Topological invariants for 1-dimensional superconductors

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Intro: Transverse field Ising model

$$H_{\mathrm{TFI}} = \sum_{i=0}^{L-1} h\sigma_i^z + \sigma_i^x \sigma_{i+1}^x$$

σ's: Pauli matrices

$[\sigma^x, \sigma^y] = 2i\sigma^z$ & cyclic

Quantum phase transition at h = 1 between two ordered phases.

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The model is solved by means of a **non-local** Jordan-Wigner transformation

Define fermionic levels: $|\uparrow\rangle = |0\rangle \qquad |\downarrow\rangle = |1\rangle$

$$\sigma_i^z = 1 - 2c_i^\dagger c_i \qquad \prod_i \sigma_i^z = (-1)^F$$

$$c_i = \Big(\prod_{j<i} \sigma_i^z\Big)\sigma_i^+ \qquad c_i^\dagger = \Big(\prod_{j<i} \sigma_i^z\Big)\sigma_i^-$$

Intro: Transverse field Ising model

In terms of the fermions, the model reads

$$
\begin{aligned}
H_{TFI} = \sum_{i=0}^{L-1} h(2c_i^\dagger c_i - 1) + \sum_{i=0}^{L-2} \left(c_i c_{i+1} + c_i c_{i+1}^\dagger + c_{i+1} c_i^\dagger + c_{i+1}^\dagger c_i^\dagger\right) \\
- (-1)^F \left(c_{L-1} c_0 + c_{L-1} c_0^\dagger + c_0 c_{L-1}^\dagger + c_0^\dagger c_{L-1}^\dagger\right)
\end{aligned}
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$$- (-1)^F \left(c_{L-1} c_0 + c_{L-1} c_0^\dagger + c_0 c_{L-1}^\dagger + c_0^\dagger c_{L-1}^\dagger\right)$$

Versatile model, which is a starting point for many generalizations:

- Kitaev: fermions themselves are the fundamental degrees of freedom:
  This gives Kitaev's 'Majorana chain'

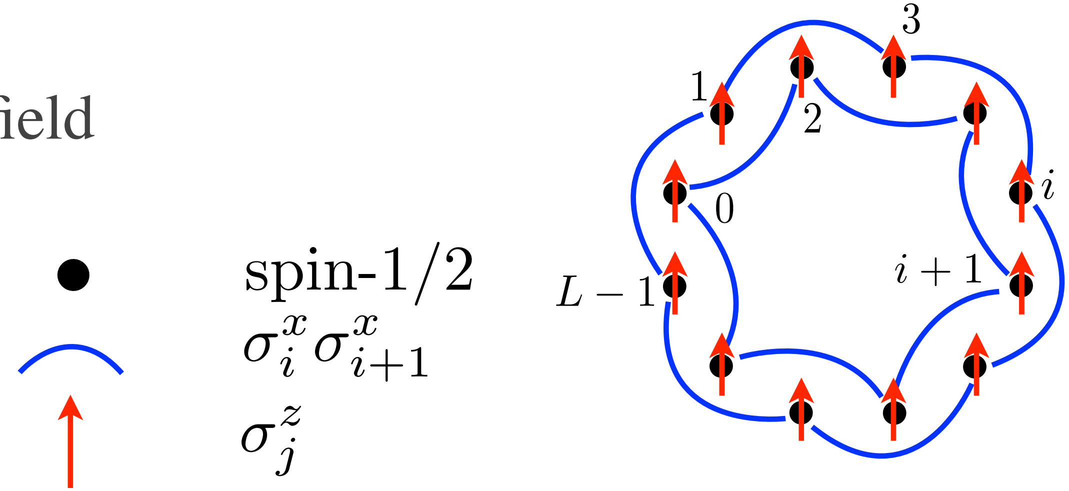
- Generalize the Majorana's to parafermions (Fendley; Shtengel, Alicea et.al)

- Realization of series of critical chains: Kitaev's 16-fold way

Advertisement: 1-d critical models

Consider n decoupled transverse field Ising models at the critical point:

$$H_{\mathrm{TFI}}^{(n)} = \sum_{i=0}^{L-1} \sigma_i^z + \sigma_i^x \sigma_{i+n}^x$$



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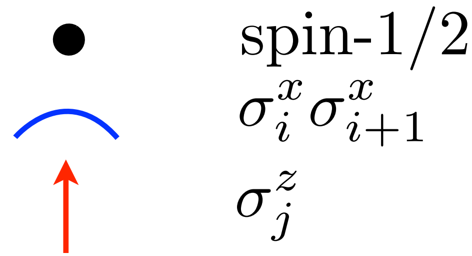

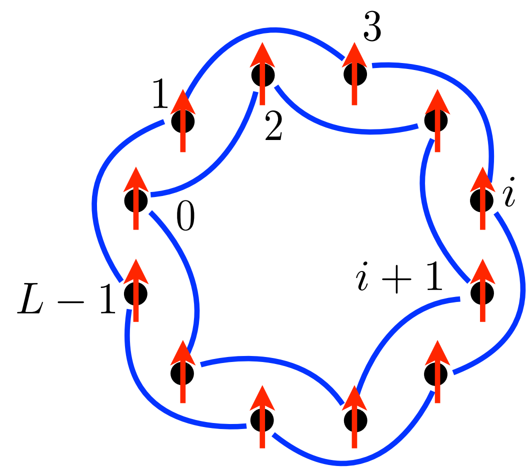

Inspired by 2-d condensation transitions between topological phases, we add an appropriate boundary term, followed by a non-local spin transformation.

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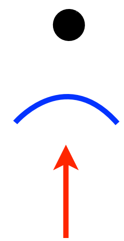

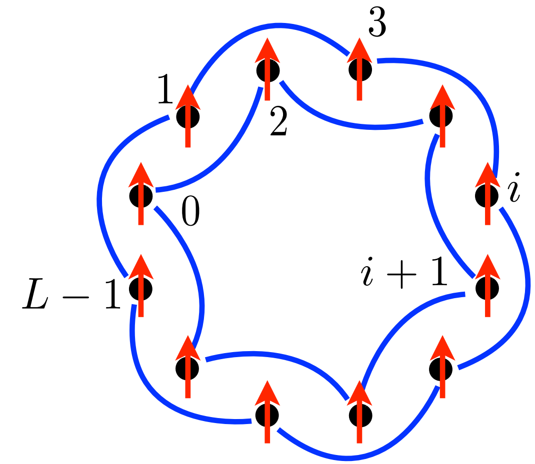

Inspired by 2-d condensation transitions between topological phases, we add an appropriate boundary term, followed by a non-local spin transformation.

We obtain a series of spin-1/2 chains, which are Jordan-Wigner solvable, and have critical $so(n)_1$ behaviour (realizing Kitaev's 16-fold way)!

n	1	2	3	4	5
$so(n)_1$	Ising	$u(1)_4$	$su(2)_2$	$u(1)_2 \times u(1)_2$	$so(5)_1$

Månsson, Lahtinen, Suorsa, EA

PRB'13 & in preparation

Kitaev's Majorana chain

In terms of the (polarized) fermions c_i , Kitaev's model reads

$$H_{\text{Kitaev}} = \sum_i -\mu\left(c_i^\dagger c_i - c_i c_i^\dagger\right) - t\left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right) + \Delta\left(c_i c_{i+1} + c_{i+1}^\dagger c_i^\dagger\right)$$

This model belongs to class D of the classification of free fermion systems

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In Bogoliubov de Gennes form, the model reads:

$$H_{\text{Kitaev}}(k) = \big(-\mu - t\cos(k)\big)\tau_z + \Delta\sin(k)\tau_y$$

τ_α: Pauli matrices in particle-hole space

Anti-unitary particle-hole 'symmetry' $\mathcal{C} = \tau_x K$, $\quad \mathcal{C}^2 = 1$
anti-commutes with the hamiltonian.

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$\mathcal{C}$ is not a real symmetry here, but a redundancy in the description, which can not be broken!

Periodic table of topological phases

Classification of topological phases of systems with time-reversal $\mathcal{T}$, particle-hole $\mathcal{C}$, and/or chiral symmetry $U_{CS} = \mathcal{T} \circ \mathcal{C}$

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Time reversal and particle-hole are anti-unitary, $\mathcal{T} = U_T K$, $\mathcal{C} = U_C K$

satisfying $[H, \mathcal{T}] = 0$, $\{H, \mathcal{C}\} = 0$ and $\mathcal{T}^2 = \pm 1$, $\mathcal{C}^2 = \pm 1$

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This gives ten different classes, with three possibilities for $\mathcal{T}$ and $\mathcal{C}$.
If both are absent, the system can be chiral or not.

Periodic table of topological phases

Class	$\mathcal{T}$	$\mathcal{C}$	U_{CS}	$d=1$	$d=2$	$d=3$	$d=4$
A	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AIII	0	0	1	$\mathbb{Z}$	0	$\mathbb{Z}$	0
BDI	$+1$	$+1$	1	$\mathbb{Z}$	0	0	0
D	0	$+1$	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
DIII	-1	$+1$	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
AII	-1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
CII	-1	-1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
C	0	-1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$
CI	$+1$	-1	1	0	0	$\mathbb{Z}$	0
AI	$+1$	0	0	0	0	0	$\mathbb{Z}$

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AII	-1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
CII	-1	-1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
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Calculating the $\mathbb{Z}_2$ invariants is typically hard, and requires a dimensional extension in general (Budich & Trauzettel)

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Subject of this talk

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Subject of this talk

Inspired by Fu & Kane
and Kitaev

Outline

- Discussion of the Kitaev's Majorana chain, and its $\mathbb{Z}_2$ invariant.
- Imposing additional time reversal symmetry
- Construction of a topological invariant for 1D superconductors in class DIII
- Applying the invariant to a 'toy-model' (p & s wave pairing and spin-orbit coupling)
- The effect of inversion symmetry: from D to DIII and back again...

Kitaev's Majorana chain

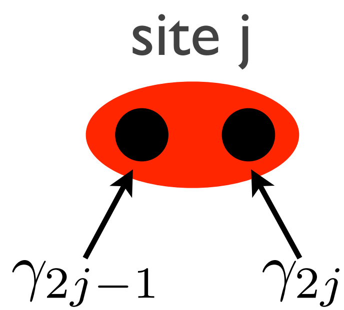
To reveal the topological nature of Kitaev's chain

$$H_{\text{Kitaev}} = \sum_j -\mu(c_j^\dagger c_j - c_j c_j^\dagger) - t(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) + \Delta(c_j c_{j+1} + c_{j+1}^\dagger c_j^\dagger)$$

we introduce Majorana fermions:

$$\gamma_{2j-1} = c_j + c_j^\dagger \;,\; \gamma_{2j} = -i(c_j - c_j^\dagger)$$

$$\{\gamma_i, \gamma_j\} = 2\delta_{i,j}$$



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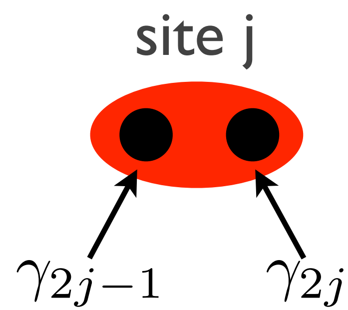

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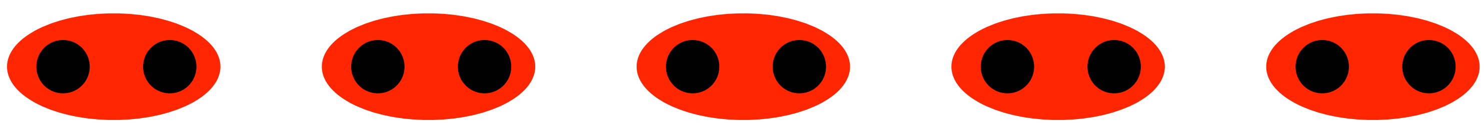

$$H_{\text{Kitaev}} = \frac{i}{2}\sum_j -(2\mu)\gamma_{2j-1}\gamma_{2j} + (t+\Delta)\gamma_{2j}\gamma_{2j+1} + (-t+\Delta)\gamma_{2j-1}\gamma_{2j+2}$$

Kitaev's Majorana chain: two phases

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For $t = \Delta = 0$ and $\mu < 0$, one finds a trivial phase:

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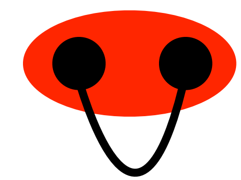

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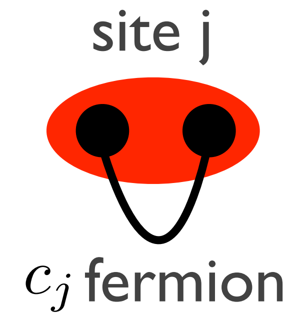

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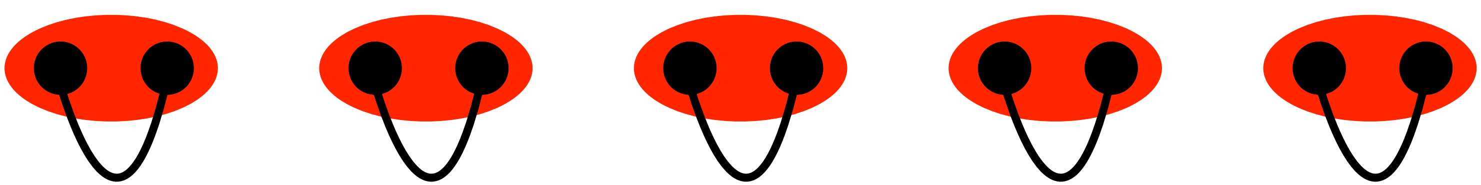
Majorana's from the same site are paired together!



The ground state is completely empty (filled for $\mu > 0$)

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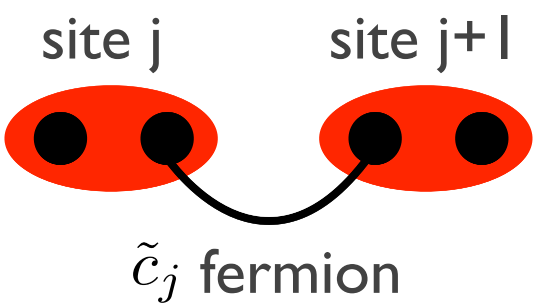

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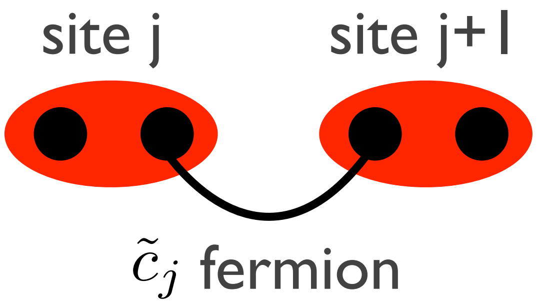

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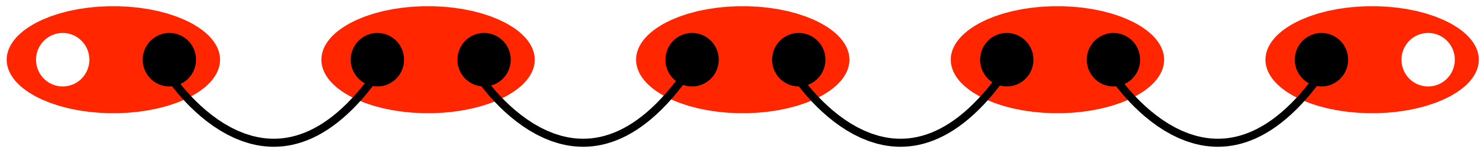

The Majorana's at the end are left unpaired. They combine into one, non-local fermionic mode **with zero energy**, which can be either filled or empty.

The pfaffian invariant

Kitaev defines a Majorana number for open chains $\mathcal{M} = \pm 1$:
$\mathcal{M} = -1$ if a Majorana bound state is present, $\mathcal{M} = +1$ if not

To define a topological invariant, we need periodic boundary conditions!
Consider the fermionic parity of the ground state of a hamiltonian H on a chain of length L: $P\big(H(L)\big)$

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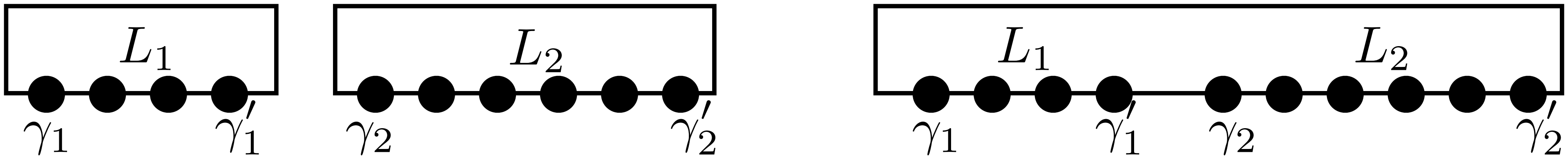

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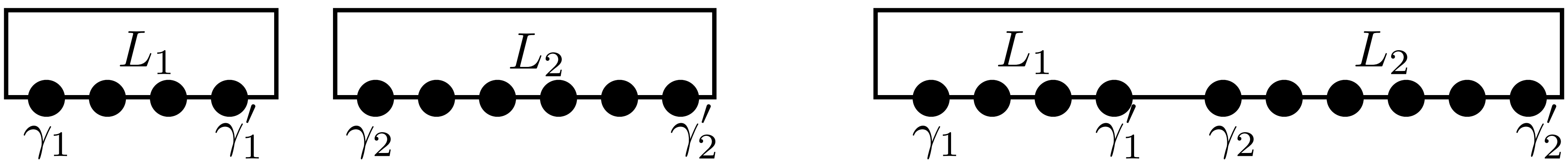

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For systems of even length: $\mathcal{M}(H) = P\big(H(L)\big)$

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A general Majorana chain has the form: $H = \dfrac{i}{2}\sum_{l,m} \gamma_l A_{l,m} \gamma_m$

where A is a real, anti-symmetric matrix.

A can be brought into Jordan form with a real, orthogonal matrix W:

$$A_J = WAW^T = \mathrm{diag}_\lambda \begin{pmatrix} 0 & \epsilon_\lambda \\ -\epsilon_\lambda & 0 \end{pmatrix}, \qquad \epsilon_\lambda > 0$$

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So we find the relation $\mathcal{M} = P(H) = \mathrm{sgn}\big(\mathrm{Pf}\, A\big) = \det W = \pm 1$

by using the relations $\mathrm{Pf}\, A_J = \prod_\lambda \epsilon_\lambda > 0$ and $\mathrm{Pf}\, A_J = \mathrm{Pf}\, A \det W$

Relation to the Berry phase

For Majorana chains with translation invariance, the invariant simplifies:

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In terms of the phases φ of the determinants, on has: $\mathcal{M} = (-1)^{\frac{\varphi_0 - \varphi_\pi}{\pi}}$

Thus, $\mathcal{M}$ is a phase winding: $\varphi_0 - \varphi_\pi = i \int_0^\pi \Big[\partial k \big(\log \det \tilde{W}(k)\big)\Big] dk$

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A calculation of the Berry phase in the Bogoliubov de Gennes picture gives exactly the same result.

Kitaev's pfaffian invariant can be seen as Berry phase (charge polarization)!

Budich, EA

What are Majorana bound states good for?

The topological phase can be found in nano-wires with SO interaction, deposited on an s-wave superconductor.

Lytchin et al., Oreg et al.

Several experimental groups have observed signatures consistent with the zero energy Majorana bound states.

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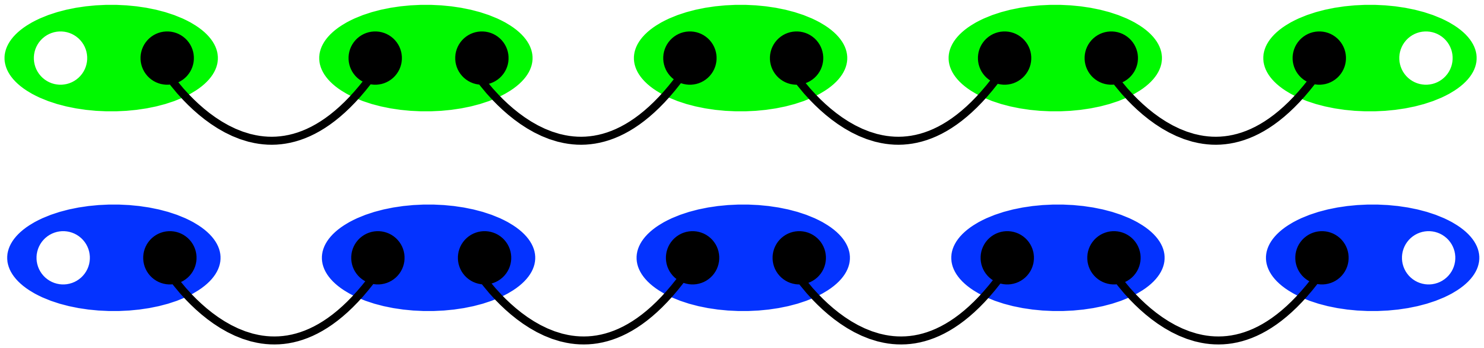
But, these anyons are not rich enough, one can not perform all gates...

Can we introduce more degrees of freedom?

If we take two spin copies of Kitaev's chain, one might be able to perform additional gates!



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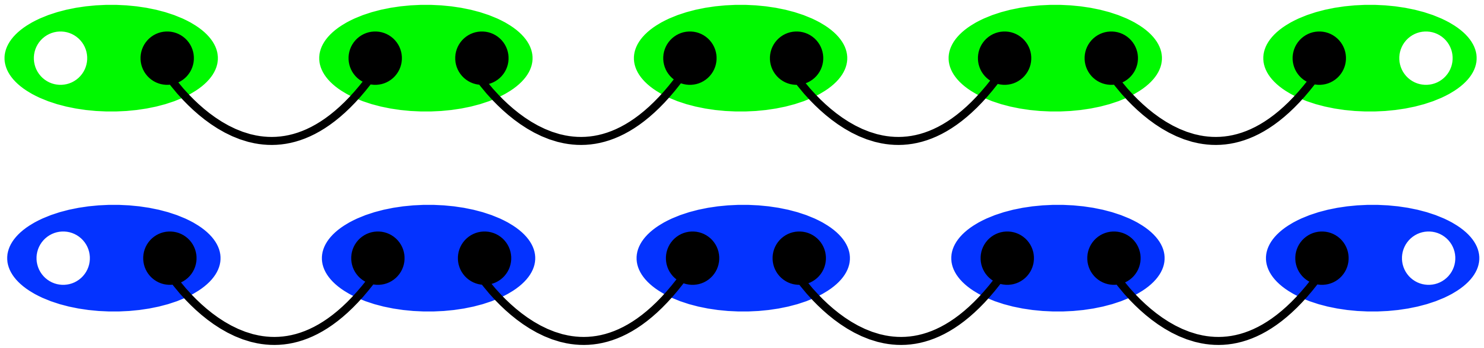

Generically, a pair of Majorana bound states at the edge will hybridize, but if time-reversal symmetry is preserved, each half of the Kramers pair has non-abelian statistics.

Liu et al.

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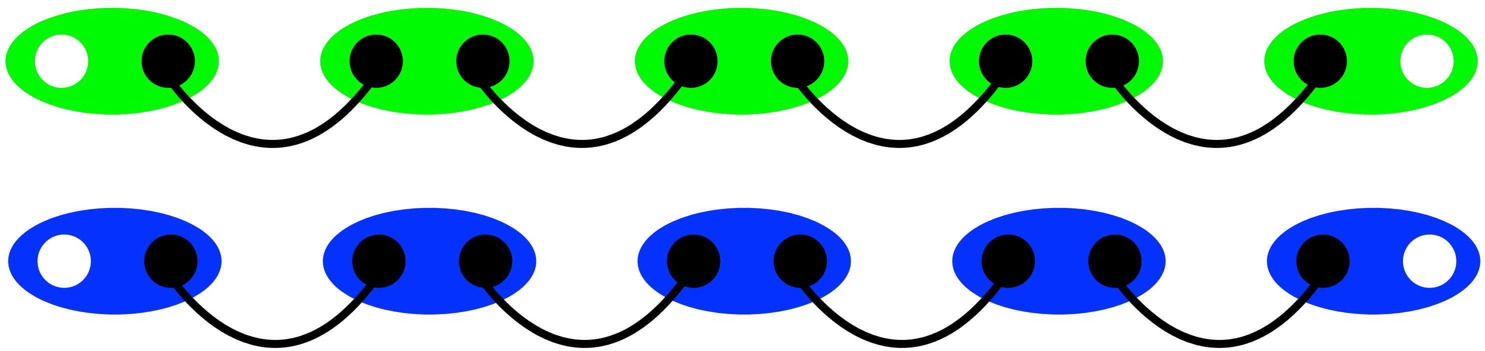

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Liu et al.

So, we will consider one-dimensional superconductors in class DIII.

Wong et al., Nakosai et al.

1-D superconductors in class DIII

In class DIII, we have both time reversal and particle-hole symmetry:
$\mathcal{T}^2 = -1 \ , \quad \mathcal{C}^2 = +1$, represented via $\mathcal{T} = i\sigma_y K \ , \quad \mathcal{C} = \tau_x K$

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Simple case: take a system h in class D, and construct its time-reversal conjugate (i.e., we have a spin-quantization axis)

$$H = \begin{pmatrix} h & 0 \\ 0 & h^* \end{pmatrix}$$

Both copies have the same value of Kitaev's invariant $\mathcal{M}(h) = \mathcal{M}(h^*) = \pm 1$

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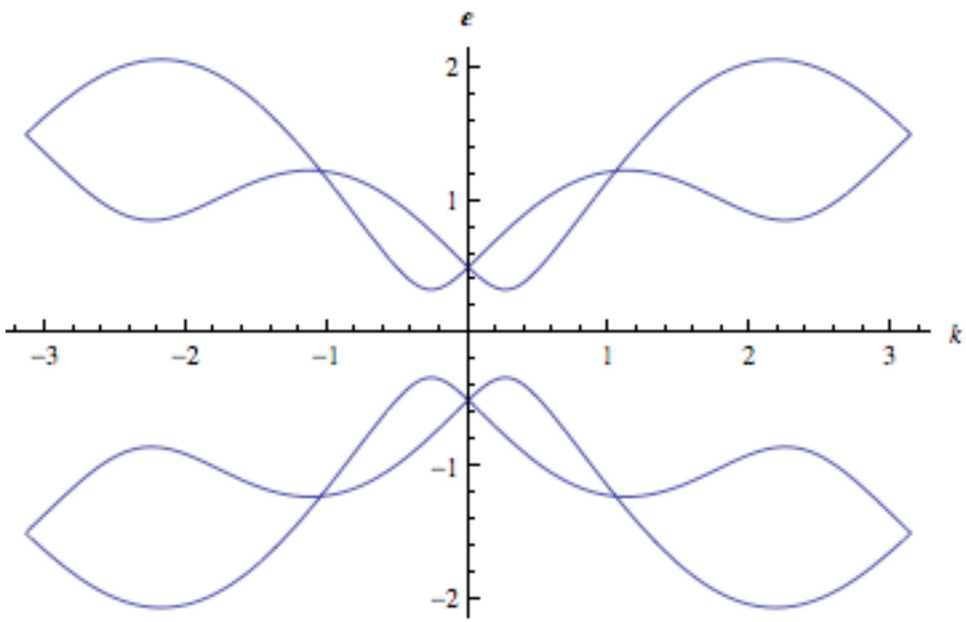
So, how do we construct an invariant in the general case?

1-D topological invariant for class DIII

Due to time-reversal symmetry, the Bloch bands come in pairs labeled by a Kramers index $\kappa = I, II$: $|u_\alpha^I(k)\rangle \ , \quad |u_\alpha^{II}(k)\rangle$

At the time-reversal symmetric (real) momenta, their energies are equal (Kramers theorem).



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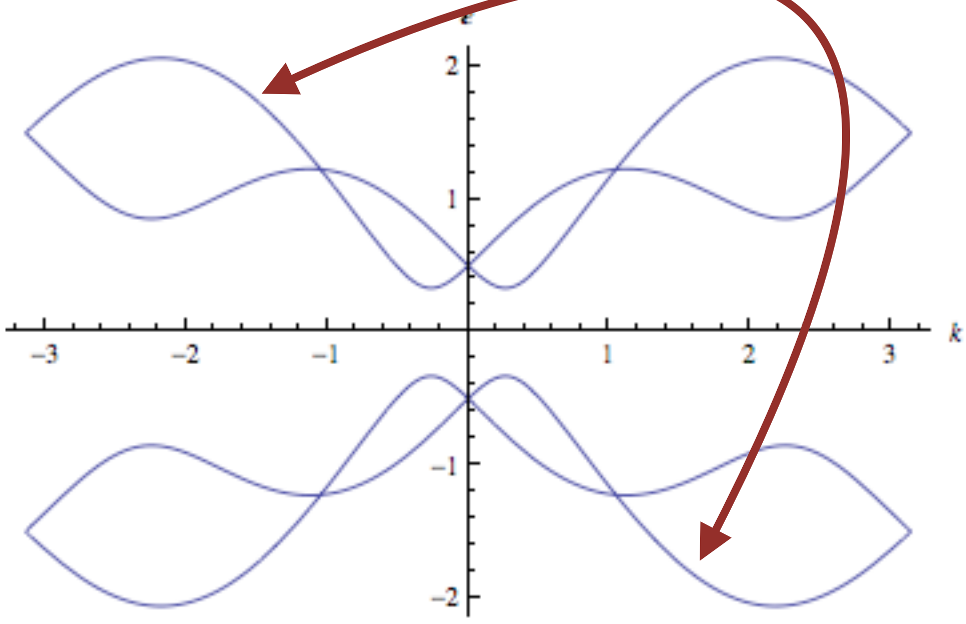

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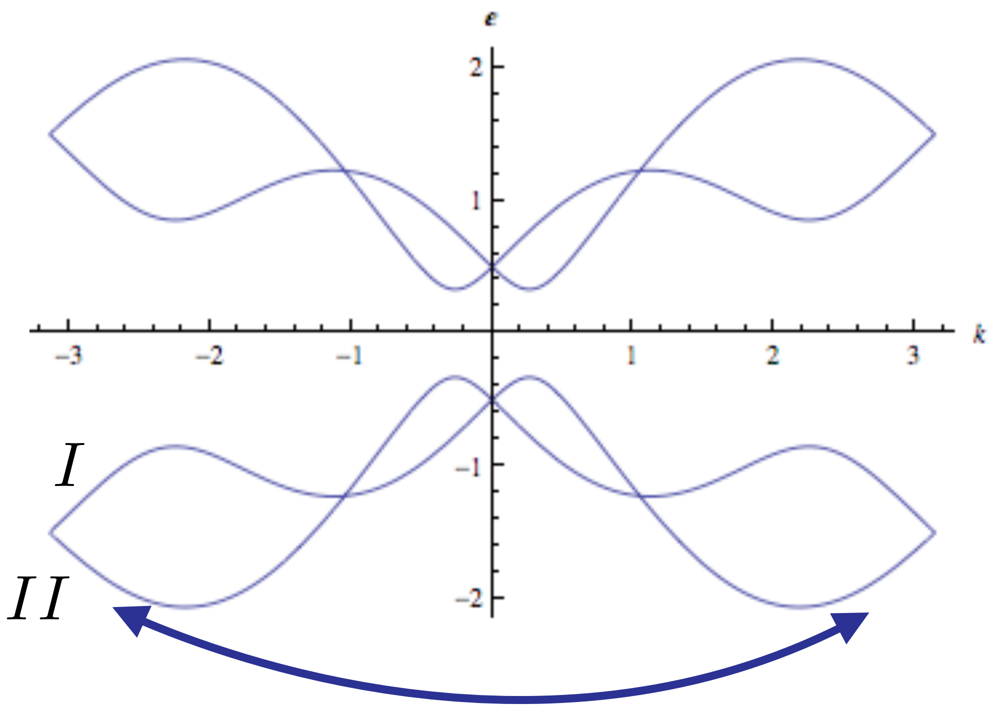

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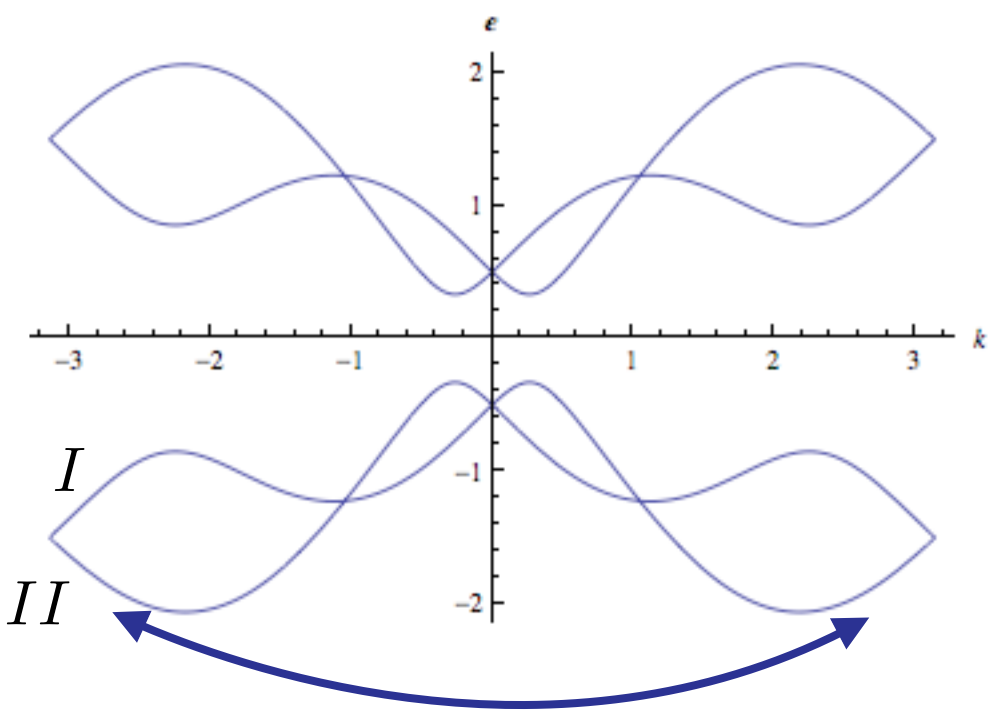

$$|u^I(-k)\rangle = -e^{i\chi(k)}\mathcal{T}|u^{II}(k)\rangle$$
$$|u^{II}(-k)\rangle = e^{i\chi(-k)}\mathcal{T}|u^I(k)\rangle$$

time-reversal symmetry

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We consider the (log of the) Berry phase (i.e., the polarization) of the occupied band I:

$$P_o^I = \frac{1}{2\pi}\int_0^{2\pi} dk \mathcal{A}_o^I(k)$$

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Berry connection

Following Fu & Kane, 2006

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Time reversal symmetry relates the Berry connection of band I and II:

$$\mathcal{A}_o^I(-k) = \mathcal{A}_o^{II}(k) - \partial_k \chi_\alpha(k)$$

It follows that P_o^I and P_o^{II} can only differ by an integer.

Following Fu & Kane, 2006

1-D topological invariant for class DIII

The polarization can be written as an integral over half the Brillouin zone

Fu & Kane, 2006

$$P_o^I = \frac{1}{2\pi}\left[\int_0^\pi \mathcal{A}_o(k)\mathrm{d}k \; + \; i\log\left(\frac{\mathrm{Pf}\;\theta_o(\pi)}{\mathrm{Pf}\;\theta_o(0)}\right)\right]$$

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In class AII, i.e., only time-reversal symmetry, P_o^I is not quantized.
In class DIII, however, the additional particle-hole symmetry implies the quantization of P_o^I, in half-integers!

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$$\nu = \mathrm{e}^{i2\pi P_o^I} = \mathrm{e}^{i\int_0^{\pi}\mathrm{d}k\mathcal{A}_o(k)}\left(\frac{\mathrm{Pf}\;\theta_o(0)}{\mathrm{Pf}\;\theta_o(\pi)}\right) = \pm 1$$

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The invariant can be calculated numerically efficiently, using Kato's gauge invariant form of the connection

Example in class DIII

As an example, we construct a non-trivial model in class DIII.
We first take two time reversal conjugate copies of a Kitaev chain:

$$H(k) = \big(-\mu - \cos(k)\big)\sigma_0 \otimes \tau_z + \Delta_p \sin(k)\, \sigma_0 \otimes \tau_y$$

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We add a Rashba term, as well as an s-wave pairing, preserving both time-reversal and particle-hole symmetry. There is no spin quantization axis!

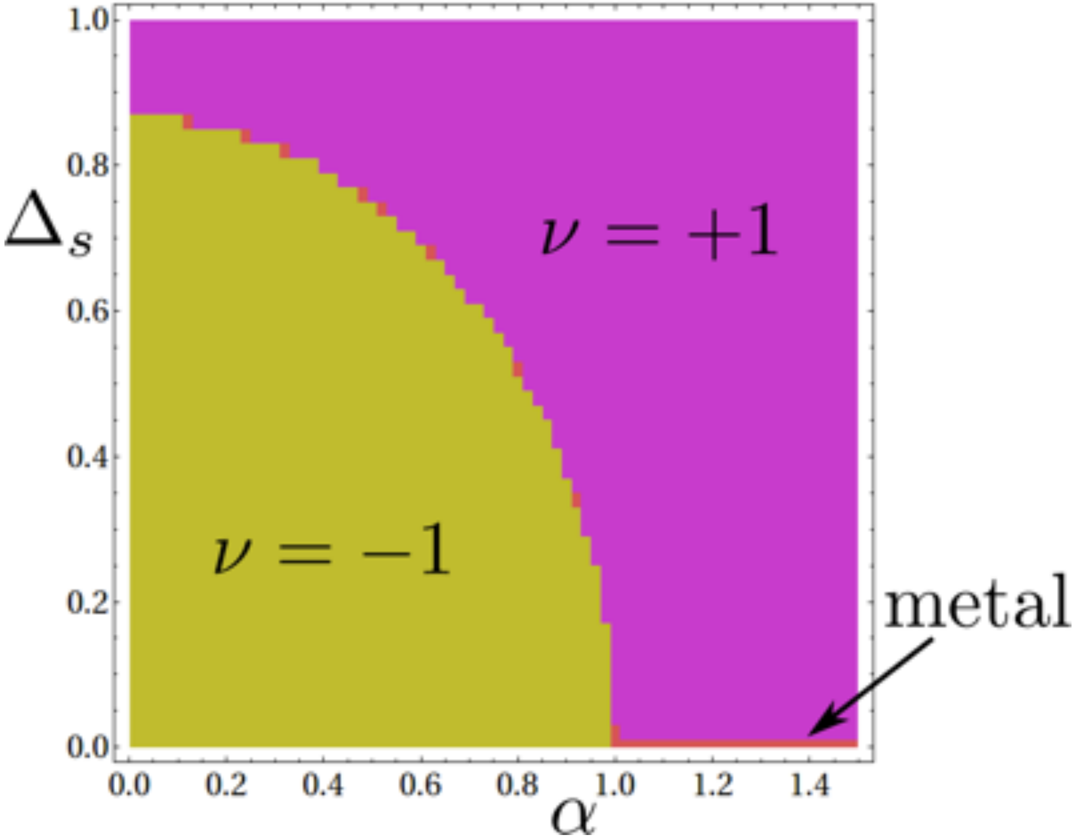
$$\begin{aligned} H(k) =& \big(-\mu - \cos(k)\big)\sigma_0 \otimes \tau_z + \Delta_p \sin(k)\, \sigma_0 \otimes \tau_y \\ &+ \alpha \sin(k)\, \sigma_x \otimes \tau_z + \Delta_s\, \sigma_y \otimes \tau_y \end{aligned}$$

The topological phase competes with both the s-wave pairing, as well as the Rashba spin-orbit coupling.

Example in class DIII

We can determine the phase diagram, by calculating the topological invariant for various parameters in the model.

For $\mu = -0.5$ and $\Delta_p = 1.0$, we obtain



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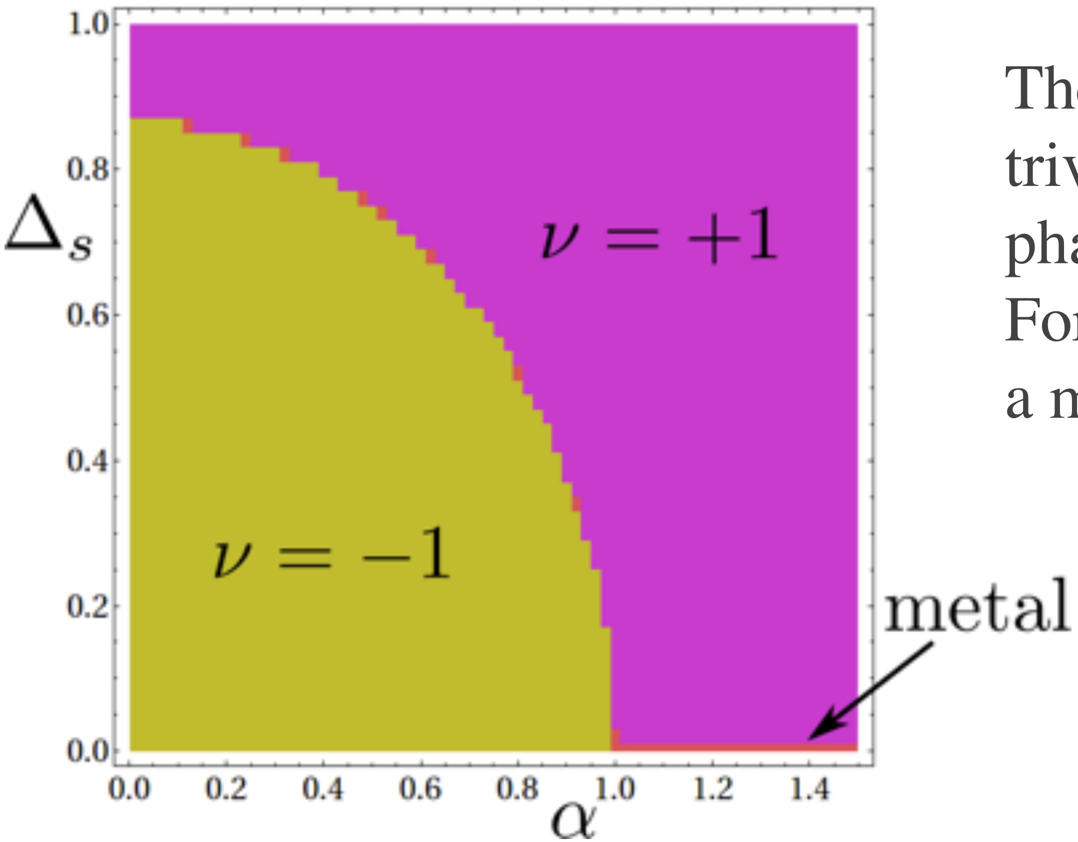

The purple region is the topolgically trivial phase, the yellow the non-trival phase.
For large $\alpha > 1.0$ and $\Delta_s = 0$, there is a metallic phase.

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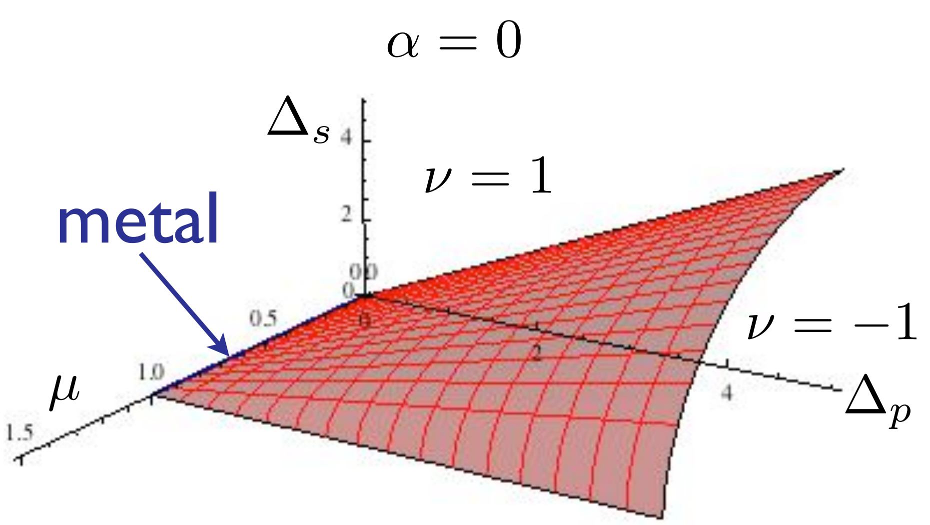

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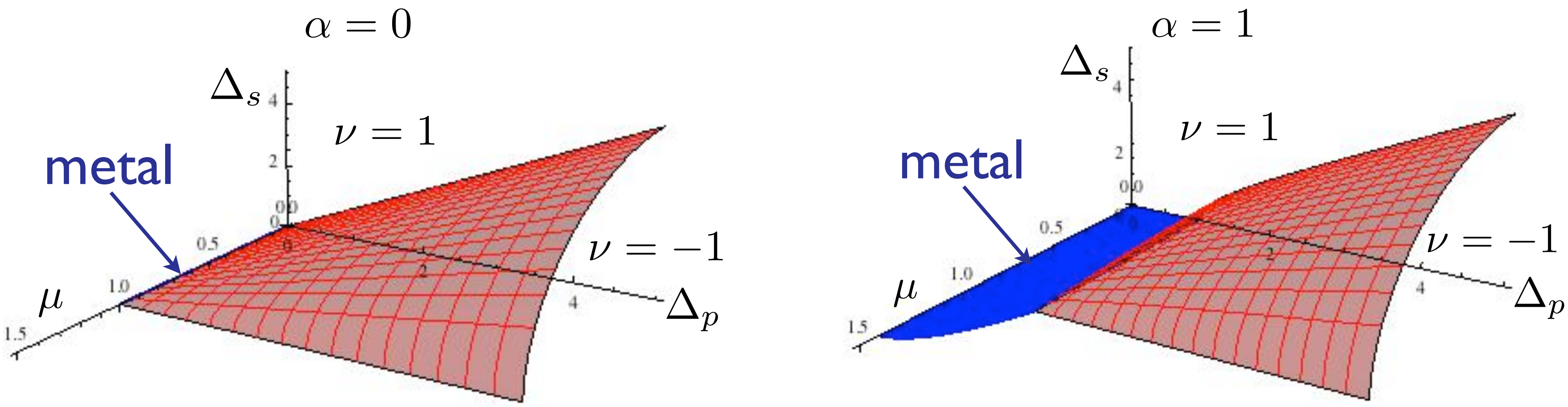

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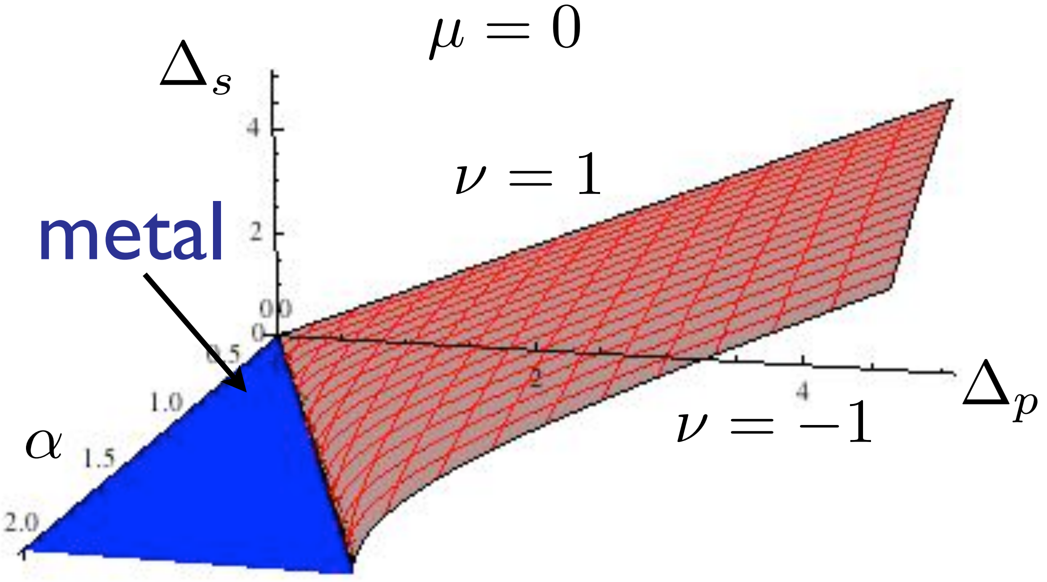

DIII invariant with inversion symmetry

In systems which also exhibit inversion symmetry, $x \mapsto -x$ the topological invariant simplifies.

Inversion symmetry is implemented by a unitary operator P_{inv} with $P_{\mathrm{inv}}^2 = 1$ satisfying $P_{\mathrm{inv}} H(k) P_{\mathrm{inv}} = H(-k)$ and $[P_{\mathrm{inv}}, \mathcal{T}] = 0$

The eigenvalues of P_{inv} are $\xi_i = \pm 1$.

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In the end of the day, the invariant is given by $\nu = \prod'_{\alpha:\,\mathrm{occ}} \xi_\alpha(0)\xi_\alpha(\pi)$

where the product is over all occupied bands, such that each Kramers pair contribute **once** to the product (both partners have the same eigenvalue due to time-reversal symmetry).

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Inversion symmetry simplifies the invariant, only knowledge about the real momenta is necessary to determine if the system is in a topological phase!

D invariant with inversion symmetry

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This relation can also be exploited for 2d systems with inversion symmetry in class A (QAH), and relate them to class AII.

Conclusion

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- We constructed the topological invariant of 1D superconductors in class DIII
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Thank you for your attention!