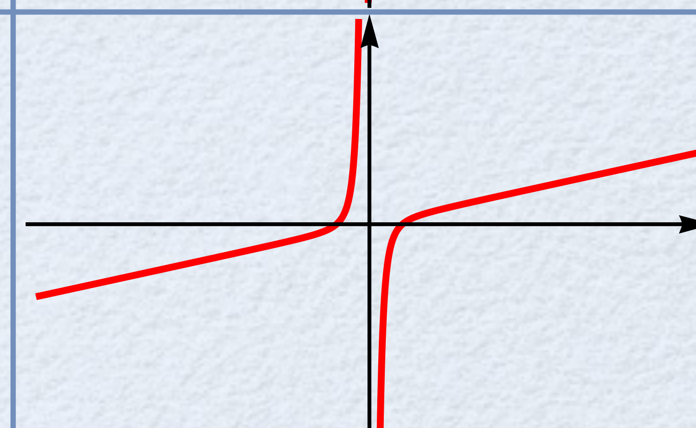
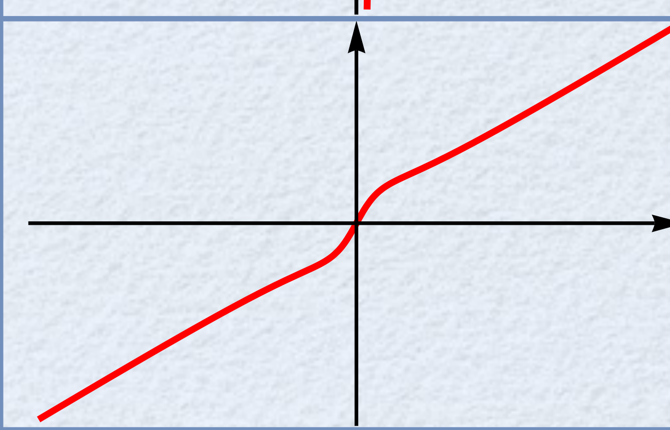
$$\Sigma(\omega) \sim \frac{1}{i\omega - P} + \frac{1}{i\omega + P}$$

$$\Sigma(\omega) \sim \frac{1}{i\omega}$$

Self-energy vs. Chern number

- Set $H_{\mathbf{k}}$ to QH state with TKNN number equals to 1
- Set several trial forms of the self-energy
- Finish the frequency-momentum integration, see what happens to n.

$\Sigma(\omega)$	n
0	1
$\dfrac{1}{i\omega}$	0
$\dfrac{1}{(i\omega)^3}$	2
$\dfrac{1}{i\omega-1}+\dfrac{1}{i\omega+1}$	1

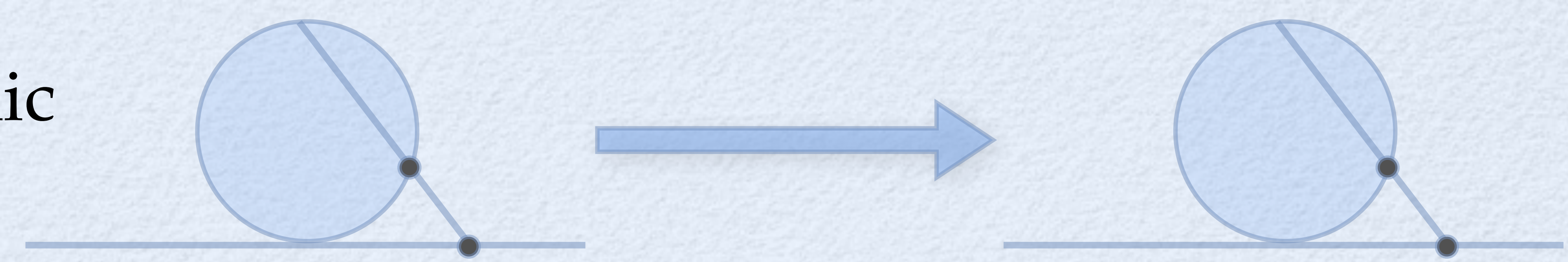
$\Sigma(\omega)$	n	$\Im G_{\text{atom}}^{-1}(\omega) = \omega - \Im\Sigma(\omega)$	$\Im G_{\text{atom}}^{-1}(\omega)$
0	1	ω	
$\dfrac{1}{i\omega}$	0	$\omega + \dfrac{1}{\omega}$	
$\dfrac{1}{(i\omega)^3}$	2	$\omega - \dfrac{1}{\omega^3}$	
$\dfrac{1}{i\omega - 1} + \dfrac{1}{i\omega + 1}$	1	$\omega + \dfrac{2\omega}{\omega^2 + 1}$	

Conjecture

Interacting Chern number = $\deg\{\Im G_{\text{atom}}^{-1}\} \times \text{TKNN}$

$$\Im G_{\text{atom}}^{-1} = \omega - \Im\Sigma(\omega) : \mathbb{R} \mapsto \mathbb{R}$$

Stereographic projection



Proof

$$H_{\mathbf{k}} = \sum_{a=1}^{5} h_{\mathbf{k}}^{a} \Gamma^{a} \qquad \hat{h}_{\mathbf{k}}^{a} \equiv h_{\mathbf{k}}^{a}/|h_{\mathbf{k}}|$$

$$G^{-1} = G_{\text{atom}}^{-1} - h_{\mathbf{k}}^{a}\Gamma^{a} \quad \partial_\omega G^{-1} = \partial_\omega G_{\text{atom}}^{-1} \quad \partial_{k_i} G^{-1} = -\partial_{k_i} H_{\mathbf{k}}$$

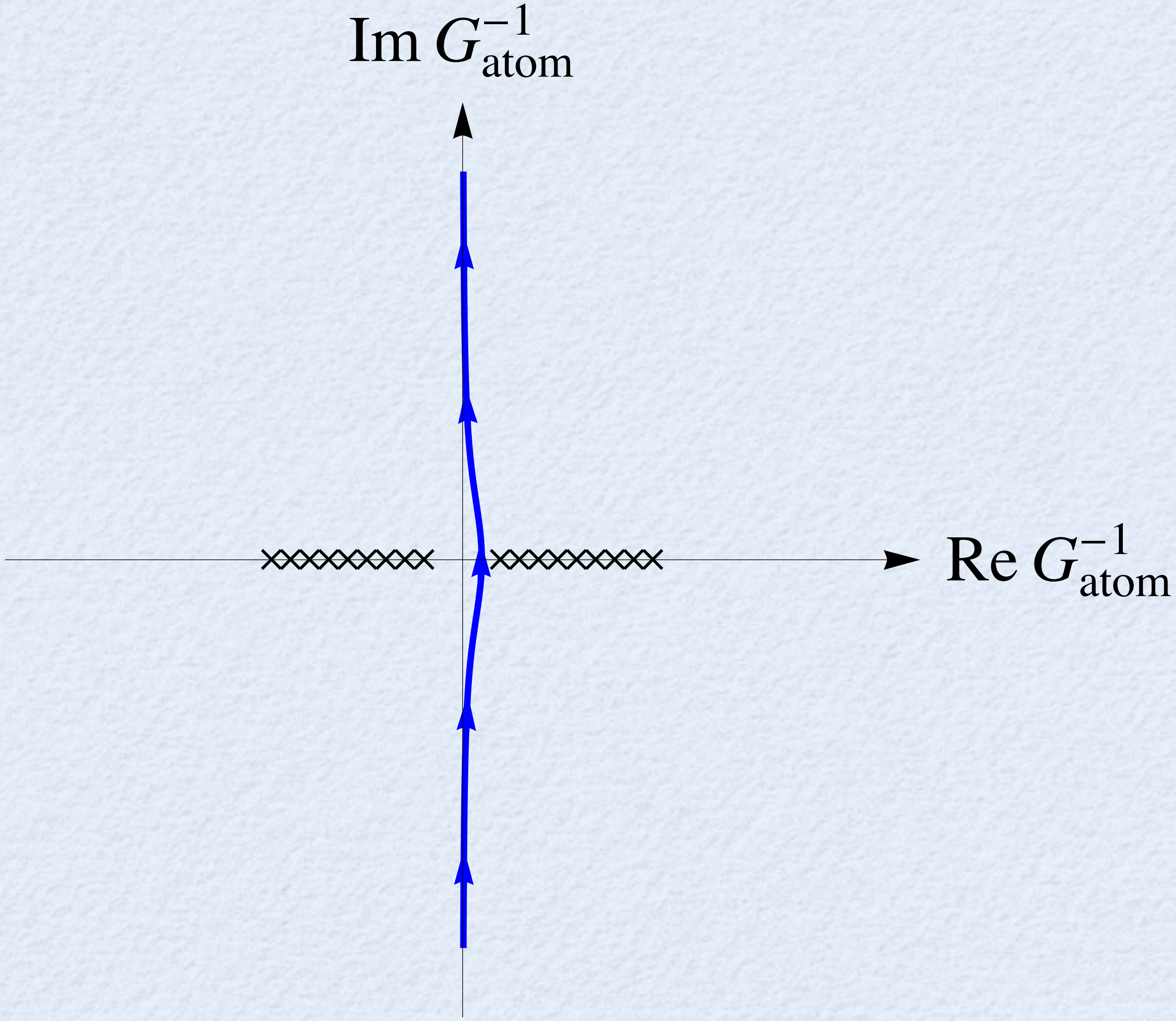
$$n = \frac{\varepsilon_{\mu\nu\rho\sigma\tau}}{15\pi^2} \mathrm{Tr} \int \frac{d^4 k d\omega}{(2\pi)^5} G\partial_\mu G^{-1} G\partial_\nu G^{-1} G\partial_\rho G^{-1} G\partial_\sigma G^{-1} G\partial_\tau G^{-1}$$

Separate integrations

$$n = \frac{2}{\pi^2} \int_{\mathrm{BZ}} \mathrm{d}^4 k \boxed{\int \frac{\mathrm{d}\omega}{2\pi i} \frac{\partial_\omega G_{\text{atom}}^{-1}}{(G_{\text{atom}}^{-2} - |h_{\mathbf{k}}|^2)^3}} \varepsilon_{abcde} h_{\mathbf{k}}^{a} \partial_{k_x} h_{\mathbf{k}}^{b} \partial_{k_y} h_{\mathbf{k}}^{c} \partial_{k_z} h_{\mathbf{k}}^{d} \partial_{k_\lambda} h_{\mathbf{k}}^{e}$$

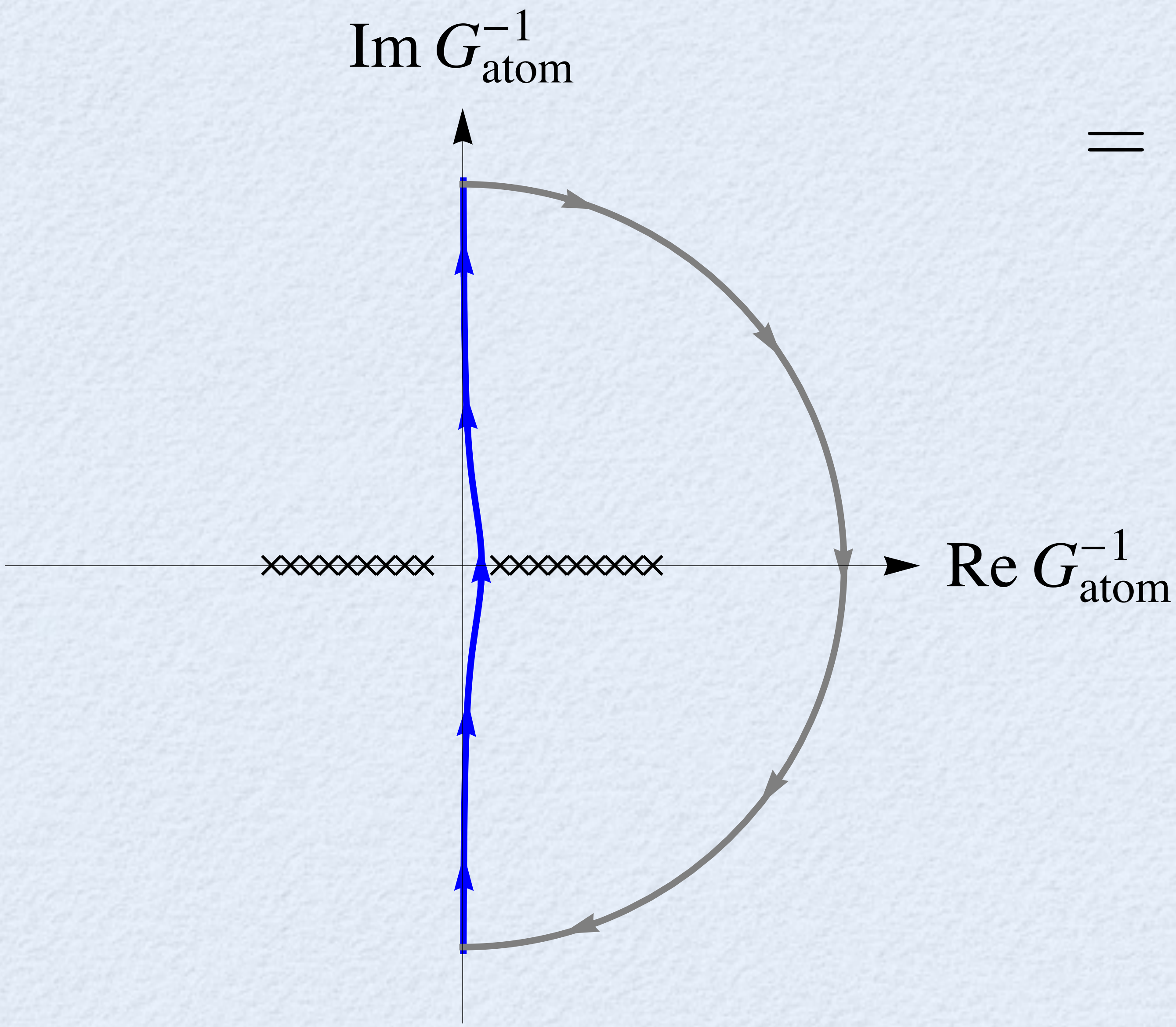
Proof (cont.)

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi i} \frac{\partial_\omega G_{\mathrm{atom}}^{-1}}{(G_{\mathrm{atom}}^{-2} - |h_{\mathbf{k}}|^2)^3} = \int_{z(-\infty)}^{z(\infty)} \frac{\mathrm{d}z}{2\pi i} \frac{1}{(z^2 - |h_{\mathbf{k}}|^2)^3}$$



Proof (cont.)

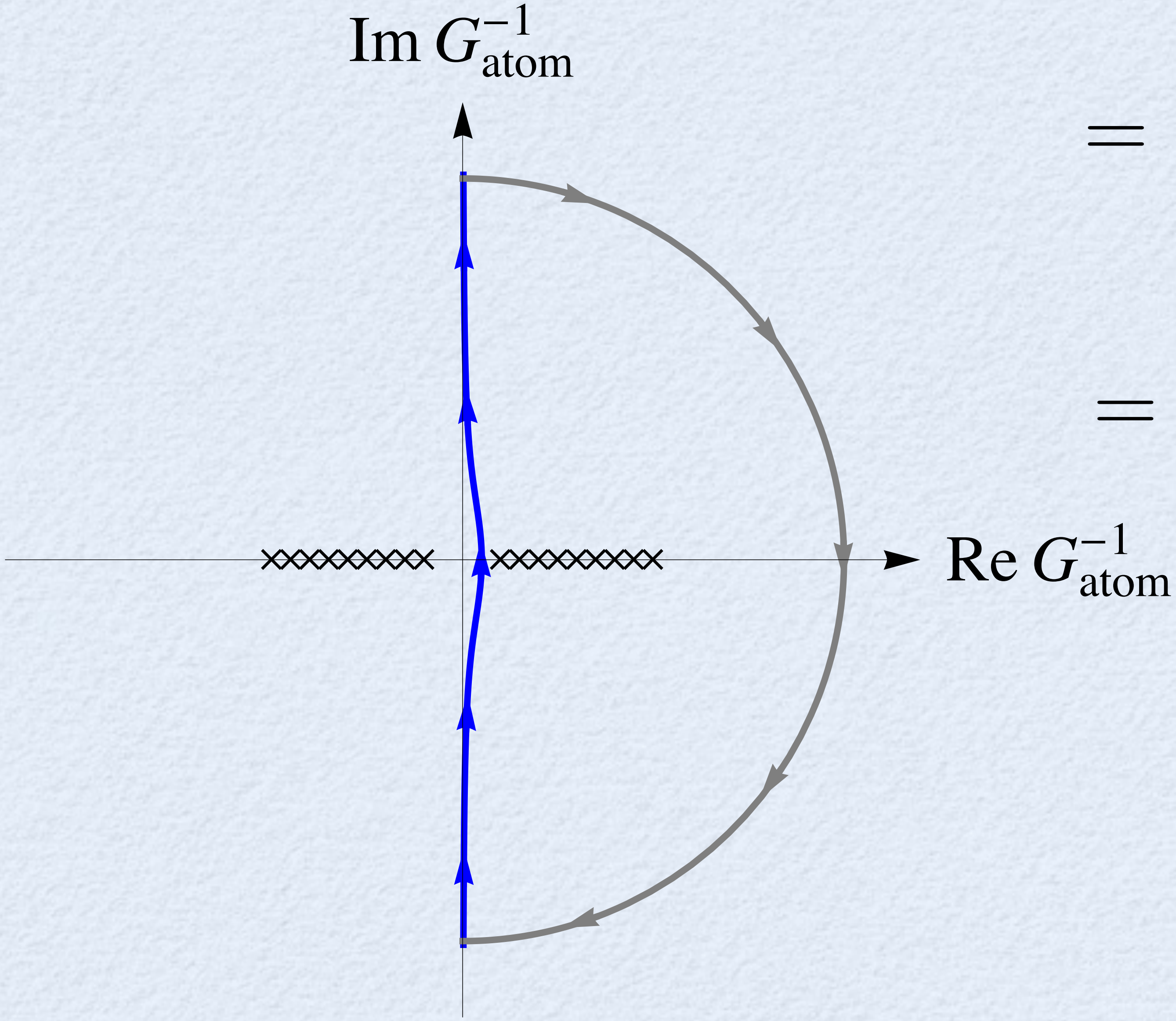
$$\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi i} \frac{\partial_\omega G_{\mathrm{atom}}^{-1}}{(G_{\mathrm{atom}}^{-2} - |h_{\mathbf{k}}|^2)^3} = \int_{z(-\infty)}^{z(\infty)} \frac{\mathrm{d}z}{2\pi i} \frac{1}{(z^2 - |h_{\mathbf{k}}|^2)^3}$$



$$= \oint_{\mathcal{C}} \frac{\mathrm{d}z}{2\pi i} \frac{1}{(z^2 - |h_{\mathbf{k}}|^2)^3}$$

Proof (cont.)

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi i} \frac{\partial_\omega G_{\mathrm{atom}}^{-1}}{(G_{\mathrm{atom}}^{-2} - |h_{\mathbf{k}}|^2)^3} = \int_{z(-\infty)}^{z(\infty)} \frac{\mathrm{d}z}{2\pi i} \frac{1}{(z^2 - |h_{\mathbf{k}}|^2)^3}$$



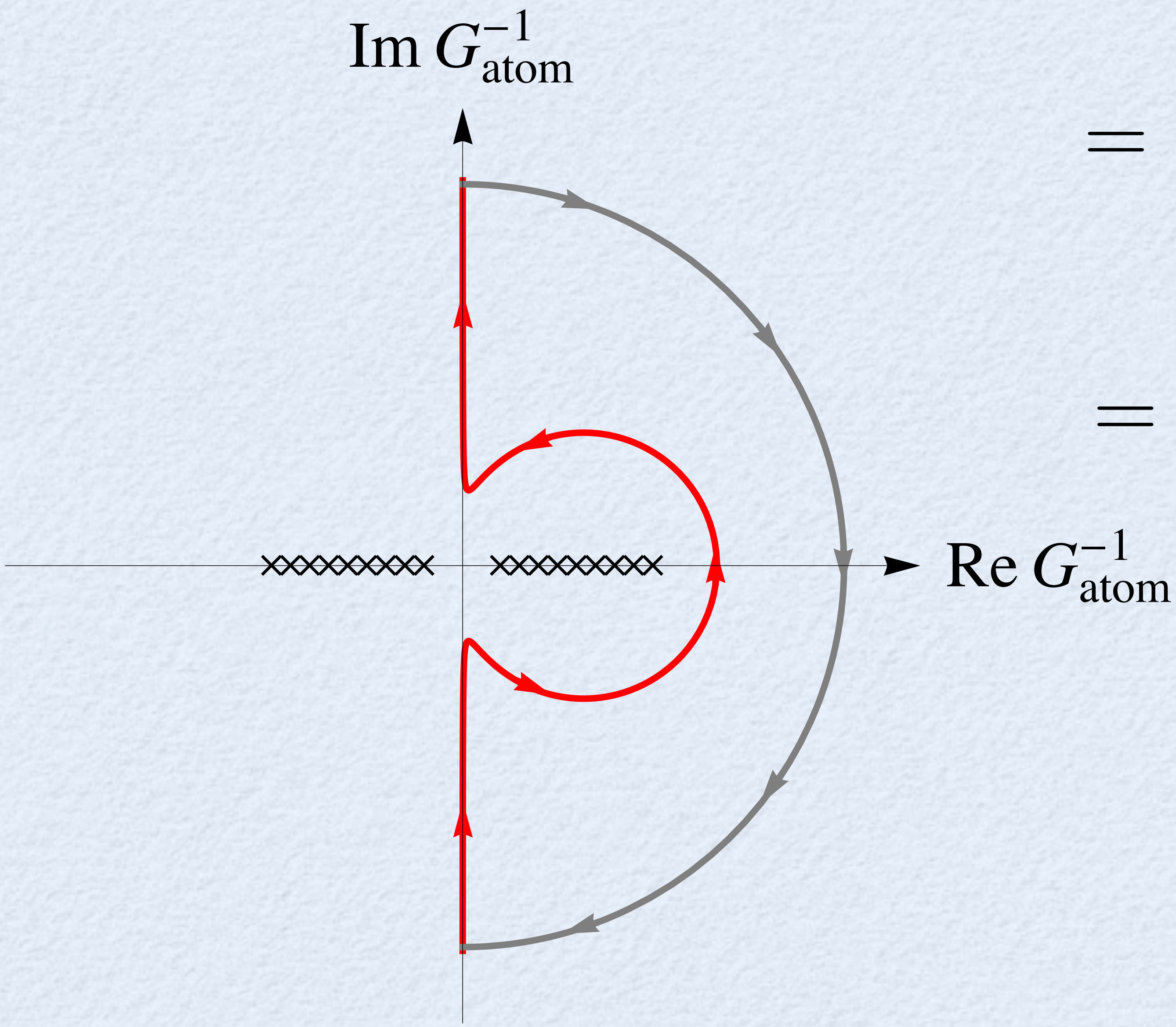
$$= \oint_{\mathcal{C}} \frac{\mathrm{d}z}{2\pi i} \frac{1}{(z^2 - |h_{\mathbf{k}}|^2)^3}$$

$$= \frac{3}{16|h_{\mathbf{k}}|^5}\gamma$$

γ = # left - # right

Proof (cont.)

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi i} \frac{\partial_\omega G_{\mathrm{atom}}^{-1}}{(G_{\mathrm{atom}}^{-2} - |h_{\mathbf{k}}|^2)^3} = \int_{z(-\infty)}^{z(\infty)} \frac{\mathrm{d}z}{2\pi i} \frac{1}{(z^2 - |h_{\mathbf{k}}|^2)^3}$$



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Proof (cont.)

$$n = \frac{2}{\pi^2}\int_{\mathrm{BZ}} \mathrm{d}^4k \boxed{\int \frac{\mathrm{d}\omega}{2\pi i}\frac{\partial_\omega G_{\mathrm{atom}}^{-1}}{(G_{\mathrm{atom}}^{-2} - |h_{\mathbf{k}}|^2)^3}} \varepsilon_{abcde} h_{\mathbf{k}}^a \partial_{k_x} h_{\mathbf{k}}^b \partial_{k_y} h_{\mathbf{k}}^c \partial_{k_z} h_{\mathbf{k}}^d \partial_{k_\lambda} h_{\mathbf{k}}^e$$

$$\Downarrow$$

$$n = \gamma \times \frac{3}{8\pi^2}\int_{\mathrm{BZ}} d^4k \varepsilon_{abcde} \hat{h}_{\mathbf{k}}^a \partial_{k_x} \hat{h}_{\mathbf{k}}^b \partial_{k_y} \hat{h}_{\mathbf{k}}^c \partial_{k_z} \hat{h}_{\mathbf{k}}^d \partial_{k_\lambda} \hat{h}_{\mathbf{k}}^e$$

Interacting Chern number = FDWN $\times$ TKNN

3D TI: dimension reduction

$$H_{\mathbf{k}} + k_\lambda \Gamma^4 \to H_{\mathbf{k}}$$

$$n = \frac{\varepsilon_{\mu\nu\rho\sigma\tau}}{15\pi^2} \mathrm{Tr} \int_{\mathrm{BZ}} \frac{\mathrm{d}^3 k}{(2\pi)^3} \boxed{\int_0^\infty \frac{dk_\lambda}{2\pi}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} G\partial_\mu G^{-1} G \partial_\nu G^{-1} \ldots$$

$$= \gamma \times \frac{1}{8\pi^2} \int_{\mathrm{BZ}} \mathrm{d}^3 k \frac{2|h_{\mathbf{k}}| + h^4_{\mathbf{k}}}{(|h_{\mathbf{k}}| + h^4_{\mathbf{k}})^2 |h_{\mathbf{k}}|^3} \varepsilon_{abcd} h^a_{\mathbf{k}} \partial_{k_x} h^b_{\mathbf{k}} \partial_{k_y} h^c_{\mathbf{k}} \partial_{k_z} h^d_{\mathbf{k}}$$

Interacting Z_2 = FDWN $\times Z_2$

Qi, Hughes, Zhang, PRB (2008), Wang, Qi, Zhang, PRL (2010), Li, Wang, Qi, Zhang, NatPhys (2010)

3D TI: dimension reduction

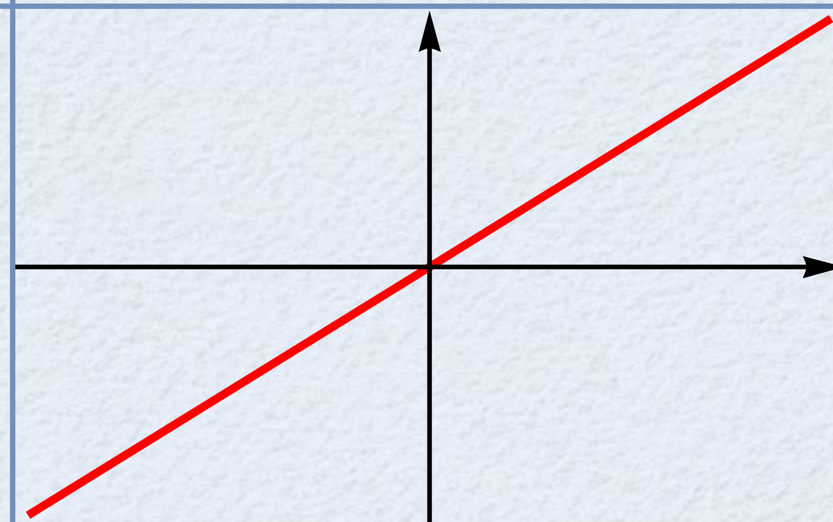
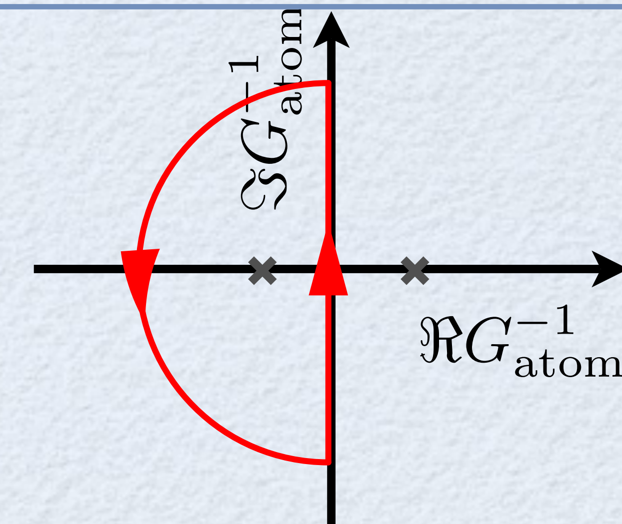
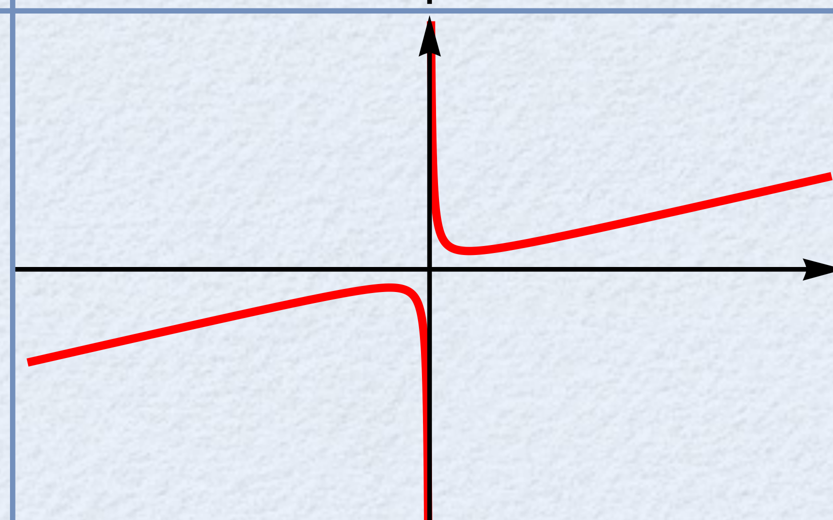
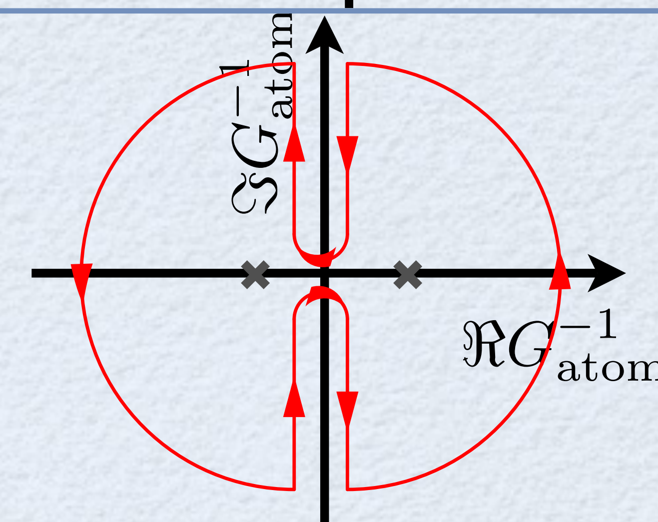
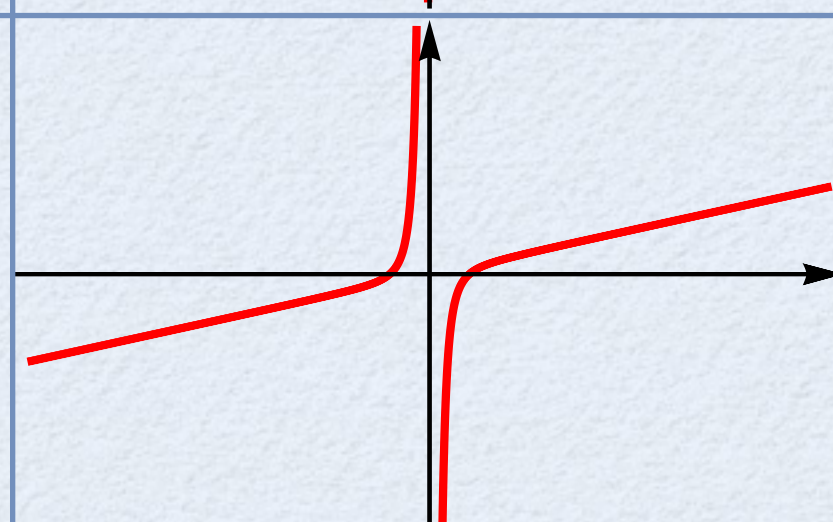
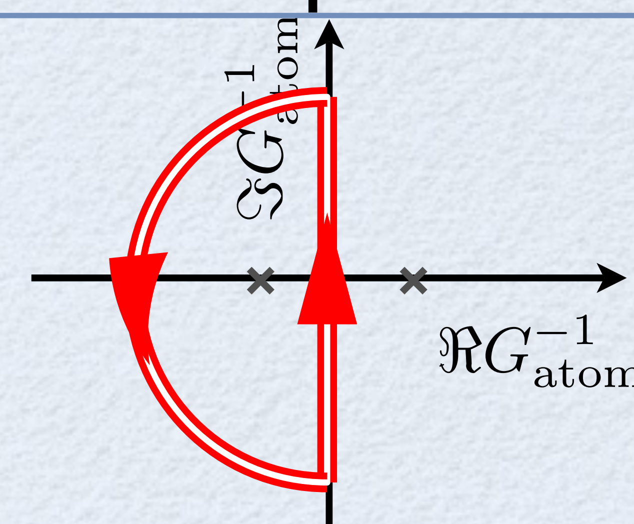
$$H_{\mathbf{k}} + k_\lambda \Gamma^4 \to H_{\mathbf{k}}$$

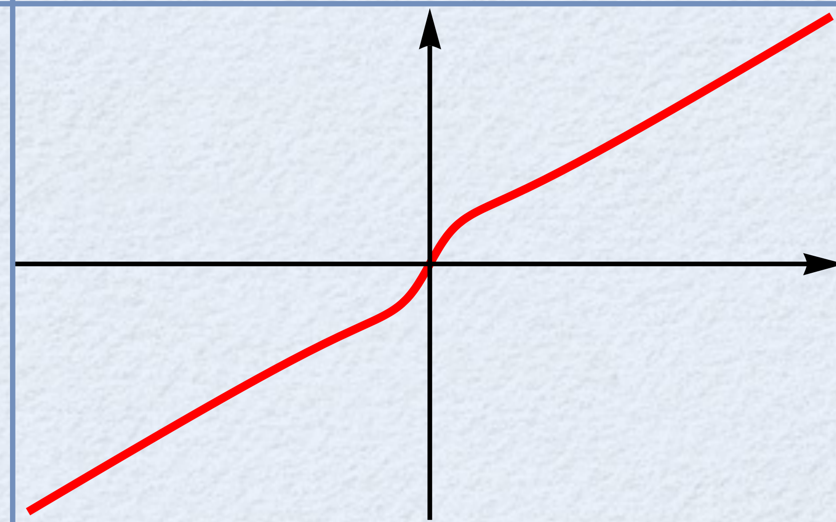
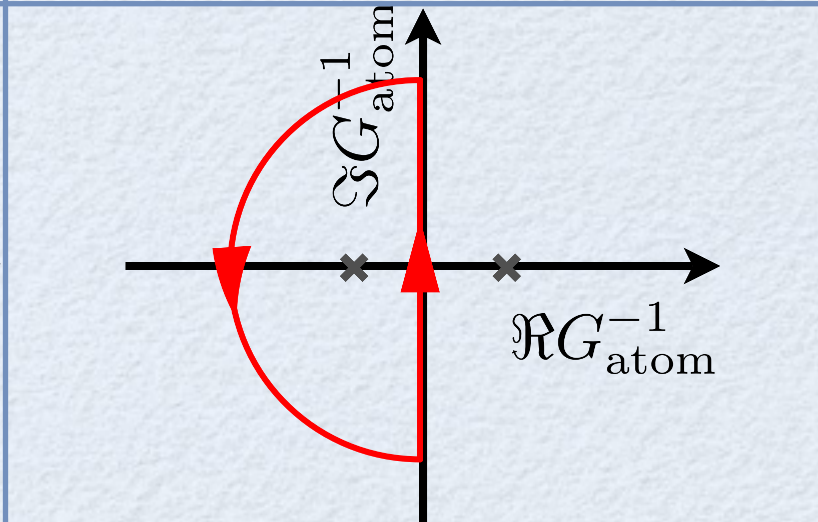
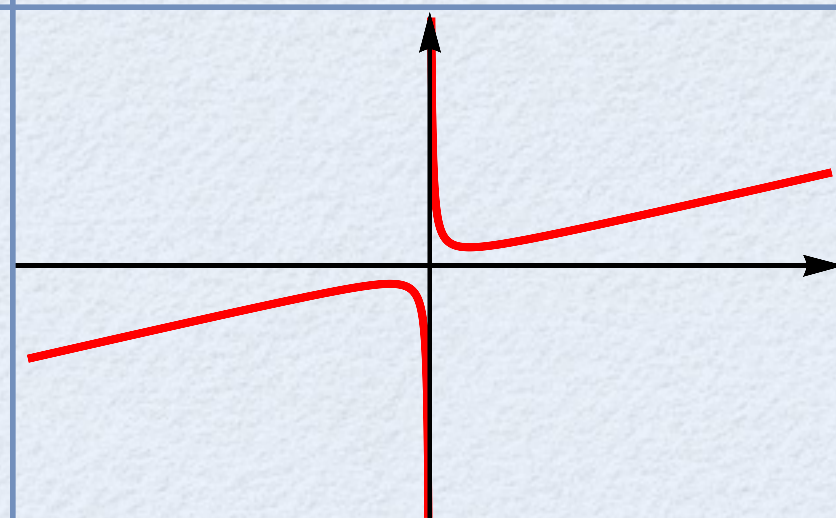
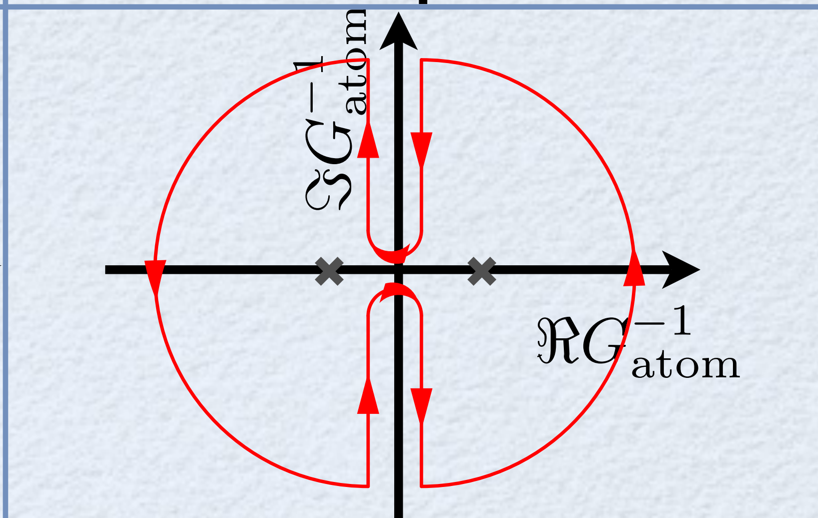
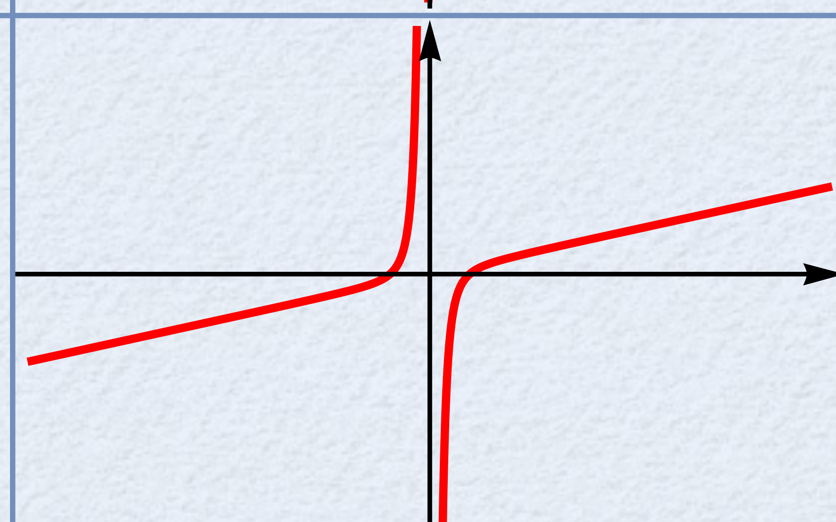
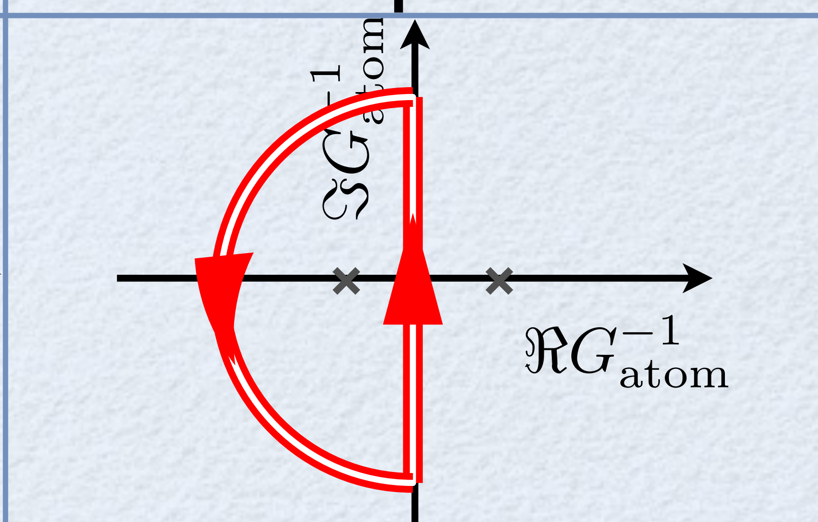
$$n = \frac{\varepsilon_{\mu\nu\rho\sigma\tau}}{15\pi^2} \mathrm{Tr} \int_{\mathrm{BZ}} \frac{\mathrm{d}^3 k}{(2\pi)^3} \int_0^\infty \frac{dk_\lambda}{2\pi} \boxed{\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}} G\partial_\mu G^{-1} G\partial_\nu G^{-1} \ldots$$

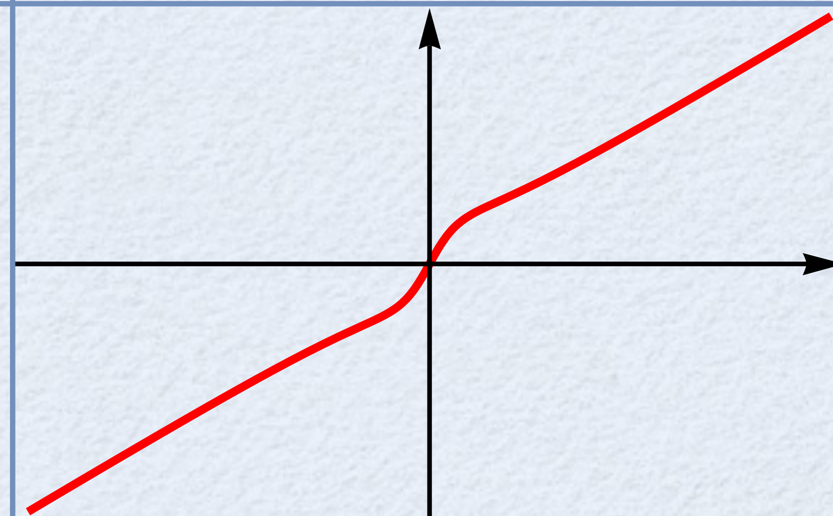
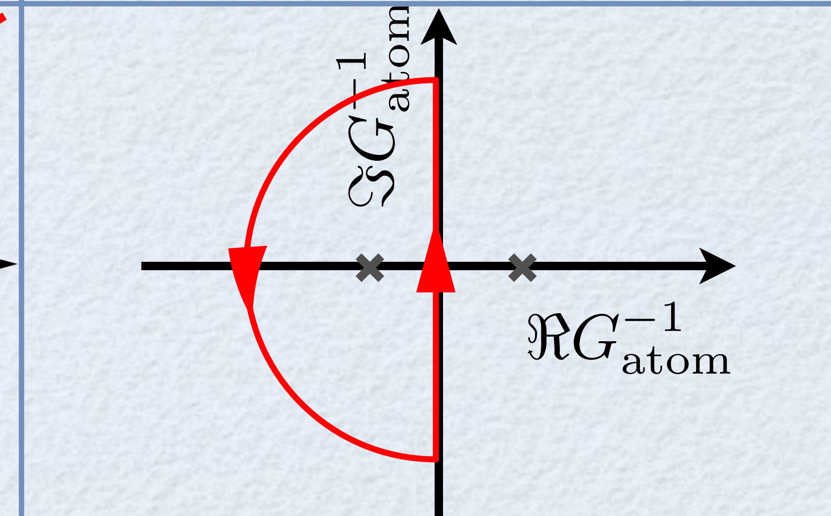
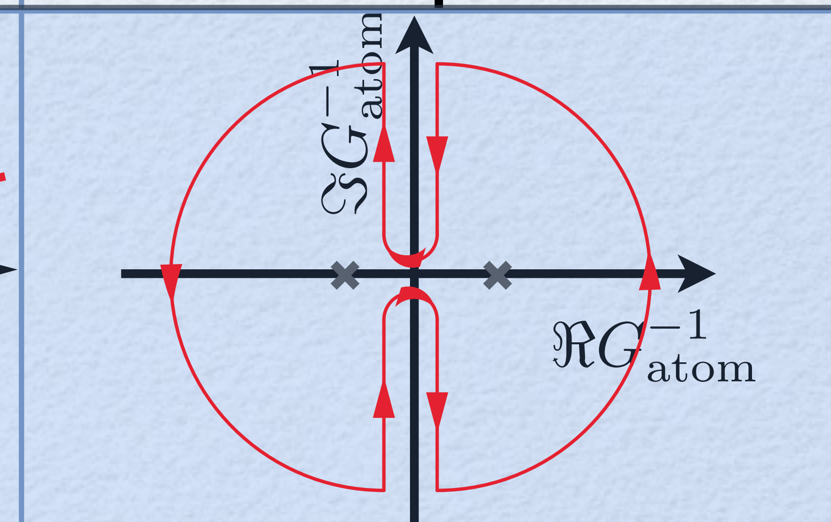
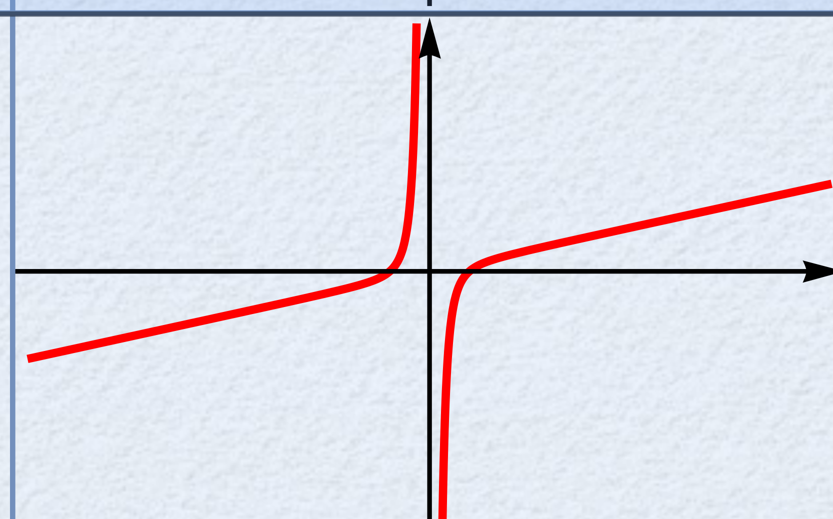
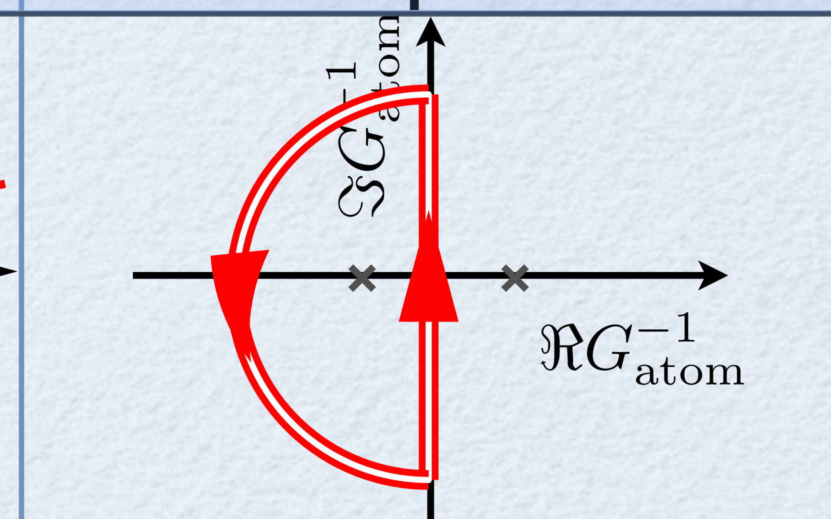
$$= \gamma \times \frac{1}{8\pi^2} \int_{\mathrm{BZ}} \mathrm{d}^3 k \frac{2|h_{\mathbf{k}}| + h^4_{\mathbf{k}}}{(|h_{\mathbf{k}}| + h^4_{\mathbf{k}})^2 |h_{\mathbf{k}}|^3} \varepsilon_{abcd} h^a_{\mathbf{k}} \partial_{k_x} h^b_{\mathbf{k}} \partial_{k_y} h^c_{\mathbf{k}} \partial_{k_z} h^d_{\mathbf{k}}$$

Interacting Z_2 = FDWN $\times Z_2$

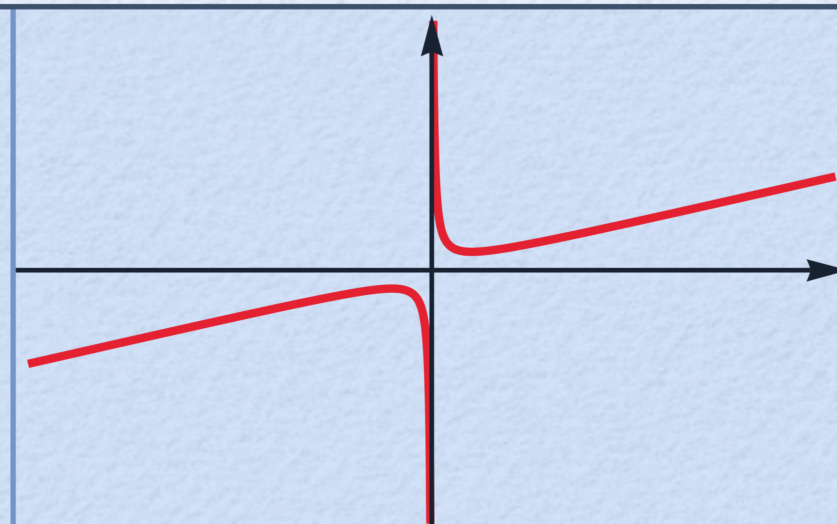
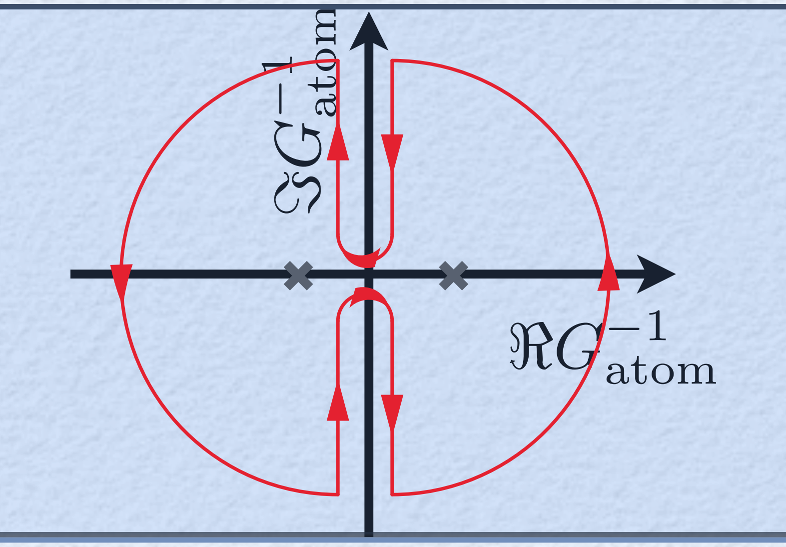
Qi, Hughes, Zhang, PRB (2008), Wang, Qi, Zhang, PRL (2010), Li, Wang, Qi, Zhang, NatPhys (2010)

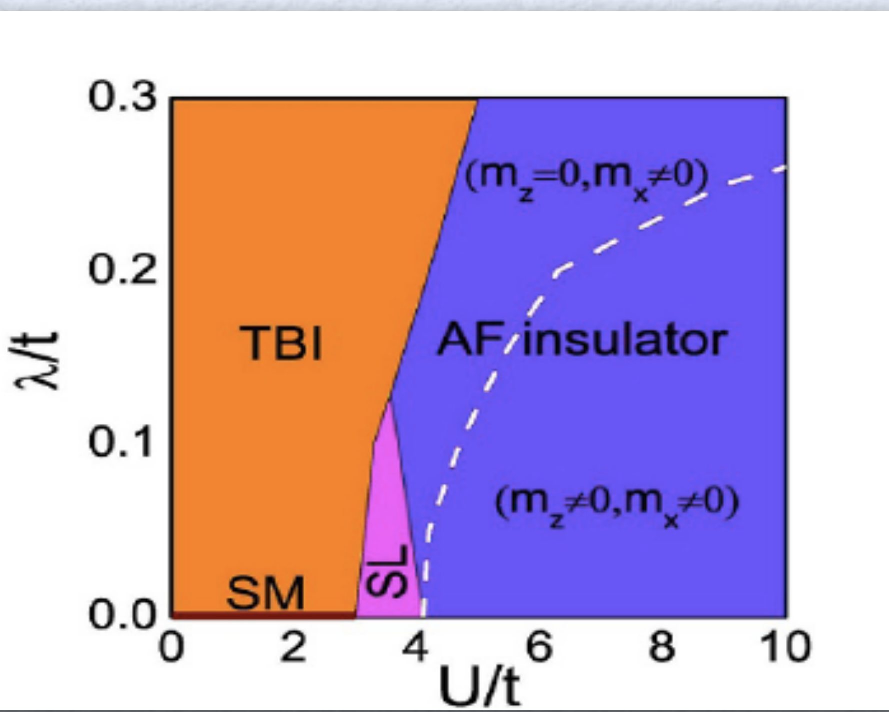
$\Sigma(\omega)$	FDWN	$\Im G_{\text{atom}}^{-1}(\omega)$	$\omega \mapsto G_{\text{atom}}^{-1}(\omega)$
0	1		
$\frac{1}{i\omega}$	0		
$\frac{1}{(i\omega)^3}$	2		

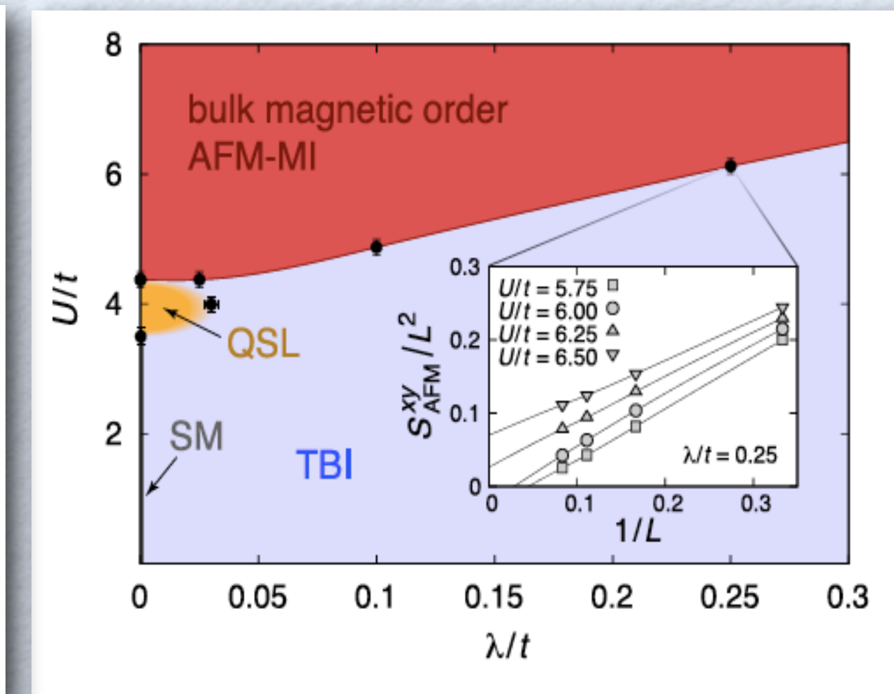
$\Sigma(\omega)$	FDWN	$\Im G^{-1}_{\mathrm{atom}}(\omega)$	$\omega \mapsto G^{-1}_{\mathrm{atom}}(\omega)$
$\dfrac{1}{i\omega - 1} + \dfrac{1}{i\omega + 1}$	1		
$\dfrac{1}{i\omega}$	0		
$\dfrac{1}{(i\omega)^3}$	2		

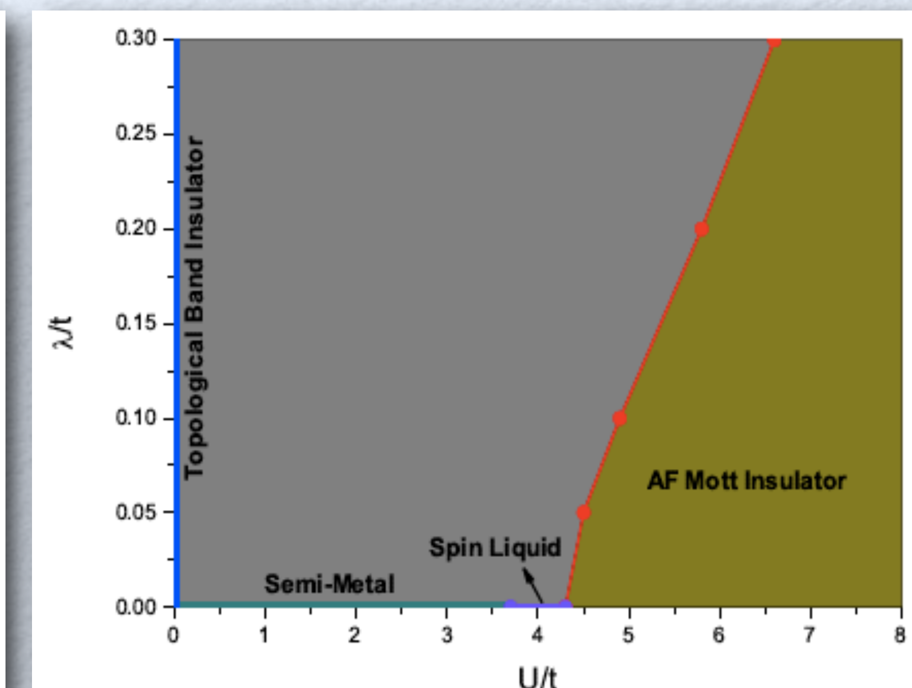
$\Sigma(\omega)$	FDWN	$\Im G^{-1}_{\text{atom}}(\omega)$	$\omega \mapsto G^{-1}_{\text{atom}}(\omega)$
$\frac{1}{i\omega - 1} + \frac{1}{i\omega + 1}$	1		
$\frac{1}{i\omega}$	0		
$\frac{1}{(i\omega)^3}$	2		

Are they related ?

$\frac{1}{i\omega}$	0		







Assumptions

(1). Momentum-independent self-energy

(2). Diagonal and orbital-independent self-energy

(3). Hamiltonian expanded by Gamma matrix

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Band flatten

Qi, Hughes, and Zhang, PRB, **78**, 195424 (2008)

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~~(2). Diagonal and orbital-independent self-energy~~

(3). Hamiltonian expanded by Gamma matrix

Pole-expansion

Savrasov, Haule and Kotliar, PRL, **96**, 036406 (2006)

Pole expansion and Pseudo-Hamiltonian

$$\hat{\Sigma}(\omega) = \hat{\Sigma}(\infty) + \hat{V}^{\dagger}(i\omega - \hat{P})^{-1}\hat{V}$$

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=& \begin{pmatrix} \boxed{[i\omega - H_{\mathbf{k}} - \hat{\Sigma}(\infty) - \hat{V}^\dagger (i\omega - \hat{P})^{-1}\hat{V}]^{-1}} & \cdots \\ \vdots & \ddots \end{pmatrix}
\end{aligned}$$

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Links interaction to non-interaction

$$G = \mathcal{P}^\dagger \tilde{G} \mathcal{P}$$

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$$\mathrm{Tr} G\partial_\omega G^{-1} G\partial_{k_x} G^{-1} G\partial_{k_y} G^{-1} G\partial_{k_z} G^{-1} G\partial_{k_\lambda} G^{-1}$$
$$= \mathrm{Tr} \tilde{G}\partial_\omega \tilde{G}^{-1} \tilde{G}\partial_{k_x} \tilde{G}^{-1} \tilde{G}\partial_{k_y} \tilde{G}^{-1} \tilde{G}\partial_{k_z} \tilde{G}^{-1} \tilde{G}\partial_{k_\lambda} \tilde{G}^{-1}$$

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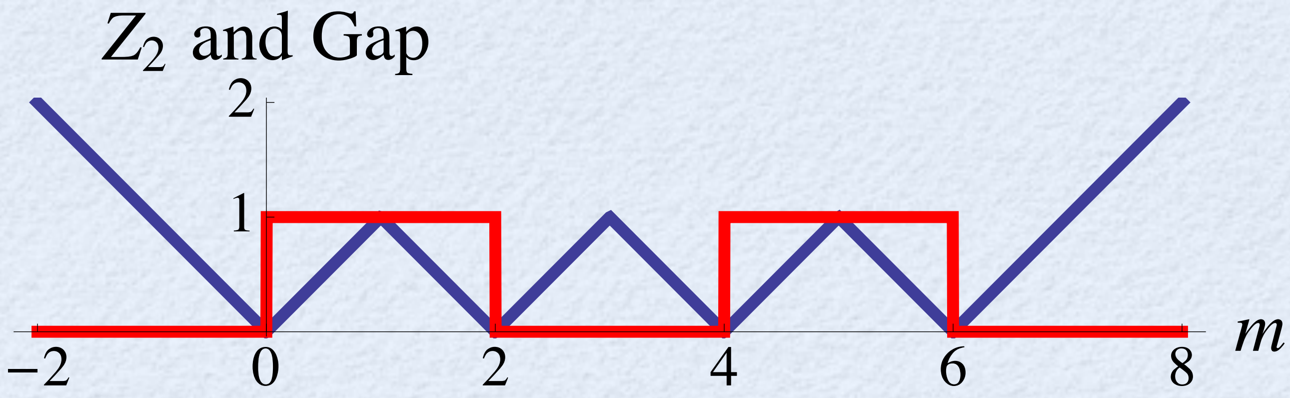
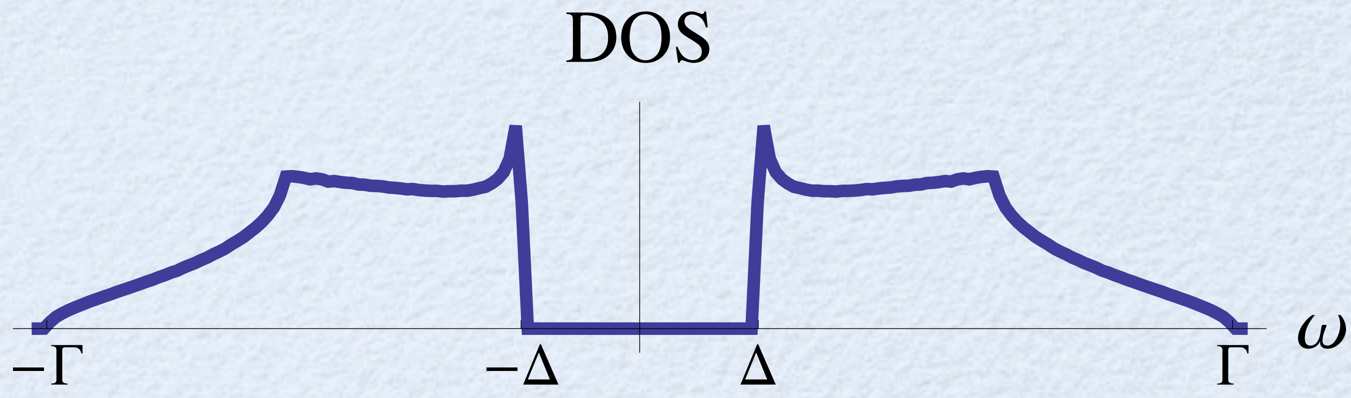
$$n[G] = n[\tilde{G}] = n[\tilde{H}_{\mathbf{k}}]$$

Toy model: 3D TI

$$H_{\mathbf{k}} = \sin k_x \Gamma^1 + \sin k_y \Gamma^2 + \sin k_z \Gamma^3 + \mathcal{M}(\mathbf{k})\Gamma^5$$

$$\mathcal{M}(\mathbf{k}) = m - 3 + (\cos k_x + \cos k_y + \cos k_z)$$





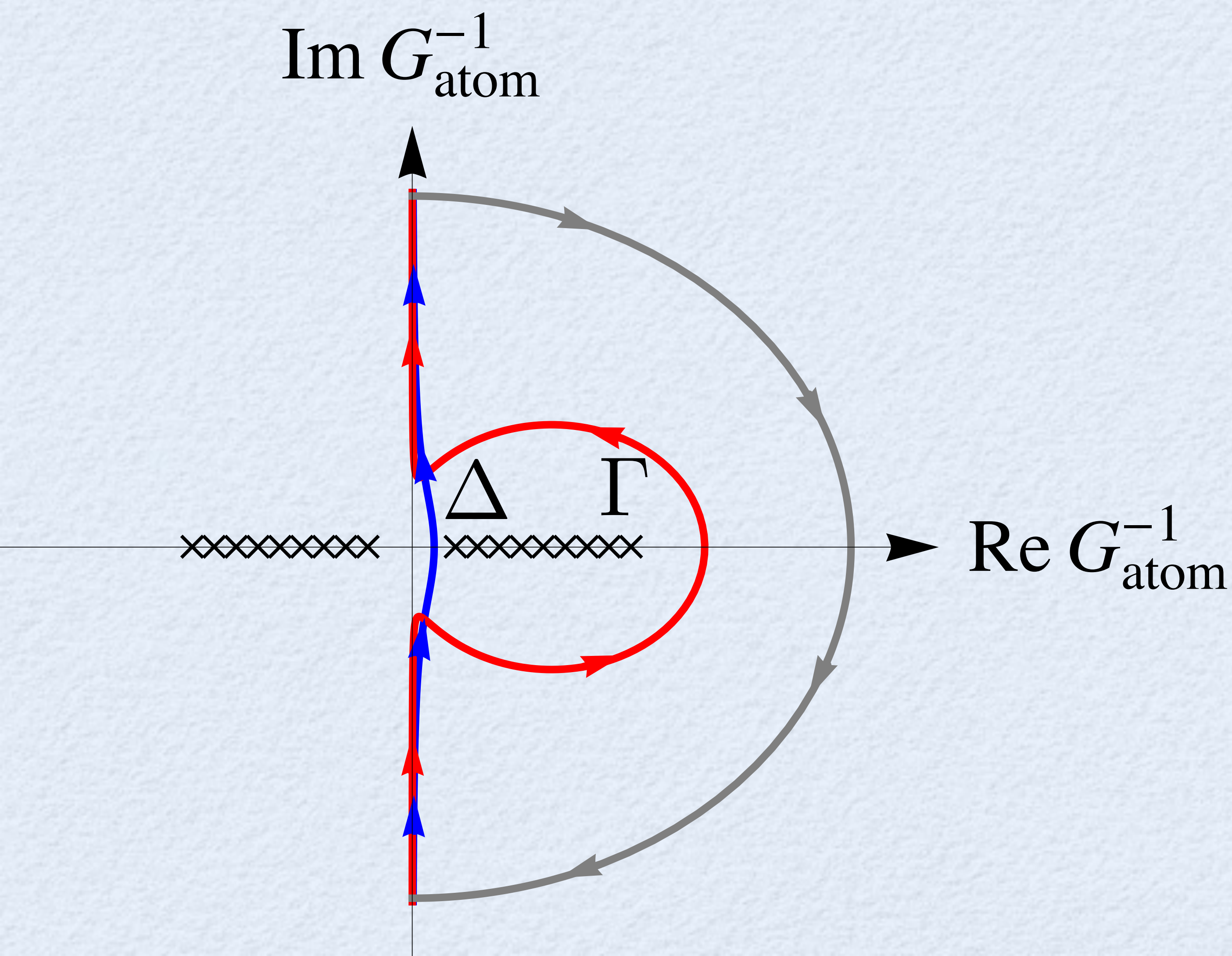
$H_{\mathbf{k}}$+ Interaction ?

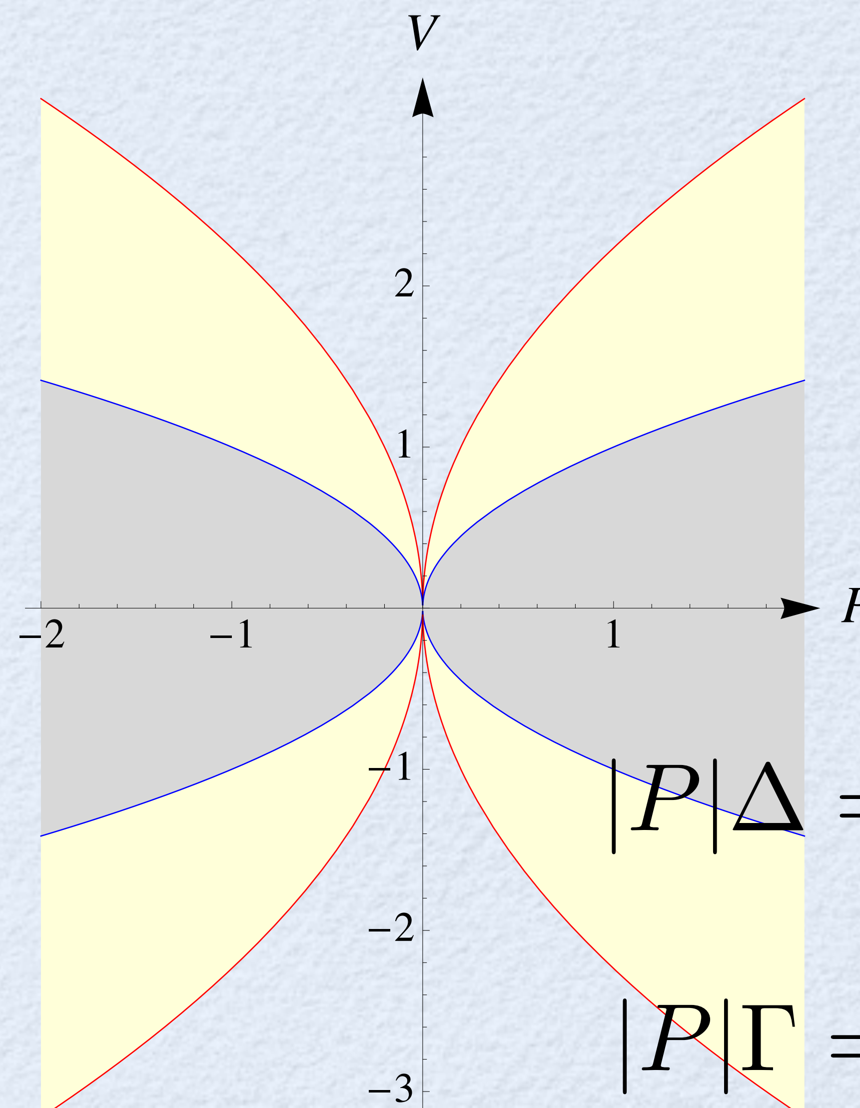
FDWN and Z_2 calculation

$$\Sigma(\omega) = \frac{V^2}{i\omega - P}$$

$$\omega \mapsto G_{\text{atom}}^{-1}(\omega) = i\omega - \Sigma(\omega)$$

$$\tilde{H}_{\mathbf{k}} = \begin{pmatrix} H_{\mathbf{k}} & V\mathbb{I}_4 \\ V\mathbb{I}_4 & P\mathbb{I}_4 \end{pmatrix}$$





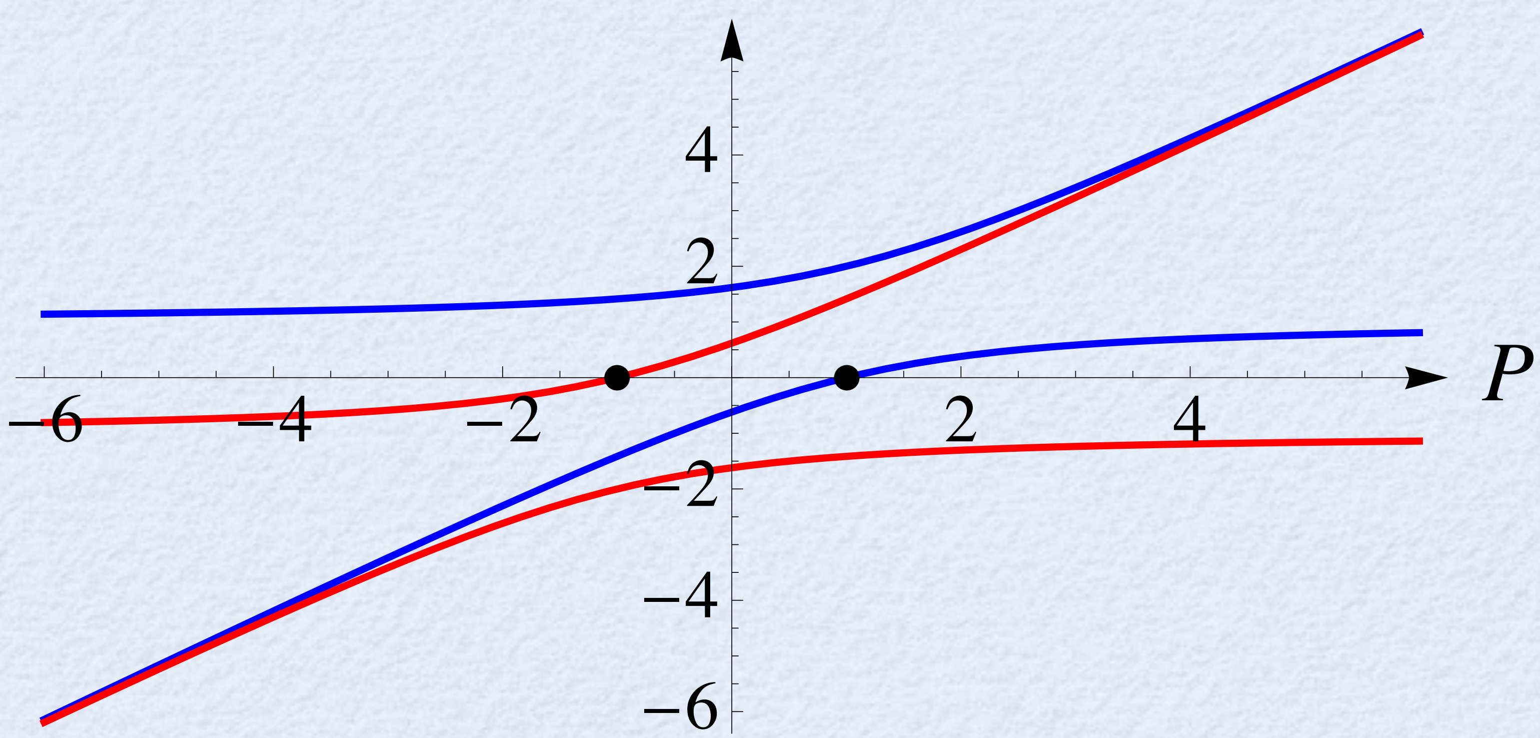
$$|P|\Delta = V^2$$

$$|P|\Gamma = V^2$$

Gap closing of pseudo-Hamiltonian

$$\tilde{H}_{\mathbf{k}} = \begin{pmatrix} H_{\mathbf{k}} & V\mathbb{I}_4 \\ V\mathbb{I}_4 & P\mathbb{I}_4 \end{pmatrix} \rightarrow \begin{pmatrix} E_{\mathbf{k}}\mathbb{I}_4 \otimes \sigma_z & V\mathbb{I}_4 \\ V\mathbb{I}_4 & P\mathbb{I}_4 \end{pmatrix}$$

$$\rightarrow \frac{(\pm E_{\mathbf{k}}) + P}{2} \pm \sqrt{[\frac{(\pm E_{\mathbf{k}}) - P}{2}]^2 + V^2}$$



$$E_{\mathbf{k}} P = V^2$$

Bonus: surface states

$$G = \mathcal{P}^\dagger \tilde{G} \mathcal{P}$$

$$\mathrm{Tr} G\partial_\omega G^{-1} G\partial_{k_x} G^{-1} G\partial_{k_y} G^{-1} G\partial_{k_z} G^{-1} G\partial_{k_\lambda} G^{-1}$$
$$= \mathrm{Tr} \tilde{G}\partial_\omega \tilde{G}^{-1} \tilde{G}\partial_{k_x} \tilde{G}^{-1} \tilde{G}\partial_{k_y} \tilde{G}^{-1} \tilde{G}\partial_{k_z} \tilde{G}^{-1} \tilde{G}\partial_{k_\lambda} \tilde{G}^{-1}$$

$$n[G] = n[\tilde{G}] = n[\tilde{H}_{\mathbf{k}}]$$

Bonus: surface states

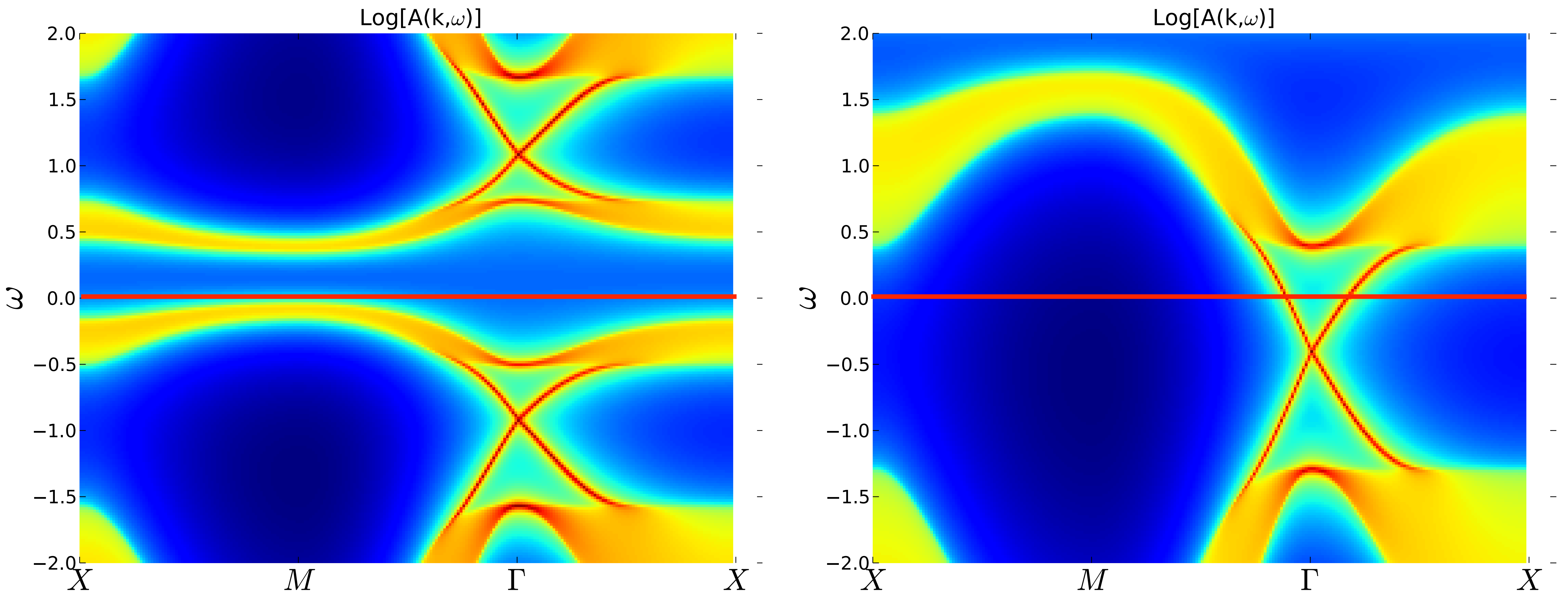
$$G = \mathcal{P}^\dagger \tilde{G} \mathcal{P} \quad \Rightarrow \quad G^{\text{surf}} = \mathcal{P}^\dagger \tilde{G}^{\text{surf}} \mathcal{P}$$

$$\mathrm{Tr} G \partial_\omega G^{-1} G \partial_{k_x} G^{-1} G \partial_{k_y} G^{-1} G \partial_{k_z} G^{-1} G \partial_{k_\lambda} G^{-1}$$
$$= \mathrm{Tr} \tilde{G} \partial_\omega \tilde{G}^{-1} \tilde{G} \partial_{k_x} \tilde{G}^{-1} \tilde{G} \partial_{k_y} \tilde{G}^{-1} \tilde{G} \partial_{k_z} \tilde{G}^{-1} \tilde{G} \partial_{k_\lambda} \tilde{G}^{-1}$$

$$n[G] = n[\tilde{G}] = n[\tilde{H}_{\mathbf{k}}]$$

Surface spectral functions

$$\Sigma(\omega) = \frac{V^2}{i\omega - P} \qquad V = 1$$



$P = 0.15$ $\qquad$ $P = 2$

Practical calculations

- Three and four dims: DMFT calculations
  - Only overall shape matters FDWN: simple IPT solver
  - Only Matsubara Green's function needed: exact CTQMC solver

Practical calculations (cont.)

- Two dim cases:
  - Spatial fluctuations: **k** dependence of self-energy
  - FLEX, DCA and diagrammatic MC
- Numerical integration: VEGAS algorithm-by Dr. Peter Lepage has been used for multi-dimensional quadrature in high energy physics for more than 30 years.

Summary

- Self-energy contains the topological signature of interacting TI
- Local self-energy approximation:
  - Frequency domain winding number
  - Pole expansion of self-energy
- Breaking down the topological phases without developing LRO: relevant to “spin liquid” phase?
- It's interesting to see the synergies of many-body numerical methods with the study of interacting topological insulators though the calculation of their Green's functions

Thank you for your attention:)