

Seminar @ Tsinghua, Dec.5/2012

# Topological states of matter in correlated electron systems

Qiang-Hua Wang

National Lab of Solid State Microstructures, Nanjing  
University, Nanjing 210093, China

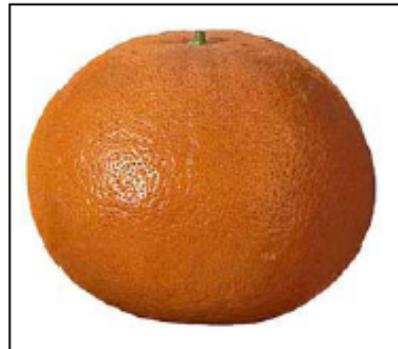
Collaborators: Dunhai Lee (Berkeley), F Wang (MIT), F Yang (Beijing)  
Students: Wan-Sheng Wang and Yuan-Yuan Xiang

Wang WS, et al, PRB 2012; Xiang YY, et al, PRB 2012

# Outline

- Introduction and motivation
- T-breaking topological phases in doped Graphene and kagome lattices
- T-invariant topological superconductors
- Conclusions

# Topology in daily life



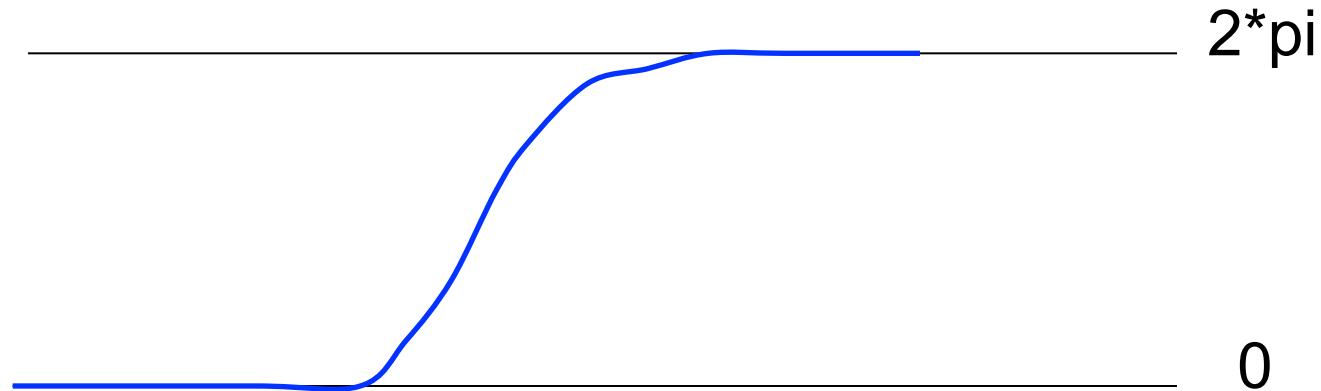
Zero handle



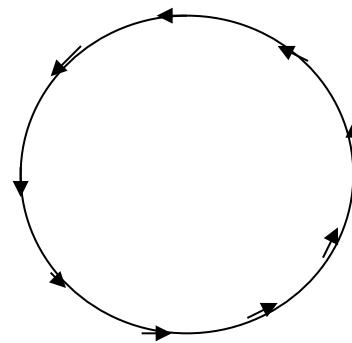
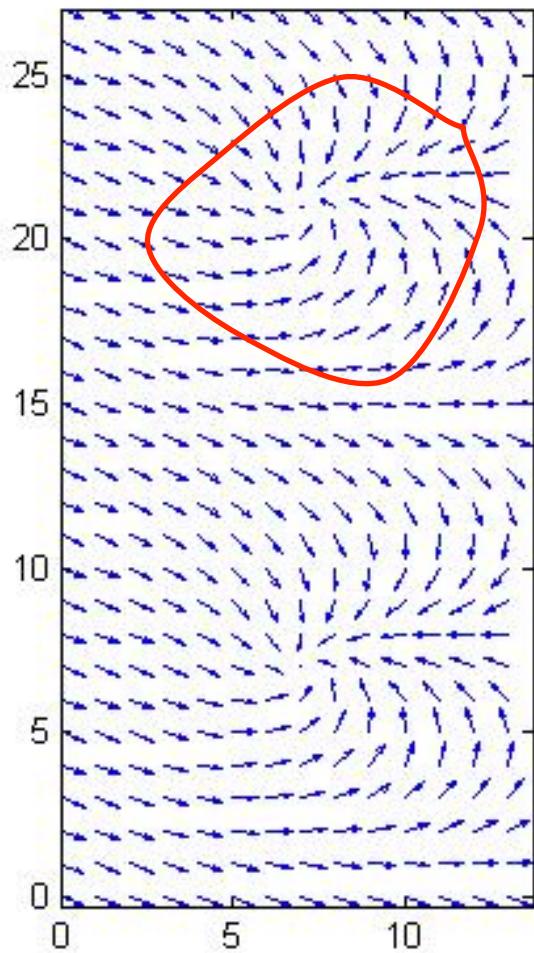
One handle

# Topological states in 1D: kink and soliton

$$H = \int dx [K(\partial_x \phi)^2 + 1 - \cos \phi]$$

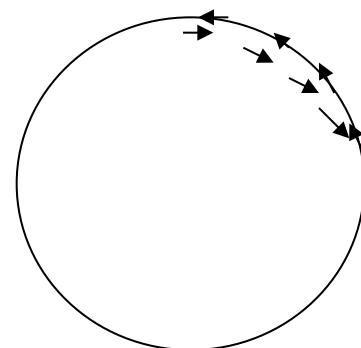
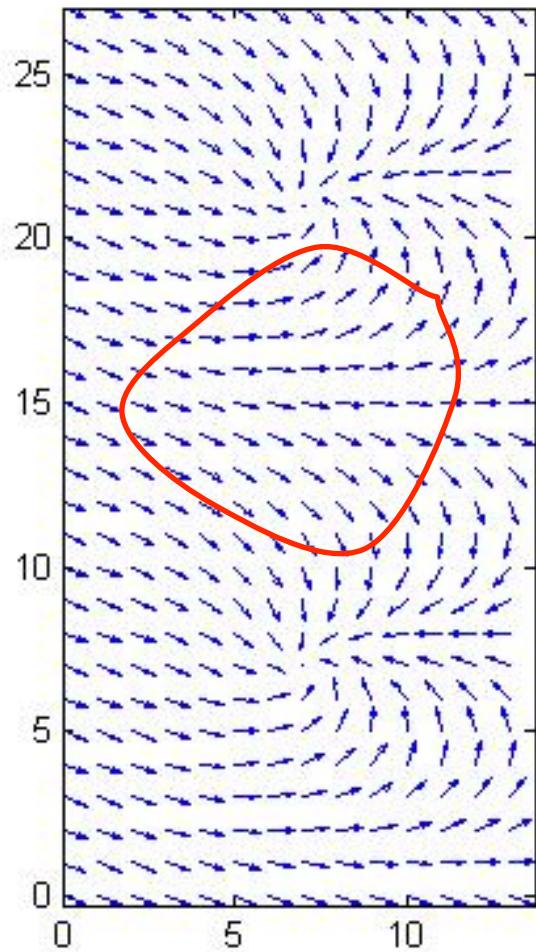


# Topological states in 2D: vortex



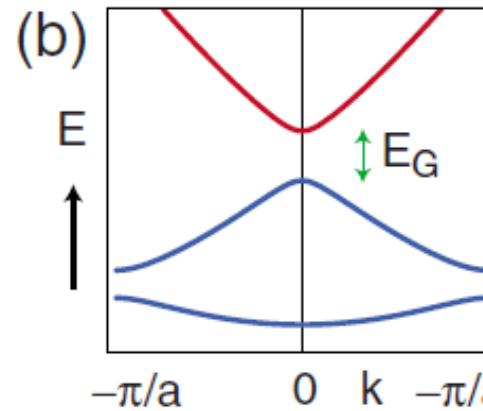
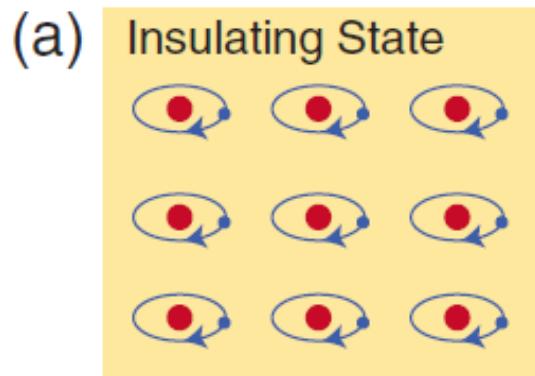
$W=1$

# Topological states in 2D: vortex

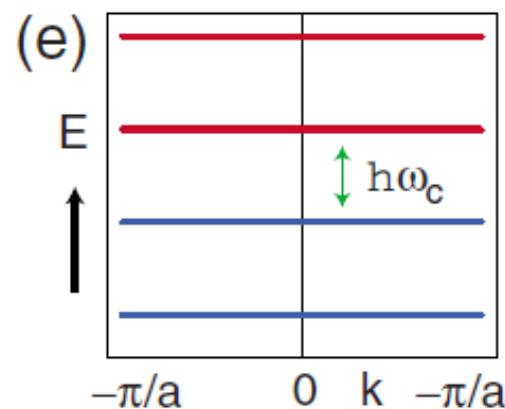
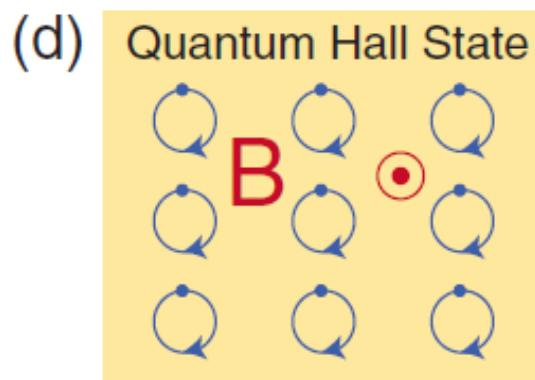


$W=0$

# Topology and topological states of matter



(c)

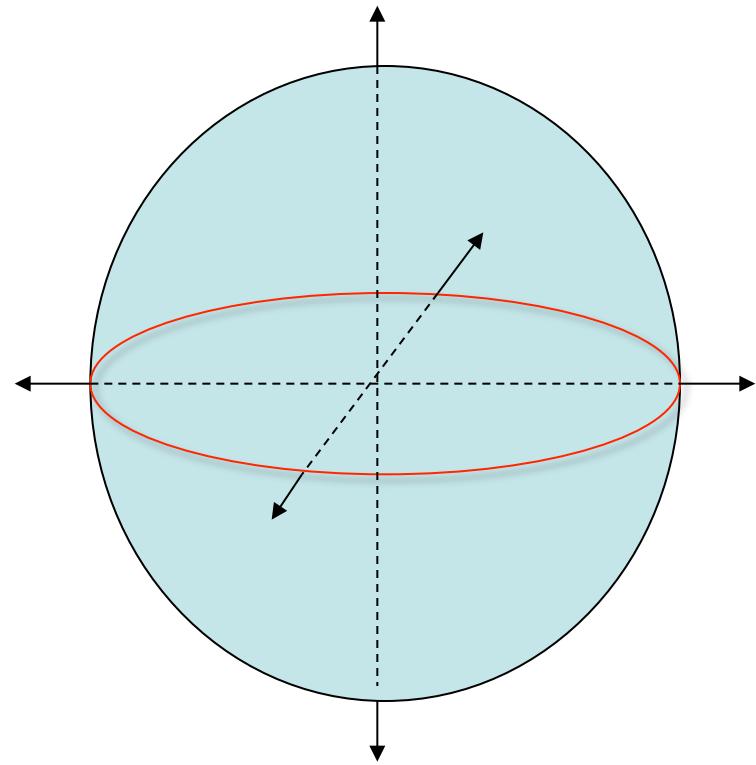
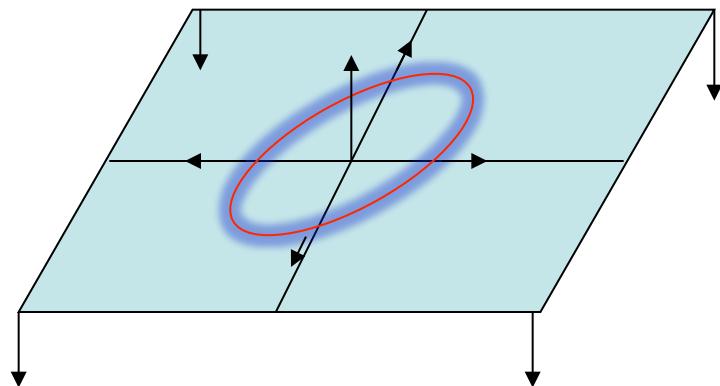


(f)

# Topology and mapping $\mathbf{k} \rightarrow H(\mathbf{k})$

$$H = \sum_k \psi_k^+ [\vec{B}(k) \cdot \Gamma + \varepsilon_k I] \psi_k, \quad C_1 = \frac{1}{4\pi} \int dk_x \int dk_y \hat{\mathbf{d}} \cdot \frac{\partial \hat{\mathbf{d}}}{\partial k_x} \times \frac{\partial \hat{\mathbf{d}}}{\partial k_y}.$$

$$\{\Gamma_\alpha, \Gamma_\beta\} = 2\delta_{\alpha\beta}.$$



# TKNN invariant, Chern number and edge states

Thouless, Kohmoto, Nightingale, and den Nijs 1982

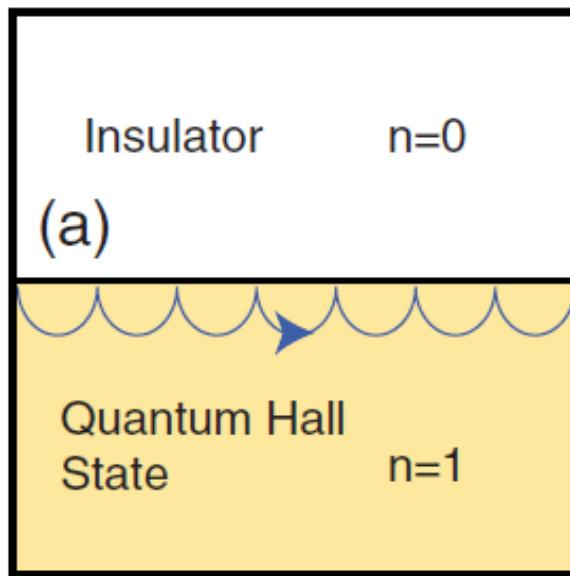
Topological number can not change smoothly.

Topologically distinct phases are connected by a) gap closing in the quantum phase transition point in parameter space, or b) gapless edge states in real space.

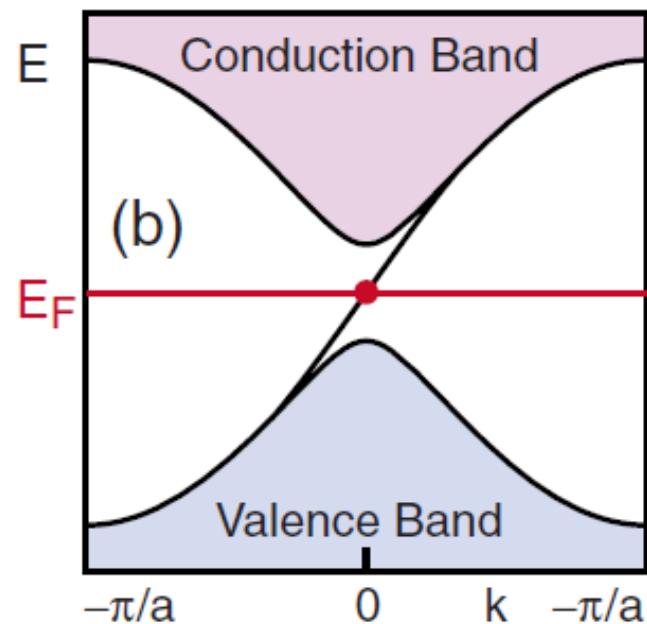
There is a 1 to 1 correspondence between the change of  $Z$  across the boundary and the number of edge states.

# TKNN invariant, Chern number and edge states

Skippy cyclotron orbits



Edge state in the Haldane model



# Spin polarized p+ip superconductor, Z=1

$$H = \frac{1}{2} \sum_p (c_{\mathbf{p}}^\dagger, c_{-\mathbf{p}}) \begin{pmatrix} \epsilon_{\mathbf{p}} & \Delta p_+ \\ \Delta^* p_- & -\epsilon_{\mathbf{p}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{p}} \\ c_{-\mathbf{p}}^\dagger \end{pmatrix}$$

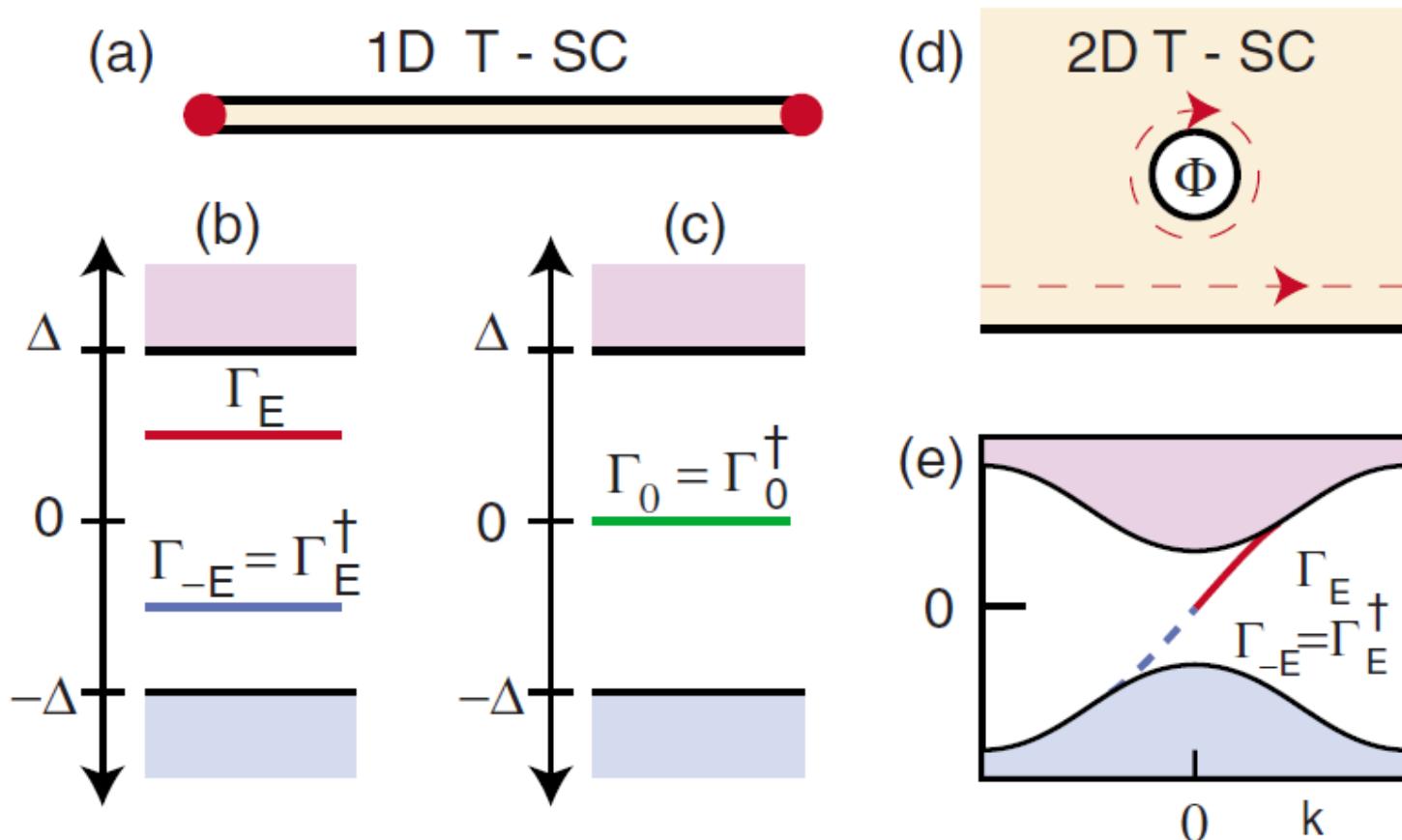
$$p_\pm = p_x \pm i p_y$$

$$\mathcal{H}_{\text{BdG}}(\mathbf{k}) = [\mathcal{H}_0(\mathbf{k}) - \mu] \tau_z + \Delta_1(\mathbf{k}) \tau_x + \Delta_2(\mathbf{k}) \tau_y.$$

The effective field  $\mathbf{B}(\mathbf{k})$  cover the Bloch sphere once.

Read and Green 2000

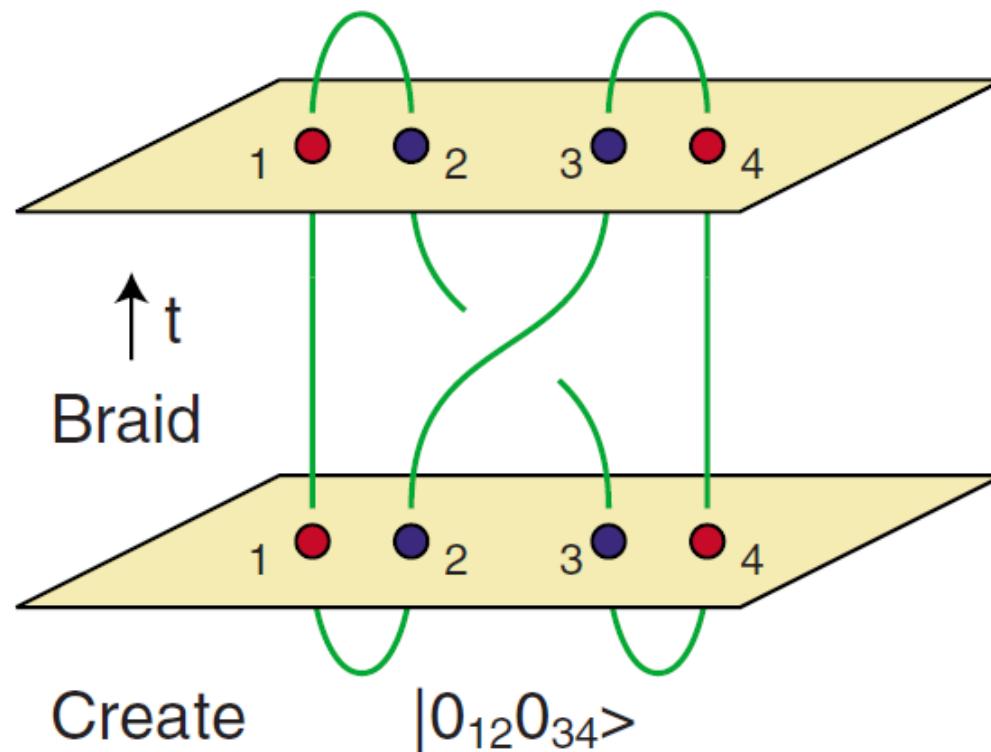
# Majorana fermions in 1d and 2d cases



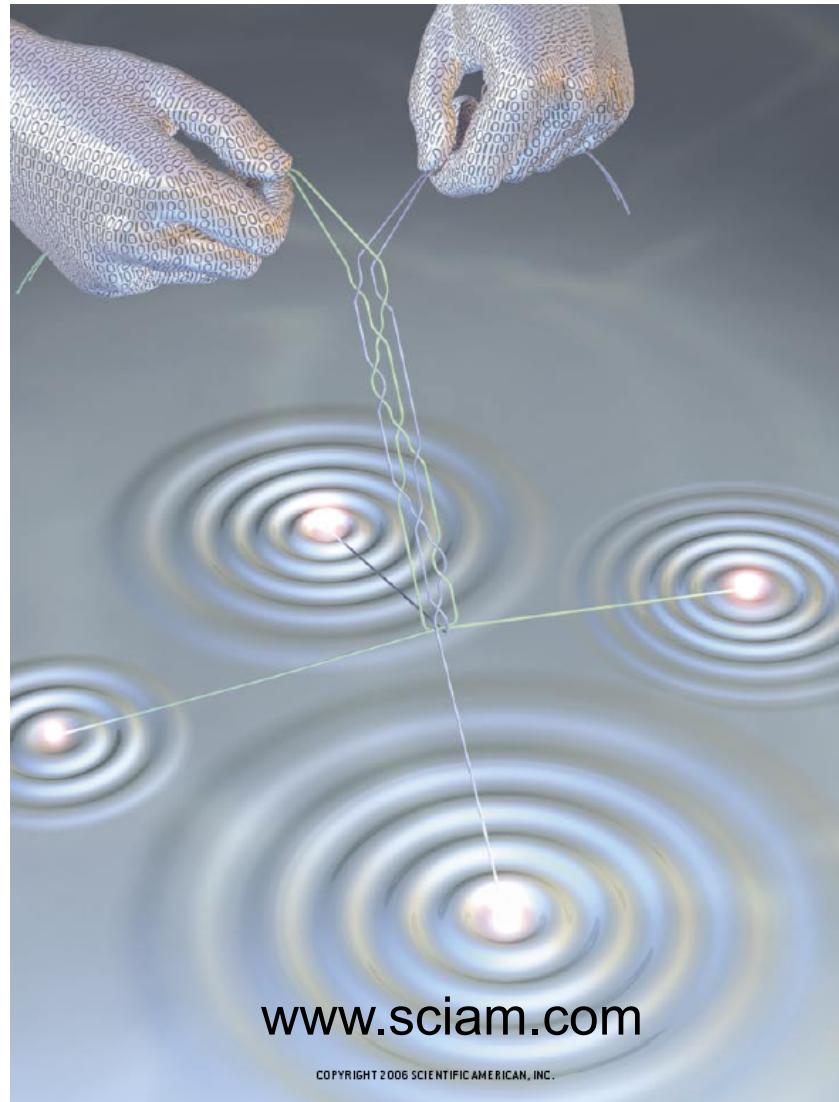
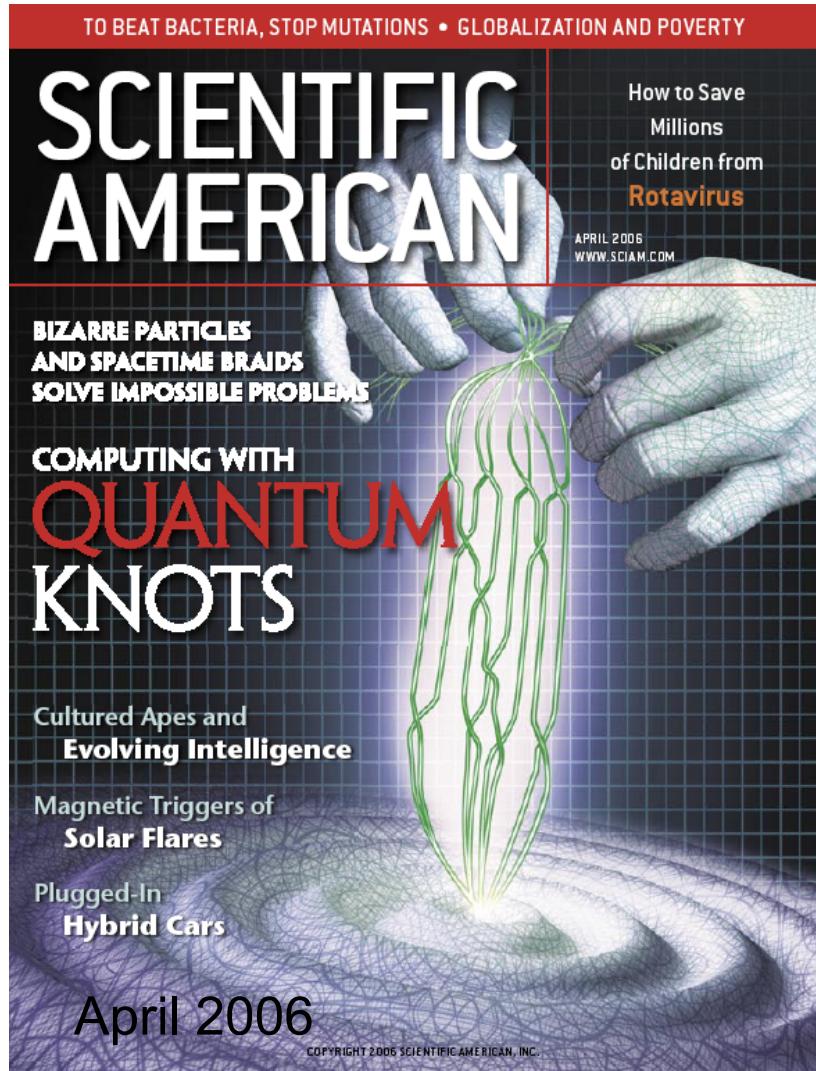
$+\mathcal{E}$  and  $-\mathcal{E}$  forms a canonical fermion, not protected  
 $\mathcal{E}=0$  comes in pair and sit on opposite edges, protected

# Majorana fermion and non-Abelian statistics

Measure  $(|0_{12}0_{34}\rangle + |1_{12}1_{34}\rangle)/\sqrt{2}$



# Topological quantum computing



[www.sciam.com](http://www.sciam.com)

COPYRIGHT 2006 SCIENTIFIC AMERICAN, INC.

# Spin singlet d+id superconductor

$$H = \sum_k \psi_k^+ \begin{pmatrix} H_0(k) - \mu & \Delta d_+(k) \\ \Delta^* d_-(k) & \mu - H_0(k) \end{pmatrix} \psi_k^-,$$

$$\psi_k^+ = (c_{k\uparrow}^+, c_{-k\downarrow}^+)^T,$$

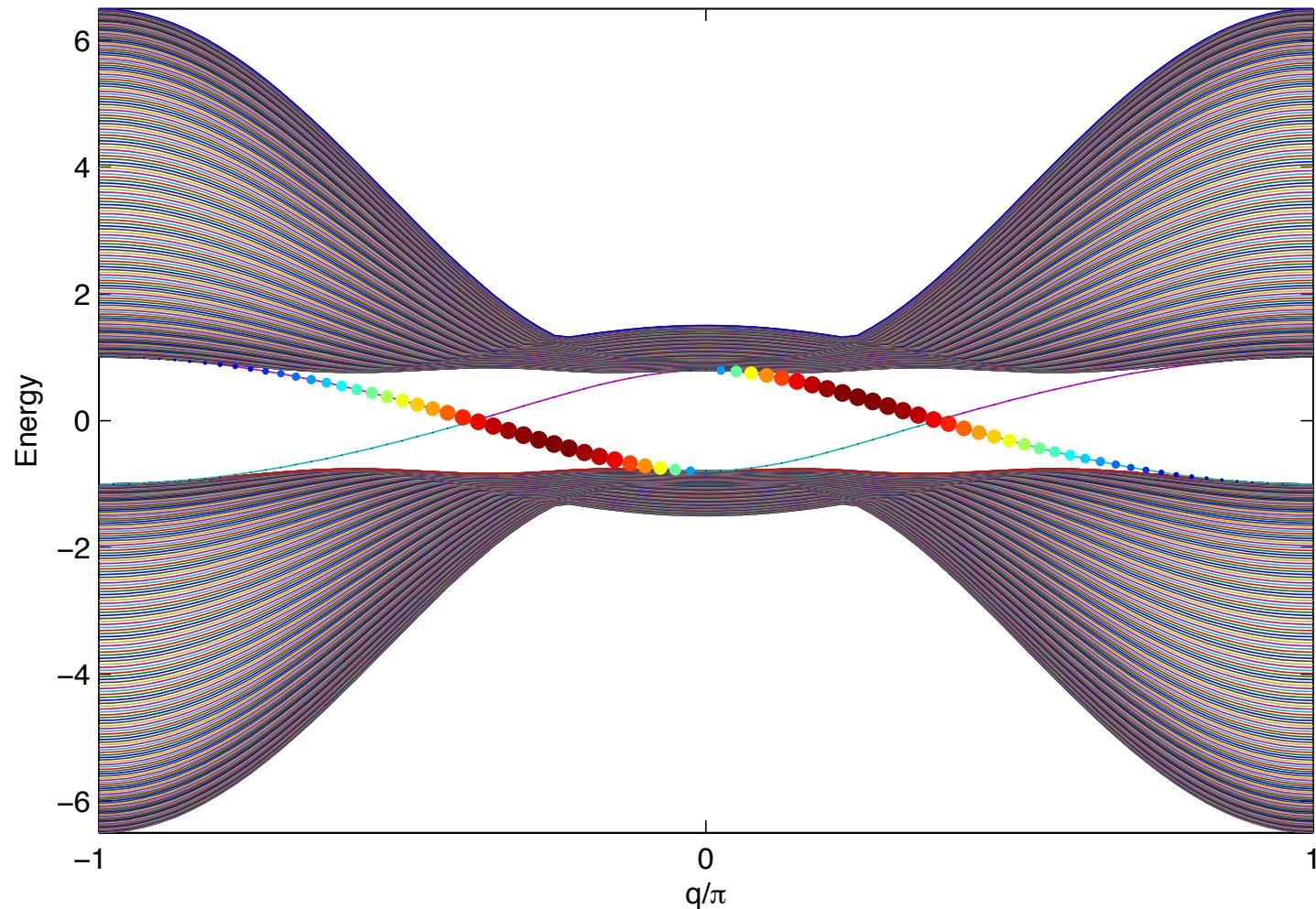
$$\psi_k^- = (c_{k\uparrow}, c_{-k\downarrow}^+)^T,$$

$$d_+(k) \sim \exp(2i\theta_k)$$

$$\mathcal{H}_{\text{BdG}}(\mathbf{k}) = [\mathcal{H}_0(\mathbf{k}) - \mu] \tau_z + \Delta_1(\mathbf{k}) \tau_x + \Delta_2(\mathbf{k}) \tau_y.$$

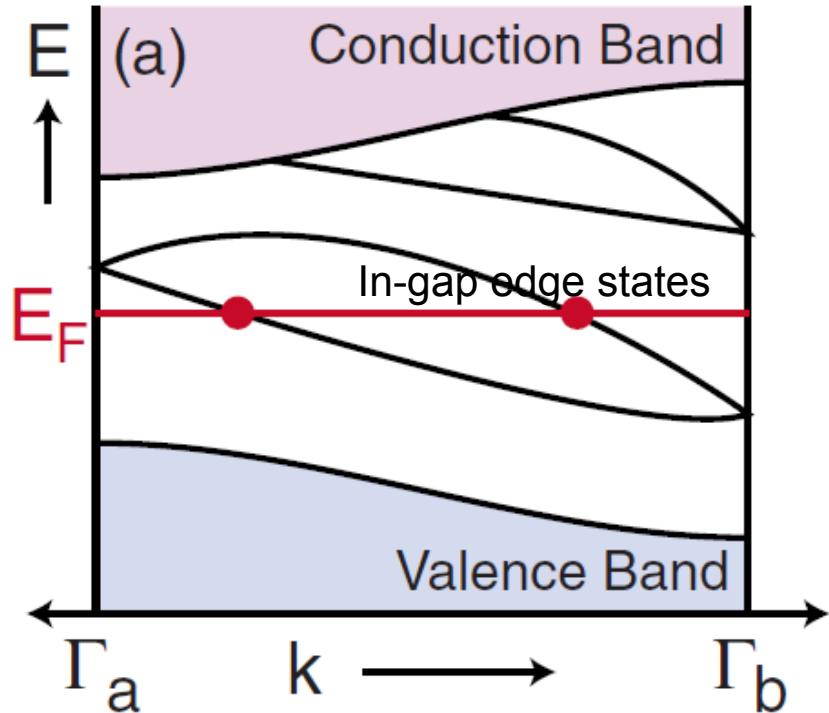
The effective field  $\mathbf{B}(\mathbf{k})$  cover the Bloch sphere twice, thus  $Z=2$

# Edge states for d+id pairing ( $Z=2$ )

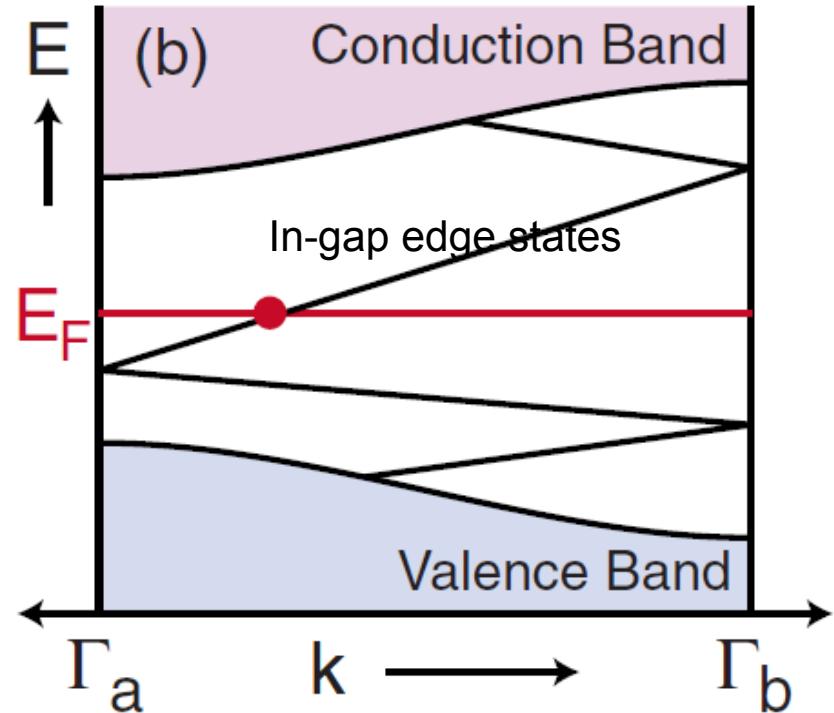


# $Z_2$ number in T-invariant insulators

Kramers degeneracy on T-invariant momenta  $\Gamma$

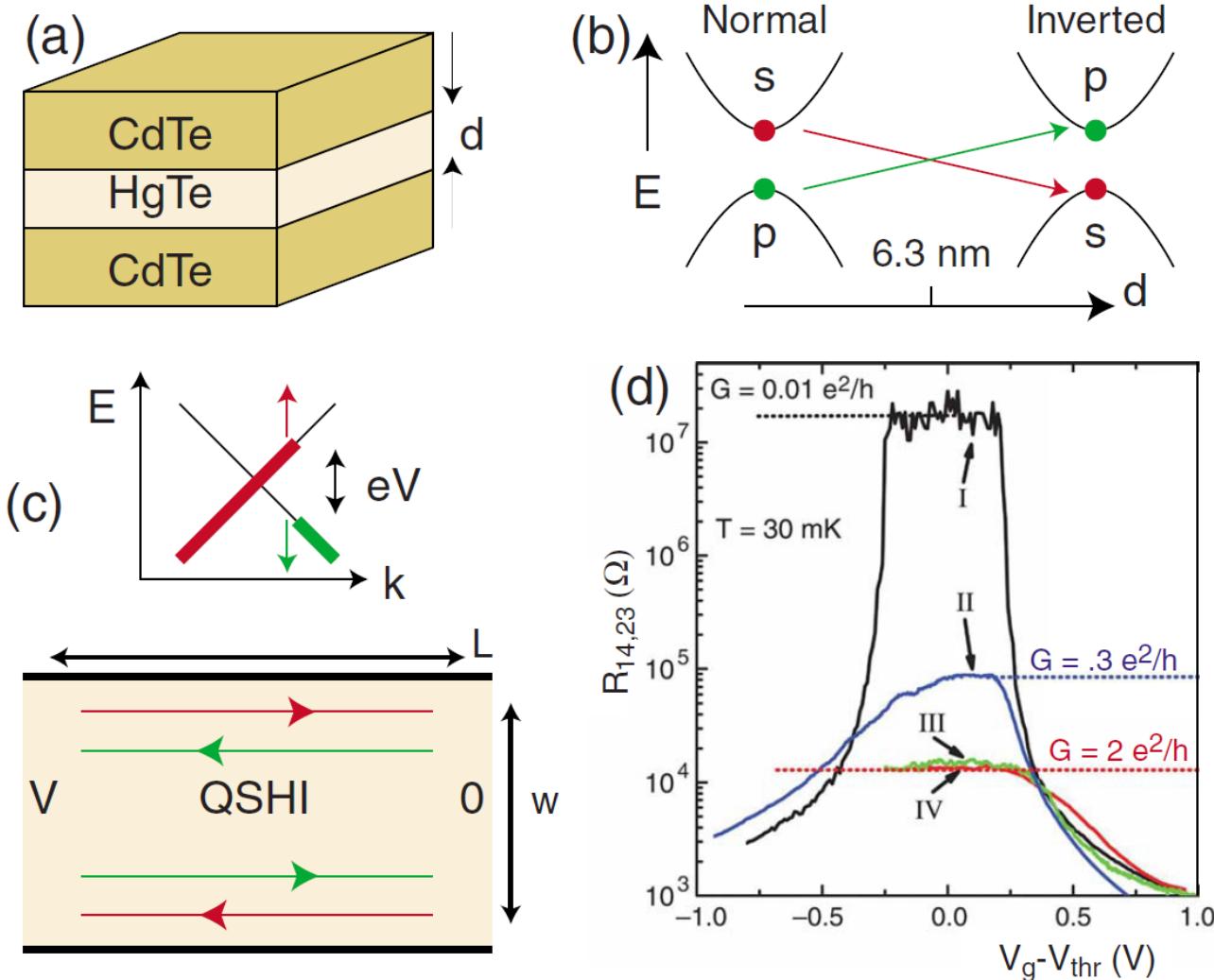


Even crossings:  $Z_2=0$



Odd crossings:  $Z_2=1$

# Quantum spin Hall system



Konig et al, 2007

# T-invariant topological insulator /superconductor

$$H = \frac{1}{2} \sum_p \tilde{\Psi}^\dagger \begin{pmatrix} \epsilon_{\mathbf{p}} & \Delta p_+ & 0 & 0 \\ \Delta^* p_- & -\epsilon_{\mathbf{p}} & 0 & 0 \\ 0 & 0 & \epsilon_{\mathbf{p}} & -\Delta^* p_- \\ 0 & 0 & -\Delta p_+ & -\epsilon_{\mathbf{p}} \end{pmatrix} \tilde{\Psi}$$

$$p_\pm = i(p_x + ip_y)$$

For a topological insulator,

$$\psi_k^+ = (a_{k\uparrow}^+, b_{k\uparrow}^+, a_{k\downarrow}^+, b_{k\downarrow}^+) \\ \psi_k^- = (a_{k\uparrow}^-, b_{k\uparrow}^-, a_{k\downarrow}^-, b_{k\downarrow}^-)^T .$$

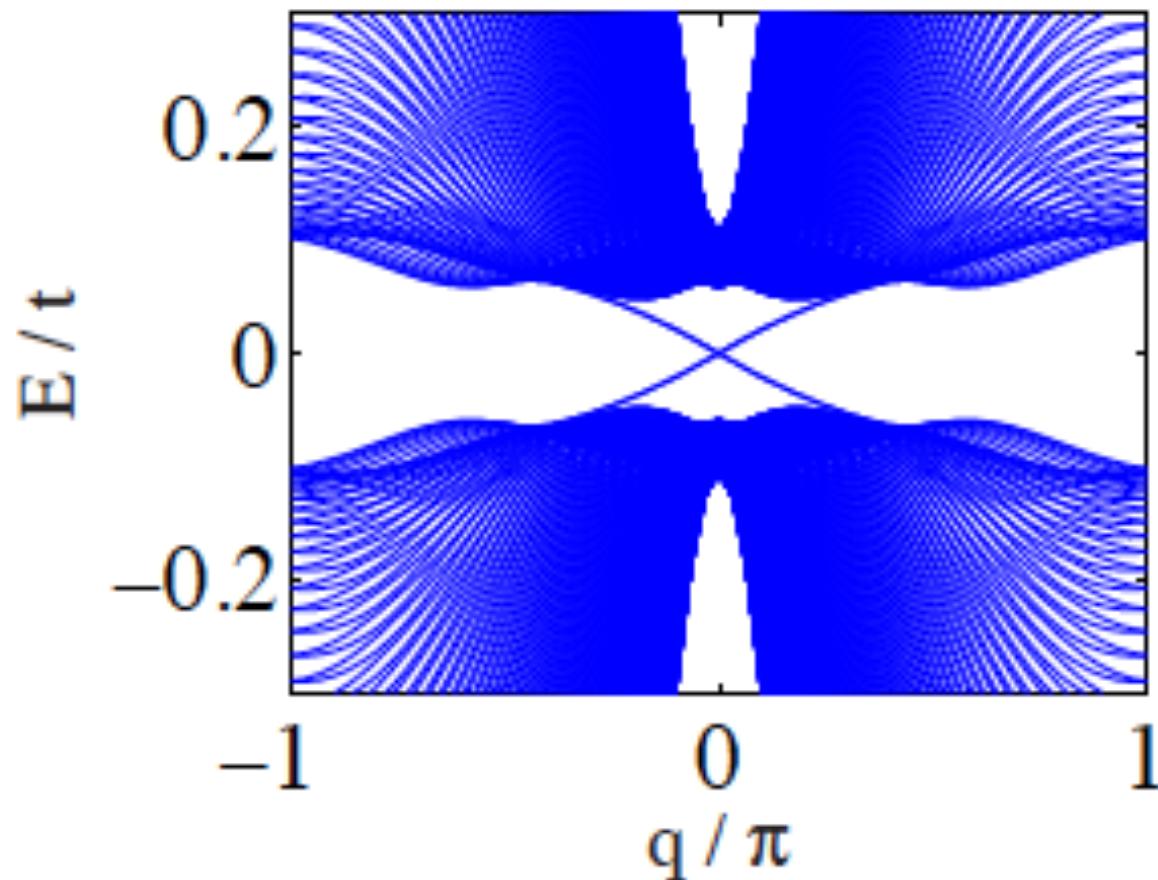
For a superconductor,

$$\psi_k^+ = (a_{k\uparrow}^+, a_{-k\uparrow}^+, a_{k\downarrow}^+, a_{-k\downarrow}^+) \\ \psi_k^- = (a_{k\uparrow}^-, a_{-k\uparrow}^-, a_{k\downarrow}^-, a_{-k\downarrow}^-)^T .$$

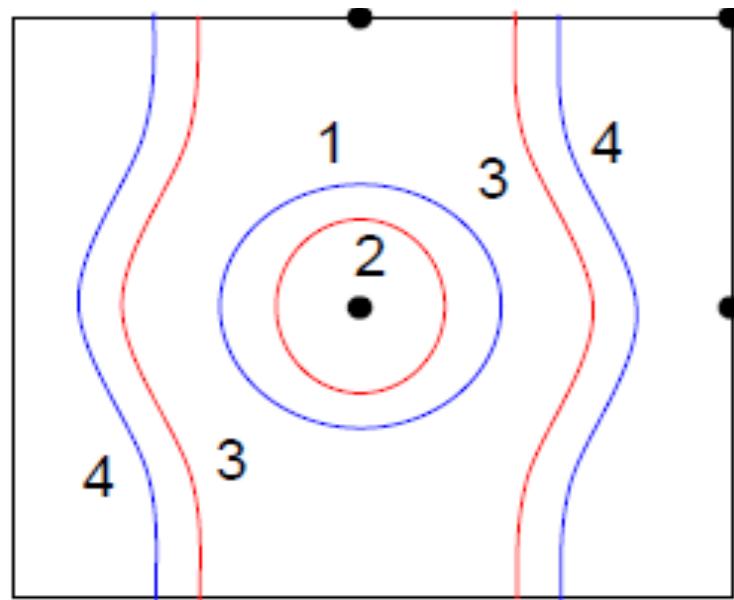
Roy et al 2008; Schnyder et al 2008

Kitaev 2009; Qi et al 2009; Qi et al, RMP 2011

# Edge state in a T-invariant topological superconductor

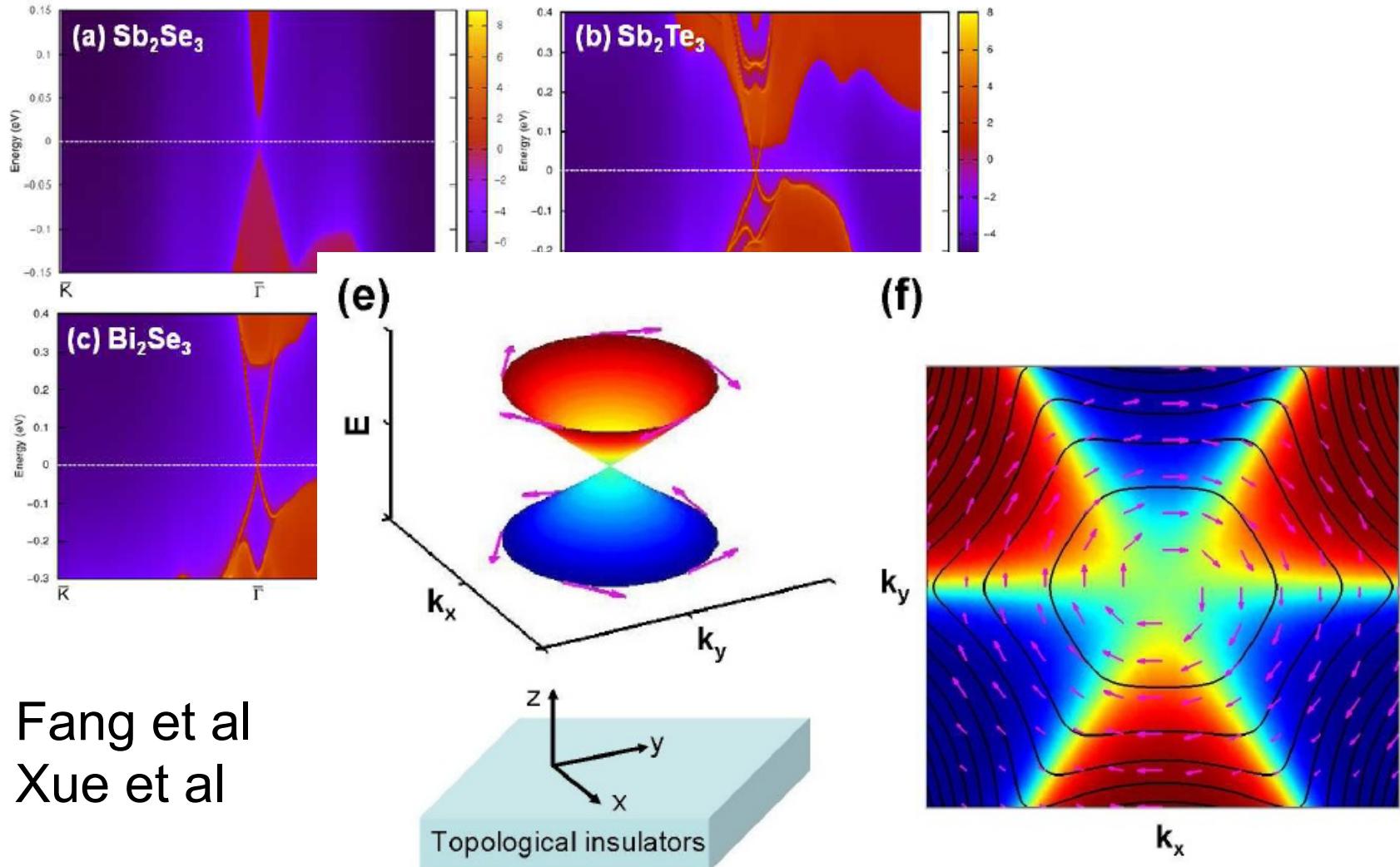


# A convenient criterion for T-invariant topological superconductor

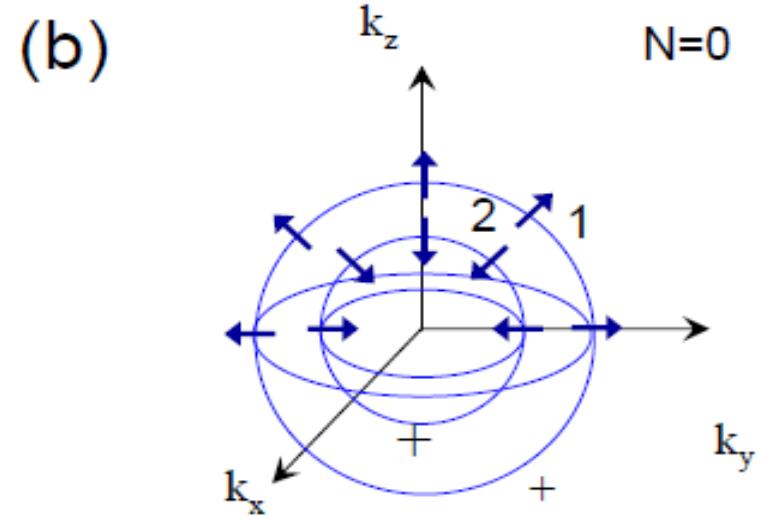
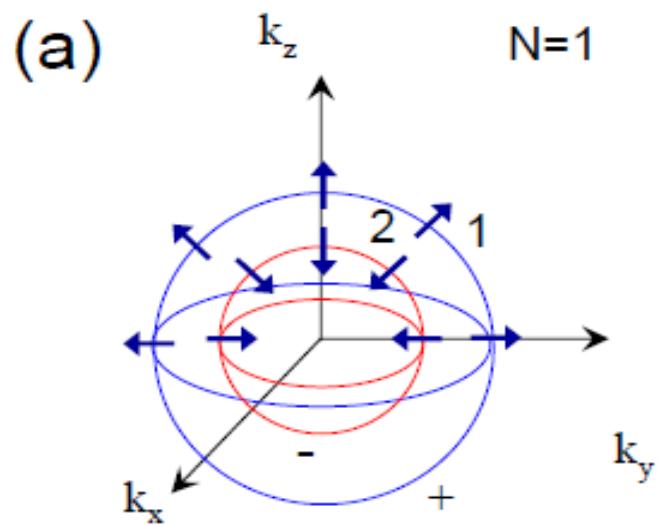


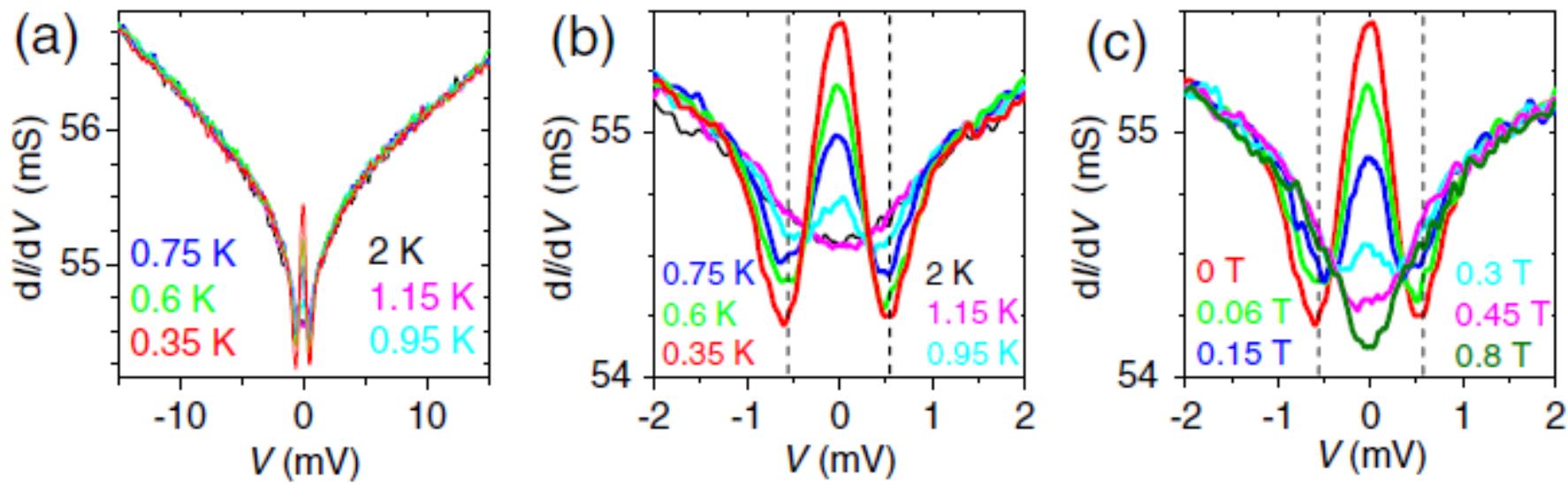
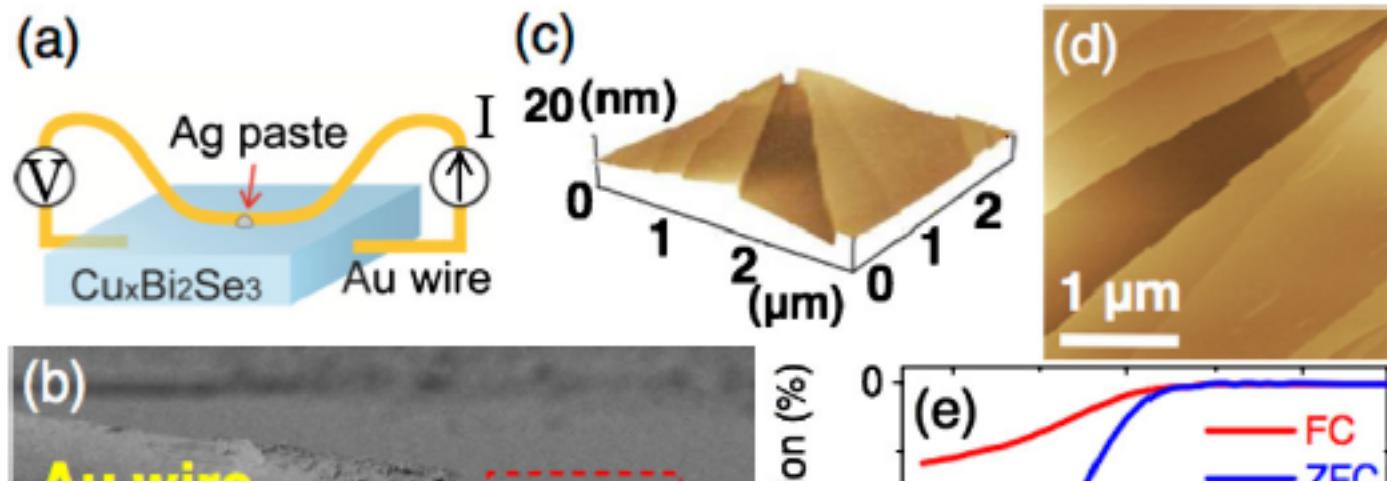
Roy et al 2008; Schnyder et al 2008  
Kitaev 2009; Qi et al 2009; Qi et al, RMP 2011

# 3d topological insulators

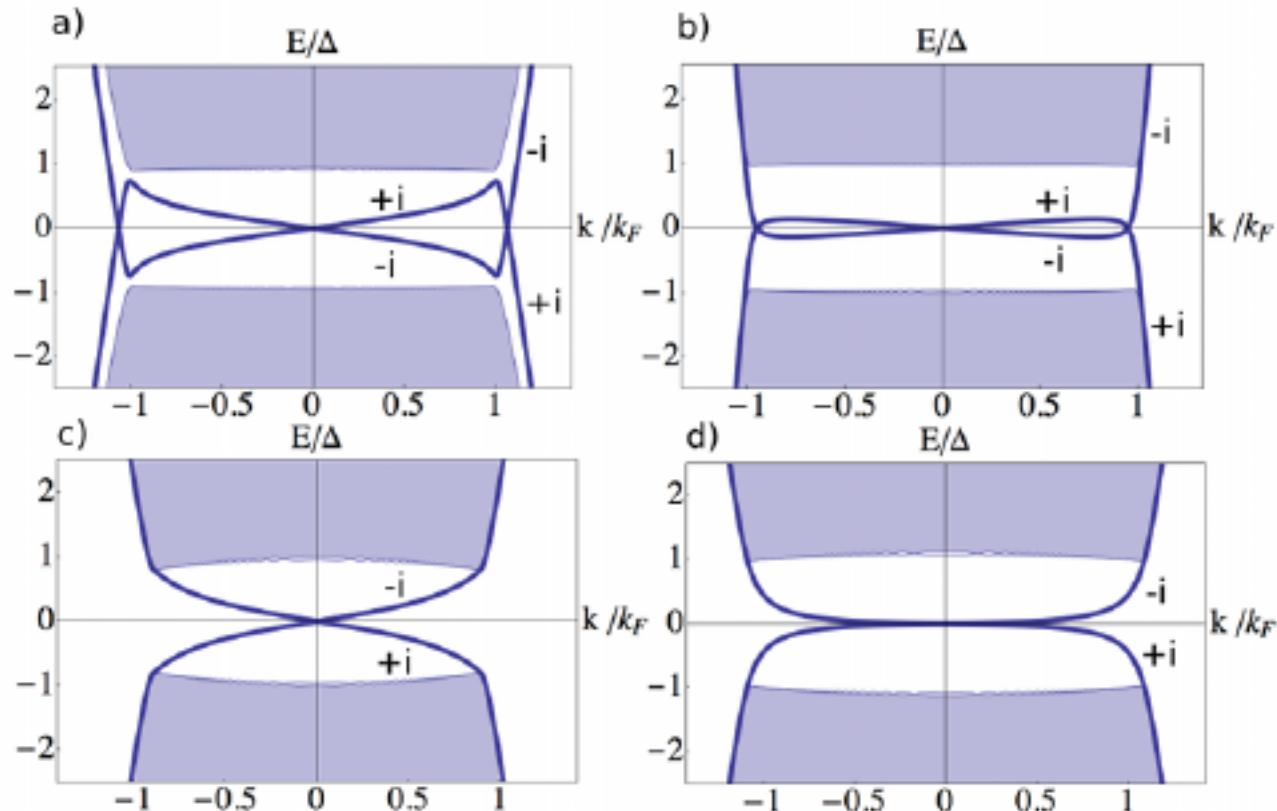


# 3d topological superconductors





Ando et al, PRL 2010



$$H_{\text{MF}} = H + \sum_{\langle i \in 1, j \in 2 \rangle} \frac{\Delta}{2} (c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger) + h.c.$$

Fu and Berg, PRL 2010

# Periodic table of topology

TABLE I. Periodic table of topological insulators and superconductors. The ten symmetry classes are labeled using the notation of Altland and Zirnbauer (1997) (AZ) and are specified by presence or absence of  $T$  symmetry  $\Theta$ , particle-hole symmetry  $\Xi$ , and chiral symmetry  $\Pi = \Xi\Theta$ .  $\pm 1$  and 0 denote the presence and absence of symmetry, with  $\pm 1$  specifying the value of  $\Theta^2$  and  $\Xi^2$ . As a function of symmetry and space dimensionality  $d$ , the topological classifications ( $\mathbb{Z}$ ,  $\mathbb{Z}_2$ , and 0) show a regular pattern that repeats when  $d \rightarrow d+8$ .

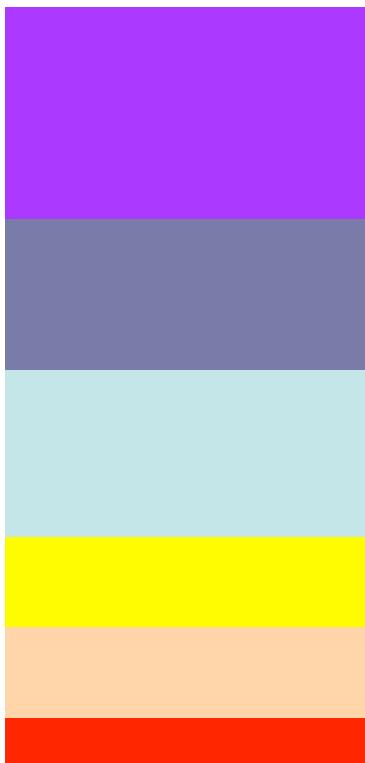
Symmetry				$d$							
AZ	$\Theta$	$\Xi$	$\Pi$	1	2	3	4	5	6	7	8
A	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AIII	0	0	1	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AI	1	0	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
BDI	1	1	1	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$
DIII	-1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0
AII	-1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$
CII	-1	-1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
C	0	-1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
CI	1	-1	1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0

# Challenges in the search of (intrinsic) topological superconductors

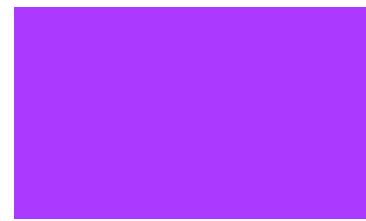
- Energy scale of topological insulators: eV
- Finding a BdG hamiltonian finishes only a half of the job
- Proximity effect generated topological superconductor depends solely on the edge (surface) states of topological insulator (many literatures in this direction)
- Intrinsic topological superconductor relies on the system itself, such as Sr<sub>2</sub>RuO<sub>4</sub> and He-III B-phase.
- In repulsive systems, the energy scale involved in superconducting transition:  $1 \sim 40\text{meV}$ . Energy hierarchy requires RG treatment.

# Ideas of RG and FRG

Wilson RG



Wetterich FRG



Energy Scale



# Ideas of RG and FRG

Wilson RG



Wetterich FRG

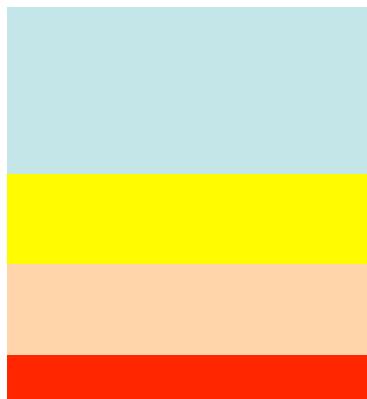


Energy Scale

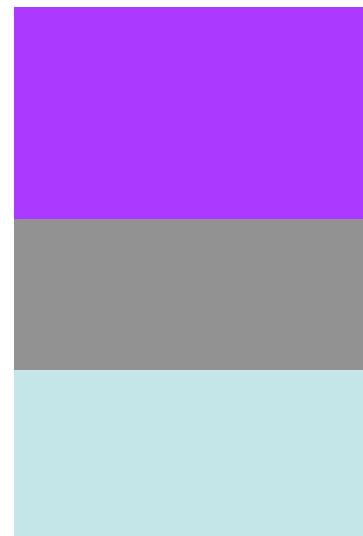


# Ideas of RG and FRG

Wilson RG



Wetterich FRG

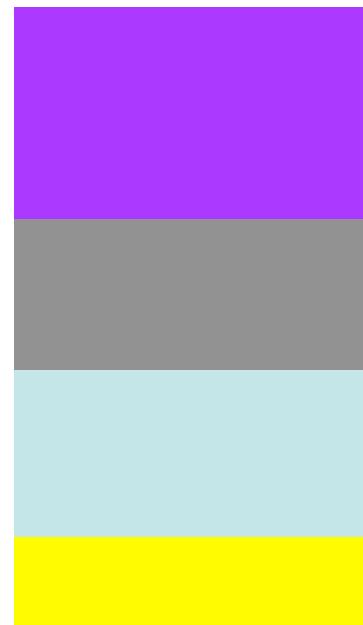


# Ideas of RG and FRG

Wilson RG



Wetterich FRG



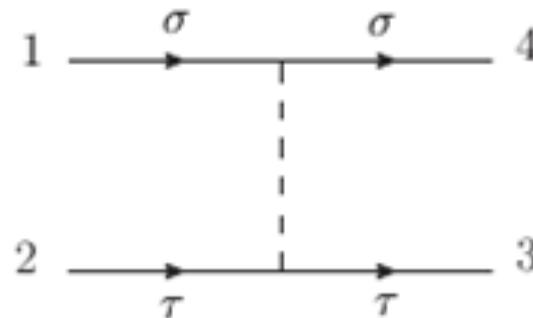
Energy Scale



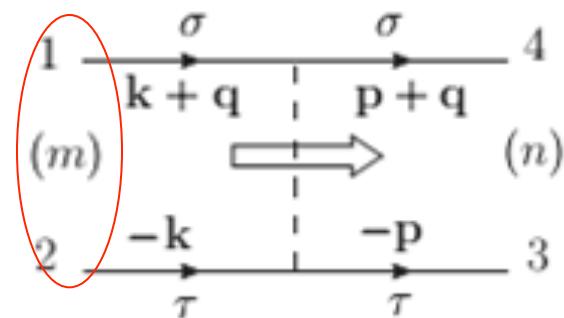
# Singular-mode FRG

Cf: Husemann and Salmhofer

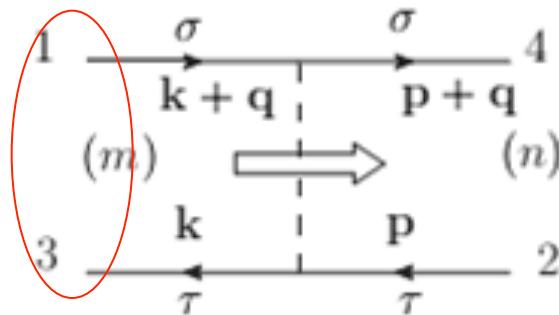
$$c_1^\dagger c_2^\dagger (-\Gamma_{1234}) c_3 c_4$$



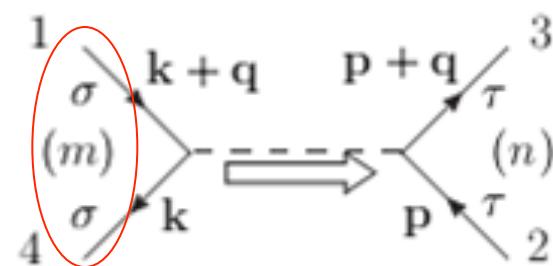
P



C

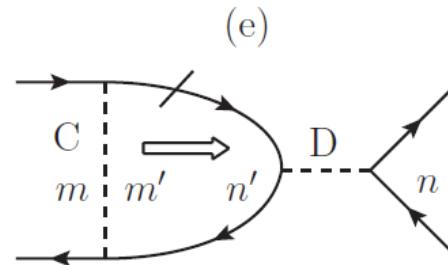
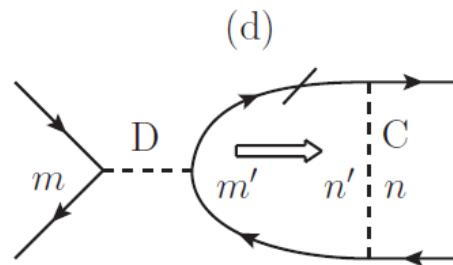
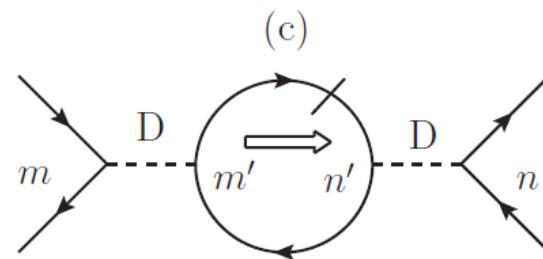
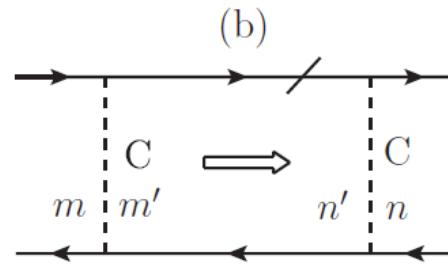
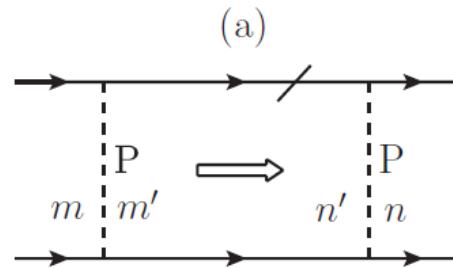


D



$\{f_m\}$ : orthonormal form factors

# FRG flow



# FRG flow

$$\partial P / \partial \Lambda = P \chi'_{pp} P,$$

$$\partial C / \partial \Lambda = C \chi'_{ph} C,$$

$$\partial D / \partial \Lambda = (C - D) \chi'_{ph} D + D \chi'_{ph} (C - D),$$

# FRG flow

$$\begin{aligned} dP/d\Lambda &= \partial P/\partial\Lambda + \hat{P}(\partial C/\partial\Lambda + \partial D/\partial\Lambda), \\ dC/d\Lambda &= \partial C/\partial\Lambda + \hat{C}(\partial P/\partial\Lambda + \partial D/\partial\Lambda), \\ dD/d\Lambda &= \partial D/\partial\Lambda + \hat{D}(\partial P/\partial\Lambda + \partial C/\partial\Lambda), \end{aligned}$$

# A simple view of mode-mode coupling

$$\pm c_{i\sigma}^+ c_{i\sigma} c_{j\tau}^+ c_{j\tau} \Leftrightarrow \pm c_{i\sigma}^+ c_{j\tau}^+ c_{j\tau} c_{i\sigma}$$

$$S_i \cdot S_j \Leftrightarrow -\frac{1}{2}(c_{i\uparrow}^+ c_{j\downarrow}^+ - c_{i\downarrow}^+ c_{j\uparrow}^+)(c_{j\downarrow} c_{i\uparrow} - c_{j\uparrow} c_{i\downarrow}) + \dots \Rightarrow \uparrow\downarrow - \downarrow\uparrow$$

Singlet pair

$$-S_i \cdot S_j \Leftrightarrow -\frac{1}{4}c_{i\uparrow}^+ c_{j\uparrow}^+ c_{j\uparrow} c_{i\uparrow} + \dots \Rightarrow \uparrow\uparrow, \quad \downarrow\downarrow, \quad \uparrow\downarrow + \downarrow\uparrow$$

Triplet pair

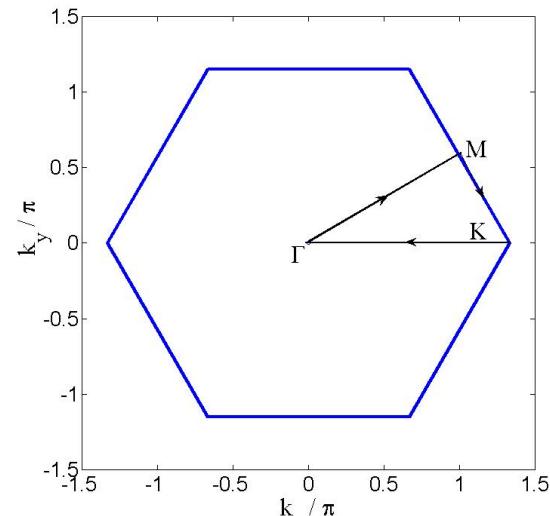
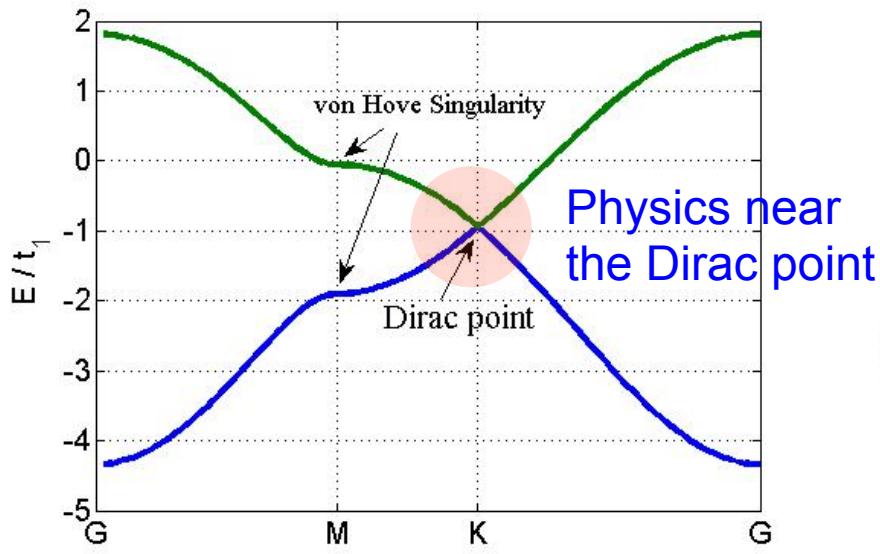
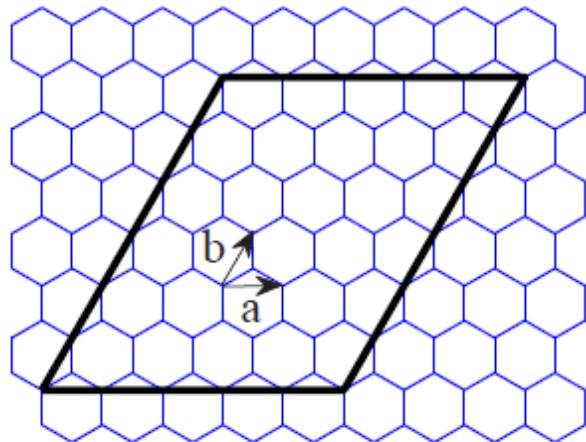
+ more general bond-type density wave interactions

# Instabilities

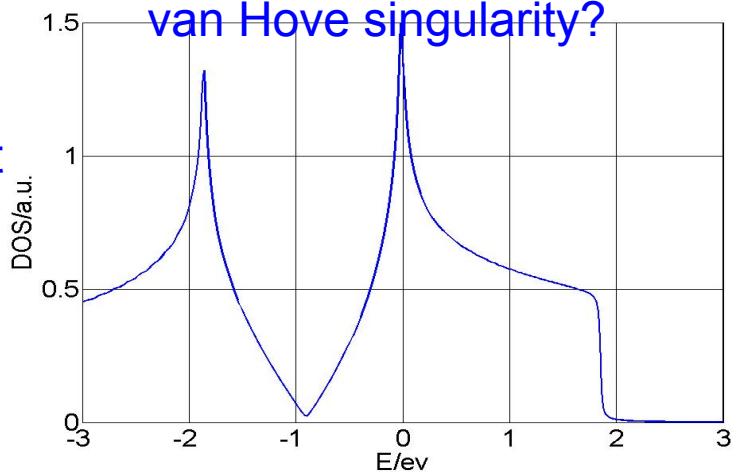
- $Q=0$  p-p susceptibility always logarithmically divergent → universal Cooper instability wrt infinitesimal attraction
- p-h susecptibility usually finite (unless in case of perfect nesting or van Hove singularity) → Stoner instability wrt finite interaction

- Introduction and motivation
- T-breaking topological phases in doped Graphene and kagome lattices
- T-invariant topological superconductors
- Conclusions

# Band structure of graphene



Physics near  
van Hove singularity?



The band structure of graphene with  
 $t_1=2.8$  eV,  $t_2=0.1$  eV,  $t_3=0.07$  eV at  $\frac{1}{4}$  doping

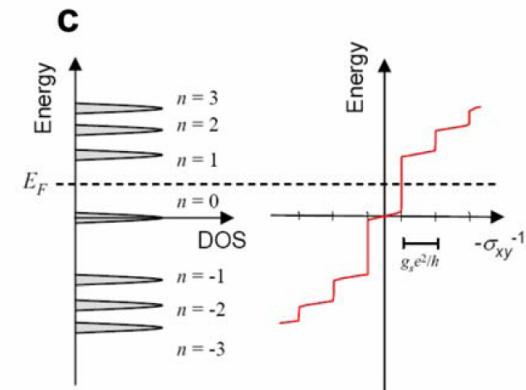
# Relativistic quantum mechanics near the Dirac point

Semenoff, PRL53,2449,1984

$$-iv_F \boldsymbol{\sigma} \cdot \nabla \psi(\mathbf{r}) = E \psi(\mathbf{r}).$$

$$\psi_{\pm, \mathbf{K}}(\mathbf{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta_{\mathbf{k}}/2} \\ \pm e^{i\theta_{\mathbf{k}}/2} \end{pmatrix} \quad \psi_{\pm, \mathbf{K}'}(\mathbf{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta_{\mathbf{k}}/2} \\ \pm e^{-i\theta_{\mathbf{k}}/2} \end{pmatrix}$$

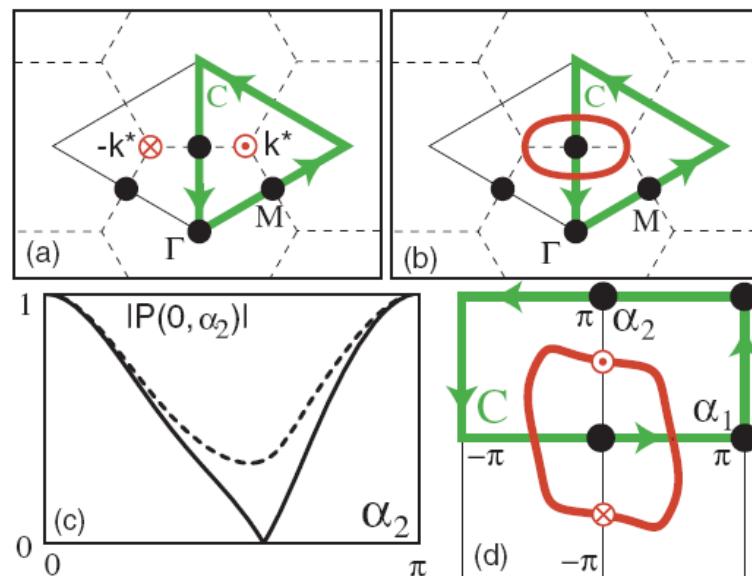
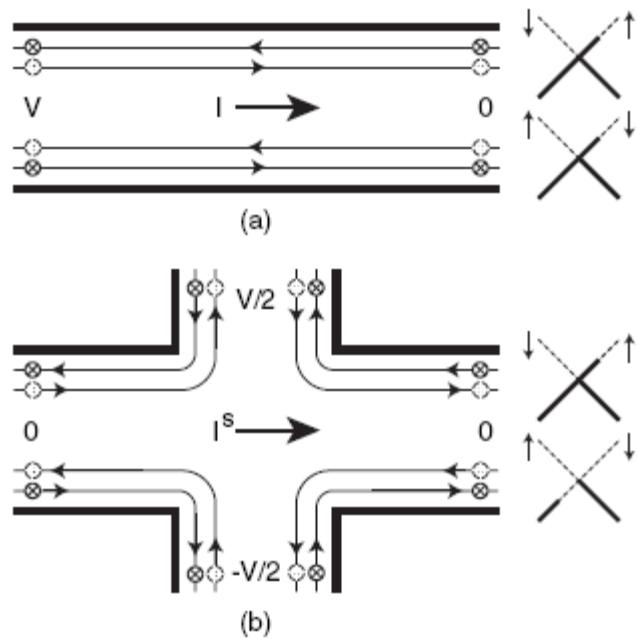
$$\sigma_{xy} = \frac{I}{V_H} = \frac{c}{V_H} \frac{\delta E}{\delta \Phi} = \pm 2(2N+1) \frac{e^2}{h},$$



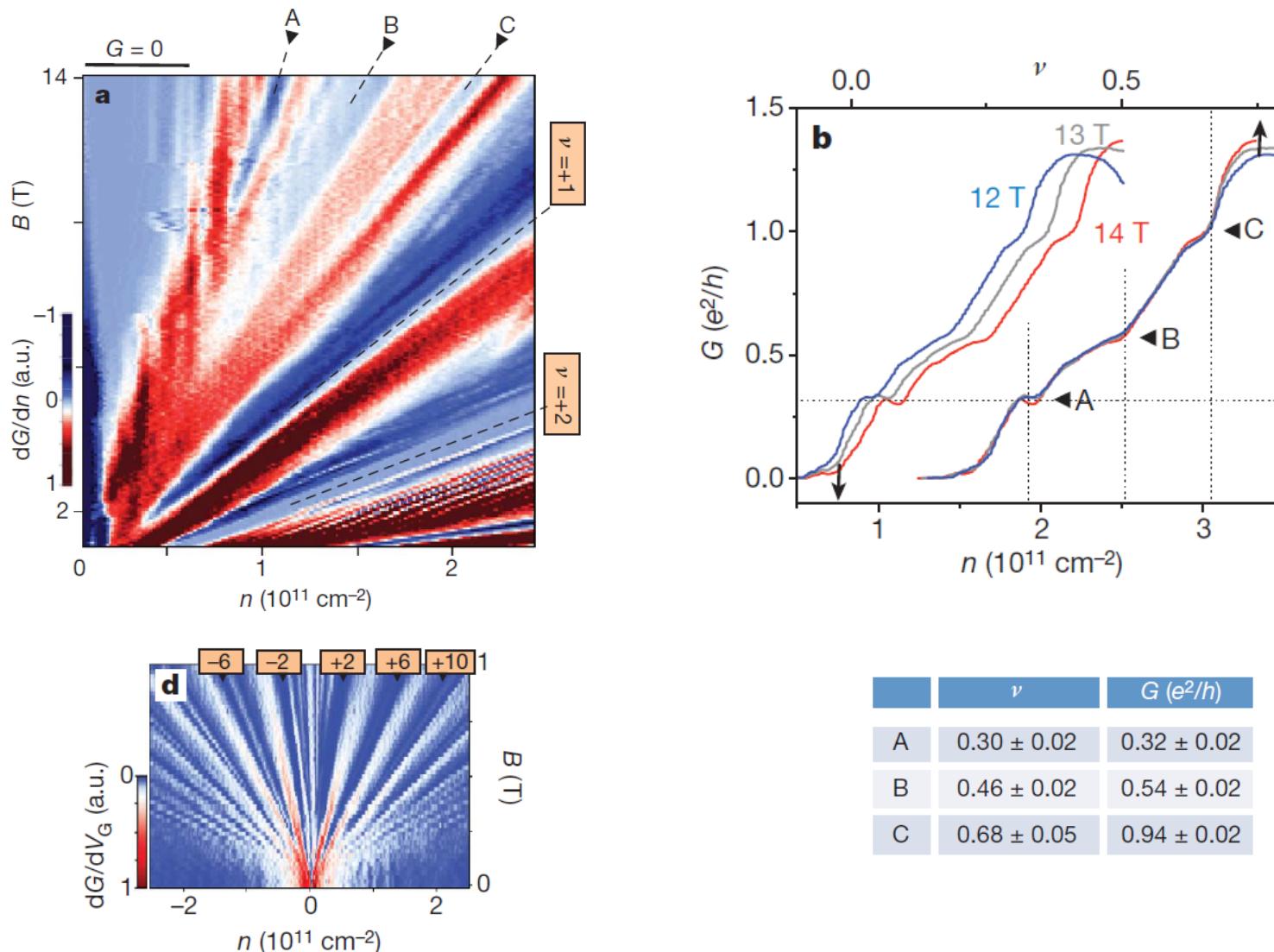
# Spin quantum Hall effect?

C. L. Kane and E.J. Mele , QSHE in Graphene , PRL95,226801(2005)

C. L. Kane and E. J. Mele, Z2 topological Order and the QSHE,  
PRL95, 146802 (2005)



# Correlations revealed by fractional QH



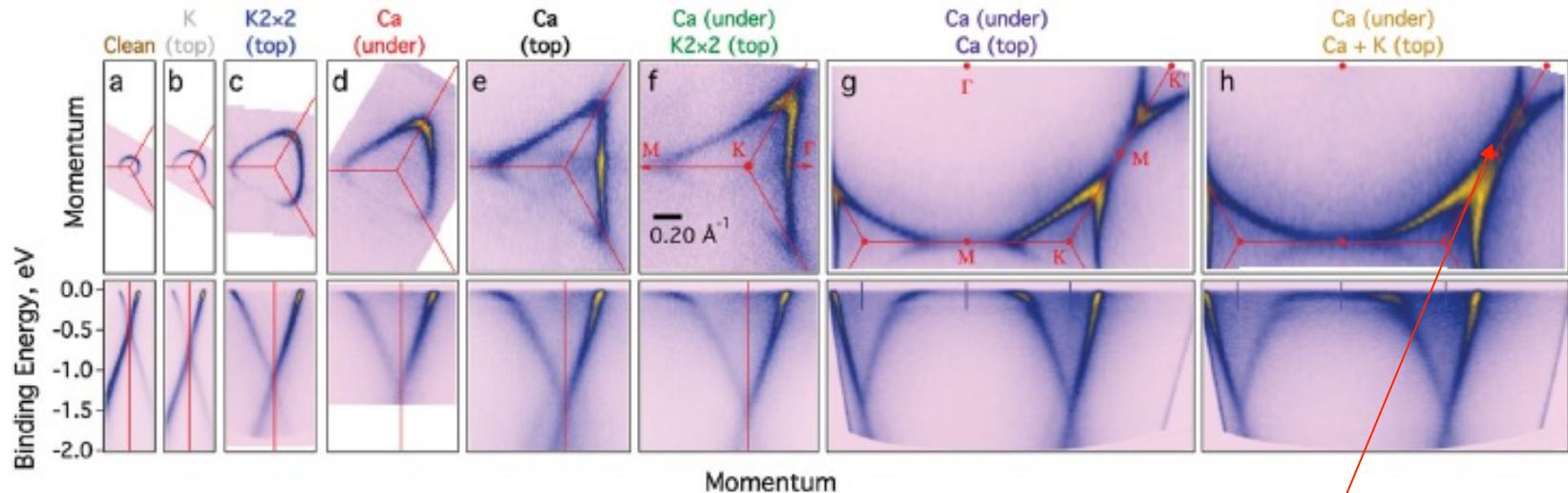
# Doping graphene...

Eli Rotenberg

PRL 104, 136803 (2010)

PHYSICAL REVIEW LETTERS

week ending  
2 APRIL 2010



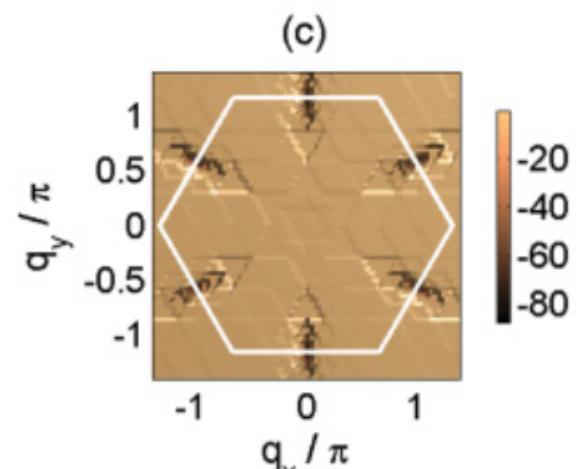
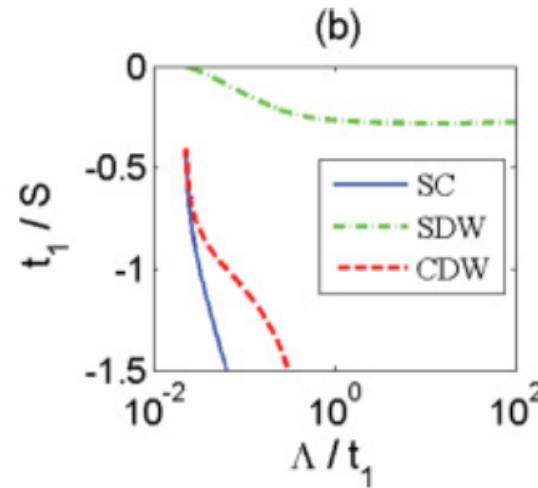
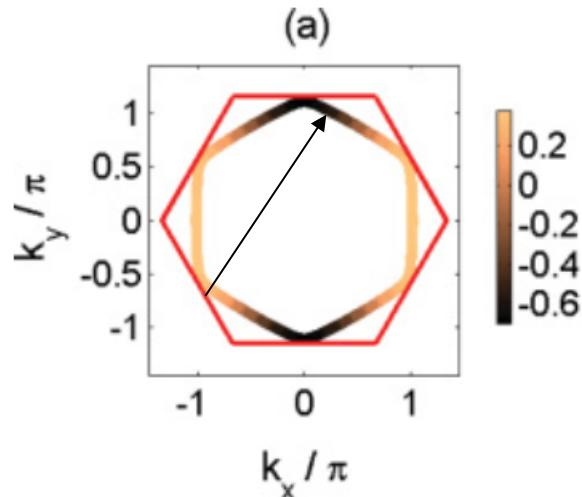
Extended van Hove singularity

# What's so special of graphene

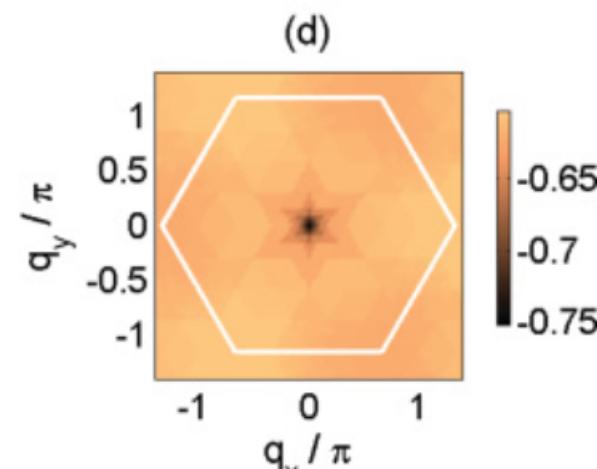
- van Hove singularity and correlation effect
- Under  $C_{6v}$  point group,  $(x^2 - y^2, xy)$  and  $(x, y)$  are doublets. Candidates for the gap function.
- T-breaking mixing of degenerate pairing gaps very likely, leading to a full gap
- Possible pairing symmetries: s, d+id, p+ip, f

$x=1/4$ ,  $U=3.6t$ ,  $V=0$

Van Hove singularity and perfect nesting



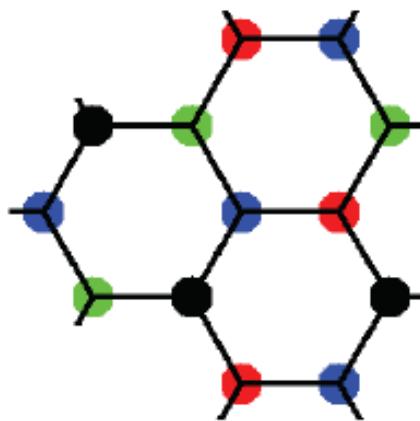
$V_{\text{sdw}}$



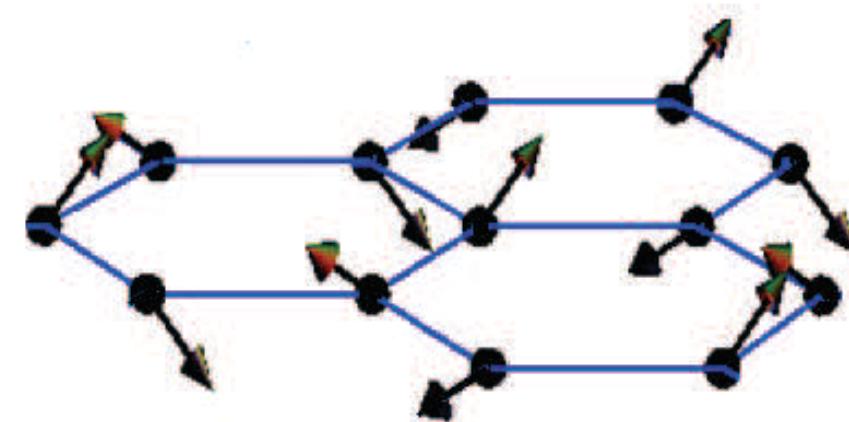
$V_{\text{sc}}$

# Chiral SDW

(a)

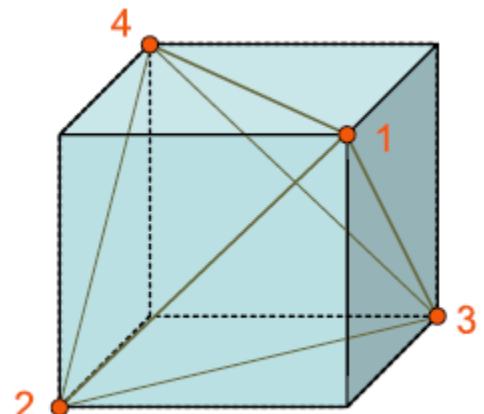


(b)

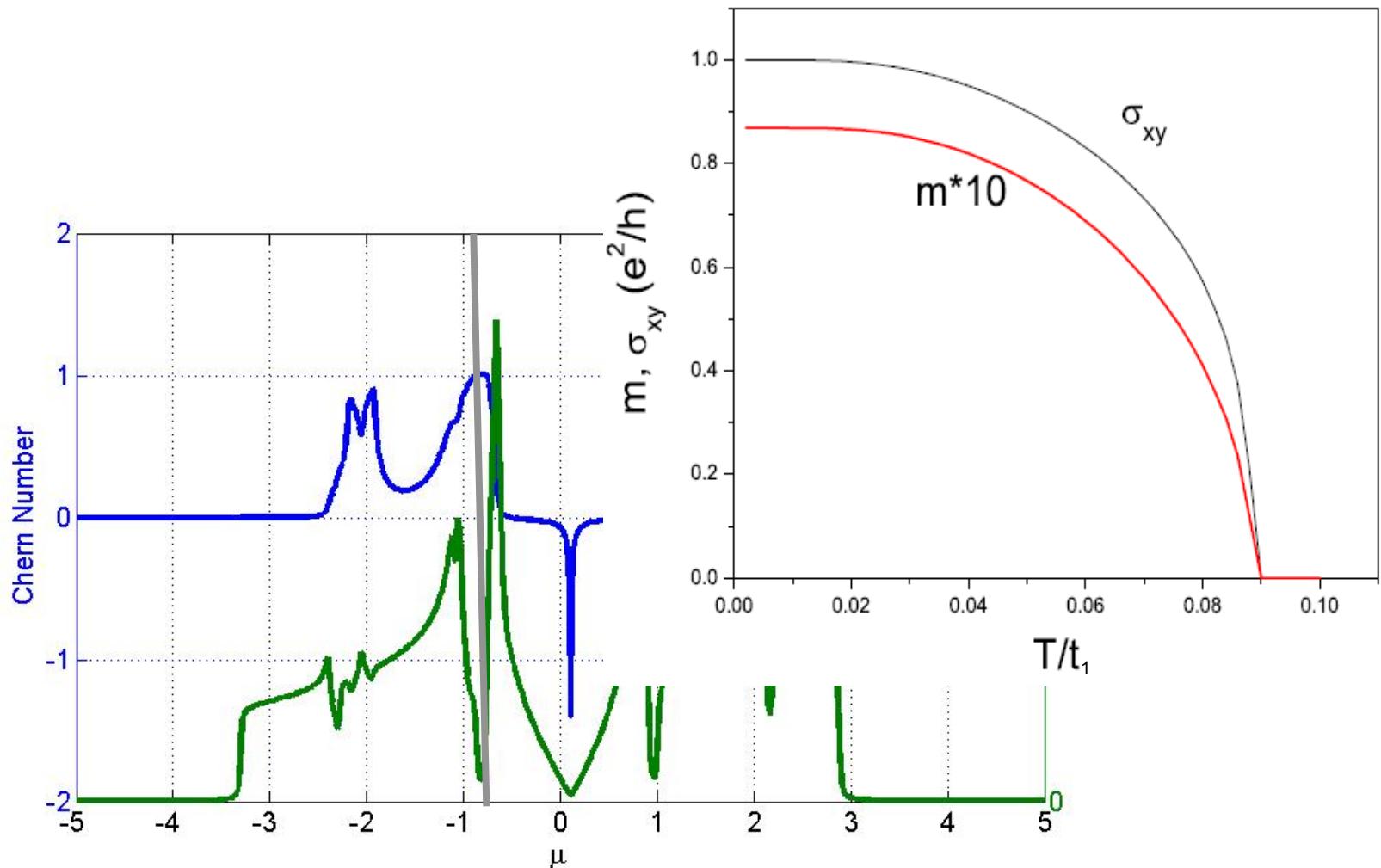


LiTao, arxiv 1103.2420, honeycomb lattice

Martin and Batista, PRL101,156402, triangle lattice



# Chern number and quantized anomalous Hall conductivity



# Non-perturbative quantum Monte Carlo

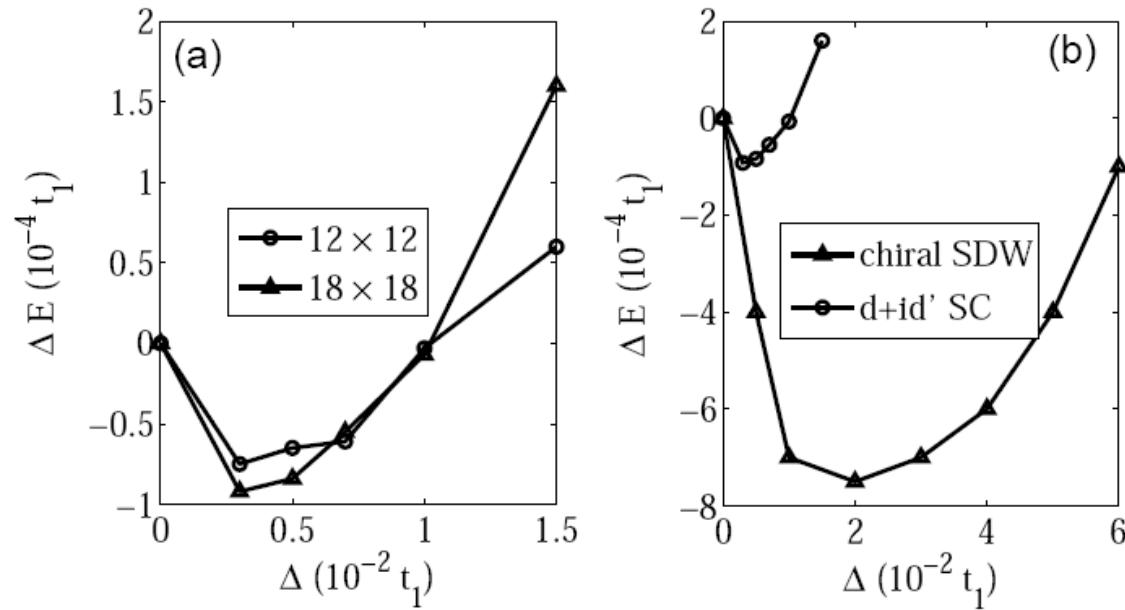
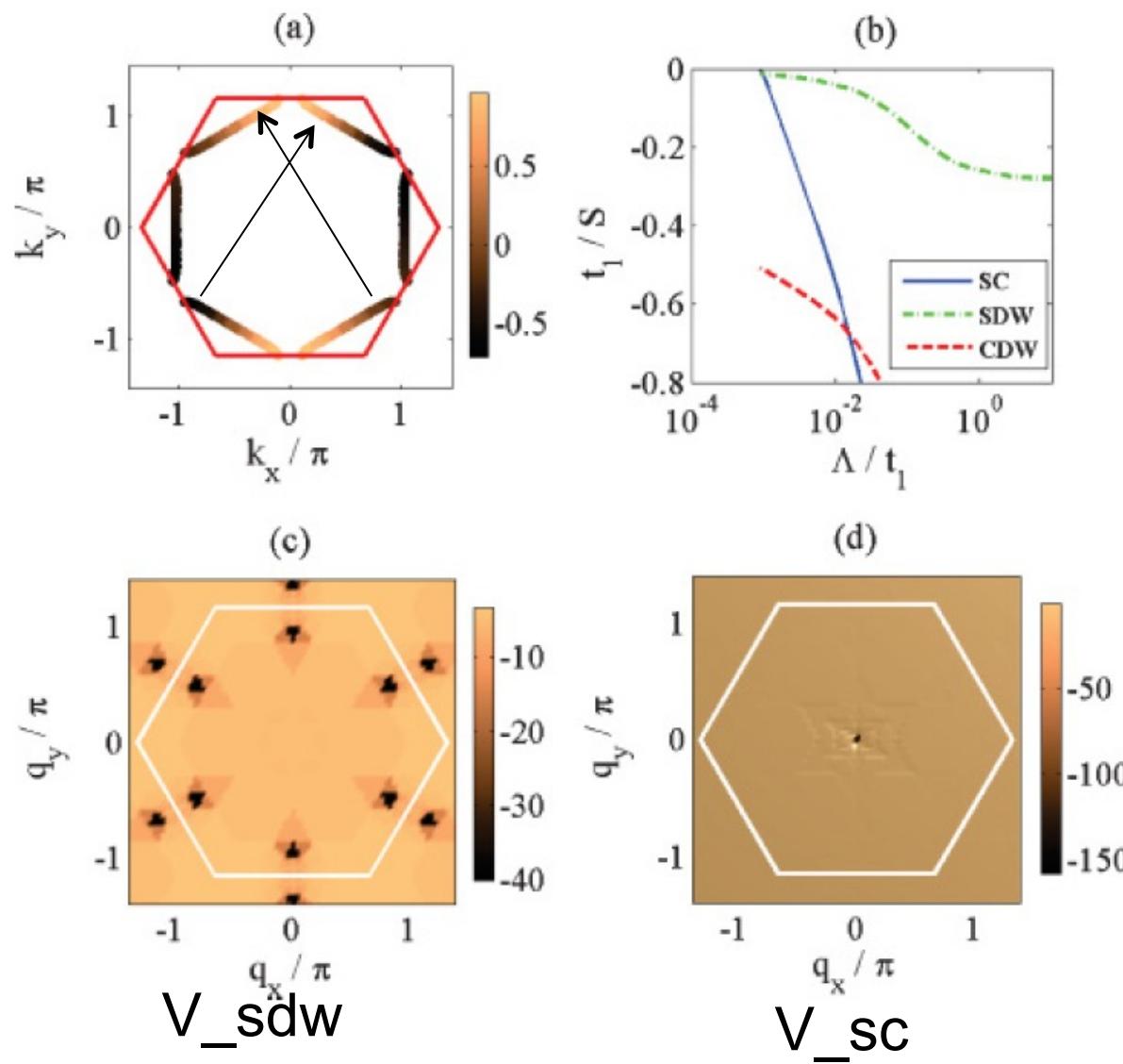


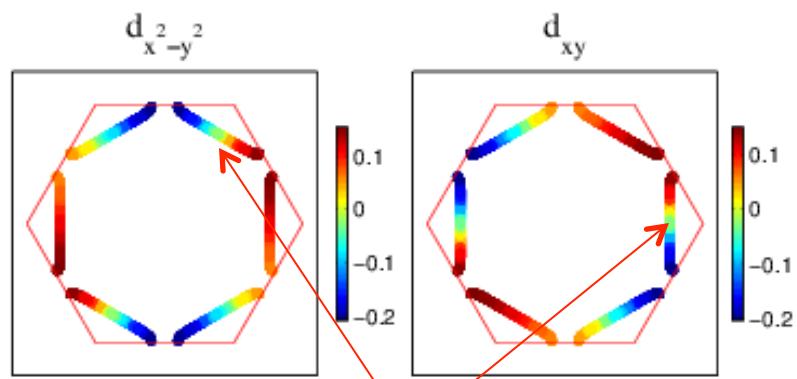
FIG. 3: Variational Monte Carlo results for  $\delta = 1/4$ . (a) The energy gain per site due to  $d+id'$  SC order on  $12 \times 12$  (circles) and  $18 \times 18$  (triangles) lattices, showing negligible finite-size effect.(b) The energy gain per site due to  $d+id'$  SC (circles) and chiral SDW (triangles) order parameters on an  $18 \times 18$  lattice.

$x=0.211$ ,  $U=3.6t$ ,  $V=0$

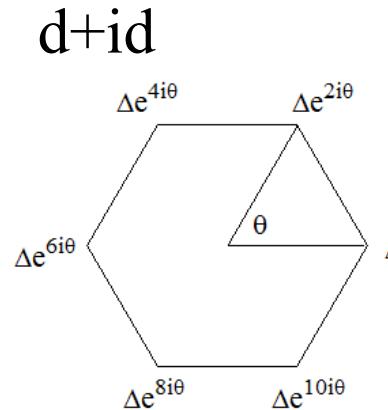


# T-breaking d+id

Two degenerate d-wave pairing:



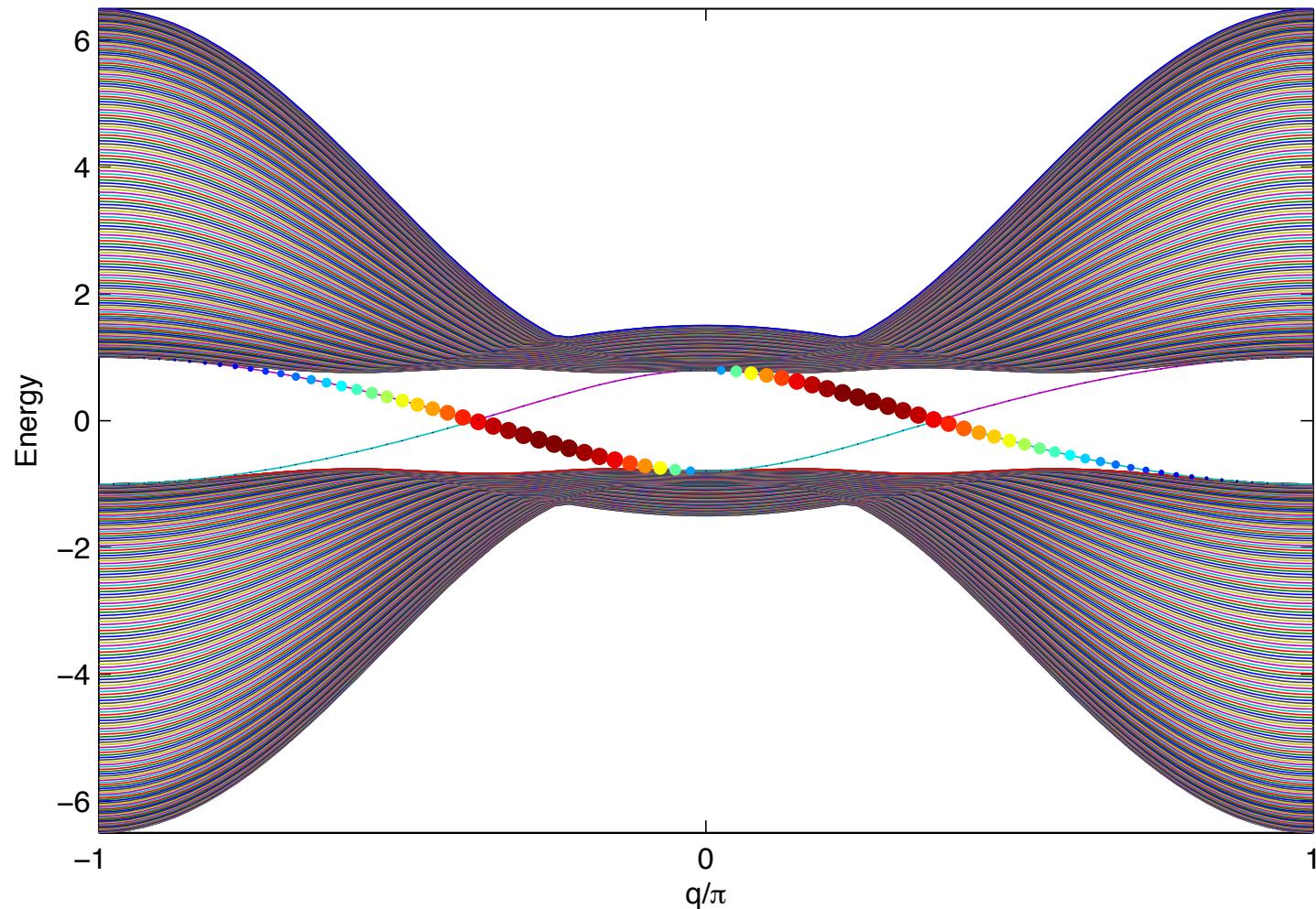
Nodal gap



MF or GL theory predict that the d+id pairing is energetically more favorable

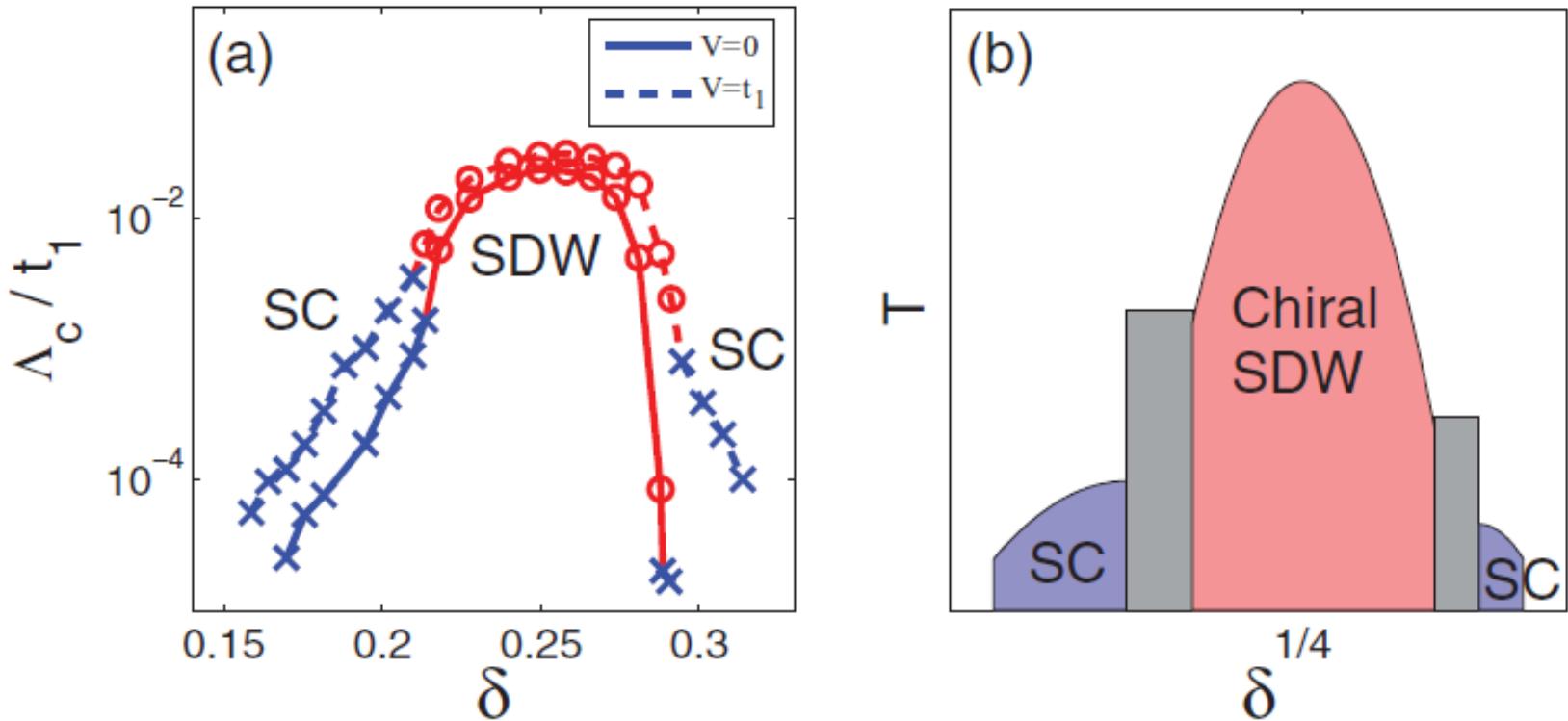
R Nandkishore et al, Nature Physics 8, 158 (2012)

# Edge states for d+id pairing ( $Z=2$ )



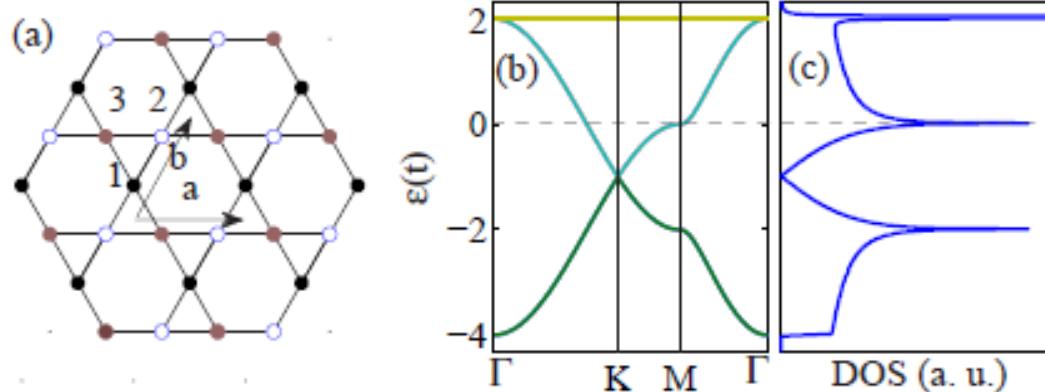
Cf: Keisel et al, arxiv 1109.2953

# Phase diagram

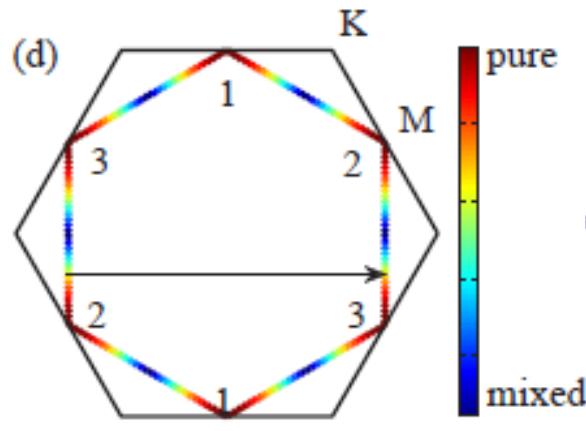


Both chiral SDW and chiral d+id are topological.

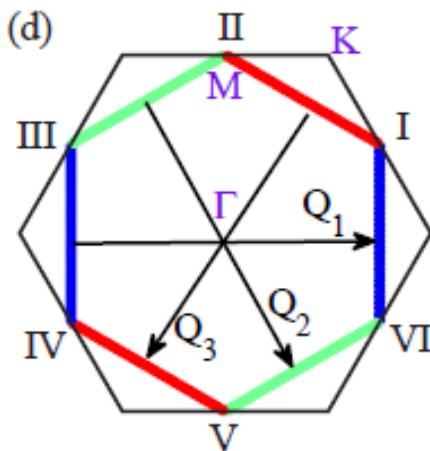
# Kagome lattice



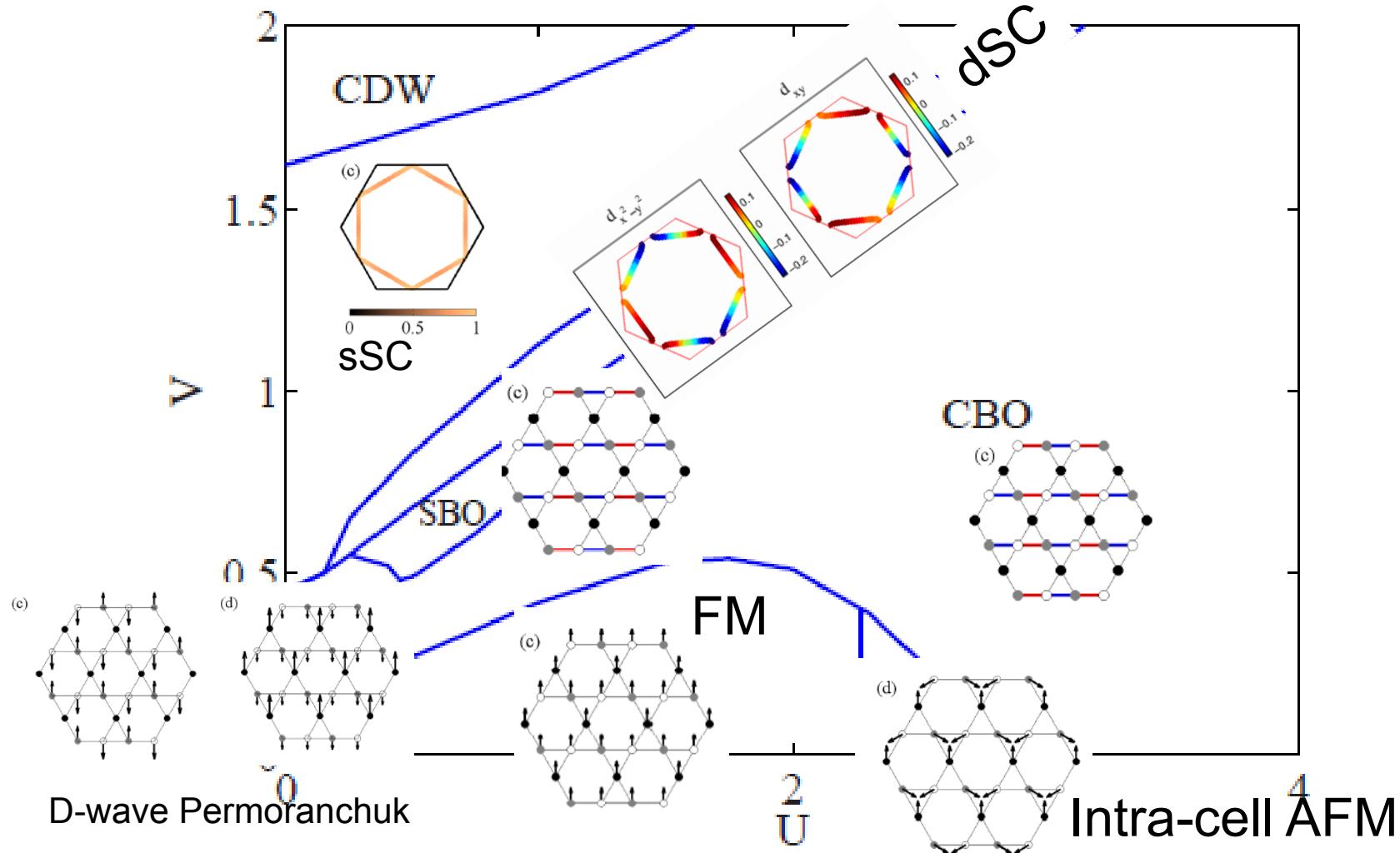
Upper van Hove filling



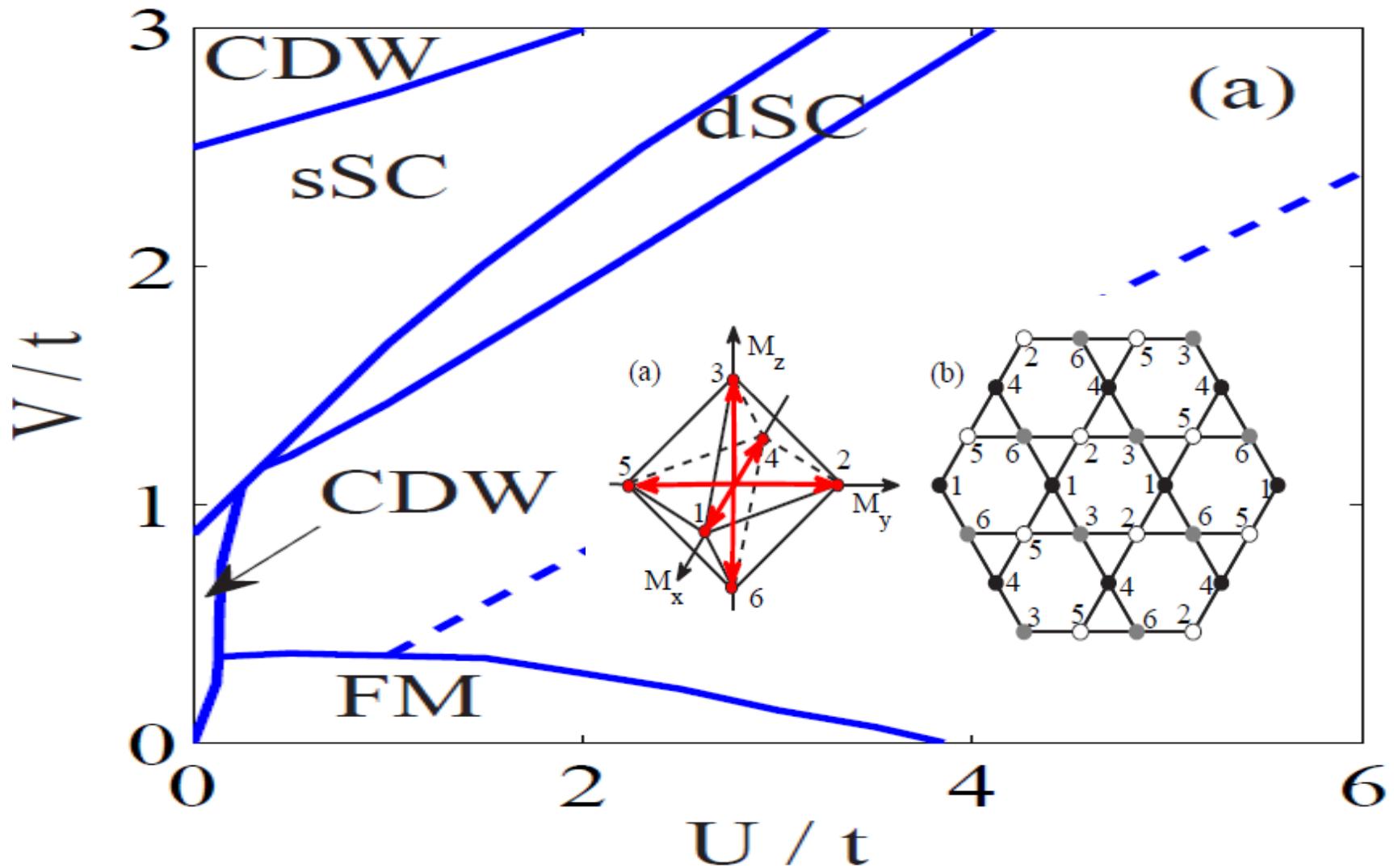
Lower van Hove filling



# Upper van Hove filling



# Lower van Hove filling



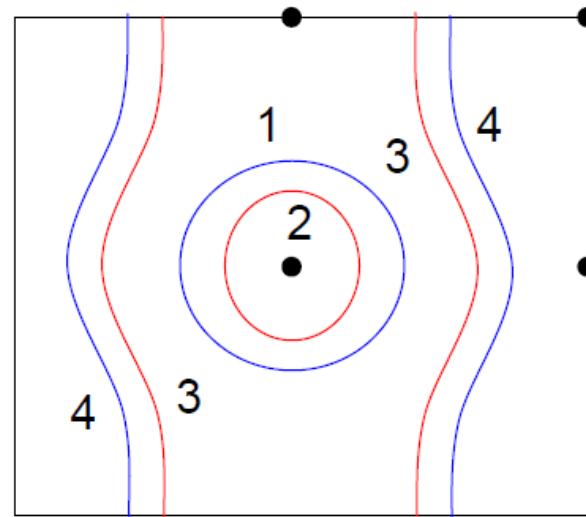
- Topological states of matter and challenges of the search of intrinsic topological superconductors
- T-breaking topological phases in doped Graphene
- T-invariant topological superconductors, a road map
- Conclusions

# Gap function of a T-invariant superconductor

$$B^\dagger = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \Delta_{\mathbf{k}} \Psi_{-\mathbf{k}}^{\dagger T}$$

$$\Delta(\mathbf{k}) = [\phi(\mathbf{k})\sigma_0 + \vec{d}(\mathbf{k}) \cdot \vec{\sigma}] i\sigma_2,$$

singlet                    triplet



Qi et al, Kitaev et al:

- 1) Even number of spin-split pockets, each encircles an odd number of T-invariant momenta.
- 2) Number of pockets with + and - signs: Even = Odd + Odd

# Gap-function of a T-invariant superconductor

$$\underline{\gamma_k = (-\sin k_y, \sin k_x, 0)}$$

$$H_0 = \Psi_k^+ (\varepsilon_k \sigma_0 + \lambda \gamma_k \cdot \sigma) \Psi_k \rightarrow \psi_k^+ (\varepsilon_k \pm \lambda |\gamma_k|) \psi_k,$$

$$|-k, a\rangle = i\sigma_2 K |k, a\rangle$$

If  $d_k \sim \gamma_k$ ,  $T$ -invariant, and

$$\begin{aligned} H_P &= \Psi_k^+ (\phi_k \sigma_0 + d_k \cdot \sigma) i\sigma_2 (\Psi_{-k}^+)^T \\ &\rightarrow -\psi_{k,a}^+ (\phi_k \pm |d_k|) (\psi_{-k,b}^+)^T \delta_{a,b} \end{aligned}$$

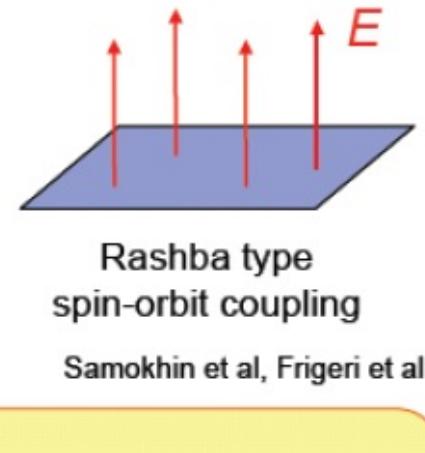
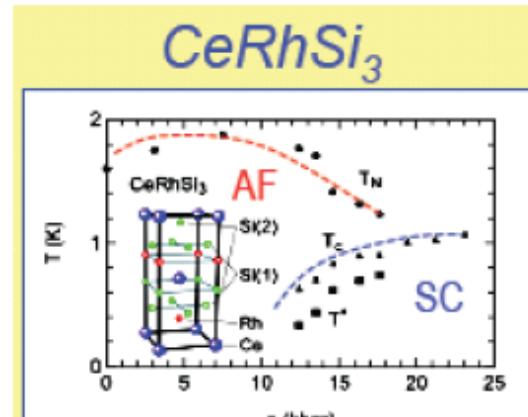
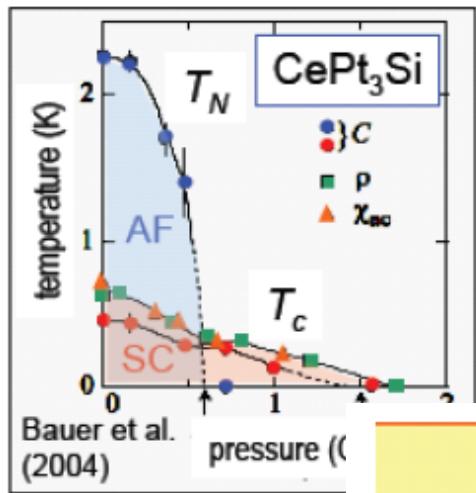
$$i(p_x+ip_y)\downarrow\downarrow+i(p_x-ip_y)\uparrow\uparrow$$

# Our road map

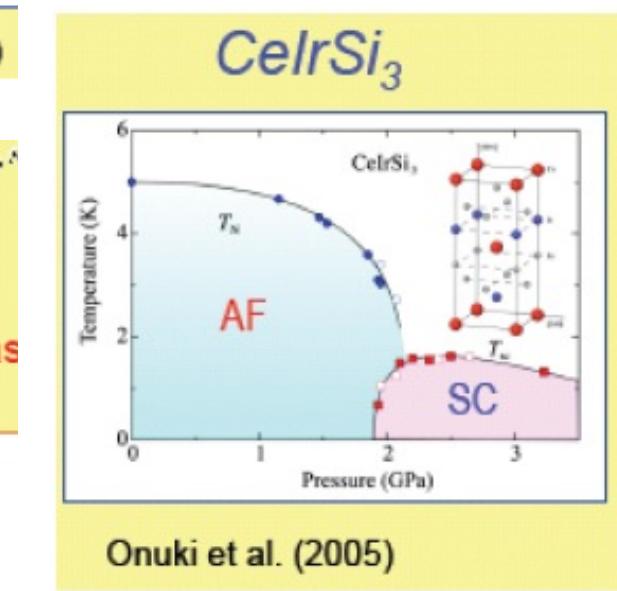
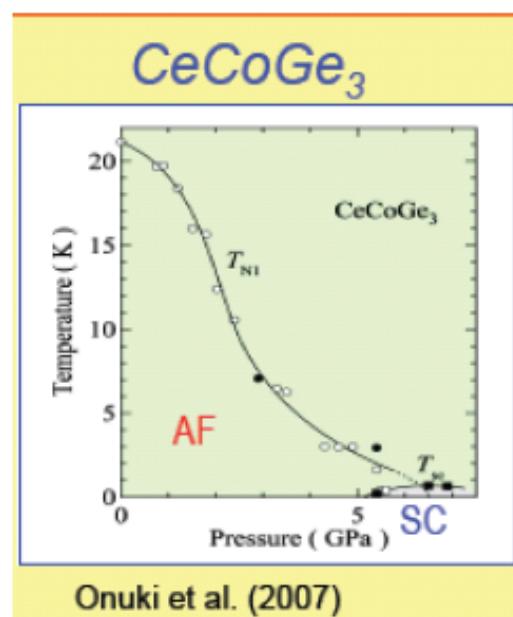
- Seek ferromagnetic spin fluctuations to favor triplet pairing
- Seek point group with odd parity degenerate irreducible representation (such as  $C_{4v}$  and  $C_{6v}$ )
- Seek a system with  $2(2n+1)$  spin-split pockets
- Rashba coupling causes degenerate triplets to recombine into a T-invariant gap, plus small induced singlet component.

# Non-centrosymmetric systems

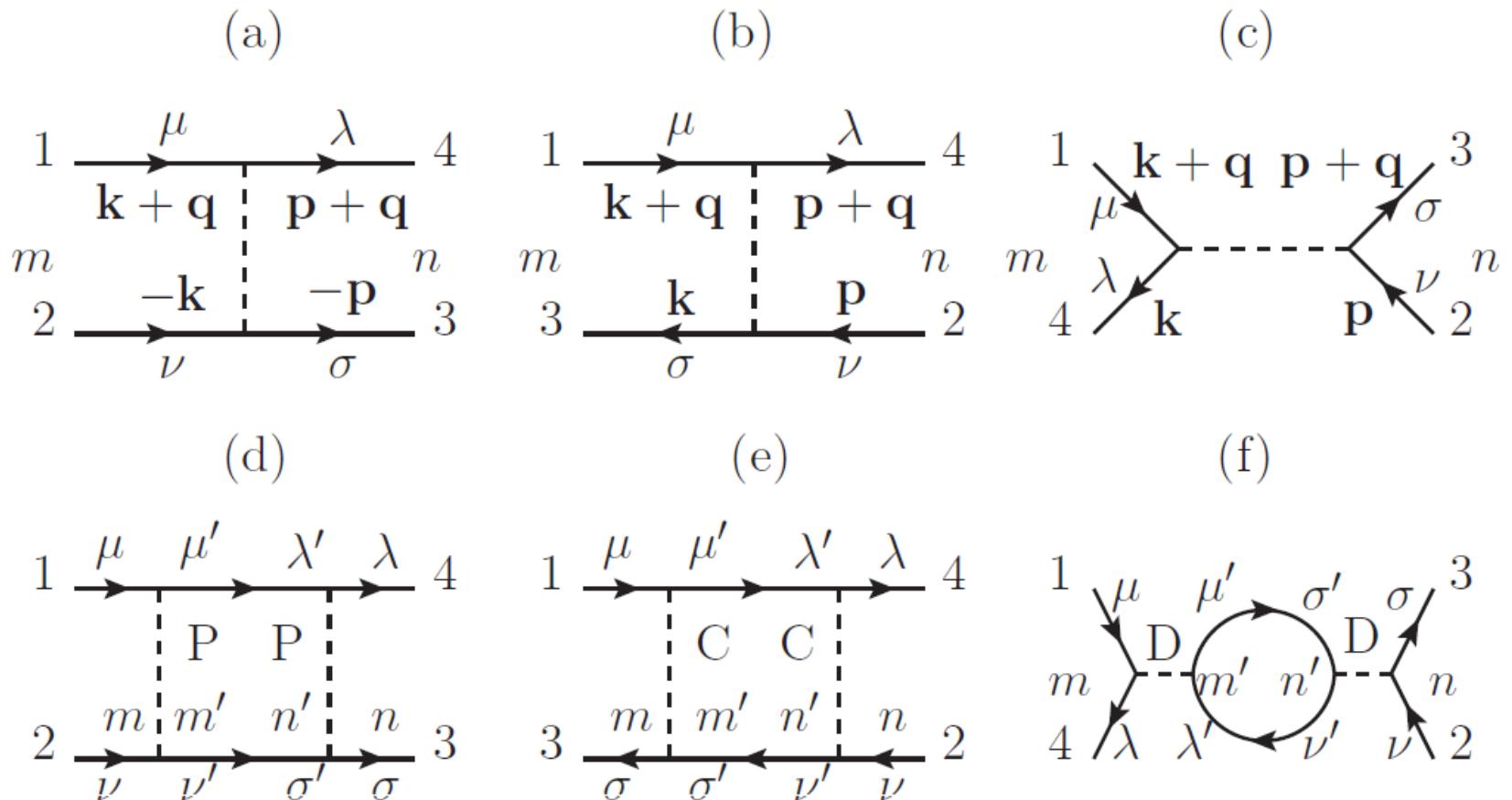
Ce-based heavy Fermion SC



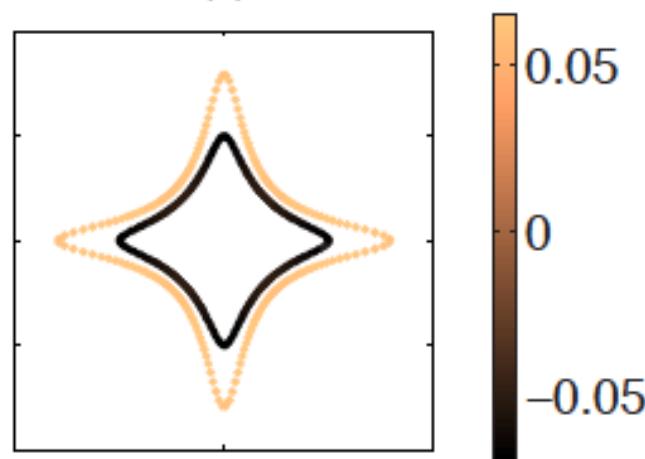
standard  
non-r  
band struc



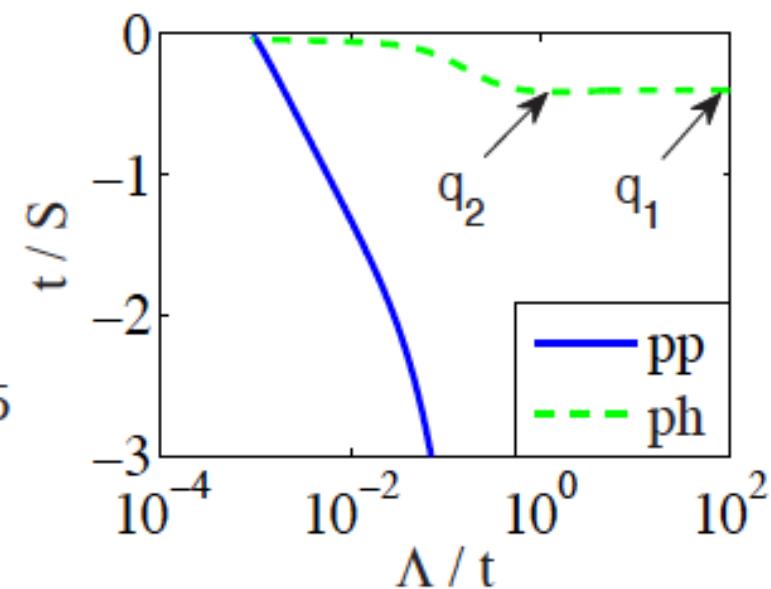
# Spin-resolved fully anti-symmetrized SM-FRG



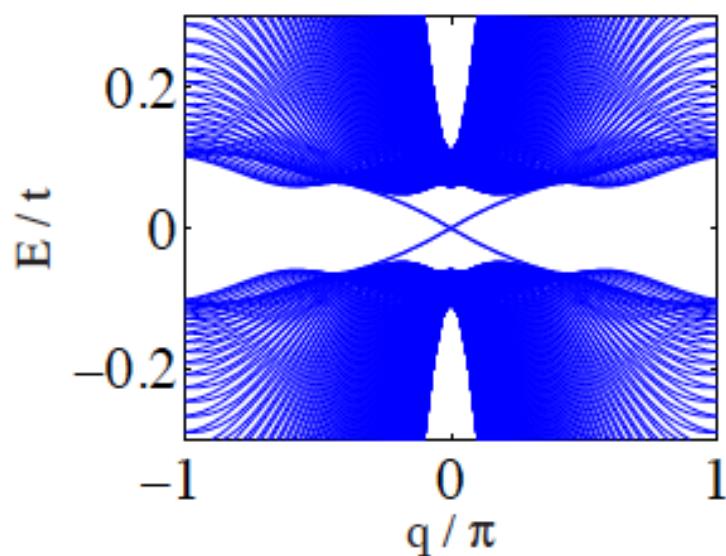
(a)



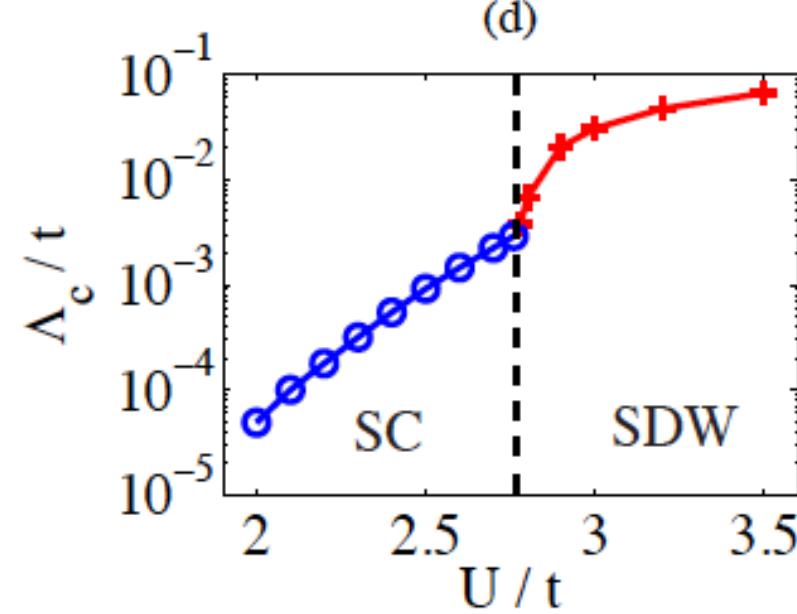
(b)



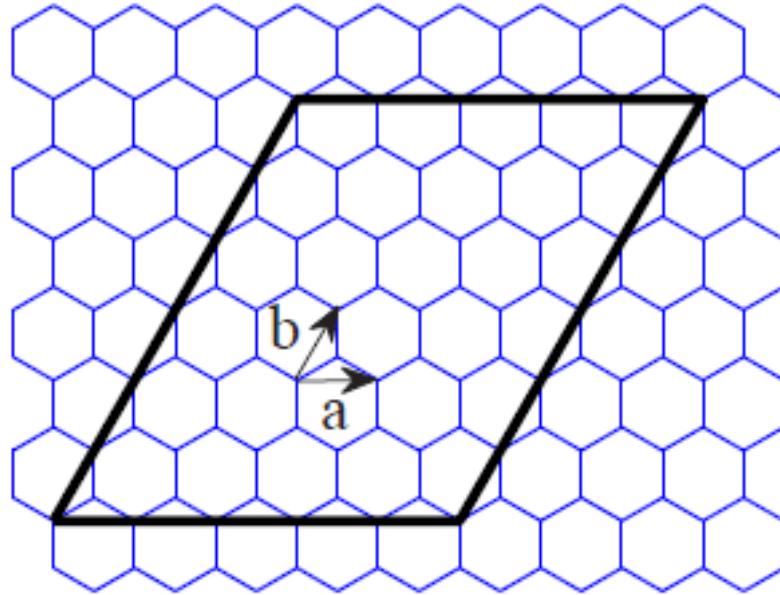
(c)



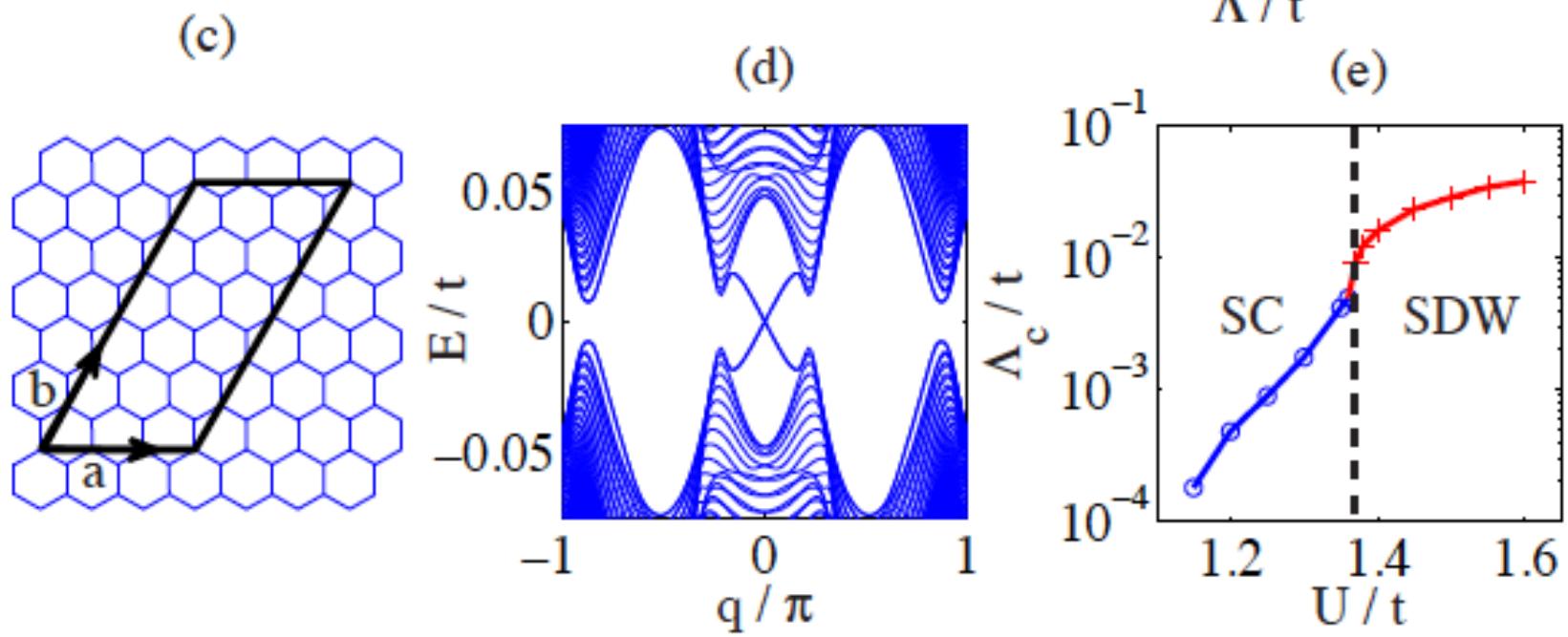
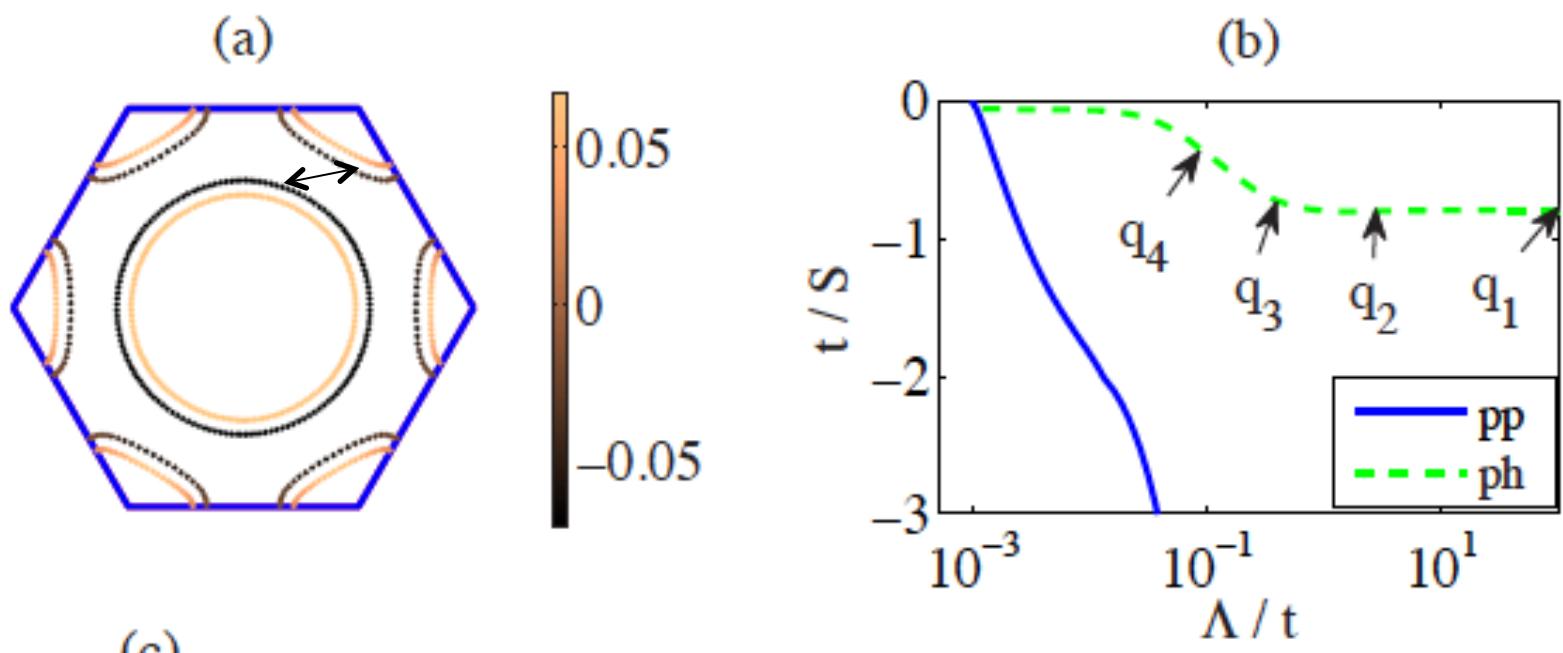
(d)



# Topological pairing triggered by small-q inter-pocket scattering



$$H_0 = - \sum_{i\delta} \Psi_i^\dagger t_\delta \Psi_{i+\delta} - i\lambda \sum_{i\delta_{nn}} \Psi_i^\dagger (\hat{z} \times \vec{\delta}_{nn} \cdot \vec{\sigma}) \Psi_{i+\delta_{nn}} - \mu \sum_i \Psi_i^\dagger \Psi_i. \quad (3)$$



# Possible candidates with ferromagnetic spin fluctuations

$\text{Li}_2\text{Pd}_3\text{B}$ ,  $\text{Li}_2\text{Pt}_3\text{B}$ ,  $\text{URhGe}$ ,  $\text{HoMo}_6\text{Se}_8$ ,  $\text{ErRh}_4\text{B}_4$ .  
Aoki and Flouquet, JPSJ 81, 011003 (2012).

Iron under high pressure  
Shimizu et al, NATURE 412, 316 (2001).

$\text{LaAlO}_3/\text{SrTiO}_3$   
Reyren, et al, Science 317, 1196 (2007).

- Motivation
- T-breaking topological phases in doped Graphene
- T-invariant topological superconductors, a road map
- Conclusions

# Conclusions

- Graphene near  $\frac{1}{4}$  doping is either a Chern insulator or a chiral  $d+id$  superconductor.
- Ferromagnetic instability is the key to T-invariant topological insulator, plus Rashba coupling and  $2(2n+1)$  spin split fermi pockets (encircling T-invarint momenta).
- T-invariant topo-SC can be triggered by 1) proximity to van Hove singularity and 2) by small-q inter-pocket scattering

Thank you for your attention