HUNGARIAN ACADEMY OF SCIENCES
WIGNER RESEARCH CENTRE FOR PHYSICS

MŰEGYETEM 1782

Topological superconductors – connections to 1st semester

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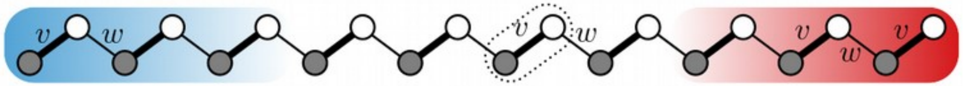
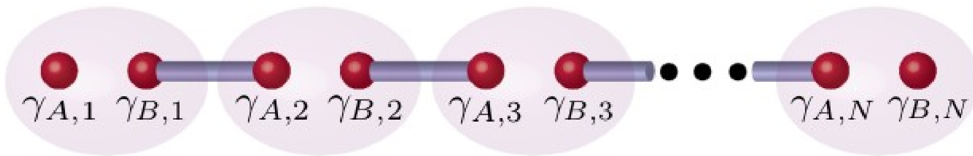
Budapest, 2020 April 22

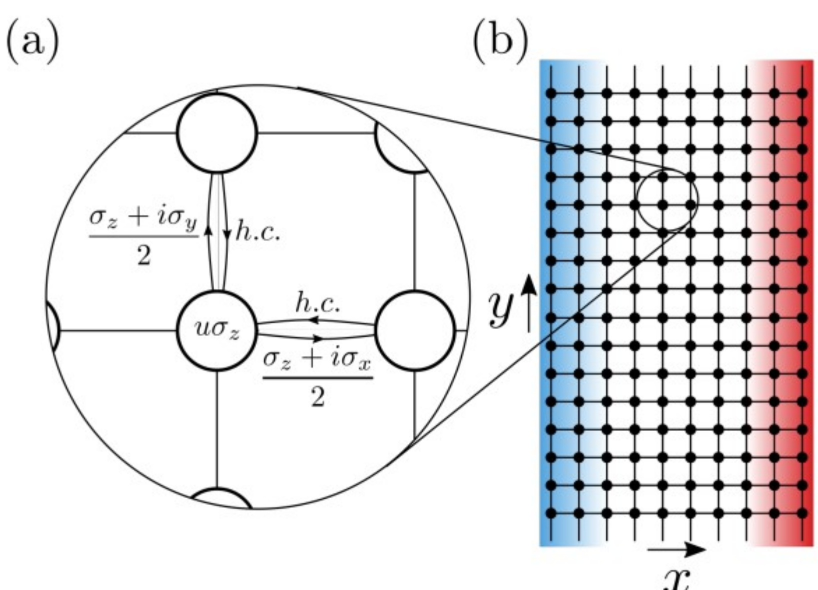
Single-particle topological Hamiltonians 1st semester can be understood as BdG Hamiltonians



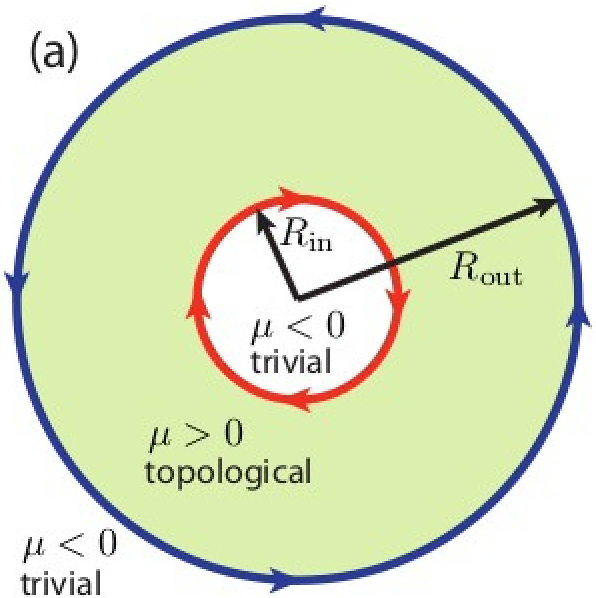
Su-Schrieffer-Heeger model
topological nanowire



Kitaev model for topological
superconductor nanowire
with / without chiral symmetry



Qi-Wu-Zhang model
2D Chern insulator



Lattice model for p+ip topological
superconductor

Superconductors are described by single-body mean-field insulating Bogoliubov-de Gennes Hamiltonians

$$\hat{H} = \sum_{m,l=1}^{N} \hat{c}_m^\dagger h_{ml} \hat{c}_l + \frac{1}{2} \sum_{m,l=1}^{N} \hat{c}_m^\dagger \Delta_{ml} \hat{c}_l^\dagger - \frac{1}{2} \sum_{m,l=1}^{N} \hat{c}_m \Delta_{ml}^* \hat{c}_l$$

Double degrees of freedom for better numerics:

$$\hat{H} = \frac{1}{2} \begin{pmatrix} \hat{\mathbf{c}}^\dagger & \hat{\mathbf{c}} \end{pmatrix} \mathcal{H} \begin{pmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{pmatrix} + \frac{1}{2} \mathrm{Tr} h; \qquad \mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$$

Diagonalize single-particle Bogoliubov-de Gennes Hamiltonian:

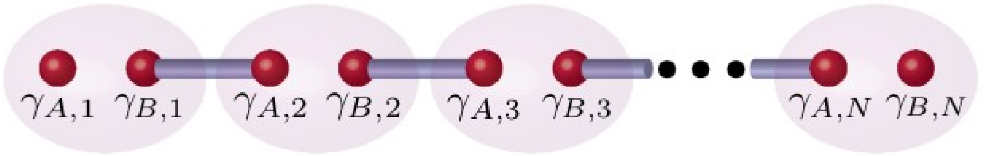
$$\mathcal{H} \begin{pmatrix} u_n^* \\ v_n^* \end{pmatrix} = E_n \begin{pmatrix} u_n^* \\ v_n^* \end{pmatrix}, \quad \text{with } E_n \geq 0 \text{ for } n = 1, \ldots, N;$$

$$\mathcal{H} \begin{pmatrix} v_n \\ u_n \end{pmatrix} = -E_n \begin{pmatrix} v_n \\ u_n \end{pmatrix}, \quad \text{for } n = 1, \ldots, N,$$

Obtain eigenmodes of system (particle-hole superpositions):

$$\hat{H} = \sum_{n=1}^{N} E_n \hat{d}_n^\dagger \hat{d}_n + \text{const} \qquad \hat{d}_n = \sum_m u_{nm} \hat{c}_m + v_{nm} \hat{c}_m^\dagger$$

1) Kitaev wire



The Kitaev wire in position-first-particle-hole-second basis

$$\hat{H}_K = \sum_{m=1}^{N} \left(\frac{\epsilon_m}{2} \hat{c}_m^\dagger \hat{c}_m - w_m \hat{c}_m^\dagger \hat{c}_{m+1} + \Delta_m \hat{c}_{m+1}^\dagger \hat{c}_m^\dagger \right) + h.c.$$

Including position dependence of onsite energies, hopping, superconductivity.

$$\underline{\hat{\mathbf{c}}}^\dagger = (\hat{c}_1^\dagger, \hat{c}_1, \hat{c}_2^\dagger, \hat{c}_2, \ldots, \hat{c}_N^\dagger, \hat{c}_N)$$

Example, N=5:

$$\mathcal{H} = \begin{pmatrix}
\epsilon_1 & 0 & -w_1 & -\Delta_1 & 0 & 0 & 0 & 0 & -w_N^* & \Delta_N \\
0 & -\epsilon_1 & \Delta_1^* & w_1^* & 0 & 0 & 0 & 0 & -\Delta_N^* & w_N \\
-w_1^* & \Delta_1 & \epsilon_2 & 0 & -w_2 & -\Delta_2 & 0 & 0 & 0 & 0 \\
-\Delta_1^* & w_1 & 0 & -\epsilon_2 & \Delta_2^* & w_2^* & 0 & 0 & 0 & 0 \\
0 & 0 & -w_2^* & \Delta_2 & \epsilon_3 & 0 & -w_3 & -\Delta_3 & 0 & 0 \\
0 & 0 & -\Delta_2^* & w_2 & 0 & -\epsilon_3 & \Delta_3^* & w_3^* & 0 & 0 \\
0 & 0 & 0 & 0 & -w_3^* & \Delta_3 & \epsilon_4 & 0 & -w_4 & -\Delta_4 \\
0 & 0 & 0 & 0 & -\Delta_3^* & w_3 & 0 & -\epsilon_4 & -\Delta_4^* & w_4 \\
-w_N & -\Delta_N & 0 & 0 & 0 & 0 & -w_3^* & \Delta_3 & \epsilon_N & 0 \\
\Delta_N^* & w_N^* & 0 & 0 & 0 & 0 & -\Delta_3^* & w_3 & 0 & -\epsilon_N
\end{pmatrix}$$

Bulk momentum-space BdG Hamiltonian → Bands
Berry phases of bands have a symmetry!

$$\mathcal{H}(k)\begin{pmatrix}u(k)\\ v(k)\end{pmatrix} = E(k)\begin{pmatrix}u(k)\\ v(k)\end{pmatrix}$$

$$\mathcal{H}(k) = \begin{pmatrix}-2\,|w|\cos(k-\chi)-\mu & -2i\Delta\sin k\\ 2i\Delta^{*}\sin k & 2\,|w|\cos(k+\chi)+\mu\end{pmatrix}$$

More generally, any number of bands, Berry phase:

$$\mathcal{H}(k)\left|n(k)\right\rangle = E_n(k)\left|n(k)\right\rangle \qquad \gamma_n = \frac{1}{2\pi i}\int_{-\pi}^{\pi} dk\,\left\langle n(k)\right|\partial_k\left|n(k)\right\rangle$$

Particle-hole symmetry connects positive and negative energy bands (like chiral symmetry)

$$-\mathcal{H}(k)\hat{\sigma}_x\left|n(-k)\right\rangle^{*} = E_n(k)\hat{\sigma}_x\left|n(-k)\right\rangle^{*}$$

$$\Rightarrow \quad \boxed{\gamma_n = \frac{1}{2\pi i}\int_{-\pi}^{\pi} dk\,\left\langle n(k)\right|\partial_k\left|n(k)\right\rangle = \gamma_{-n}}$$

Bulk topological invariant is "polarization": sum of all negative energy Berry phases. 0=trivial; π=topological.

Lattice Hamiltonians:

$$\sum_{n<0} \gamma_n + \sum_{n>0} \gamma_n = 0 \quad (\mathrm{mod} 2\pi)$$

Particle-hole symmetry
of BdG Hamiltonians:

$$\sum_{n<0} \gamma_n = \sum_{n>0} \gamma_n$$

$$\text{trivial:} \quad \sum_{n<0} \gamma_n = 0 \quad (\mathrm{mod} 2\pi)$$

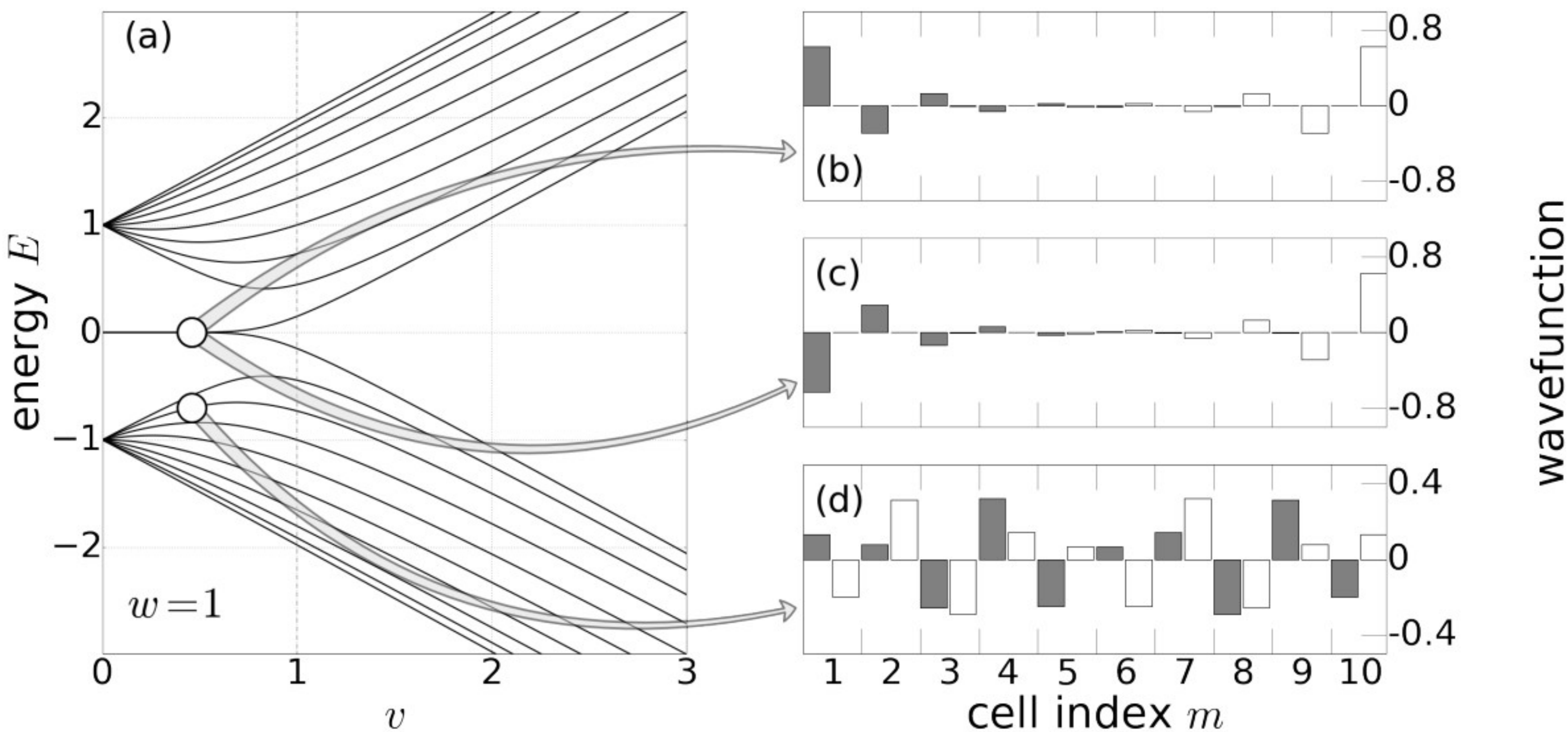
$$\text{topological:} \quad \sum_{n<0} \gamma_n = \pi \quad (\mathrm{mod} 2\pi)$$

Like polarization in Hamiltonians. Obstruction against adiabatic deformation to atomic limit.
Same as ground-state fermion parity of rings of even number of sites.

Topological invariant determines whether there are unpaired Majorana Zero Modes at chain ends

We can find and analyze edge states in the BdG Hamiltonian of the Kitaev wire in the same way as we did for the SSH model.

1) Flat-band limit: edge states
2) Moving away from the flat-band limit: topological protection
3) General bulk–boundary correspondence argument: using polarization.



Zero-energy edge states, particle-hole-symmetric partners of themselves

→ Majorana Zero Mode fermionic zero-energy excitations

If hopping w and pair potential Δ have no complex phases, the Kitaev wire maps onto the SSH model

$$\mathcal{H}(k) = \begin{pmatrix} -2\,|w|\cos(k-\chi) - \mu & -2i\Delta\sin k \\ 2i\Delta^*\sin k & 2\,|w|\cos(k+\chi) + \mu \end{pmatrix}$$

$$H(k) = \begin{pmatrix} 0 & v + we^{-ik} \\ v + we^{ik} & 0 \end{pmatrix}$$

Do a unitary transformation to rotate $\sigma_z \rightarrow \sigma_x$ (almost the Majorana Fermion basis)

$$\mathcal{H}' = e^{i\pi/4\,\sigma_y}\mathcal{H}e^{-i\pi/4\,\sigma_y} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\mathcal{H}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} i(\operatorname{Im}h + \operatorname{Im}\Delta) & -\operatorname{Re}h + \operatorname{Re}\Delta \\ -\operatorname{Re}h - \operatorname{Re}\Delta & i(\operatorname{Im}h - \operatorname{Im}\Delta) \end{pmatrix}$$

Take χ=0, Δ real:

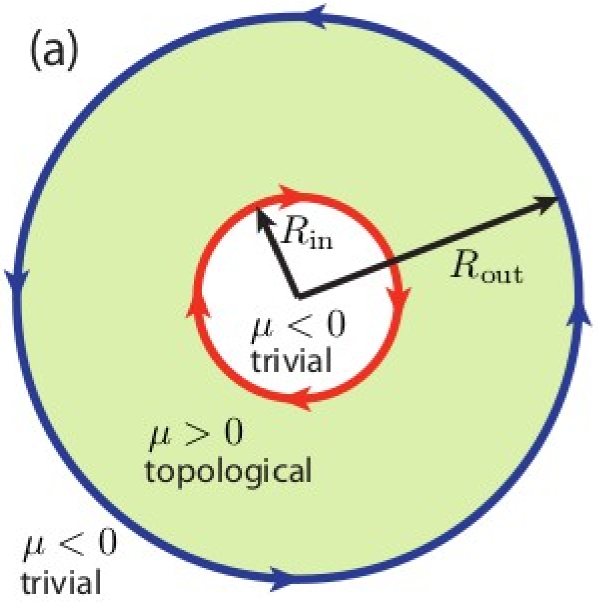
$$\boxed{\mathcal{H}'(k) = \begin{pmatrix} 0 & -2w\cos k - \mu - 2i\Delta\sin k \\ -2w\cos k - \mu + 2i\Delta\sin k & 0 \end{pmatrix}}$$

Relations between Kitaev wire and SSH model, summarized:

For real parameters, Kitaev wire also has time-reversal symmetry: class BDI

	Kitaev	SSH	Kitaev MF
PHS (+1)	$\sigma_x \mathcal{H}^* \sigma_x = -\mathcal{H}$	$\sigma_z H^*_{\mathrm{SSH}} \sigma_z = -H_{\mathrm{SSH}}$	$\mathcal{A}^* = \mathcal{A}$
TRS (+1)	$\mathcal{H}^* = \mathcal{H}$	$H^*_{\mathrm{SSH}} = H_{\mathrm{SSH}}$	$\sigma_z \mathcal{A}^* \sigma_z = -\mathcal{A}$
CS	$\sigma_x \mathcal{H} \sigma_x = -\mathcal{H}$	$\sigma_z H_{\mathrm{SSH}} \sigma_z = -H_{\mathrm{SSH}}$	$\sigma_z \mathcal{A} \sigma_z = -\mathcal{A}$

2) 2-dimensional p+ip superconductor



Exploit connections to topological insulators: QWZ model as a superconductor

$$\hat{H}(k_x, k_y) = \sin k_x \hat{\sigma}_x + \sin k_y \hat{\sigma}_y + [u + \cos k_x + \cos k_y]\hat{\sigma}_z$$

We are lucky: this has particle-hole symmetry!

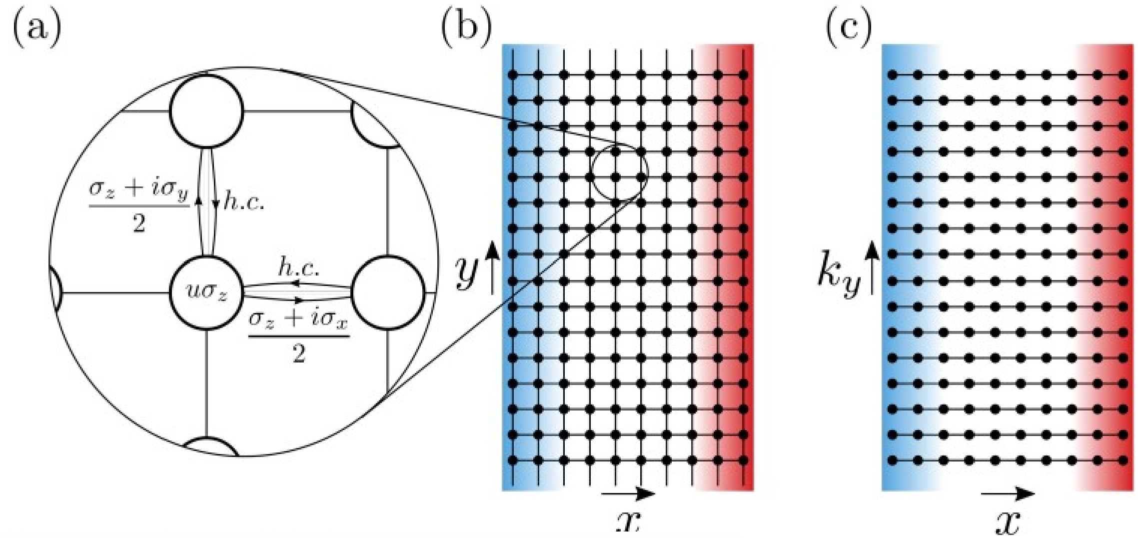
$$\hat{\sigma}_x \mathcal{K}\mathcal{H}(k)\mathcal{K}\hat{\sigma}_x = -\mathcal{H}(k)$$

$$\mathcal{K}\mathcal{H}(k)\mathcal{K} = \mathcal{H}(-k)^*$$

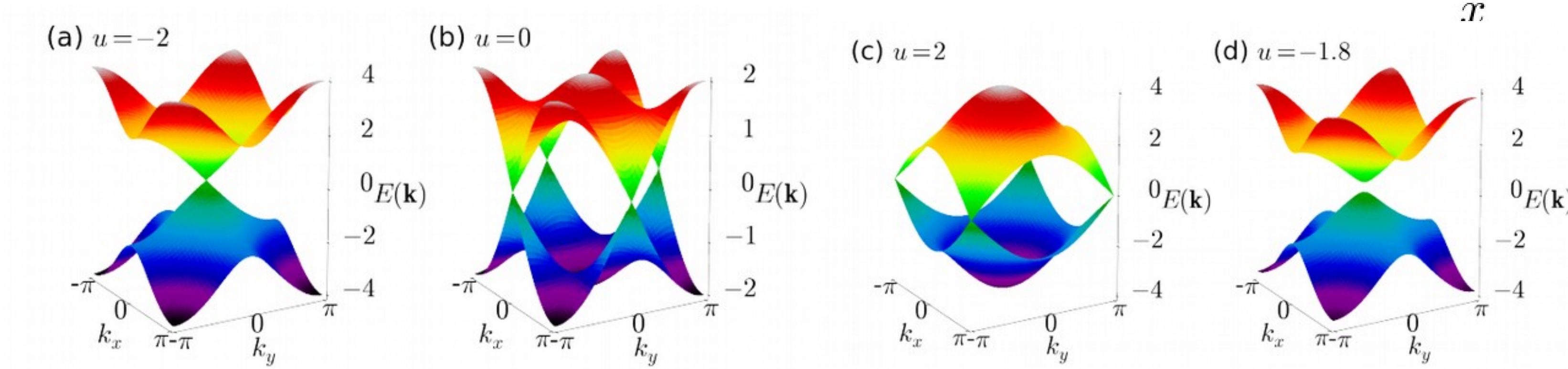
→ Can be interpreted as a BdG Hamiltonian of a superconductor

– How is the pair potential Δ special?
– What are the chiral edge states?

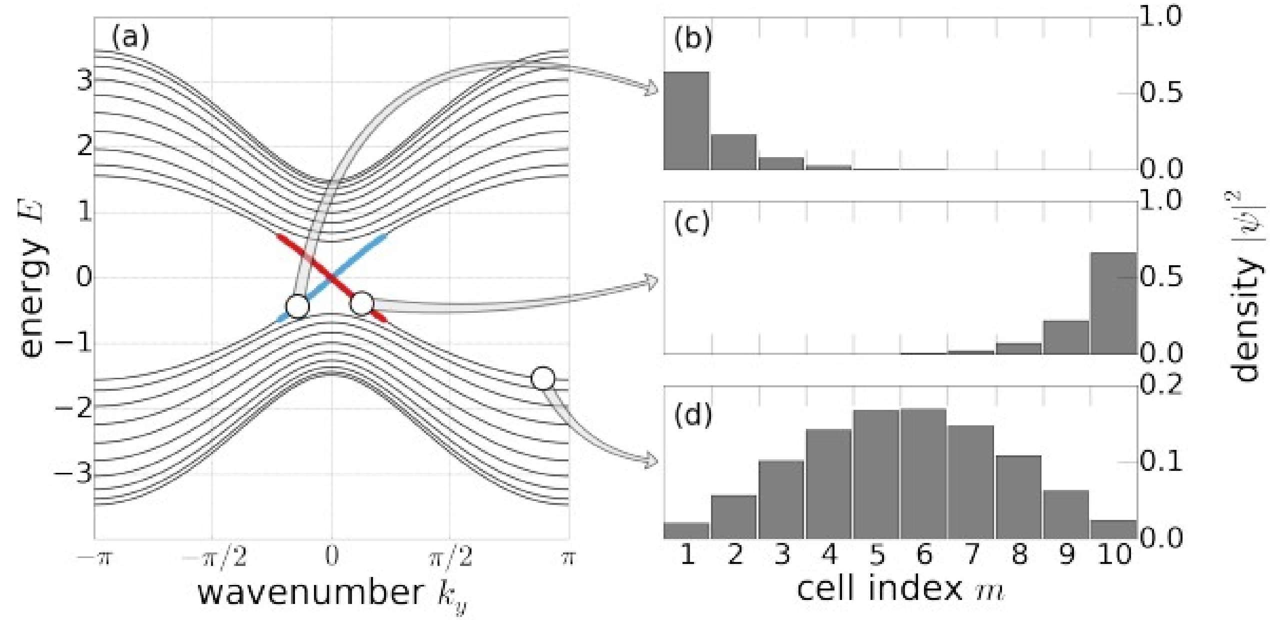
Reminder: QWZ model



bulk Chern number
chiral edge modes



$$
\begin{aligned}
u < -2 \quad &: \quad Q = 0; \\
-2 < u < 0 \quad &: \quad Q = -1; \\
0 < u < 2 \quad &: \quad Q = +1; \\
2 < u \quad &: \quad Q = 0.
\end{aligned}
$$



The superconducting version of the Qi-Wu-Zhang model is a p+ip (p_x+ip_y) topological superconductor

$$\hat{H}(k_x,k_y) = \sin k_x \hat{\sigma}_x + \sin k_y \hat{\sigma}_y + [u + \cos k_x + \cos k_y]\hat{\sigma}_z$$

$$\hat{H}_{QWZ}(k) = \begin{pmatrix} w\cos k_x + w\cos k_y + u & w\sin k_x + iw\sin k_y \\ w\sin k_x - iw\sin k_y & -w\cos k_x - w\cos k_y - u \end{pmatrix}$$

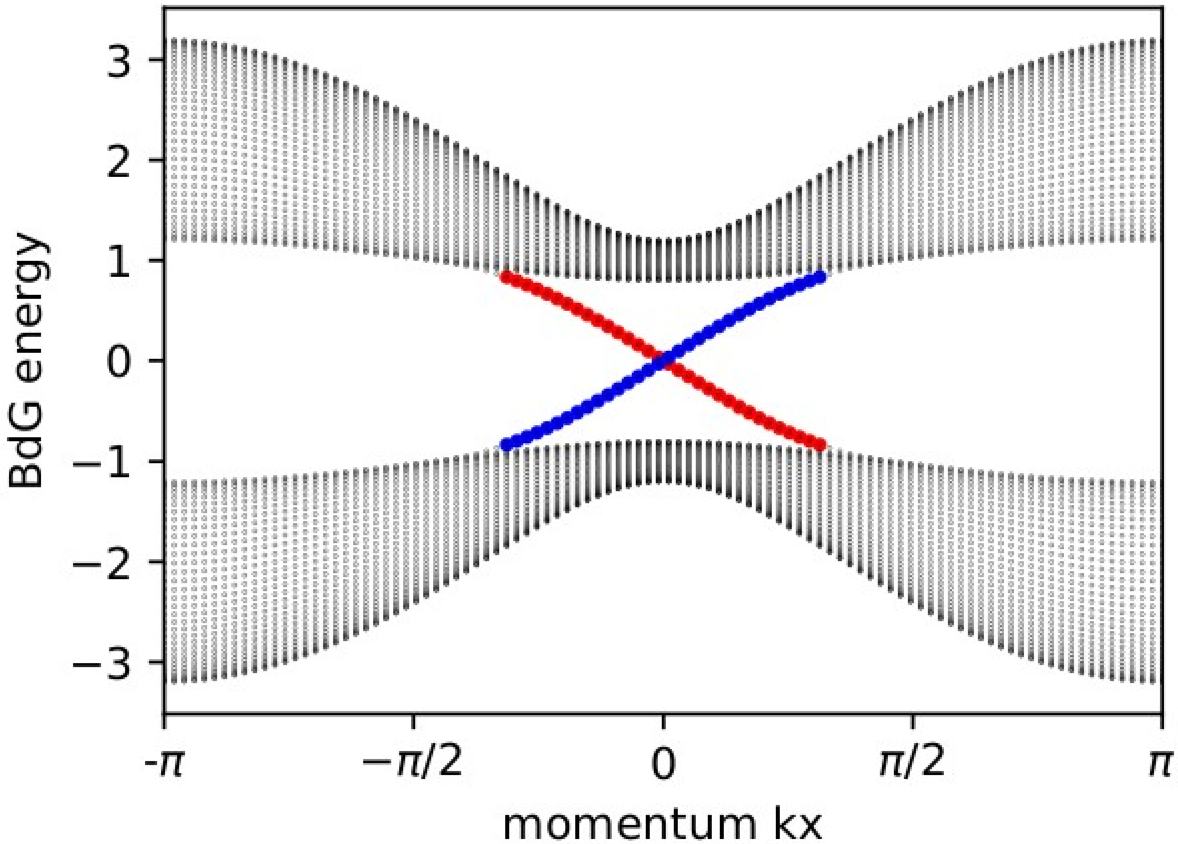
$$\hat{H}_{p+ip}(k) = \begin{pmatrix} -w\cos k_x - w\cos k_y - \mu & -i\Delta_0 \sin k_x + \Delta_0 \sin k_y \\ i\Delta_0^* \sin k_x + \Delta_0^* \sin k_y & w\cos k_x + w\cos k_y + \mu \end{pmatrix}$$

Δ(k) = -Δ(-k) → p-wave; relative phase → p_x+ip_y

$$\hat{H}_{p+ip} = \sum_{m,l=1}^{N} \Big(- w\hat{c}^\dagger_{m,l}\hat{c}_{m+1,l} - w\hat{c}^\dagger_{m,l}\hat{c}_{m,l+1} + h.c.\Big) - \mu \sum_{m,l=1}^{N} \hat{c}^\dagger_{m,l}\hat{c}_{m,l}$$

$$+ \sum_{m,l=1}^{N} \Big(\Delta_0 \hat{c}^\dagger_{m+1,l}\hat{c}^\dagger_{m,l} + i\Delta_0 \hat{c}^\dagger_{m,l+1}\hat{c}^\dagger_{m,l} + h.c.\Big).$$

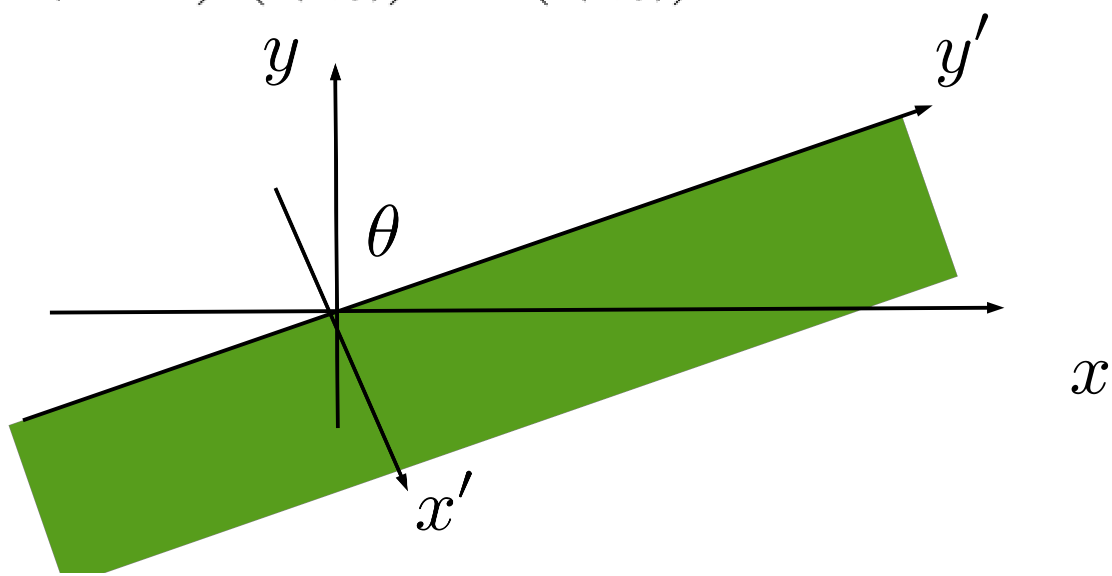
Edge modes on boundaries are "Majorana fermions", equal superpositions of particle and hole



$$
\begin{aligned}
2w < \mu : &\quad Q = 0; \\
0 < \mu < 2w : &\quad Q = 1; \\
-2w < \mu < 0 : &\quad Q = -1; \\
\mu < -2w : &\quad Q = 0.
\end{aligned}
$$

Long-wavelength approximation reveals Nambu polarization of edge modes locked to phase of Δ

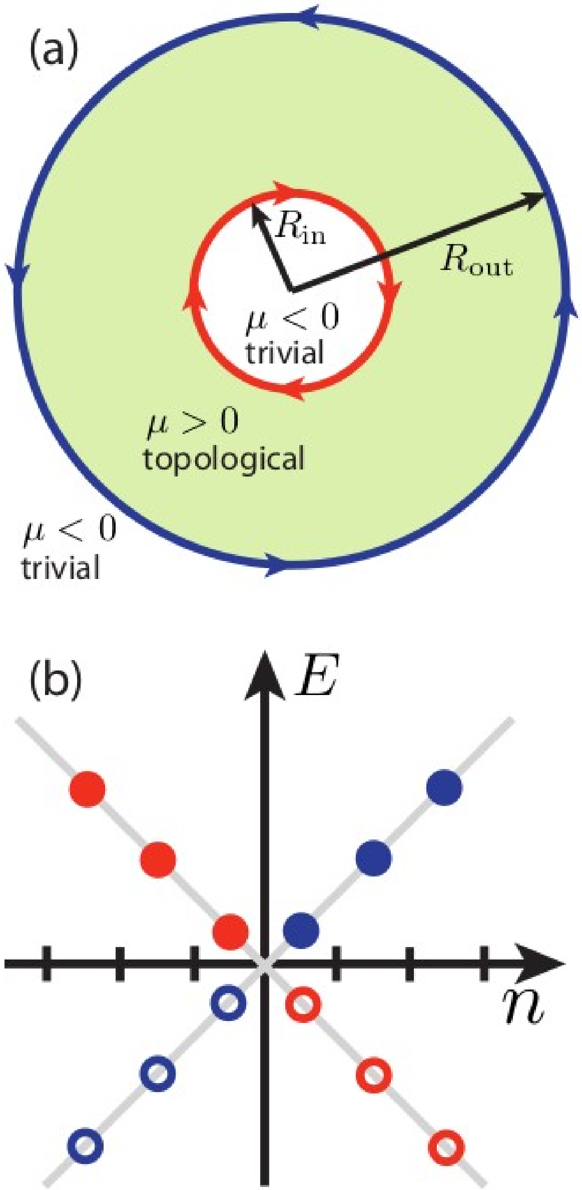
$$\begin{pmatrix} -\mu & \Delta(-\partial_x - i\partial_y) \\ \Delta^*(\partial_x - i\partial_y) & \mu \end{pmatrix} \begin{pmatrix} u(x,y) \\ v(x,y) \end{pmatrix} = E \begin{pmatrix} u(x,y) \\ v(x,y) \end{pmatrix}$$



$$\pm |\Delta| \, k = E;$$
$$-2\mu v(x') \mp 2 |\Delta| \, \partial_{x'} v(x') = 0.$$

$$\Psi(x', y') = \begin{pmatrix} \pm e^{i(\phi - \theta)} \\ 1 \end{pmatrix} \exp\left[\int_0^{x'} \frac{\pm \mu(x'')}{|\Delta|} dx'' \right] e^{iky'}$$

Corbino disk of p+ip: has Majorana fermion edge modes on inside and outside, but no Majorana Zero Mode



Nambu spin locked to phase of Δ(k)

→ Nambu spin rotates around perimeter

→ boundary conditions for edge mode antiperiodic

→ no Majorana Zero Mode at k=0, E=0

→ if hole is shrunk away: nothing special

New directions in the pursuit of Majorana fermions in solid state systems

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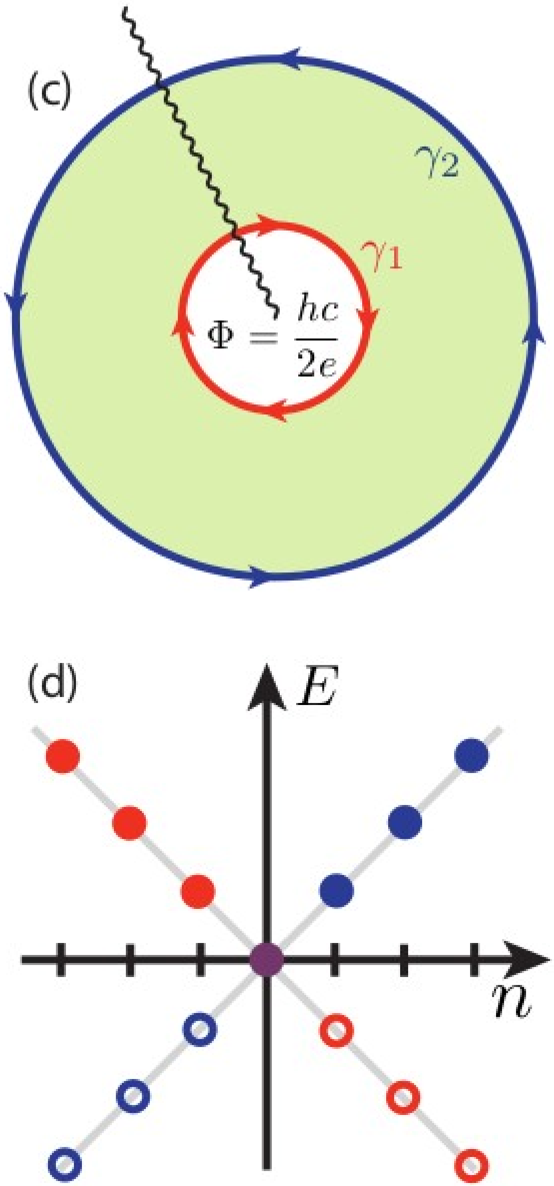
[1]*Department of Physics and Astronomy, University of California, Irvine, California 92697*

(Dated: February 8, 2012)

We can create a Majorana Zero Mode in Corbino disk by threading magnetic flux through hole



Magnetic field only through hole (e.g. with solenoid):
- no magnetic field in superconductor
- Aharonov-Bohm effect:

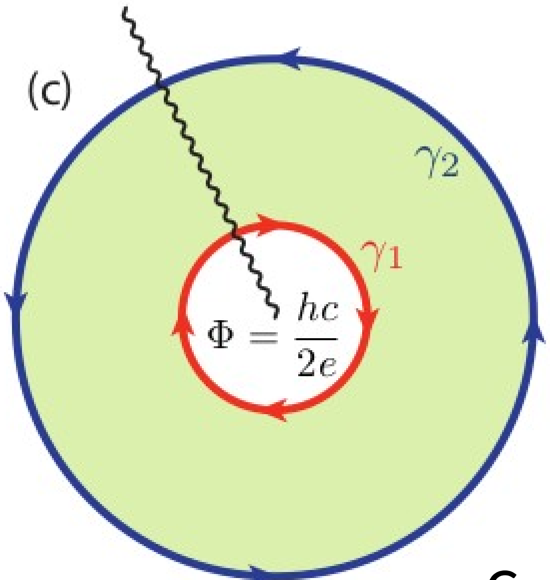
$$\Delta(x = r\cos\theta, y = r\sin\theta) = e^{i\Phi/\Phi_0\theta}\Delta(x = r, y = 0)$$

→ Δ(x,y,k):
position-dependence: winds around origin
momentum dependence: winds around k=0

Position dependence can cancel momentum dependence for edge states!

Nambu spin locked to phase of Δ(k)
→ Nambu spin does not rotate around perimeter
→ boundary conditions for edge mode periodic
→ Majorana Zero Mode at k=0, E=0
→ if hole is shrunk away: 1 Majorana Zero Mode left at the vortex core → unpaired Majorana

In a conveniant gauge, the branch cuts represent lines, across which all hoppings are multiplied by -1



$$\hat{c}_{\mathbf{r}} \to \hat{c}_{\mathbf{r}} e^{i\Lambda_{\mathbf{r}}} \qquad \hat{c}^\dagger_{\mathbf{r}} \to \hat{c}^\dagger_{\mathbf{r}} e^{-i\Lambda_{\mathbf{r}}}$$

$$w_{\mathbf{r}',\mathbf{r}} \hat{c}^\dagger_{\mathbf{r}'} \hat{c}_{\mathbf{r}}; \quad w_{\mathbf{r}',\mathbf{r}} \to w_{\mathbf{r}',\mathbf{r}} e^{-i(\Lambda_{\mathbf{r}} - \Lambda_{\mathbf{r}})};$$

$$\Delta_{\mathbf{r}',\mathbf{r}} \hat{c}^\dagger_{\mathbf{r}'} \hat{c}^\dagger_{\mathbf{r}}; \quad \Delta_{\mathbf{r}',\mathbf{r}} \to \Delta_{\mathbf{r}',\mathbf{r}} e^{-i(\Lambda_{\mathbf{r}} + \Lambda_{\mathbf{r}'})},$$

Convenient gauge transformation:

$$\Lambda(x = r\cos\theta, y = r\sin\theta) = \theta$$

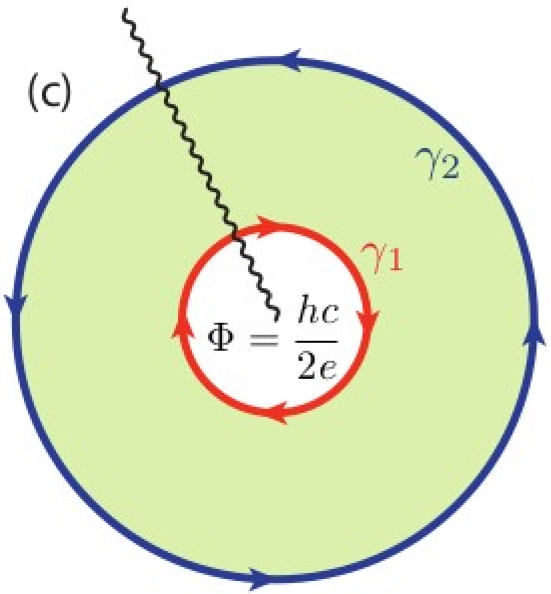
→ Δ(k,x,y) no longer winds in position (still depends on momentum!)

→ both hopping w and nonlocal pair potential Δ have extra – sign across wavy line (“Dirac string”)

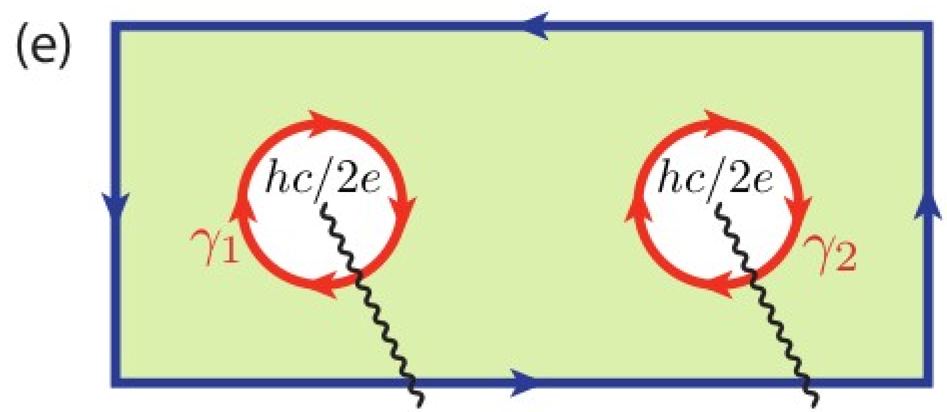
- position of wavy line gauge dependent

Majorana Zero Modes always come in pairs

Vortex core – outer edge



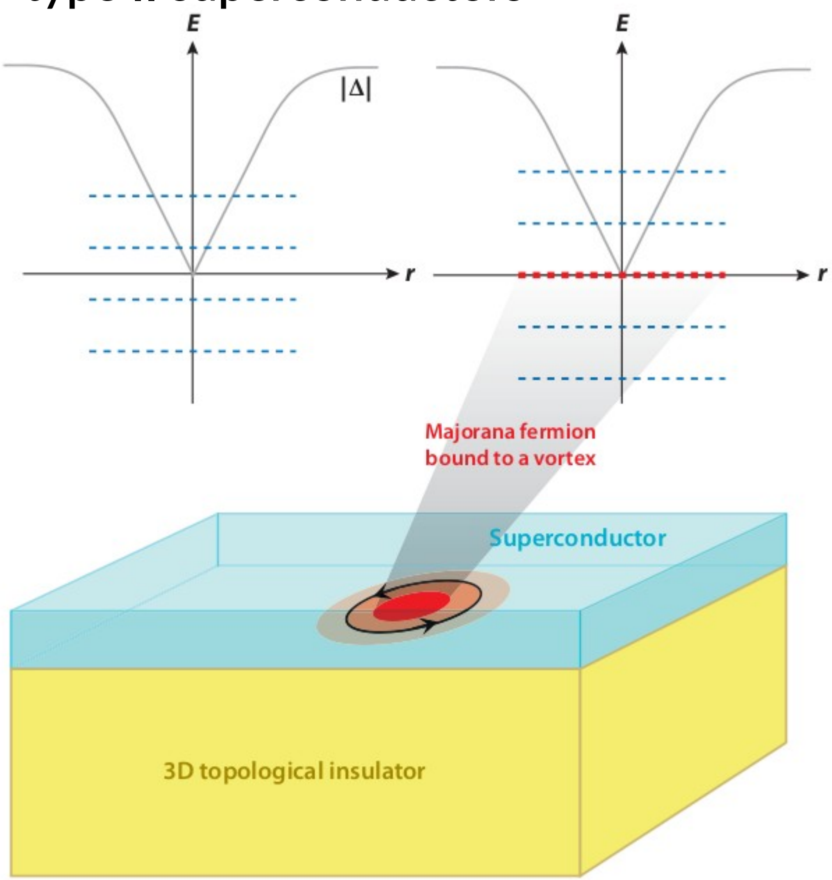
Vortex 1 core – Vortex 2 core



Topologically protected 0-energy bound states of BdG Hamiltonians are Majorana Zero Modes – each of them is half of a nonlocal fermion

Zero modes at end of nanowire

Zero modes also in centers of vortices of type II superconductors



Beenakker: Search for Majorana fermions in superconductors, Annu. Rev. Con. Mat. Phys (2013)

Single Majorana Zero Mode:
single mode of doubled BdG Hamiltonian
→ particle-hole symmetry eigenstate
→ its own symmetry partner
→ pinned to 0 energy,
→ fermion parity switch operator
→ no charge, no spin, no mass

$$\hat{\gamma}_j^2 = 1$$

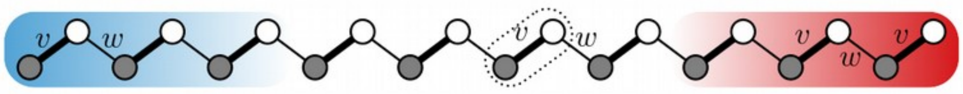
Any two Majoranas can be combined into a complex fermion, which represents a 0-energy excitation of the system.

$$\frac{1}{2}(\hat{\gamma}_1 + i\hat{\gamma}_2) = \hat{d}_{12}$$

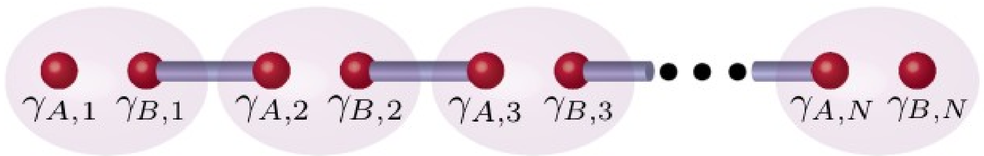
Pairs of topological defects in topological superconductors host nonlocal zero-energy fermions

Electrons torn apart into half fermions

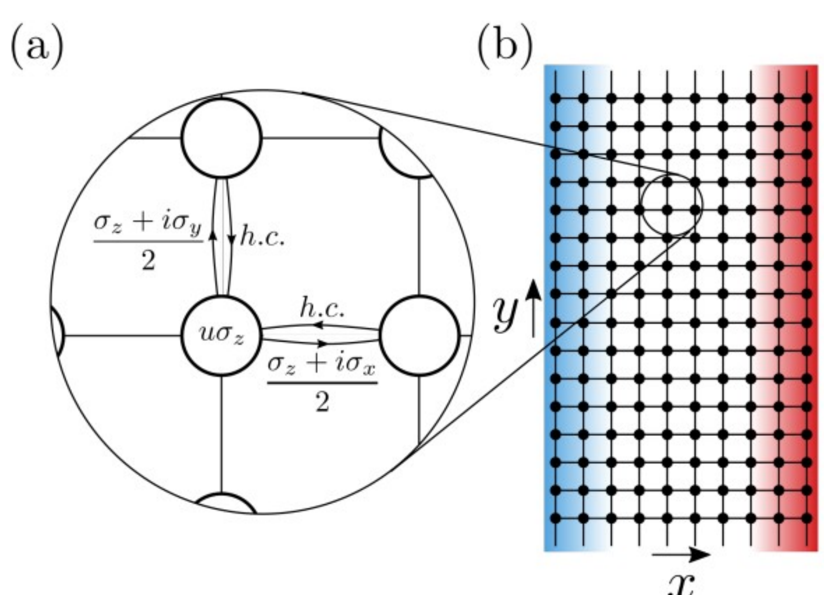
Single-particle topological Hamiltonians 1st semester can be understood as BdG Hamiltonians



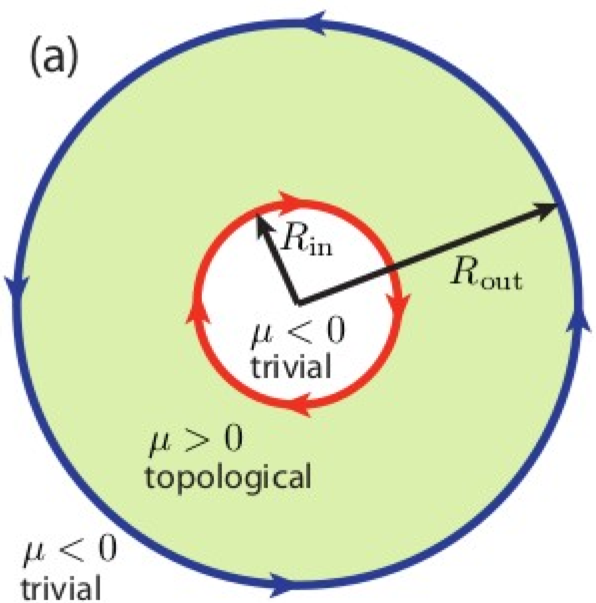
Su-Schrieffer-Heeger model
topological nanowire



Kitaev model for topological
superconductor nanowire
with / without chiral symmetry



Qi-Wu-Zhang model
2D Chern insulator



Lattice model for p+ip topological
superconductor

Exercises

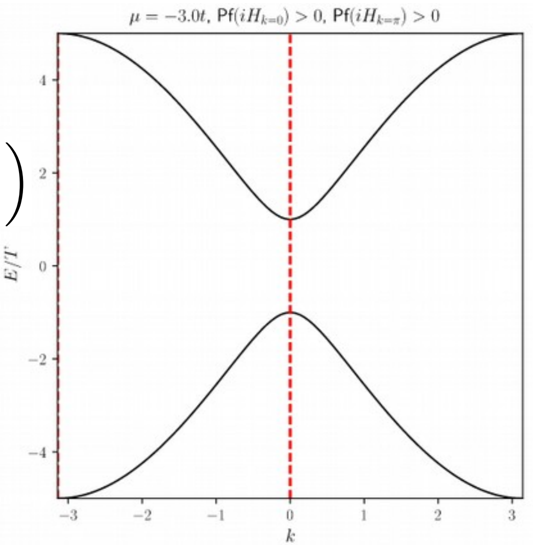
For superconducting wires, how is the Z2 Pfaffian invariant related to the bulk polarization?

Z2 Pfaffian invariant

$$Q = \mathrm{sign}\left(\mathrm{Pf}[i\tilde{H}(k=0)]\mathrm{Pf}[i\tilde{H}(k=\pi)]\right)$$

trivial: Q=+1

topological: Q=-1



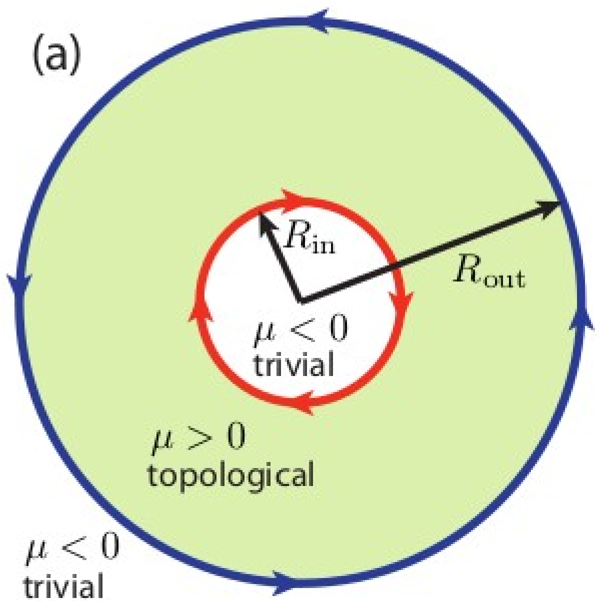
Bulk polarization

$$\text{trivial:} \quad \sum_{n<0} \gamma_n = 0 \quad (\mathrm{mod} 2\pi)$$

$$\text{topological:} \quad \sum_{n<0} \gamma_n = \pi \quad (\mathrm{mod} 2\pi)$$

1) They give the same classification (why?)
2) They give different classification (example?)
3) The bulk polarization is more general, the Pfaffian invariant is only for two-level systems
4) The bulk polarization is more general, the Pfaffian requires antisymmetry of the BdG Hamiltonian

Do edge states on a QWZ disk also not have a mode with 0 angular momentum, “k=0”?



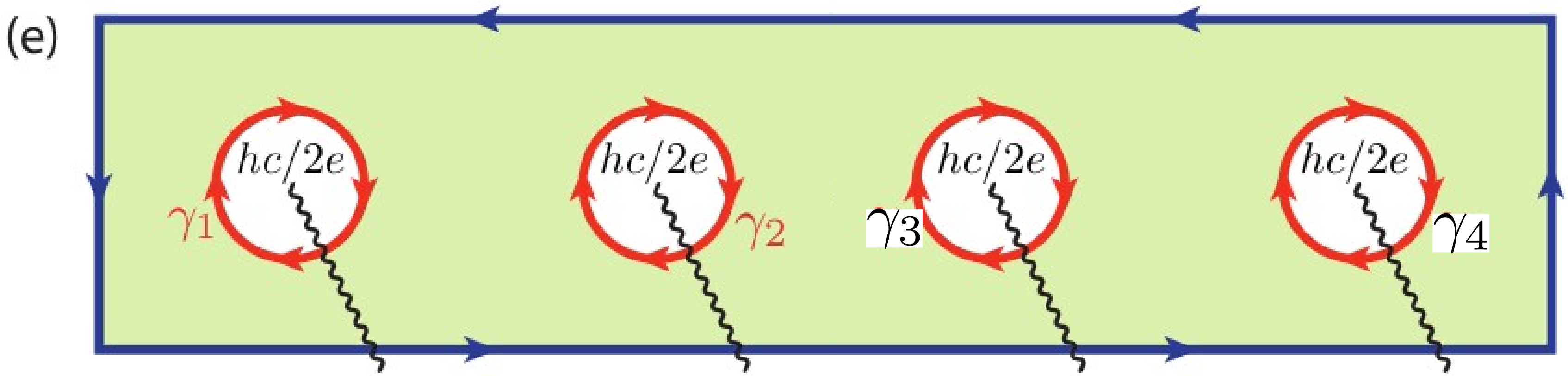
1) No, there the hoppings are all real-valued
→ no pseudospin-momentum locking
→ no extra rotation phase of (-1)

2) Yes, the same story holds as in p+ip

3) No, QWZ edge states are complex fermions
→ represent two particles
→ two phases of (-1) cancel

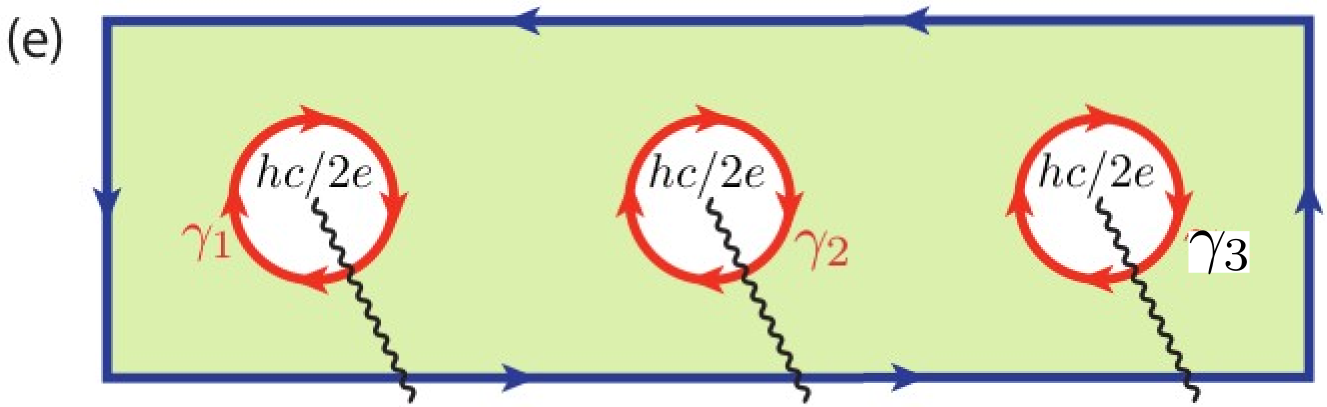
4) No, because the QWZ model does not have particle-hole symmetry

What is the ground state degeneracy here, and why? (assuming large enough bulk regions)



1) 1: nondegenerate (even number of vortices)
2) 4: 2^(number of Majorana Zero Modes / 2)
3) 4: number of vortices
4) 5: the number of vortices + the outside edge

What is the ground state degeneracy here, and why? (assuming large enough bulk regions)



1) impossible, cannot have odd number of vortices
2) 2√2: 2^(number of Majorana Zero Modes / 2)
3) 4: number of vortices + outside edge
4) 4: 2^(number of Majorana Zero Modes, including edge / 2)