Majorana edge states and level crossings in chains of Co adatoms

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Scope

- Chains of cobalt adatoms

  → XY model with in-plane magnetic field

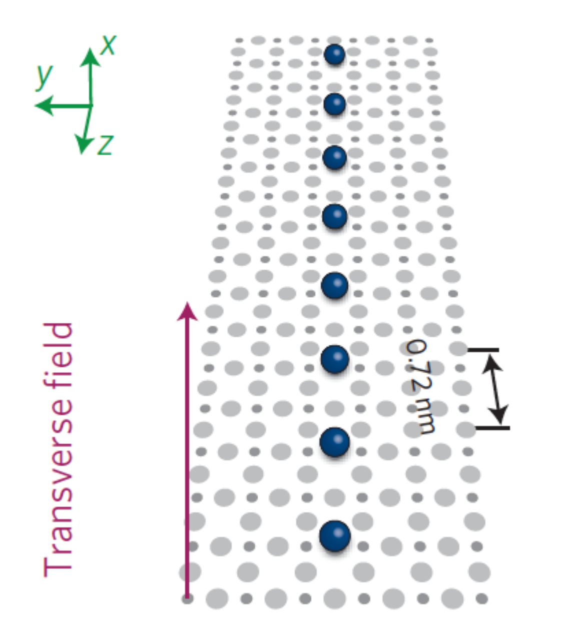
  → Series of level crossings
- The 1D Kitaev model of p-wave superconductor

  → Majorana wave-function oscillations

  → level crossings as a function of μ
- Transverse field Ising model with longitudinal coupling

  → Mapping on Kitaev
- Conclusions

Chains of Co adatoms on Cu_2N



$$\mathcal{H}_{3/2} = J\sum_{i=1}^{N-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + D\sum_{i=1}^{N} (S_i^z)^2 - g\mu_B B_x \sum_{i=1}^{N} S_i^x$$

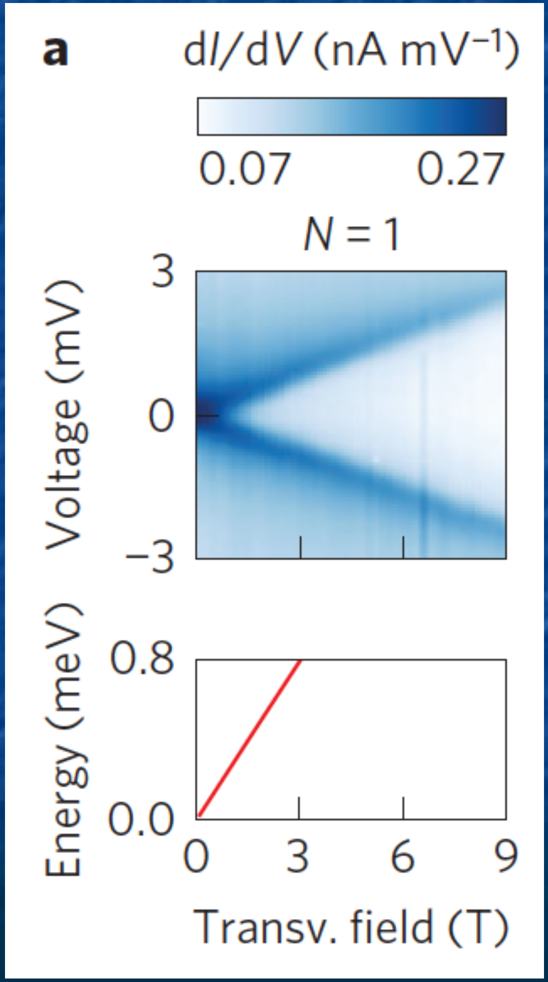
$$J = 0.24 \text{ meV}, \ D = 2.75 \text{ meV}$$

J/D expansion

$$\mathcal{H}_{1/2} \simeq \sum_{i=1}^{N-1} J_\perp (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) - \mu_B B_x \sum_{i=1}^{N} g_i S_i^x$$

Teskovic, van den Berg, Spinelli, Eliens, van den Toorn, Bryant, Caux, Otte, Nat. Phys. 2016

STM results: single site



Zeeman effect

↓

Splitting of Kondo resonance

↓

V shape spectrum

STM results: up to 9 sites

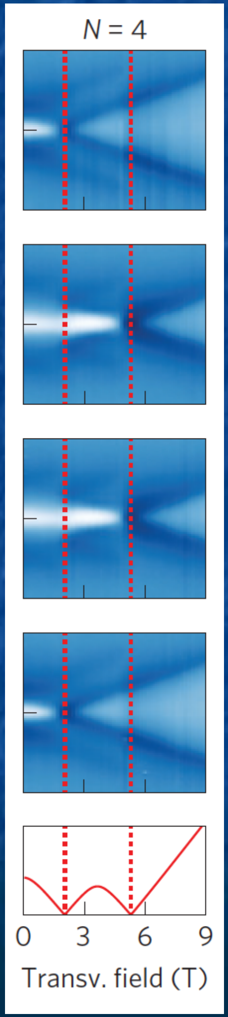
4 sites

Site 1

Site 2

Site 3

Site 4

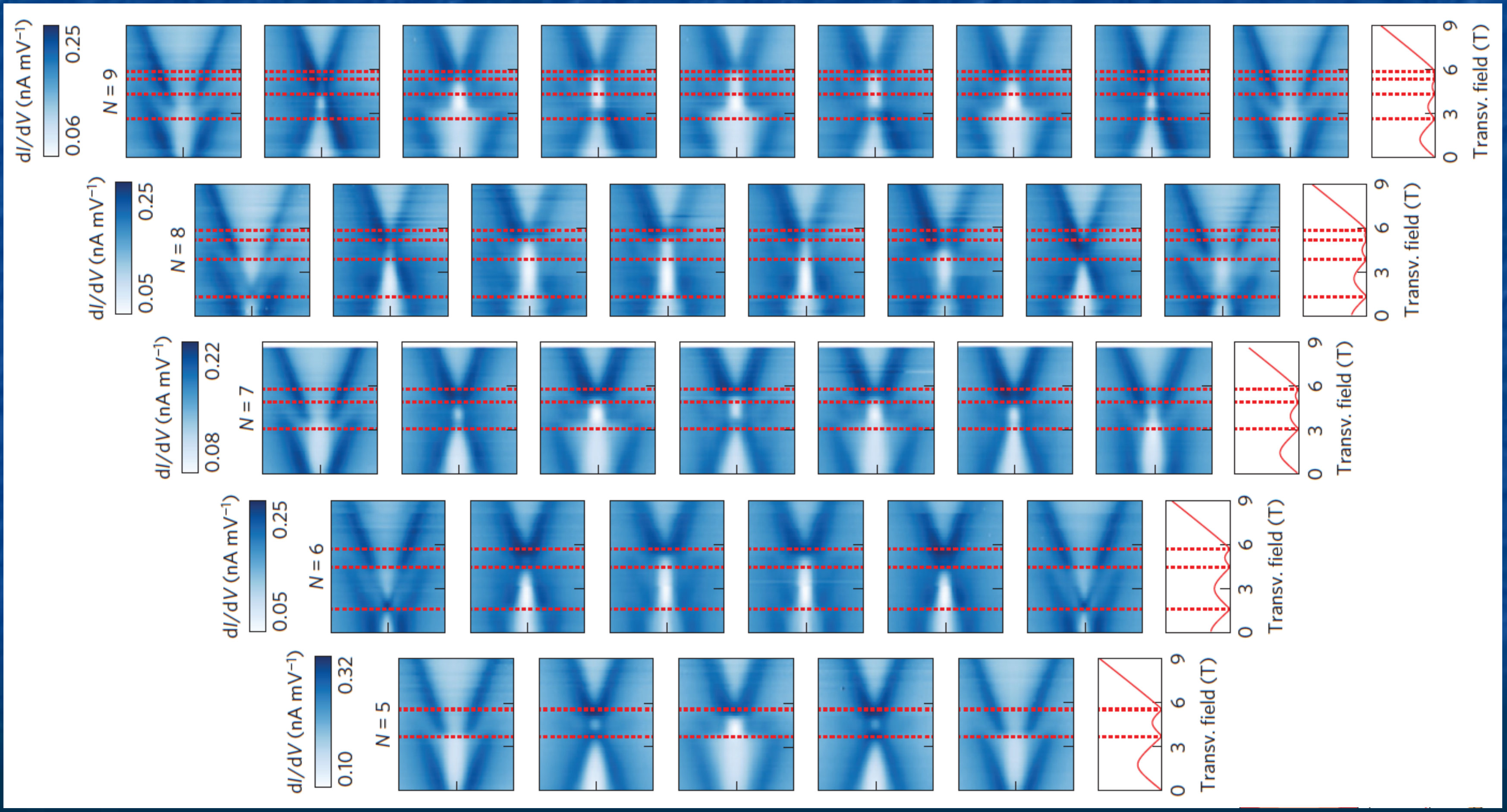


V shape

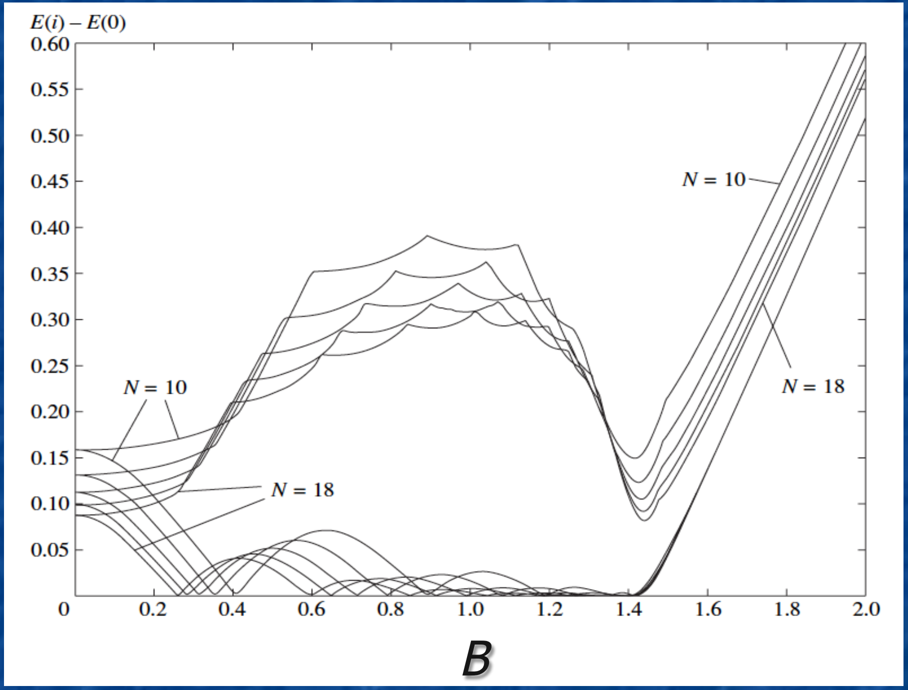
↓

Level crossing at the tip of the V

Results from 5 to 9 sites



Exact diagonalization



N/2 level crossings for B>0

↓

N level crossings

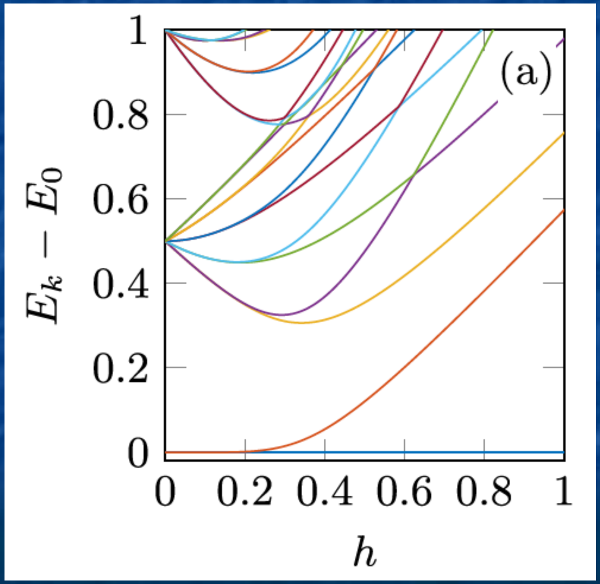
Dmitriev, Krivnov, Ovchinnikov, Langari, JETP 2002

Physical origin?

Effect of longitudinal coupling

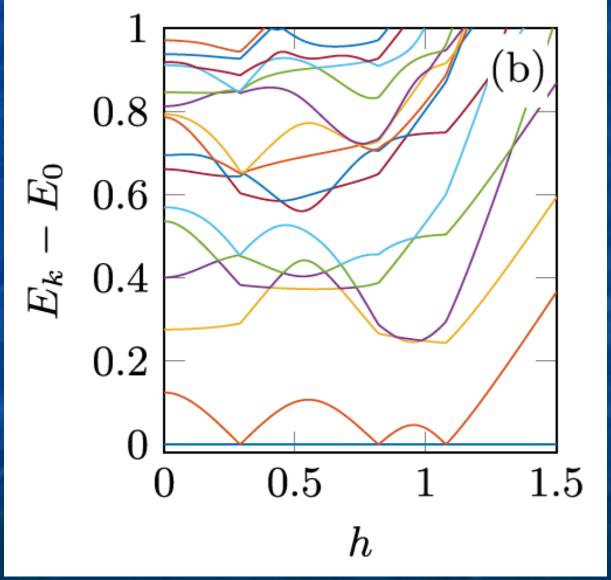
$$H = J_x \sum_{i=1}^{N-1} S_i^x S_{i+1}^x + J_z \sum_{i=1}^{N-1} S_i^z S_{i+1}^z - h \sum_{i=1}^{N} S_i^z$$

J_z=0 (Ising)



No crossing

J_z=0.75



Several crossings

Link to Majorana edge states

FM, Nat. Phys. 2016

Transverse field Ising model $\longleftrightarrow$ (Jordan-Wigner) Kitaev chain with $\Delta=t$

+ Longitudinal coupling $\longrightarrow$ Level crossings between GS?

Mapping of TFI onto Kitaev

Transverse field
Ising model

$$H = J_x \sum_{i=1}^{N-1} S_i^x S_{i+1}^x - h \sum_{i=1}^{N} S_i^z$$

Jordan-Wigner transformation

$$\begin{cases} S_i^x = \frac{1}{2}(c_i^\dagger + c_i) \exp\left(\mathrm{i}\pi \sum_{j<i} c_j^\dagger c_j\right) \\ S_i^y = \frac{1}{2\mathrm{i}}(c_i^\dagger - c_i) \exp\left(\mathrm{i}\pi \sum_{j<i} c_j^\dagger c_j\right) \\ S_i^z = c_i^\dagger c_i - \frac{1}{2}, \end{cases}$$

$$\mathcal{H} = t \sum_{i=1}^{N-1} (c_i^\dagger c_{i+1} + \mathrm{H.c.}) - \Delta \sum_{i=1}^{N-1} (c_{i+1}^\dagger c_i^\dagger + \mathrm{H.c.}) - \mu \sum_{i=1}^{N} c_i^\dagger c_i$$

$$\text{with } \Delta = t = J_x/4, \; \mu = h$$

Pfeuty, 1970

Kitaev model with Δ=t

Kitaev p-wave SC chain

Kitaev, 2001

$$\mathcal{H} = -t \sum_{i=1}^{N-1} (c_i^\dagger c_{i+1} + \mathrm{H.c.}) + \Delta \sum_{i=1}^{N-1} (c_{i+1}^\dagger c_i^\dagger + \mathrm{H.c.}) - \mu \sum_{i=1}^{N} c_i^\dagger c_i$$

- $|\mu| < 2t$
  → topological phase
  → 2-fold degenerate ground state
- $|\mu| > 2t$
  → trivial phase
  → unique ground state

Majorana formulation

Majorana fermions

$$\begin{cases} \gamma_i' = c_i + c_i^\dagger \\ \gamma_i'' = -\mathrm{i}(c_i - c_i^\dagger) \end{cases}$$

$$\gamma_i''^\dagger = \gamma_i'' \qquad \gamma_i'^\dagger = \gamma_i'$$

$$\{\gamma_i', \gamma_j''\} = 0 \qquad \{\gamma_i', \gamma_j'\} = \{\gamma_i'', \gamma_j''\} = 2\delta_{ij}$$

$$\mathcal{H} = \frac{i}{2} \sum_{i=1}^{N-1} (\Delta + t)\gamma_i''\gamma_{i+1}' + (\Delta - t)\gamma_i'\gamma_{i+1}'' - \frac{i\mu}{2} \sum_{i=1}^{N} \gamma_i'\gamma_i''$$

Majorana edge states

$$\Delta = t, \mu = 0 \quad \rightarrow \quad \mathcal{H} = it \sum_{i=1}^{N-1} \gamma_i'' \gamma_{i+1}'$$

γ_1' and γ_N'' do not appear in $\mathcal{H}$ → **Perfectly localized states**

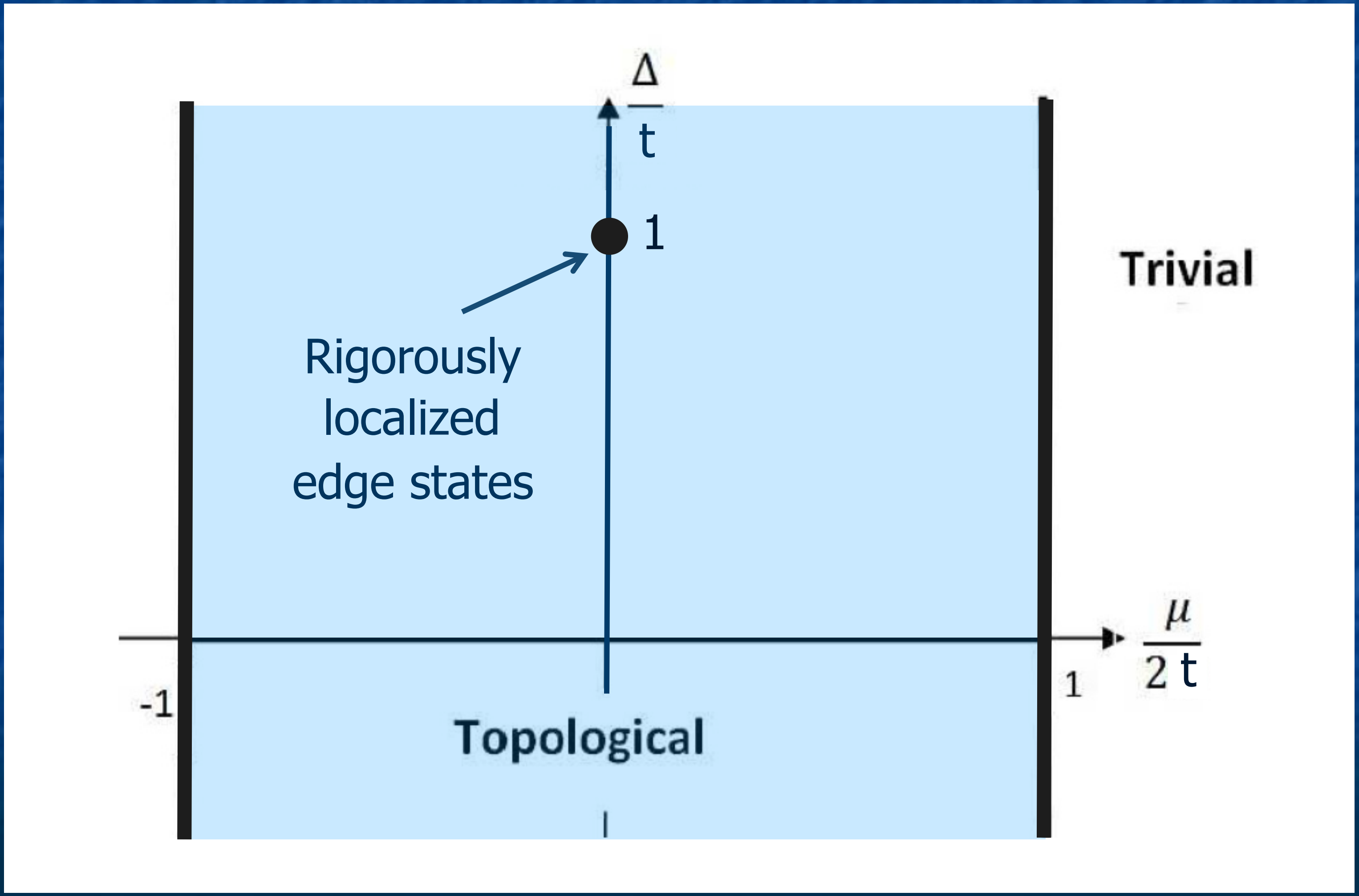
$$\begin{cases} c^\dagger = \gamma_1' + i\gamma_N'' \\ c = \gamma_1' - i\gamma_N'' \end{cases} \rightarrow \text{fermion, can be empty or occupied}$$

→ **Two-fold GS degeneracy**

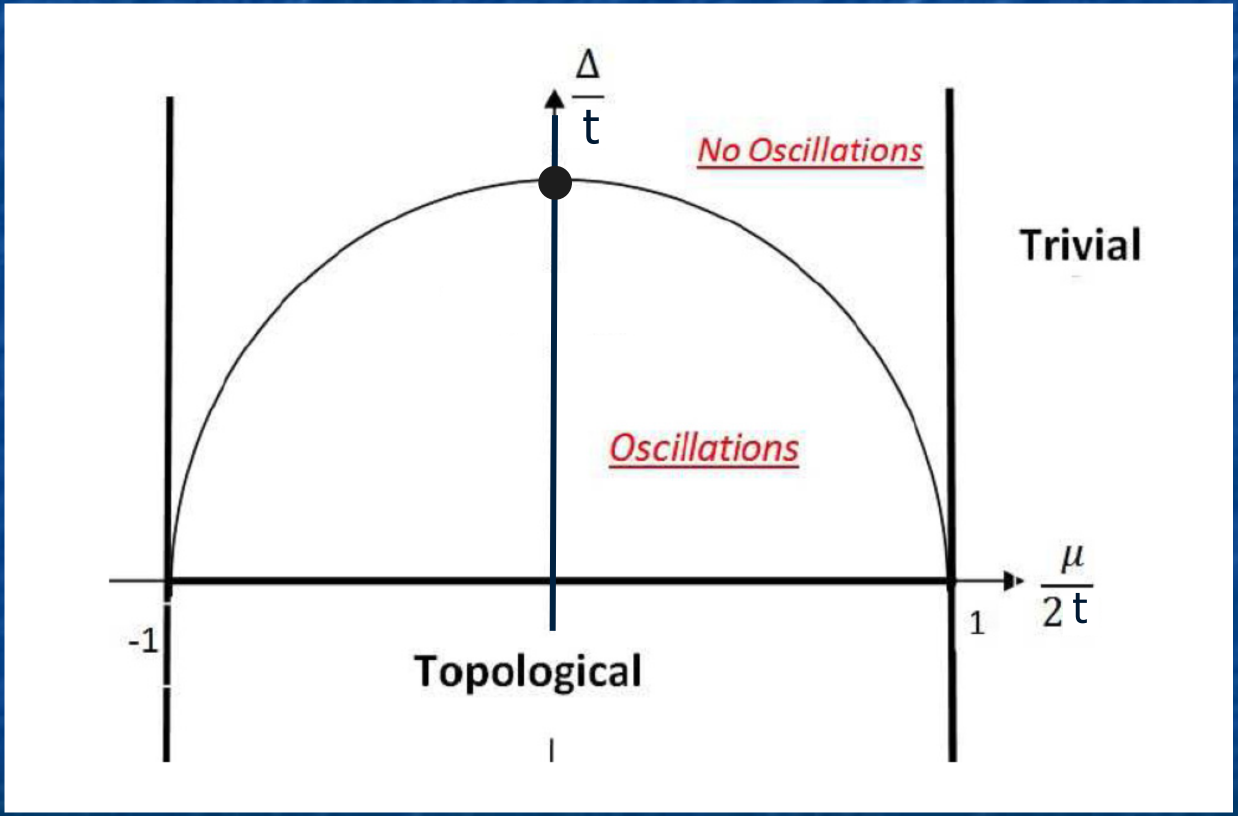
General properties of topological phase

- Localized Majorana edge states
- Quasi-degeneracy
  → splitting of the order of $\exp(-Na/\xi)$
  → ξ= localization length of Majorana edge states
- Detection of Majorana edge states
  → STM at the end of the chain
  Mourik et al, Science 2012; Nadj-Perge et al, Science 2014
- Other way of detecting them? YES!

Phase diagram



Majorana oscillations



Kao, PRB 2014; Hedge and Vishveshwara, PRB 2016

Majorana wave-functions

Diagonalization of H $\longrightarrow$

$$\mathcal{H} = \frac{i}{2}\sum_{k=1}^{N} \epsilon_k \tilde{\gamma}'_k \tilde{\gamma}''_k$$

$$\tilde{\gamma}'_k = \sum_j (a_+ x_+^j + a_- x_-^j + b_+ x_+^{N+1-j} + b_- x_-^{N+1-j})\gamma'_j$$

$$\tilde{\gamma}''_k = \sum_j (a_+ x_+^{N+1-j} + a_- x_-^{N+1-j} + b_+ x_+^j + b_- x_-^j)\gamma''_j$$

Smallest eigenvalue

$$\left(\frac{\mu}{2t}\right)^2 + \left(\frac{\Delta}{t}\right)^2 < 1 \rightarrow x_\pm = re^{\pm i\phi}, \phi > 0$$

Boundary conditions for zero mode

Smallest eigenvalue

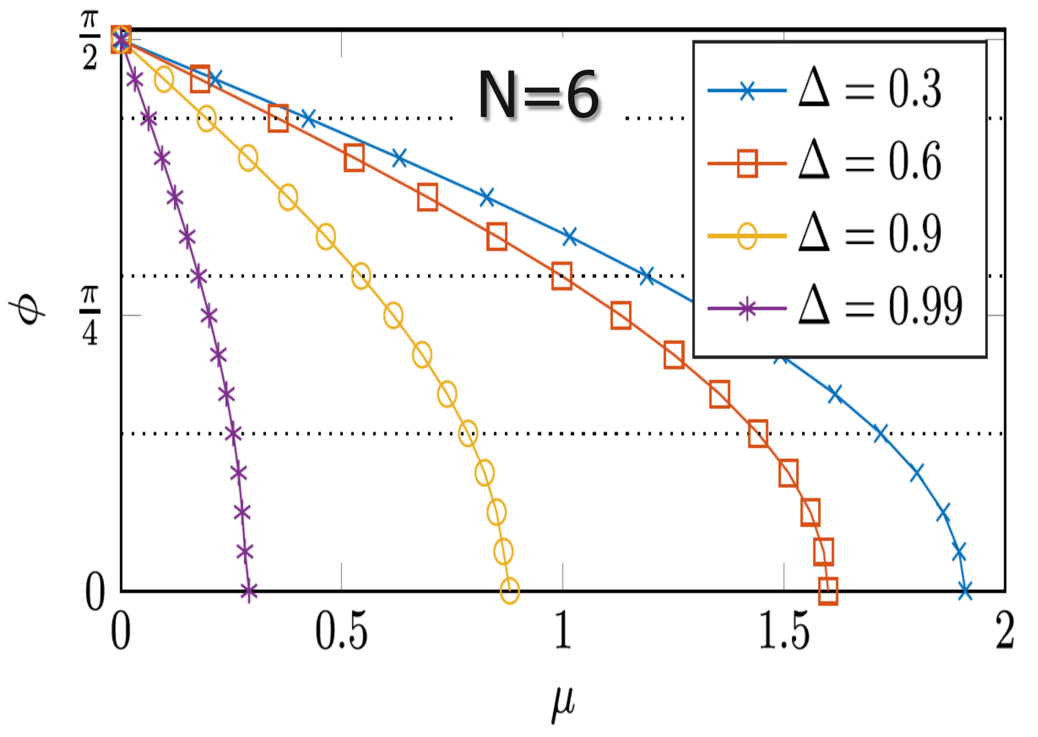
$$\epsilon_1 = 0 \longrightarrow \begin{cases} b_+ = b_- = 0 \\ a_+ + a_- = 0 \\ a_+ x_+^{N+1} + a_- x_-^{N+1} = 0 \end{cases}$$

Possible if

$$(x_+^{N+1} - x_-^{N+1}) \propto r^{N+1} \sin[(N+1)\phi] = 0$$

or $$\phi = \frac{\pi m}{N+1}$$

Phase condition



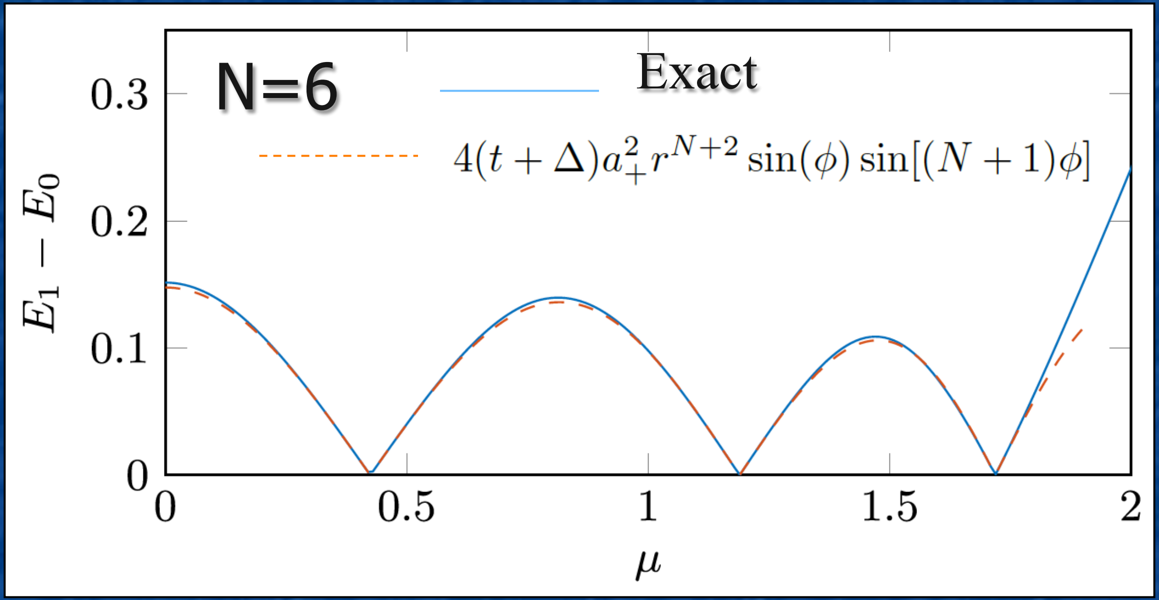
$$\tan\phi = \sqrt{(\mu_c/\mu)^2 - 1}$$

N solutions as soon as

$$\left(\frac{\Delta}{t}\right)^2 < 1$$

G. Vionnet, B. Kumar, FM, arXiv:1701.08057

Zero modes



N zero modes in the interval -2t < μ < 2t

NB: level crossings because low-lying states have different fermion parity

XY model in transverse field

$$H = J_x \sum_{i=1}^{N-1} S_i^x S_{i+1}^x + J_y \sum_{i=1}^{N-1} S_i^y S_{i+1}^y - h \sum_{i=1}^{N} S_i^z$$

$$\mathcal{H} = t \sum_{i=1}^{N-1} (c_i^\dagger c_{i+1} + \mathrm{H.c.}) - \Delta \sum_{i=1}^{N-1} (c_{i+1}^\dagger c_i^\dagger + \mathrm{H.c.}) - \mu \sum_{i=1}^{N} c_i^\dagger c_i$$

with $t = (J_x + J_y)/4, \ \Delta = (J_x - J_y)/4, \ \mu = h$

Oscillations of correlation functions

Barouch and McCoy, 1971

TFI with longitudinal coupling

$$H = J_x \sum_{i=1}^{N-1} S_i^x S_{i+1}^x + J_z \sum_{i=1}^{N-1} S_i^z S_{i+1}^z - h \sum_{i=1}^{N} S_i^z$$

$$\mathcal{H} = \mathcal{H}(J_z = 0) + J_z \sum_{i=1}^{N-1} (c_i^\dagger c_i - \frac{1}{2})(c_{i+1}^\dagger c_{i+1} - \frac{1}{2})$$

Model of interacting fermions

Symmetry: rotation by π around z

<=> fermion parity

Mean-field theory

- Simultaneous decoupling in all channels

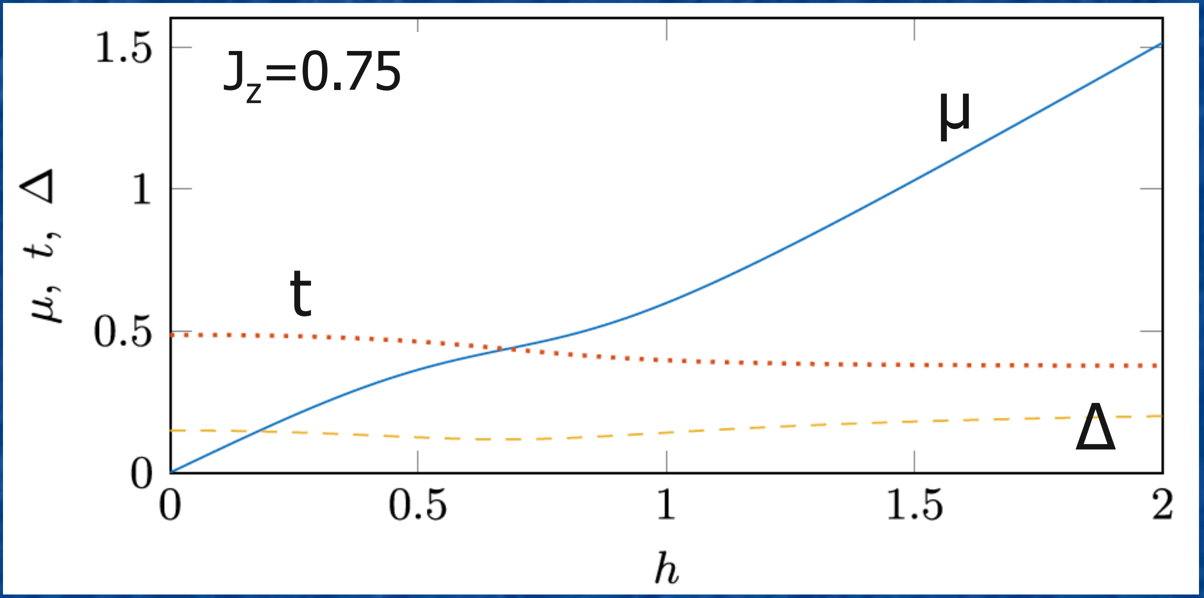
$$
\begin{aligned}
c_i^\dagger c_i c_{i+1}^\dagger c_{i+1} \simeq & \langle c_i^\dagger c_i \rangle\, c_{i+1}^\dagger c_{i+1} + \langle c_{i+1}^\dagger c_{i+1} \rangle\, c_i^\dagger c_i - \langle c_i^\dagger c_i \rangle \langle c_{i+1}^\dagger c_{i+1} \rangle \\
& - \langle c_i^\dagger c_{i+1}^\dagger \rangle\, c_i c_{i+1} - \langle c_i c_{i+1} \rangle\, c_i^\dagger c_{i+1}^\dagger + \langle c_i^\dagger c_{i+1}^\dagger \rangle \langle c_i c_{i+1} \rangle \\
& + \langle c_i^\dagger c_{i+1} \rangle\, c_i c_{i+1}^\dagger + \langle c_i c_{i+1}^\dagger \rangle\, c_i^\dagger c_{i+1} - \langle c_i^\dagger c_{i+1} \rangle \langle c_i c_{i+1}^\dagger \rangle
\end{aligned}
$$

→ Kitaev model for periodic BC with

$$\mu = h + J_z(1 - 2\langle c_i^\dagger c_i \rangle),\ t = \frac{J_x}{4} - J_z \langle c_i^\dagger c_{i+1} \rangle,\ \text{and } \Delta = \frac{J_x}{4} - J_z \langle c_i c_{i+1} \rangle$$

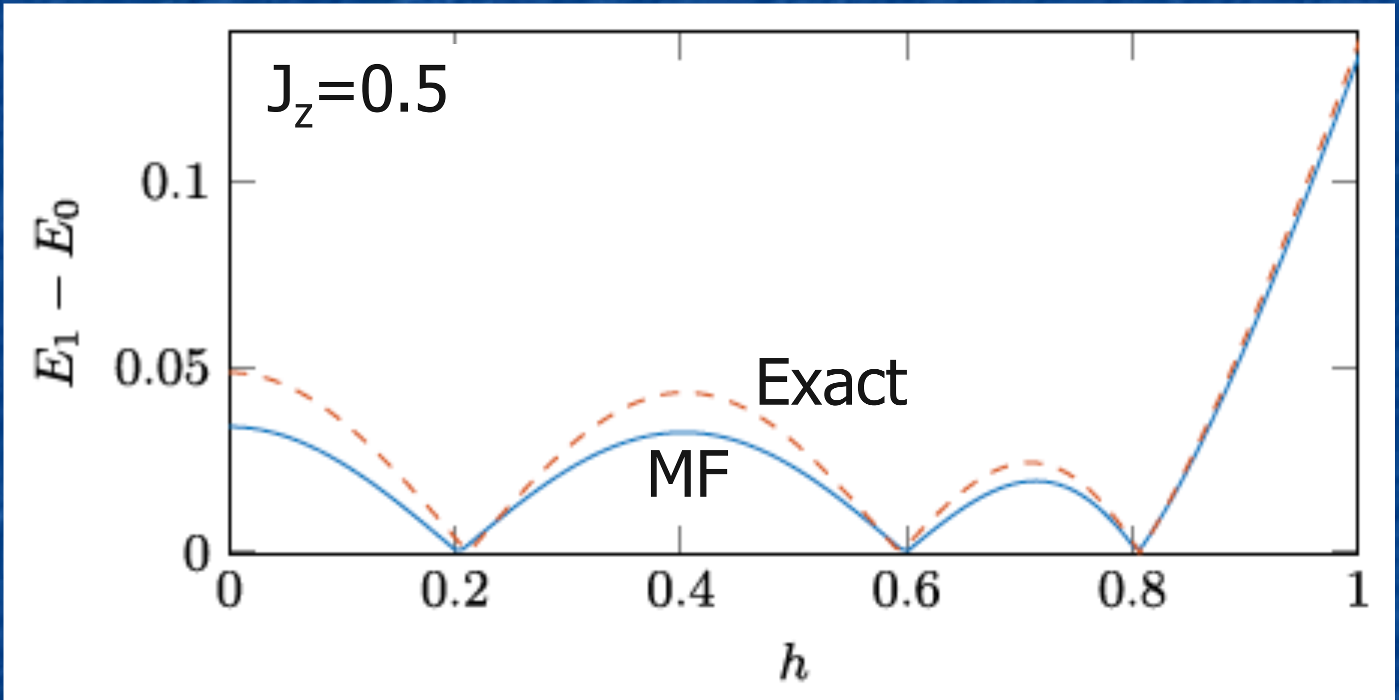
G. Vionnet, B. Kumar, FM, arXiv:1701.08057

Mean-field parameters



t and Δ nearly constant, Δ<t, μ roughly linear in h
→ qualitatively equivalent to Kitaev

MF theory of level crossings



Good agreement between ED and MF Kitaev model

Conclusion/Perspectives

- Level crossings in Co adatoms
  → evidence of two quasi-degenerate GS
  → mechanism: Majorana oscillations
- Other geometries (perpendicular field, longer chains, 2D arrangements,…)
- Level crossings in SC wires
  → see Albrecht et al, Nature 2016