# Majorana in condensed matter systems – PART II

## IV) Experimental realizations: Heuristic arguments

Recipe for realizing 1d TSC in experiment:

* Spinless fermions ⟶ spin-polarized electrons
  - half metal
  - strong Zeeman field

* Superconductivity ⟶ proximity effect w/ conventional SC
  - s-wave: spin-singlet Cooper pairs cannot enter into spin-polarized system
  - p-wave: not readily available

* Spin-orbit coupling ⟶ effectively mixes s- and p-wave order parameters in SC; p-wave component can enter into spin-polarized system

NOTE: * SO coupling can be in SC (half metal, magnetic adatoms), in normal system (semiconductor quantum wires – InAs, InSb), or both

* alternative: helical Zeeman field

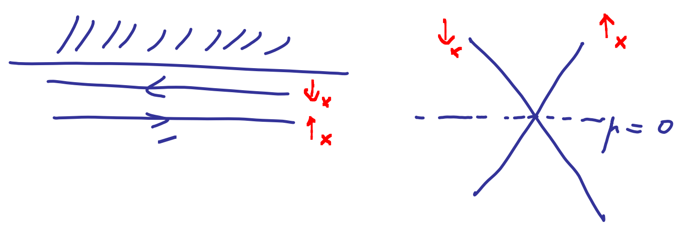
## V) Topological insulator edge

Model & phase diagram:

Can induce topological SC by proximity coupling to s-wave SC (Fu & Kane PRL 2008 & PRB 2009)

helical edge states of 2d TI (conserved $\sigma_x$; $\mu = 0$) → Kane's lecture

$$H = v_F p \sigma_x$$

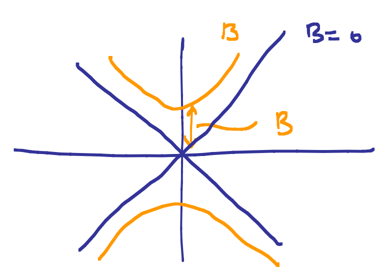



($\sigma_i$ : Pauli matrices in spin space)

gaps opened by

* Zeeman field perpendicular to $\hat{x}$, by applied B field or by proximity to magnetic insulator

$$H = v_F p \sigma_x + B \sigma_z$$




$$\rightsquigarrow \quad E_k = \pm\sqrt{(v_F k)^2 + B^2}$$

* Proximity coupling to s-wave SC

$$H = v_F p \sigma_x \tau_z + \Delta \tau_x$$

(using Nambu spinor $[\psi_\uparrow, \psi_\downarrow, \psi_\downarrow^\dagger, -\psi_\uparrow^\dagger]$; hh block in BdG Hamiltonian is minus the time reversed of the ee block; s-wave pairing is proportional to unit matrix in spin space)

Simultaneous presence of both terms: gaps compete!

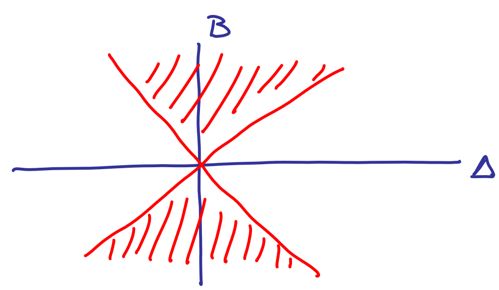
$$H = v_F p \sigma_x \tau_z + B \sigma_z + \Delta \tau_x$$

Spectrum by squaring:

$$H^2 = (v_F p)^2 + B^2 + \Delta^2 - 2B\Delta \sigma_z \tau_x$$

$$\Rightarrow \boxed{E_p^\pm = \pm\sqrt{(v_F p)^2 + (B \mp \Delta)}}$$

$\rightsquigarrow$ gap closes for $B = \pm\Delta$



Q: Which phase is topological?

actually both: model has magnetism - superconductivity duality (evident when relabeling $\sigma_x \Leftrightarrow \sigma_z$); no atomic limit due to linear spectrum

Low-energy theory near critical line & domain walls:

Project model to low energies for $B \simeq \Delta$ & $p$ small ($\mu = 0$):

low-energy subspace $|+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ $\quad |-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ 0 \\ -1 \end{bmatrix}$
($\sigma_z \tau_x = 1$)

$$\langle + | \sigma_x \tau_z | + \rangle = \frac{1}{2} (1\ 0\ 1\ 0) \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix} = 0$$

$$\langle - | \sigma_x \tau_z | - \rangle = \frac{1}{2} (0\ 1\ 0\ -1) \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} = 0$$

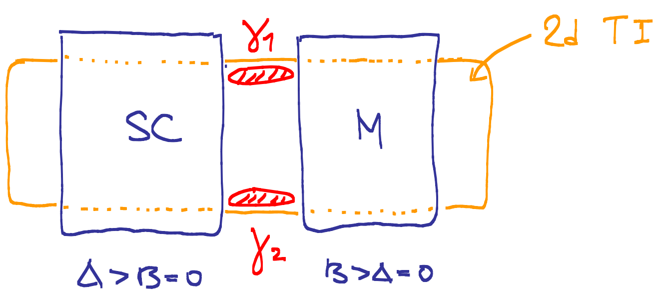
$$\langle + | \sigma_x \tau_z | - \rangle = \frac{1}{2} (1\ 0\ 1\ 0) \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} = 1$$

$$\rightsquigarrow \quad H_{eff} \approx \begin{pmatrix} \Delta - B & v_F p \\ v_F p & -(\Delta - B) \end{pmatrix}$$

exactly the same low-energy Dirac theory as for p-wave SC of spinless fermions discussed above

- domain walls: zero-energy bound state; for domain wall w/ $\Delta - B = \alpha x$ shifted harmonic oscillator spectrum as discussed above.

- "simplest" domain wall (Fu & Kane PRB 2009)




- topological critical point: $\Delta - B = 0$

$$H = \begin{pmatrix} 0 & v_F p \\ v_F p & 0 \end{pmatrix} \quad \text{w/ eigenvectors} \quad \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{ikx} \quad \& \quad \begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{ikx}$$

or, in original 4-spinors

$$\begin{pmatrix} 1 \\ 1 \\ 1 \\ -1 \end{pmatrix} e^{ikx} \longrightarrow \gamma_k^{(R)} = \psi_{k\uparrow} + \psi_{k\downarrow} + \psi^\dagger_{-k\downarrow} + \psi^\dagger_{-k\uparrow}$$

$$i\begin{pmatrix} 1 \\ -1 \\ 1 \\ 1 \end{pmatrix} e^{ikx} \longrightarrow \gamma_k^{(L)} = i\left[\psi_{k\uparrow} - \psi_{k\downarrow} + \psi^\dagger_{-k\downarrow} - \psi^\dagger_{-k\uparrow}\right]$$

i.e., modes are right (R) – and left (L) moving Majorana modes,

$$\gamma_k^\dagger = \gamma_{-k}$$

– Zero-energy bound states & Majorana operators

time reversal $\quad T = i\sigma^y K$

charge conjugation $\quad C = i\tau^y$

BdG Hamiltonian satisfies $\{CT, \mathcal{H}\} = 0$

$$\mathcal{H}|\psi\rangle = E|\psi\rangle \Rightarrow \mathcal{H}\, CT|\psi\rangle = -E\, CT|\psi\rangle$$

localized and isolated zero-energy solution $|\gamma\rangle$ :

$$|\gamma\rangle = CT|\gamma\rangle$$

i.e., with $\langle r|\gamma\rangle = [\chi_e, \chi_h]^t$, one must have

$$\chi_e = T\chi_h$$

$$CT|\gamma\rangle = \left(\begin{array}{c|c} 0 & \mathbb{1} \\ \hline -\mathbb{1} & 0 \end{array}\right)\begin{pmatrix} T\chi_e \\ T\chi_h \end{pmatrix} = \begin{pmatrix} T\chi_h \\ -T\chi_e \end{pmatrix}$$

or explicitly

$$\langle r|\gamma\rangle = [\chi_\uparrow, \chi_\downarrow, \chi_\downarrow^*, -\chi_\uparrow^*]$$

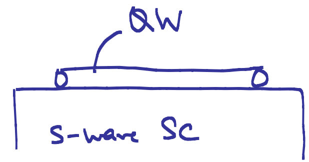
This implies $\gamma = \gamma^\dagger$ for Bogoliubov operator

$$\gamma = \int dr\, [\chi_\uparrow\ \chi_\downarrow\ \chi_\downarrow^*\ -\chi_\uparrow^*] \begin{bmatrix} \psi_\uparrow \\ \psi_\downarrow \\ \psi_\downarrow^\dagger \\ -\psi_\uparrow^\dagger \end{bmatrix}.$$

$$= \int dr \left[\left(\chi_\uparrow\psi_\uparrow + \chi_\uparrow^*\psi_\uparrow^\dagger\right) + \left(\chi_\downarrow\psi_\downarrow + \chi_\downarrow^*\psi_\downarrow^*\right)\right]$$

$\rightarrow$ $\gamma$ is necessarily Majorana!

## VI) Semiconductor quantum wires




BdG Hamiltonian: difference w/ TI above

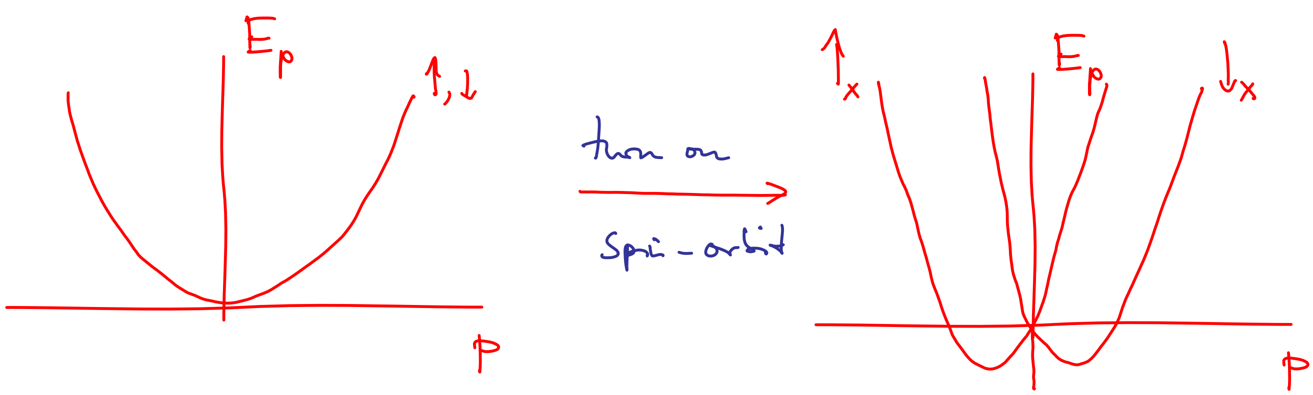
$$\mathcal{H} = \left(\frac{p^2}{2m} - \mu + u p \sigma^x\right)\tau^z - B\sigma^z + \Delta\tau^x$$

↑ Rashba SOC

Normal-state dispersion:

* $B=0$ (ignore $\mu$ since normal Hamiltonian):

$$E_p = \frac{p^2}{2m} \pm u p = \frac{1}{2m}(p \pm m u)^2 - \frac{1}{2} m u^2$$

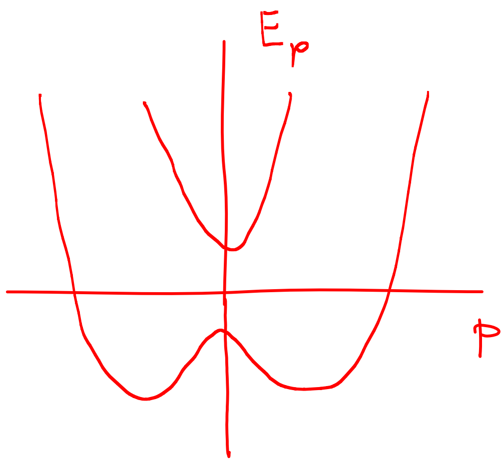



* finite $B$: $B$ mixes $\uparrow_x$ and $\downarrow_x$ & opens gap at $p=0$:

$$E_p = \frac{p^2}{2m} \pm \sqrt{(u p)^2 + B^2}$$

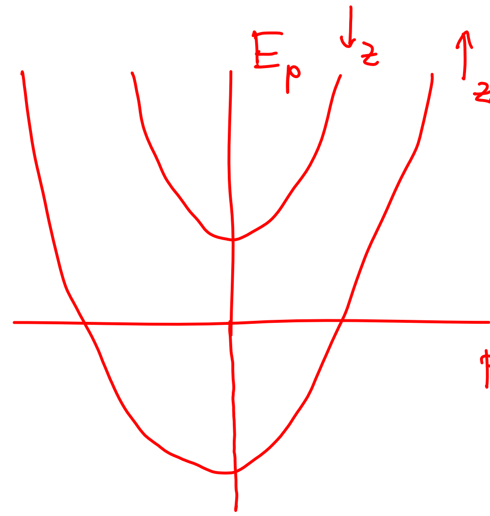
↑ effective strength of "Zeeman field" combined from $-B\sigma^z$ and $u p \sigma^x$

TI limit




$B \ll \epsilon_{so} = mu^2$

Kitaev limit




$B \gg \epsilon_{so} = mu^2$

* Kitaev limit: $B \gg \epsilon_{so}, \Delta$ — mapping to spinless p-wave SC

basic idea following heuristic discussion above: choose chemical potential such that only lower band is relevant and project BdG Hamiltonian

$$\mathcal{H} \simeq \left[ \frac{p^2}{2m} - (B+\mu) \right] \tau^z + \text{pairing term}$$

$$\xrightarrow[\text{measuring } \mu \text{ from lower band edge}]{} \left( \frac{p^2}{2m} - \mu \right) \tau^z + \text{pairing term}$$

pairing within lower band enabled by spin-orbit coupling:

- w/o SOC – eigenspinors corresponding to lower band:

$$|e\rangle = (1,0,0,0)^T \quad ; \quad |h\rangle = (0,0,0,1)^T$$

$$\langle e|\mathcal{H}_\Delta|h\rangle = (1,0,0,0)\left(\begin{array}{cc|cc} & & \Delta & 0 \\ & 0 & 0 & \Delta \\ \hline \Delta & 0 & & \\ 0 & \Delta & & 0 \end{array}\right)\begin{pmatrix}0\\0\\0\\1\end{pmatrix} = 0$$

reflects that spin singlet Cooper pair cannot enter into spin-polarized system!

- w/ SOC – include perturbatively to linear order

$$|e\rangle = \left(1, -\frac{up}{2B}, 0, 0\right)^T \qquad |h\rangle = \left(0, 0, -\frac{up}{2B}, 1\right)^T$$

$$\langle e|\mathcal{H}_\Delta|e\rangle = \langle h|\mathcal{H}_\Delta|h\rangle = 0$$

$$\langle e|\mathcal{H}_\Delta|h\rangle = -\left(\frac{up}{B}\right)\Delta$$

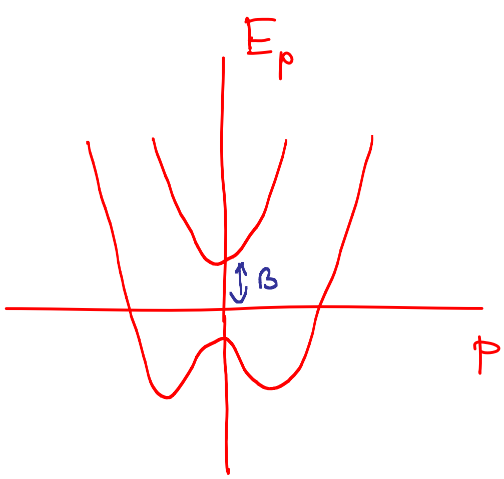
→ projected Hamiltonian:

$$\boxed{\mathcal{H} \simeq \left(\frac{p^2}{2m} - \mu\right)\tau^z + \Delta_{eff}\, p\, \tau^x}$$

i.e., just the Hamiltonian of a spinless p-wave SC w/ pairing strength $\Delta_{eff} = -u\Delta/B$.

→ **Quantum wire realizes topological superconducting phase which can host Majorana bound states.**

* TI limit: $\Delta, B \ll \epsilon_{so}$ — mapping to TI edge




- choose $\mu = 0$ : right- and left movers are spin polarized

- SC opens gap $\sim \Delta$ at origin

∘ gaps due to B and Δ at $p=0$:

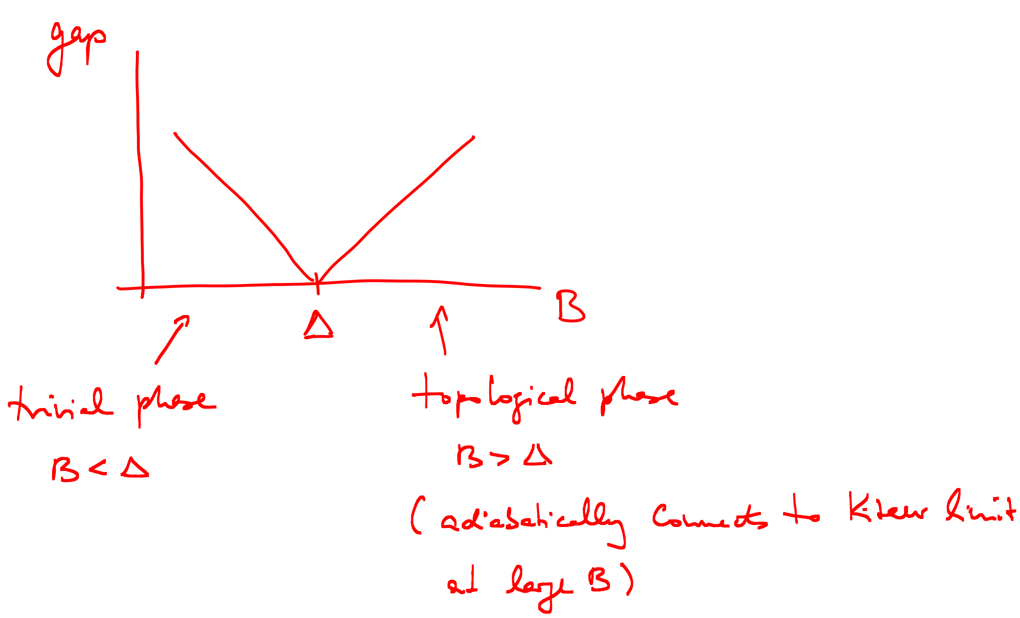
small momenta $\Rightarrow$ neglect $\frac{p^2}{2m}$-term in $\mathcal{H}$

$$\mathcal{H} \simeq u p \sigma^x \tau^z - B\sigma^z + \Delta \tau^x$$

↝ just Hamiltonian for proximity-coupled TI edge w/ excitation spectrum

$$E_p = \pm \sqrt{(up)^2 + (B \pm \Delta)^2}$$

$B \simeq \Delta$ ↝ low-energy physics dominated by small momenta & neglect of $p^2$-term is justified



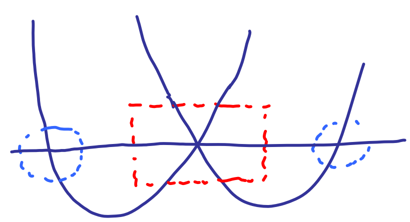
Remarks:

* phases reverse relative to TI:

e.g., $4\pi$ - periodic Josephson effect:

- $\Delta - B - \Delta$ junction for TI
- $B - \Delta - B$ junction for QW

to understand, consider limit of large $\epsilon_{so}$:



- $p \approx 0$: dispersion just like TI
- wings: also topological SC

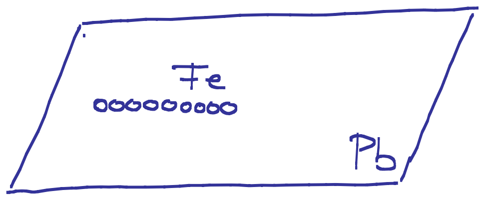
$\rightsquigarrow$ topological phase of wings reverses phase of TI!

* including $\mu$: phase boundary at $B = \sqrt{\Delta^2 + \mu^2}$

$\rightsquigarrow$ domain wall can be induced by variation of chemical potential, i.e., by gate electrodes

$\rightsquigarrow$ provides method to manipulate Majoranas

## VIII) Chains of magnetic adatoms




Yazdani group (Science 2014)
Franke group (PRL 2015)
Meyer group (arXiv 2015)

Candidate for TSC:

- proximity-induced SC: Pb substrate
- Zeeman field: exchange splitting of Fe d-bands
- Spin orbit coupling: Pb is relatively heavy element.

features:

- atomically defined system
- Majorana accessible to STM (energy & space resolution)
- in principle, broad class of systems (adatom & SC substrate)
- adatoms can sometimes be manipulated by STM (though not yet in this context!)

* Individual magnetic impurity on SC:

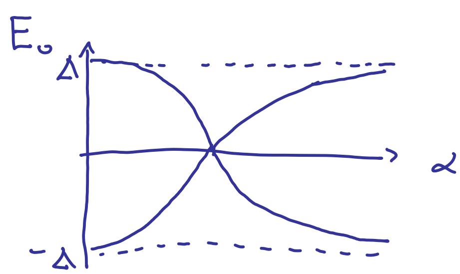
$$H = \left(\frac{p^2}{2m} - \mu\right)\tau_z - J\,\vec{S}\cdot\vec{\sigma}\,\delta(\vec{r}) + \Delta\,\tau_x$$

classical magnetic impurity w/ spin S

impurity binds Yu-Shiba-Rusinov (short: Shiba) state in SC:

- energy: $E_0 = \pm \Delta \dfrac{1-\alpha^2}{1+\alpha^2}$ $\qquad \alpha = \pi \nu_0 J S$

(see, e.g., Pientka et al. PRB 2013)

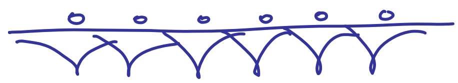



$E_0 = 0 \rightsquigarrow$ quantum phase transition from even to odd ground state.

- wave function: $\psi_+(r) \sim \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix} \dfrac{\sin(k_F r \mp \delta)}{k_F r}\, e^{-r/\xi_E}$ $\quad$ w/ $\xi_E = \dfrac{v_F}{\sqrt{\Delta^2 - E^2}}$

  - spin polarized: spin-up particles + spin down holes
  - slow decay $\propto 1/r$ on intermediate lengths

* chain of magnetic adatoms – dilute limit:




deep Shiba states: one spin-polarized state per adatom

→ Kitaev chain as (simplified) model:

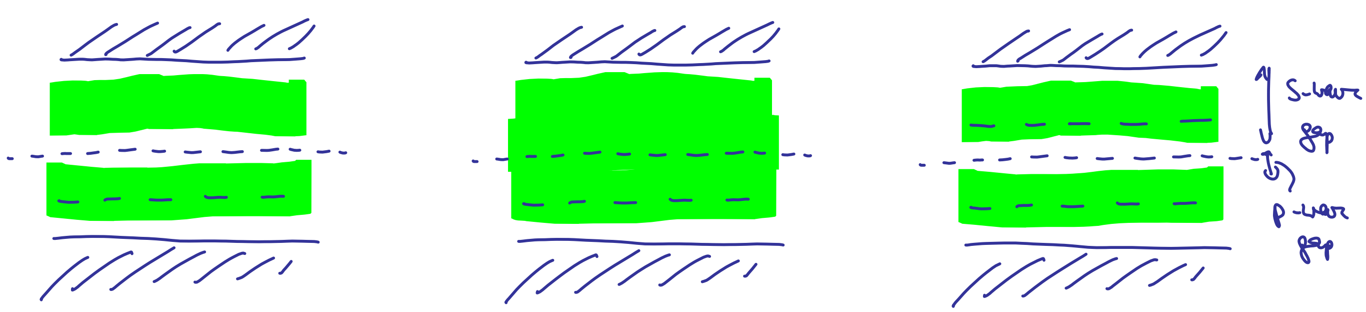
$$H = \sum_j \left\{ E_0 c_j^\dagger c_j - t \left( c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) + \Delta \left( c_j^\dagger c_{j+1}^\dagger + c_{j+1} c_j \right) \right\}$$

energy of individual Shiba states

hybridization of Shiba states

eff. p-wave pairing (SOC)

∘ lattice version of spinless p-wave SC




weak hybridization

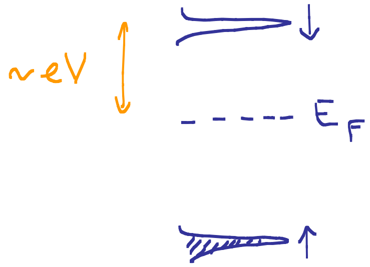
strong hybridization (no pairing)

strong hybridization (w/ pairing)

– long-range hopping due to 1/r decay of Shiba w.f.'s (see Pientka et al. PRB 2013 & 2014)

* chain of magnetic adatoms – dense limit:

individual impurity:




Fe d-levels (think spin 1/2 Anderson impurity for simplicity) far from Fermi energy of SC

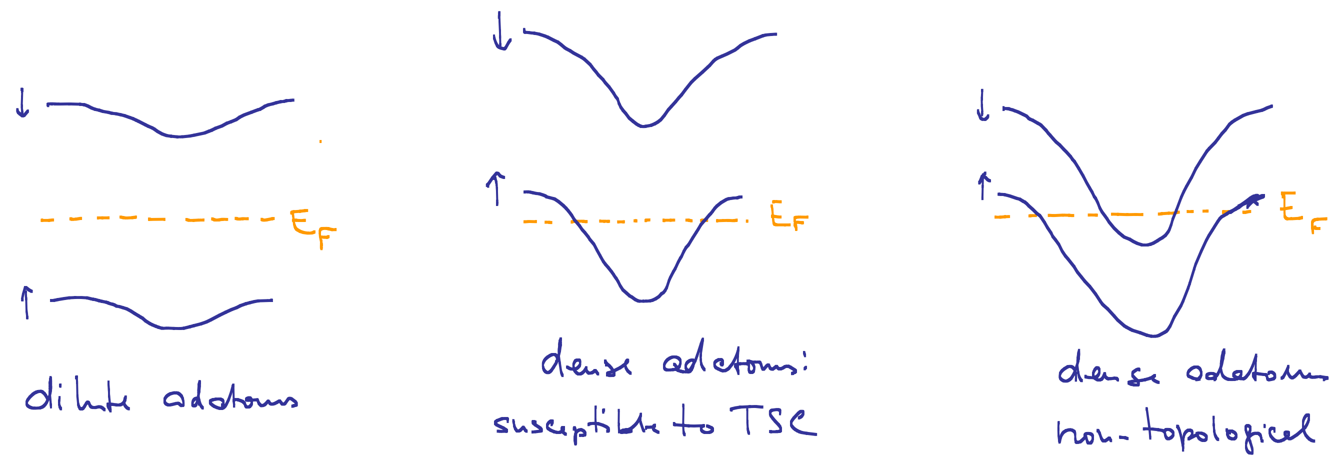
chain of impurities: d-levels form 1d bands

dilute limit: d-band weakly dispersing & stay far from Fermi energy limit of SC, i.e., d-bands remain electronically inert

↝ Shiba-state model as described above

dense limit: d-levels strongly dispersing & can cross Fermi energy of SC

↝ d-bands no longer electronically inert.




Central figure: essentially ideal realization of 1d spinless p-wave SC

- note that TSC, if present, should be very robust: band structure energy scales are of order eV
(not so favorable for manipulation of Majoranas)

minimal model capturing all regimes: chain of Anderson impurities

$$H = \sum_j \sum_\sigma \varepsilon_d d^\dagger_{j\sigma} d_{j\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow}$$ Anderson impurities

$$+ \sum_j \sum_\sigma \left\{ -w d^\dagger_{j+1,\sigma} d_{j\sigma} + h.c. \right\}$$ hopping between d-levels

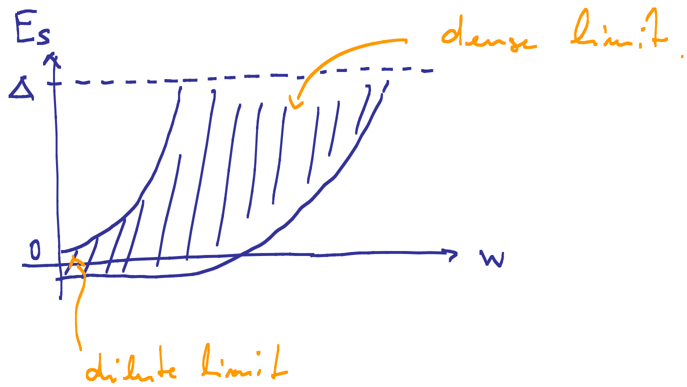
$$+ \sum_j \sum_\sigma \left\{ -t \psi^\dagger_\sigma(R_j) d_{j\sigma} + h.c. \right\}$$ hybridization w/ SC

$$+ H_{BCS}$$ SC

- treat on-site $U$'s in Anderson's mean-field approach, assuming ferromagnetic order in chain (as suggested by experiment)

(see Y. Peng et al. PRL 2015; also Princeton group including ab-initio results - Li et al. PRB 2015)

phase diagram:




Model includes superconducting proximity effect explicitly:

- detailed discussion: see Y. Peng et al. or Les Houches notes
- here: basic proximity effect between 1d normal system & 3d SC (no spin polarization or SOC) + arguments

Propagation of subgap excitation in 1d system:

$$G(k,\omega) = \frac{1}{\omega - v_F k \tau_z - \Sigma(k,\omega)}$$

w/ $$\Sigma(k,\omega) = t^2 \sum_{k_\perp} \tau_z G_{sc}(k,\omega)\tau_z \simeq -\Gamma \frac{\omega + \Delta\tau_x}{\sqrt{\Delta^2 - \omega^2}}$$

accounting for coupling to SC.

- weak coupling $\Gamma \ll \Delta$:

$$G^{-1}(k, \omega \ll \Delta) = \omega - v_F k \tau_z + \underbrace{\Gamma}_{\text{proximity-induced gap}} \tau_x$$

- strong coupling $\Gamma \gg \Delta$ (relevant for adatoms):

$$G(k, \omega \ll \Delta) = \frac{Z}{\omega - Z v_F k \tau_z - Z\Gamma\tau_x}$$

w/ quasiparticle weight $Z = \frac{1}{1+\Gamma/\Delta} \simeq 10^{-3}$ ;

adatoms

induced gap saturates at $\Delta_{ind} = Z\Gamma \simeq \Delta$,

but coherence length of proximity-induced SC scales as

$$\xi \propto \frac{v_F}{\Gamma} \ll \frac{v_F}{\Delta}$$

coherence length of proximity-providing SC

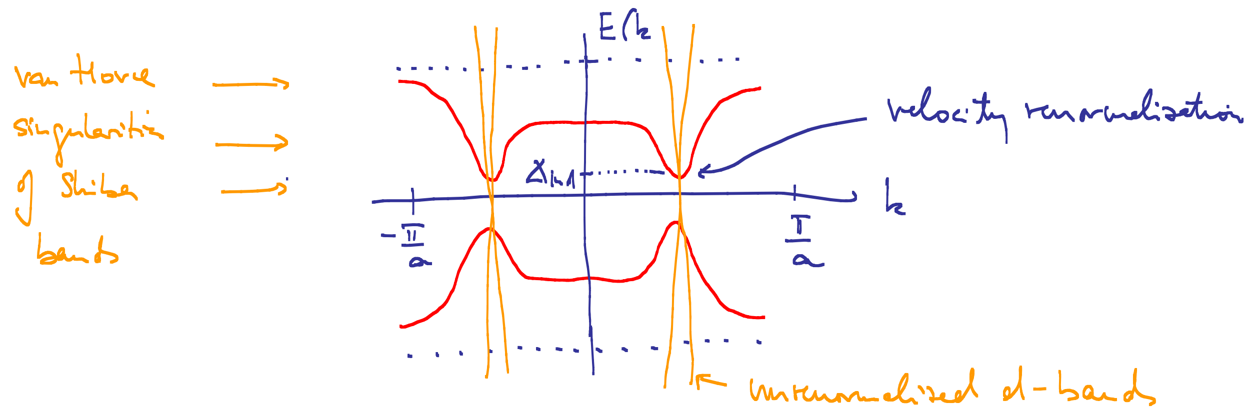
↝ $\xi$ is (almost: spin polarization & SOC) relevant for Majorana localization!

Including SOC & spin polarization:

- maximal induced gap: $\Delta_{ind} \ll \Delta$ even for $\Gamma \gg \Delta$

  need to induce pairing in spin polarized system which requires SOC.

- adatoms induce band of subgap states which reflect the large renormalization




• Majorana localization

$$\xi_M \sim \frac{v_F}{\Gamma}\,\frac{\Delta}{\Delta_{ind}} \sim \xi_{sc}\cdot\underbrace{\left(\frac{\Delta}{\Gamma}\right)}_{10^{-3}}\cdot\underbrace{\left(\frac{\Delta}{\Delta_{ind}}\right)}_{10\,?} \sim 10^{-2}\,\xi_{sc}$$

→ strong localization.