# Impurity and vortex-core states in superconducting spin-helical Dirac fermions

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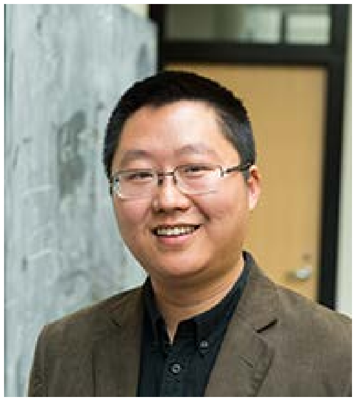
# Acknowledgment

Liang Fu



Michał Papaj

HI, M. Papaj, and L. Fu (to appear)

# Outline

2D topological surface states in proximity to *s*-wave superconductivity will host Majorana zero modes.

- We look into impurity bound states and vortex core states in detail.
- Is there a way to distinguish Majorana zero modes from another zero energy localized modes?

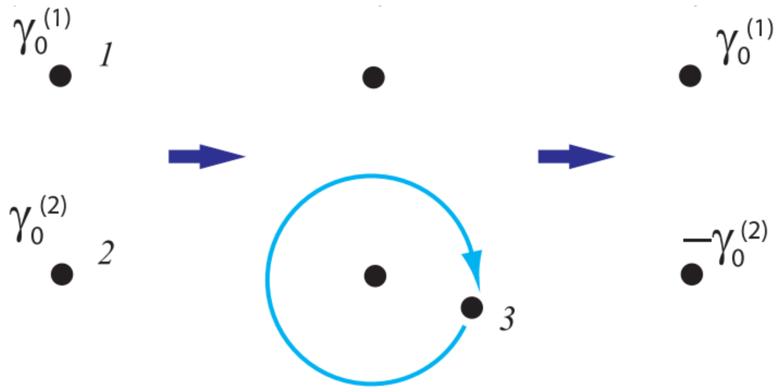
Results:

- Impurity bound states can also be zero-energy localized modes.
- However, they are different in: spatial distribution, spin configuration…

# Search for Majorana zero modes

- Majorana condition $\gamma_0 = \gamma_0^\dagger$
- Localized at an $hc/2e$ vortex in a $p + ip$ superconductor
- It necessarily lies at zero energy in superconductors.

- Non-Abelian statistics and application to quantum computation




M. Sato and Y. Ando, Reports Prog. Phys. **80**, 076501 (2017).

# Search for Majorana zero modes

However, a Majorana zero mode is not the only one localized midgap modes in superconductors.

Midgap states includes:

- Vortex-core states (Caroli-de Gennes-Matricon, 1964)
  - Include Majorana zero modes
- Impurity bound states (Yu, 1965; Shiba, 1968; Rusinov, 1969)
- Kondo impurity resonance, etc.

# Midgap states in superconductors

For conventional *s-wave* superconductors:

$$\mathcal{H}_0 = \sum_{\mathbf{k}\alpha} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\alpha} c_{\mathbf{k}\alpha} + \Delta_0 \sum_{\mathbf{k}} \{ c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \}$$

- Impurity bound states – Yu-Shiba-Rusinov states

$$H_{\mathrm{ex}} = \frac{1}{2N} \sum_{\substack{\mathbf{k},\mathbf{k}' \\ \alpha\beta}} J(\mathbf{k}-\mathbf{k}') c^{\dagger}_{\mathbf{k},\alpha} \boldsymbol{\sigma}_{\alpha\beta} \cdot \mathbf{S} c_{\mathbf{k}'\beta}. \qquad \epsilon_0 = \frac{E_0}{\Delta_0} = \frac{1-(JS\pi N_0/2)^2}{1+(JS\pi N_0/2)^2}$$

A. V. Balatsky, I. Vekhter, and J.-X. Zhu, Rev. Mod. Phys. **78**, 373 (2006).

- Vortex-core states – Caroli-de Gennes-Matricon states

$$\hat{\psi} = \exp(ik_F z \cos\alpha) \exp(i\mu\theta) \hat{f}(r)$$

$$\epsilon_{\mu\alpha} = q v_F \sin\alpha = \mu (k_F \sin\alpha)^{-1} \frac{\int_0^\infty \frac{\Delta(r)}{r} e^{-2K(r)} dr}{\int_0^\infty e^{-2K(r)} dr} \longrightarrow \mu \Delta_\infty^2 / E_F$$

$$= \mu (k_F \sin\alpha)^{-1} (d\Delta/dr)_{r=0}\, g(\alpha) \qquad (\mu \neq 0,\ \mu \ll k_F \xi)$$

C. Caroli, P. G. De Gennes, and J. Matricon, Phys. Lett. **9**, 307 (1964).

# Realization of topological superconductivity

Majorana zero modes in 2D superconductors:

- Intrinsic (*p*+*ip*)-superconductor

  $Sr_2RuO_4$

- 3D Topological insulator surface states + *s*-wave SC
  - Proximity effect
  - Intrinsic realization

  $Cu_xBi_2Se_3$, $Sn_{1-x}In_xTe$, $FeTe_{1-x}Se_x$

- 2D electron gas with Rashba + *s*-wave SC + Zeeman

See reviews, e.g., Alicea (2012), Sato and Ando (2017)

# Superconductivity proximity effect

## 2D superconductor on top of 3D topological insulator

Suppose that an $s$-wave superconductor is deposited on the surface. Because of the proximity effect, Cooper pairs can tunnel into the surface states. This can be described by adding $V = \Delta\psi_\uparrow^\dagger\psi_\downarrow^\dagger + \text{H.c.}$ to $H_0$, where $\Delta = \Delta_0 e^{i\phi}$ depends on the phase $\phi$ of the superconductor and the nature of the interface [17]. The states of the surface can then be described by $H = \Psi^\dagger \mathcal{H} \Psi/2$, where in the Nambu notation $\Psi = ((\psi_\uparrow, \psi_\downarrow), (\psi_\downarrow^\dagger, -\psi_\uparrow^\dagger))^T$ and

$$\mathcal{H} = -iv\tau^z\sigma\cdot\nabla - \mu\tau^z + \Delta_0(\tau^x\cos\phi + \tau^y\sin\phi). \tag{2}$$

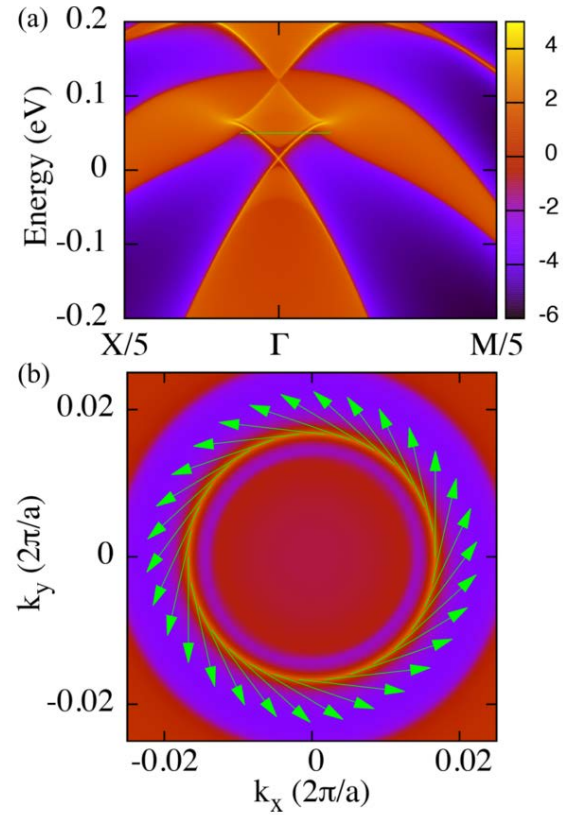
$\vec{\tau}$ are Pauli matrices that mix the $\psi$ and $\psi^\dagger$ blocks of $\Psi$. Time reversal invariance follows from $[\Theta, \mathcal{H}] = 0$, where $\Theta = i\sigma^y K$ and $K$ is complex conjugation. Particle hole symmetry is expressed by $\Xi = \sigma^y\tau^y K$, which satisfies $\{\Xi, \mathcal{H}\} = 0$. When $\Delta$ is spatially homogeneous, the excitation spectrum is $E_{\mathbf{k}} = \pm\sqrt{(\pm v|\mathbf{k}| - \mu)^2 + \Delta_0^2}$. For $\mu \gg \Delta_0$, the low energy spectrum resembles that of a spinless $p_x + ip_y$ superconductor. This analogy can be made precise by defining $c_{\mathbf{k}} = (\psi_{\uparrow\mathbf{k}} + e^{i\theta_{\mathbf{k}}}\psi_{\downarrow\mathbf{k}})/\sqrt{2}$ for $\mathbf{k} = k_0(\cos\theta_{\mathbf{k}}, \sin\theta_{\mathbf{k}})$ and $vk_0 \sim \mu$. The projected Hamiltonian is then $\sum_{\mathbf{k}}(v|\mathbf{k}| - \mu)c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + (\Delta e^{i\theta_{\mathbf{k}}} c_{\mathbf{k}}^\dagger c_{-\mathbf{k}}^\dagger + \text{H.c.})/2$. Though this is formally equivalent to a spinless $p_x + ip_y$ superconductor, there is an important difference: $\mathcal{H}$ respects time reversal symmetry, while the $p_x + ip_y$ superconductor does not.

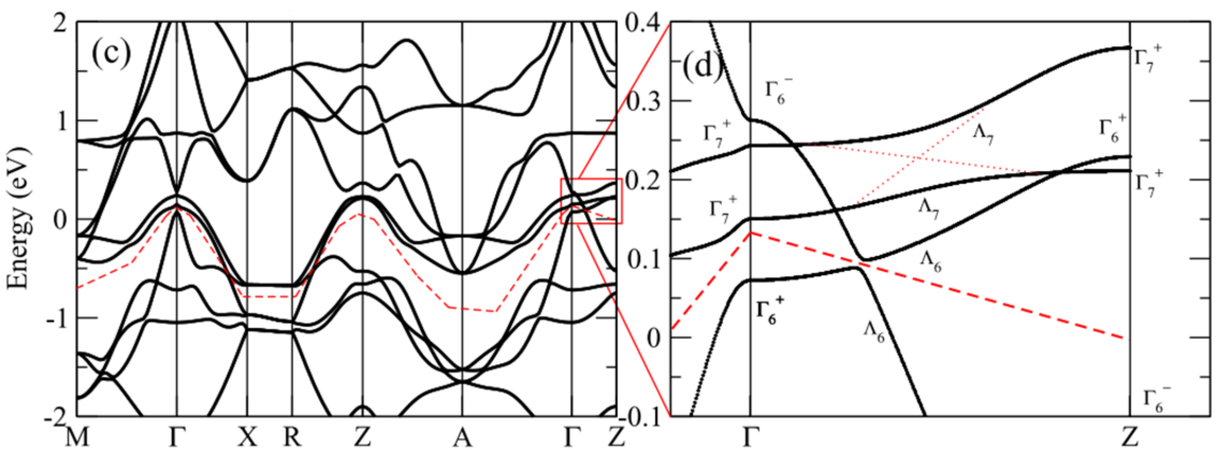
L. Fu and C. L. Kane, Phys. Rev. Lett. **100**, 096407 (2008).

# $FeSe_{1-x}Te_x$: Normal state

DFT calculations

- Band inversion along $\Gamma - Z$ line
- Topological "metal"
- Single Dirac cone on 001 surface



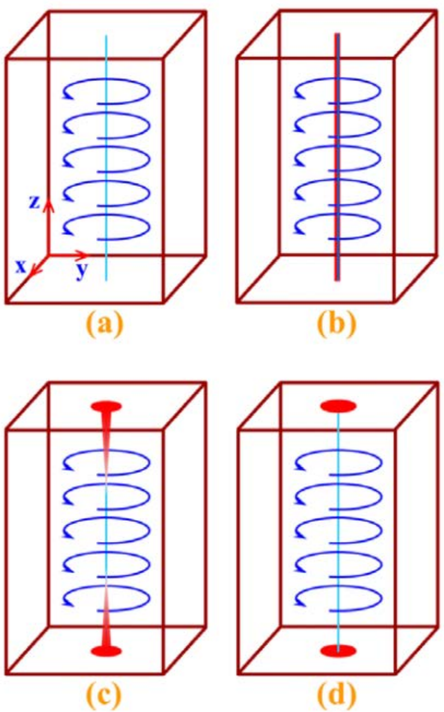



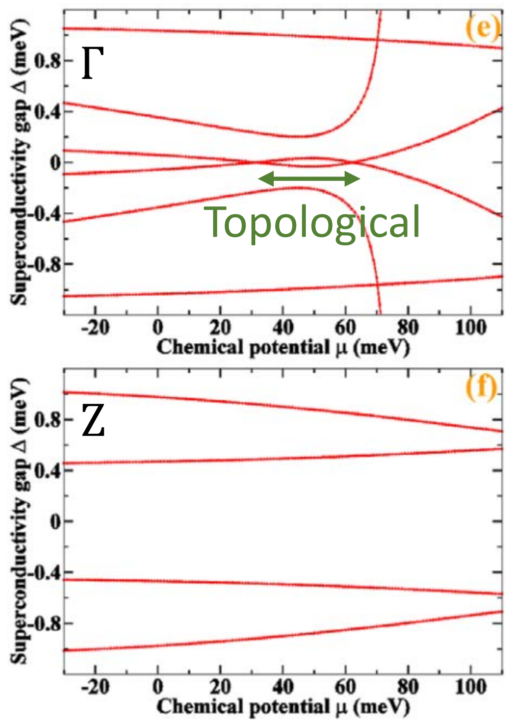

Z. Wang, P. Zhang, G. Xu, L. K. Zeng, H. Miao, X. Xu, T. Qian, H. Weng, P. Richard, A. V. Fedorov, H. Ding, X. Dai, and Z. Fang, Phys. Rev. B **92**, 115119 (2015).

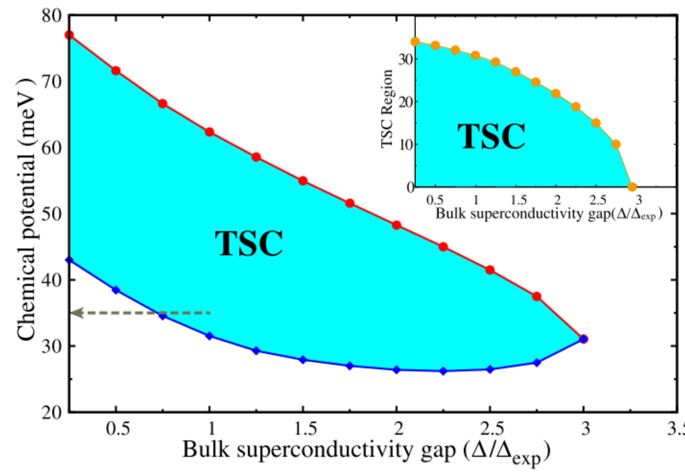
# $FeSe_{1-x}Te_x$: Superconducting state

DFT calculations

- Energy spectrum along a vortex line (like a Majorana chain)
- Self-doping by excess Fe atoms $Fe_{1+y}Se_{0.5}Te_{0.5}$ (TSC: $0.03<y<0.06$)



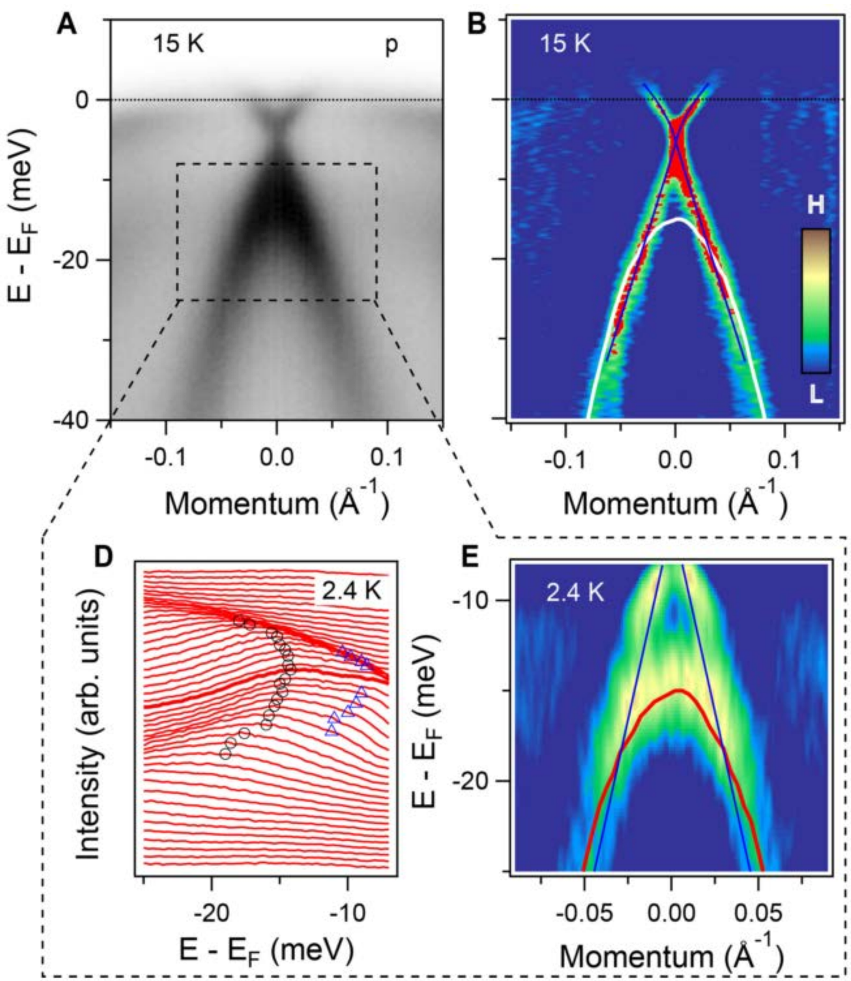



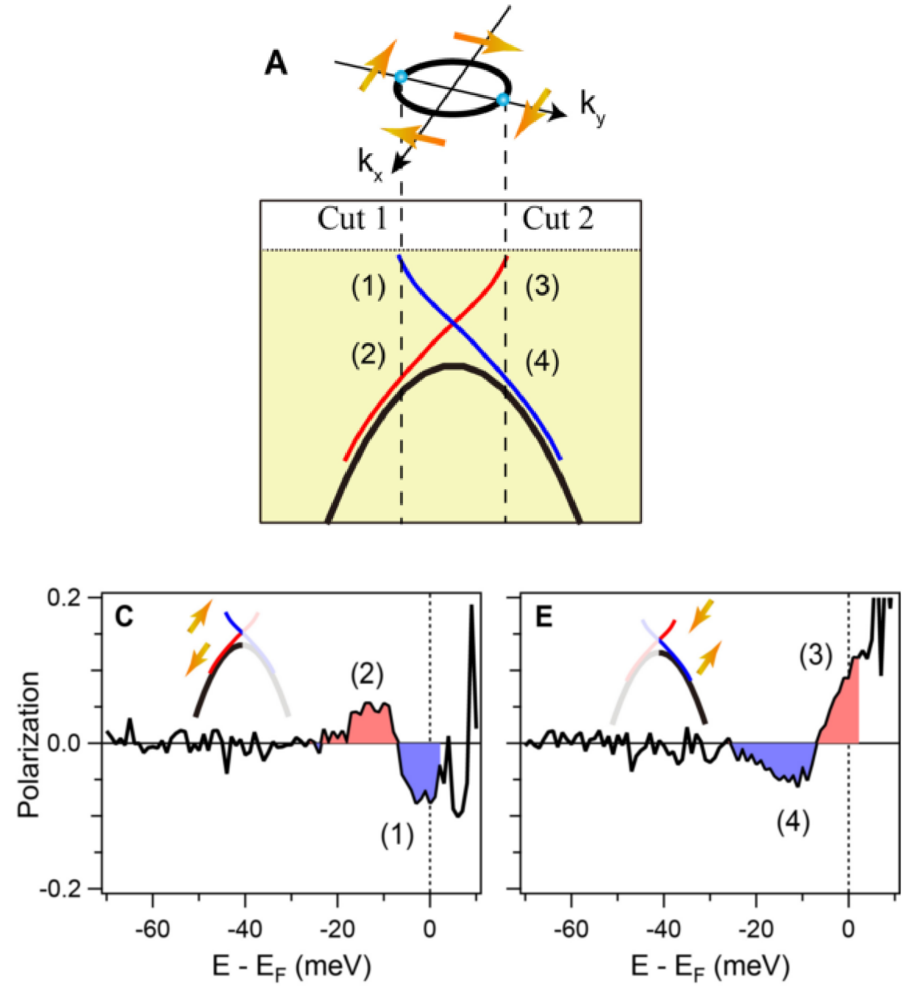

G. Xu, B. Lian, P. Tang, X.-L. Qi, and S.-C. Zhang, Phys. Rev. Lett. **117**, 047001 (2016).

# $FeSe_{1-x}Te_x$: ARPES

## $FeTe_{0.55}Se_{0.45}$ ($T_c$=14.5K)

- Spin-helical surface Dirac cone



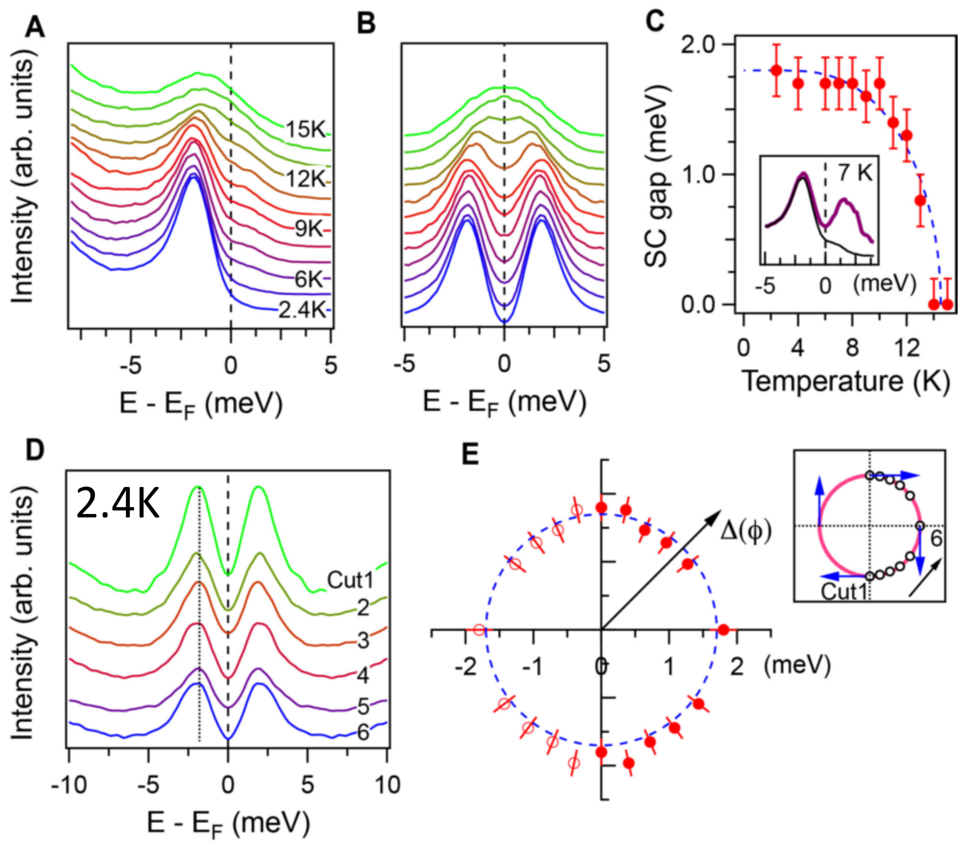




P. Zhang, K. Yaji, T. Hashimoto, Y. Ota, T. Kondo, K. Okazaki, Z. Wang, J. Wen, G. D. Gu, H. Ding, and S. Shin, arXiv:1706.05163.

# $FeSe_{1-x}Te_x$: ARPES

$FeTe_{0.55}Se_{0.45}$ ($T_c$=14.5K)

- *s*-wave superconducting gap on the surface



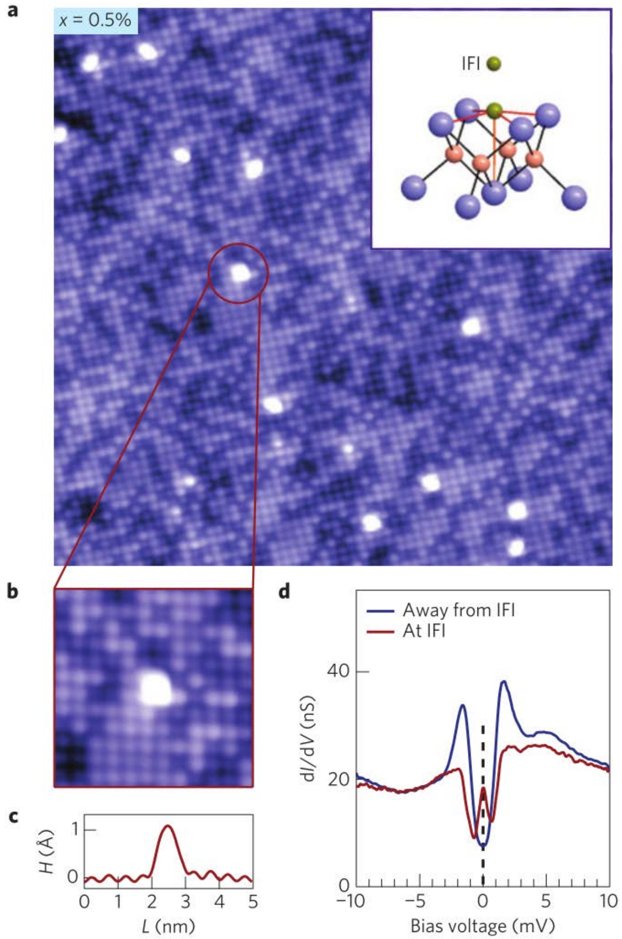

P. Zhang, K. Yaji, T. Hashimoto, Y. Ota, T. Kondo, K. Okazaki, Z. Wang, J. Wen, G. D. Gu, H. Ding, and S. Shin, arXiv:1706.05163.

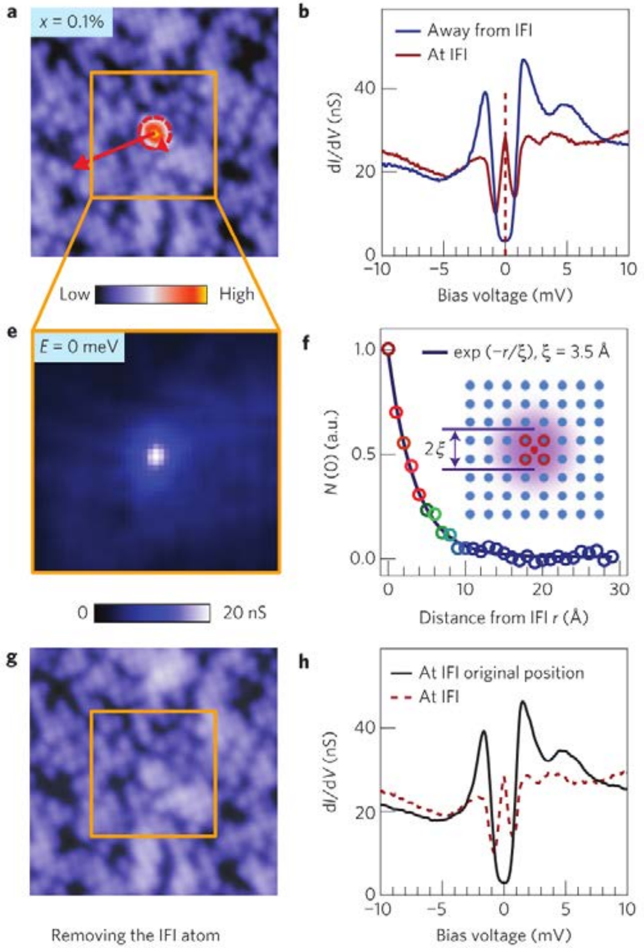
# $FeSe_{1-x}Te_x$: STM/S (impurity)

Pristine Fe(Te,Se) ($T_c$=14.5K)

At an interstitial iron impurity (excess iron atom)

Highest $T_c$ without IFIs



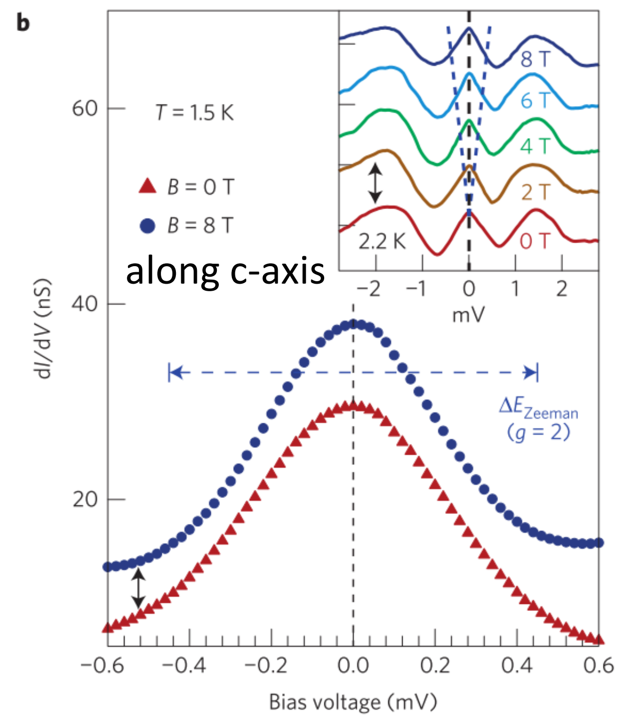




J.-X. Yin *et al.*, Nat. Phys. **11**, 543 (2015).

# $FeSe_{1-x}Te_x$: STM/S (impurity)

Possibilities for midgap states:

- Majorana zero modes
- Impurity bound states (magnetic or non-magnetic)
  - Pair of spectral peaks, symmetric around zero energy
  - Zeeman split under magnetic field
- Kondo resonance
  - Not at zero energy
  - Zeeman split
- *d*-wave pairing state with an impurity at unitary limit
  - Four-fold pattern in real space

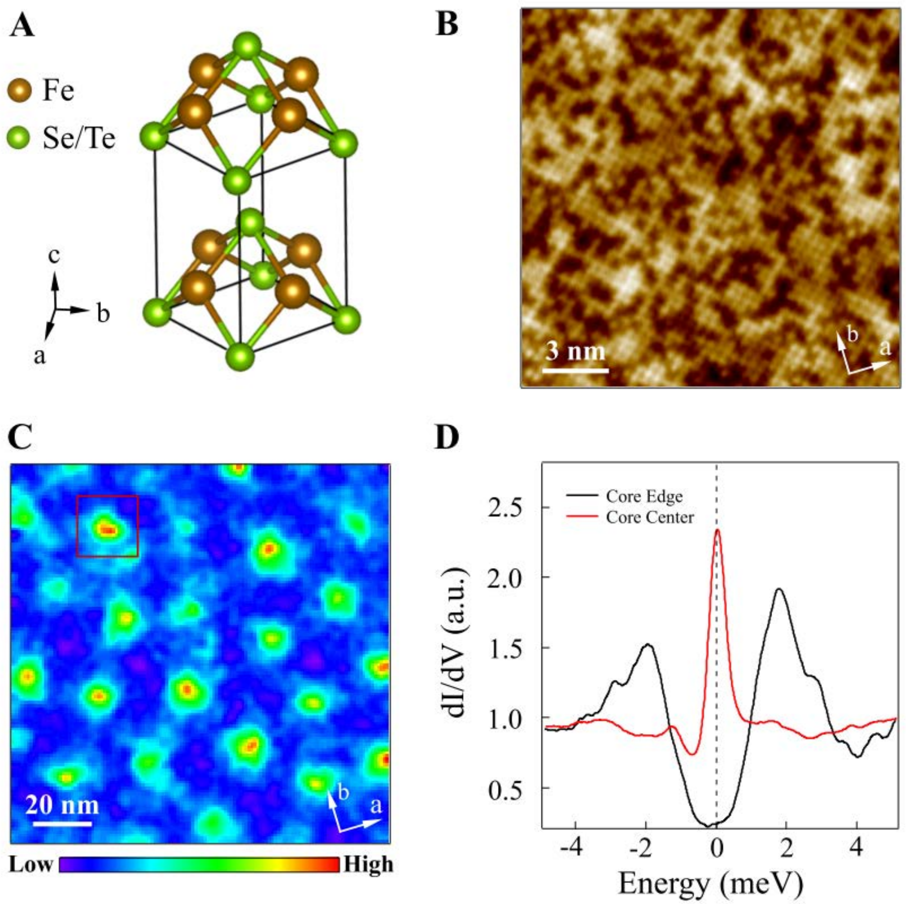


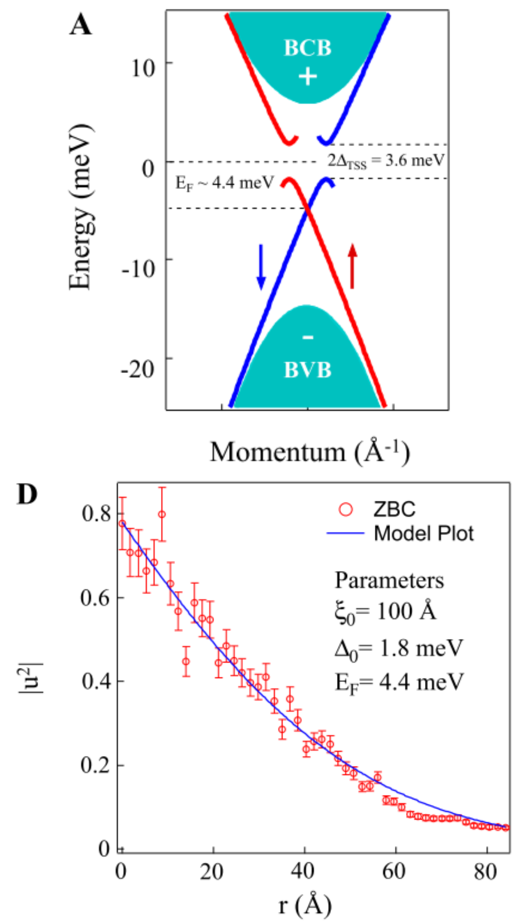

J.-X. Yin, Z. Wu, J.-H. Wang, Z.-Y. Ye, J. Gong, X.-Y. Hou, L. Shan, A. Li, X.-J. Liang, X.-X. Wu, J. Li, C.-S. Ting, Z.-Q. Wang, J.-P. Hu, P.-H. Hor, H. Ding, and S. H. Pan, Nat. Phys. **11**, 543 (2015).

# $FeSe_{1-x}Te_x$: STM/S (vortex)

$FeTe_{0.55}Se_{0.45}$ ($T$=0.55K, $T_c$=14.5K)

- Vortex lattice under magnetic field along the *c*-axis (4T)




D. Wang *et al.*, arXiv:1706.06074.

# Model

- Spin-helical Dirac fermion + *s*-wave superconductivity (2D)

$$\hat{H}_0 = \Psi^\dagger H_0 \Psi / 2$$

$$H_0(\boldsymbol{r}) = -iv\tau^z \boldsymbol{\sigma} \cdot \nabla - \mu\tau^z + \Delta_0(\tau^x \cos\phi - \tau^y \sin\phi)$$

$$\Psi(\boldsymbol{r}) = (\psi_\uparrow, \psi_\downarrow; \psi_\downarrow^\dagger, -\psi_\uparrow^\dagger)^T$$

  - Coherence length $\xi = v/\Delta_0$

- Symmetry
  - Time reversal $\Theta = i\sigma^y K$ $[\Theta, H] = 0$
  - Particle-hole $\Xi = \sigma^y \tau^y K$ $\{\Xi, H\} = 0$

# Vortex core states

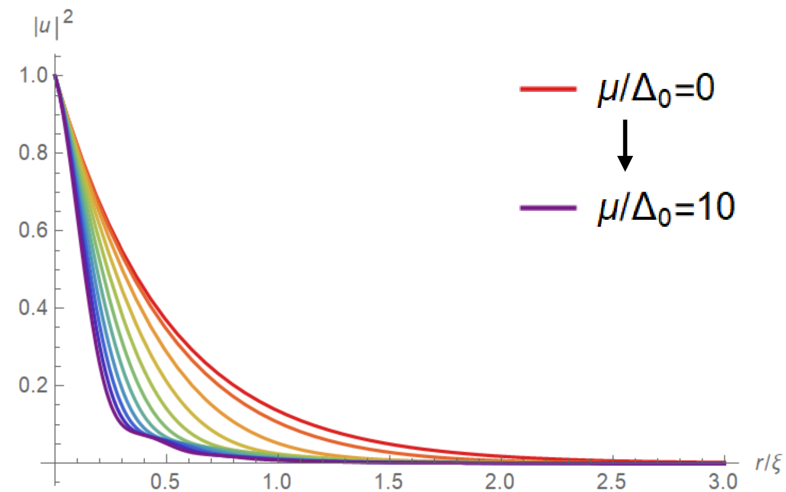
Apply magnetic field $B_{c1} < B < B_{c2}$ $l_B \gg \xi$ $l_B = \sqrt{\hbar c/eB}$

Quantized vortex $\Delta(\boldsymbol{r}) = |\Delta(r)|e^{il\theta}$ ($l$: vorticity)

- Around the vortex core, the wave function acquires the phase $2\pi\nu + \pi(l-1)$. ($\nu$: angular momentum) mod $2\pi$
  [ $2\pi\nu + \pi l$ for a conventional *s*-wave superconductor]

Majorana zero mode ($l = 1, \nu = 0$)

$$\chi(\boldsymbol{r}) = \exp\left(-\int_0^r |\Delta(r')|dr'/v\right)\begin{pmatrix} J_0(k_F r) \\ ie^{i\theta}J_1(k_F r) \\ e^{-i\theta}J_1(k_F r) \\ iJ_0(k_F r) \end{pmatrix}$$





References:
I. M. Khaymovich, N. B. Kopnin, A. S. Mel'nikov, and I. A. Shereshevskii, Phys. Rev. B **79**, 224506 (2009).
D. L. Bergman and K. Le Hur, Phys. Rev. B **79**, 184520 (2009).
M. Cheng, R. M. Lutchyn, V. Galitski, and S. Das Sarma, Phys. Rev. B **82**, 094504 (2010)

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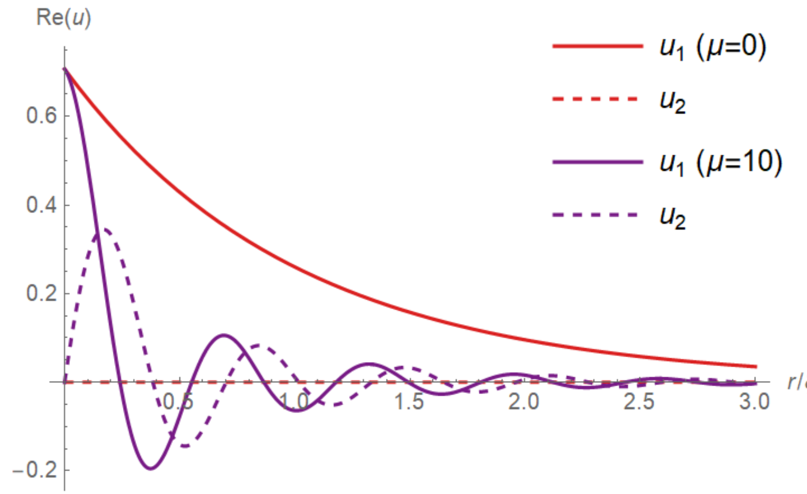



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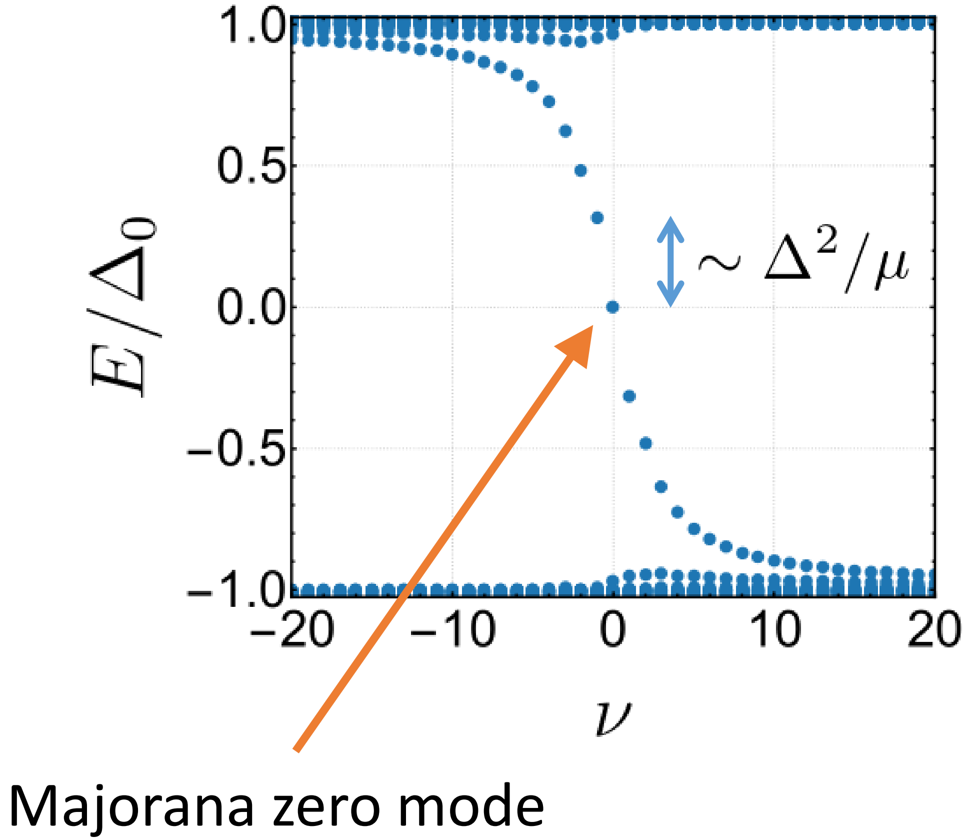
D. L. Bergman and K. Le Hur, Phys. Rev. B **79**, 184520 (2009).
M. Cheng, R. M. Lutchyn, V. Galitski, and S. Das Sarma, Phys. Rev. B **82**, 094504 (2010)

# Vortex core states

Midgap states at a vortex: $\Delta(\boldsymbol{r}) = |\Delta(r)|e^{i\theta}$



# Impurity bound state

Impurity potential $H_{\rm imp} = V\delta(\boldsymbol{r}) = (U\tau^z\sigma^0 - J\tau^0\boldsymbol{S}\cdot\boldsymbol{\sigma})\delta(\boldsymbol{r})$

- $U$: scalar potential
- $S$: classical spin $S \to \infty$ and $JS \to$ finite.

Bound state energy: pole of T-matrix $T = H_{\rm imp} + H_{\rm imp}G_0T$

$$\det[1 - H_{\rm imp}G_0(E)] = 0 \quad (-\Delta_0 < E < \Delta_0)$$

Equivalently, from the Bogoliubov-de Gennes equation

$$(H_0 + H_{\rm imp})\chi(\boldsymbol{r}) = E\chi(\boldsymbol{r})$$

$$[1 - G_0(E)H_{\rm imp}]\chi(\boldsymbol{r}) = 0$$

$$G_0(E) = (E - H_0)^{-1} \qquad \chi = (u_\uparrow, u_\downarrow; v_\downarrow, -v_\uparrow)^T$$

*Is there a zero energy state?*

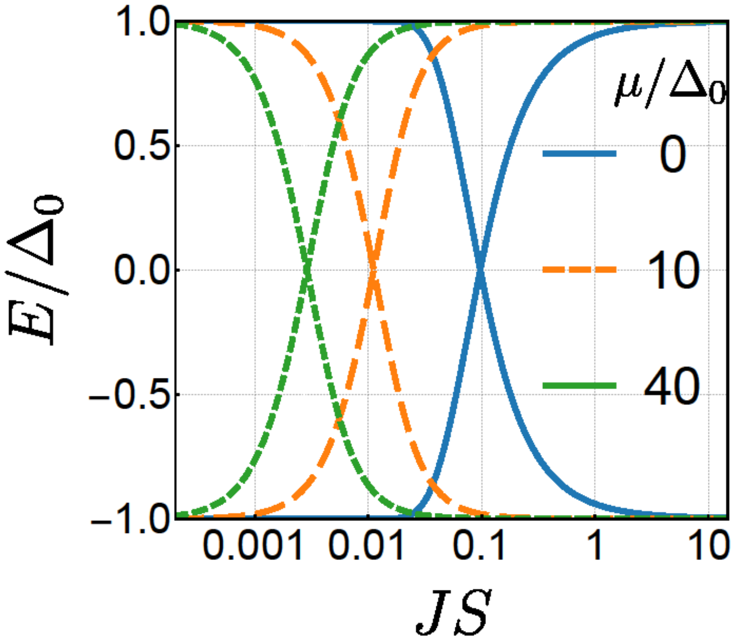
# Magnetic impurity

Impurity potential $H_{\rm imp} = V\delta(\boldsymbol{r}) = (U\tau^z\sigma^0 - J\tau^0\boldsymbol{S}\cdot\boldsymbol{\sigma})\delta(\boldsymbol{r})$

- $U = 0, JS \neq 0$

Energy spectrum of midgap states

- Pairs of states at *any* $JS$
- Accidental crossing at a certain $JS$




Energy spectrum at large $\mu$

$$E_\pm = \pm\Delta_0[1-(\pi\rho_0 JS/2)^2]/[1+(\pi\rho_0 JS/2)^2]$$

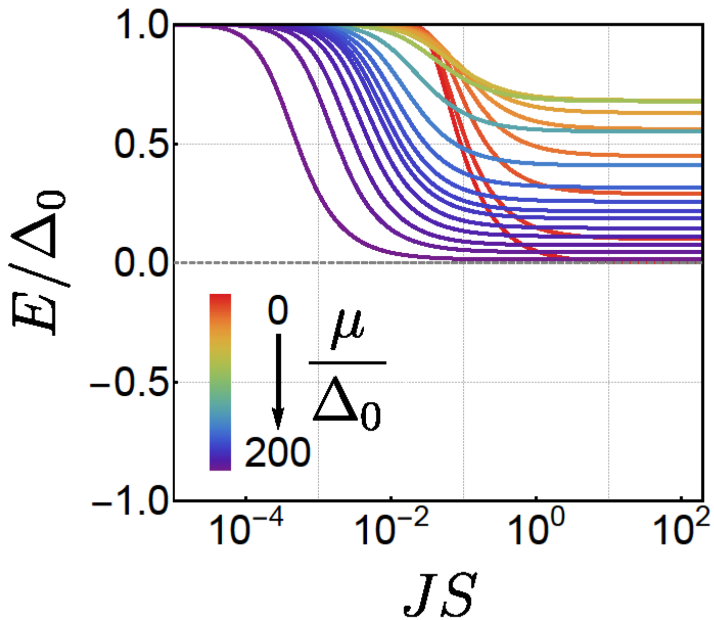
- Same form as one for conventional *s*-wave superconductors

# Magnetic + scalar impurity

Impurity potential $H_{\rm imp} = V\delta(\boldsymbol{r}) = (U\tau^z\sigma^0 - J\tau^0\boldsymbol{S}\cdot\boldsymbol{\sigma})\delta(\boldsymbol{r})$

Assume only the spin-up level is on resonance: $U = JS (= g)$.

- *Zero energy states* exist in the strong coupling limit.




(There also exist pair states with negative energy.)

# Magnetic + scalar impurity

Impurity potential $H_{\mathrm{imp}} = V\delta(\boldsymbol{r}) = (U\tau^z\sigma^0 - J\tau^0\boldsymbol{S}\cdot\boldsymbol{\sigma})\delta(\boldsymbol{r})$

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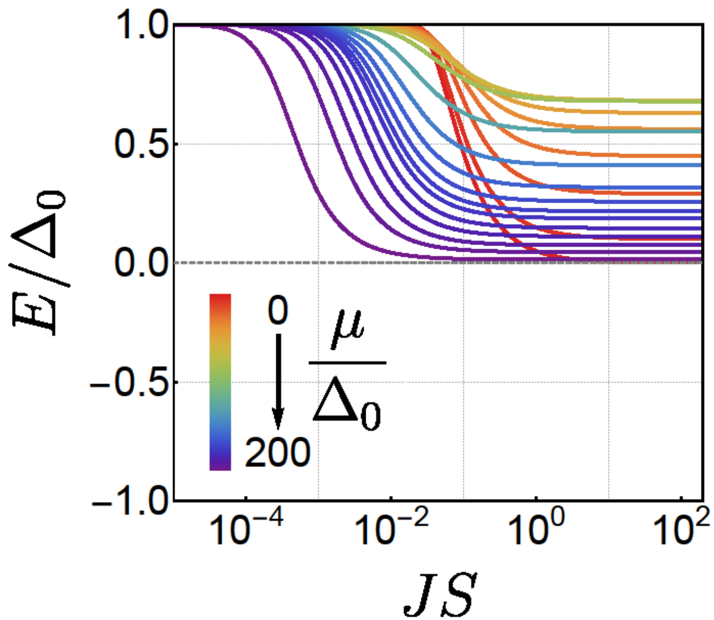



(There also exist pair states with negative energy.)

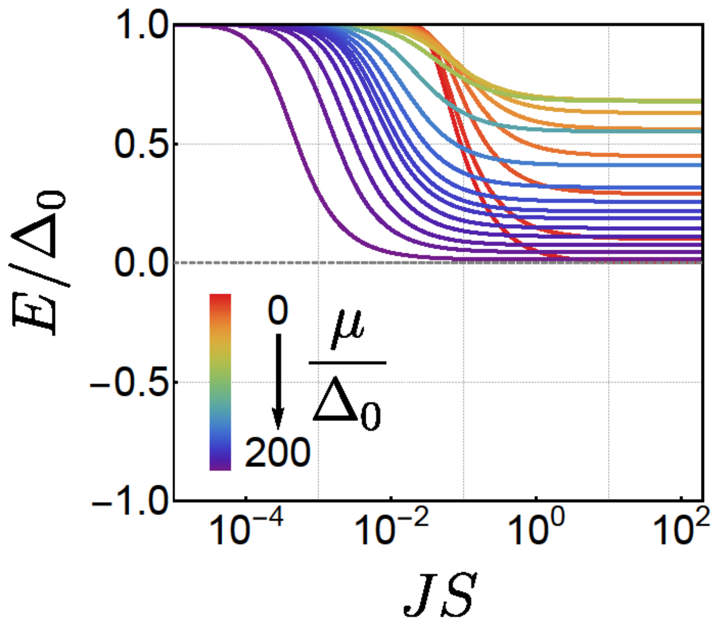
Large $\mu$ $$E_\pm = \pm\Delta_0 \frac{1}{\sqrt{1+(\pi\rho_0 g)^2}}$$

# Magnetic + scalar impurity

Impurity potential $H_{\mathrm{imp}} = V\delta(\boldsymbol{r}) = (U\tau^z\sigma^0 - J\tau^0\boldsymbol{S}\cdot\boldsymbol{\sigma})\delta(\boldsymbol{r})$

Assume only the spin-up level is on resonance: $U = JS(= g)$.

- *Zero energy states* exist in the strong coupling limit.




(There also exist pair states with negative energy.)

$\mu = 0$

$$E_{\pm} = \pm\frac{\pi v^2}{g\ln\left(\frac{v\Lambda}{\Delta_0}\right)}$$

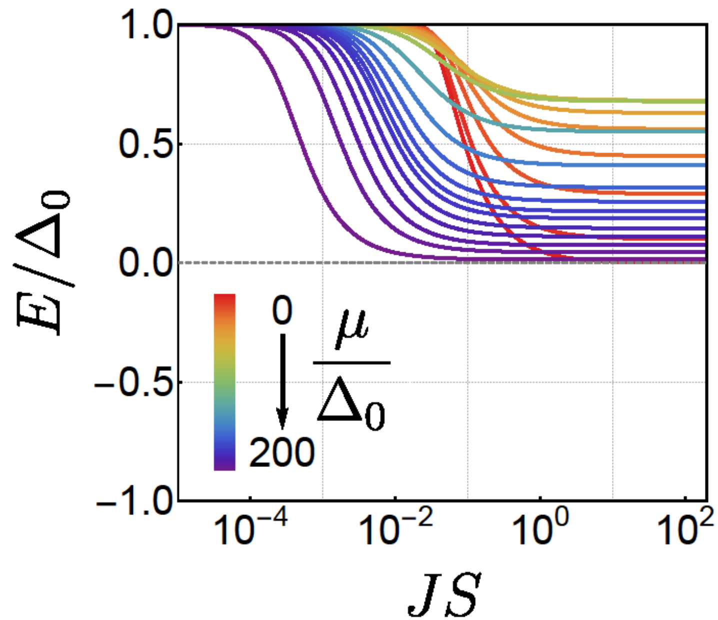
- Momentum cutoff $\Lambda(\gg \Delta_0/v)$
- Valid for large $g$

# Magnetic + scalar impurity

Impurity potential $H_{\mathrm{imp}} = V\delta(\boldsymbol{r}) = (U\tau^z\sigma^0 - J\tau^0\boldsymbol{S}\cdot\boldsymbol{\sigma})\delta(\boldsymbol{r})$

Assume only the spin-up level is on resonance: $U = JS (= g)$.

- *Zero energy states* exist in the strong coupling limit.




(There also exist pair states with negative energy.)

Intermediate $\mu$ $\lim_{g\to\infty} E_{\pm} = \pm\Delta_0\left(\frac{\Delta_0}{2\mu} - \frac{3\Delta_0^3}{8\mu^3} + O\left(\frac{\Delta_0^5}{\mu^5}\right)\right)$ $|\mu| \gg \Delta_0$

# Difference from Majorana zero modes

| | **Impurity bound states** | **Majorana zero modes** |
|---|---|---|
| Localized at … | Impurity | Vortex (magnetic flux) |
| Locked at zero energy? | No | Yes |
| Appear in pairs? | Yes | No |

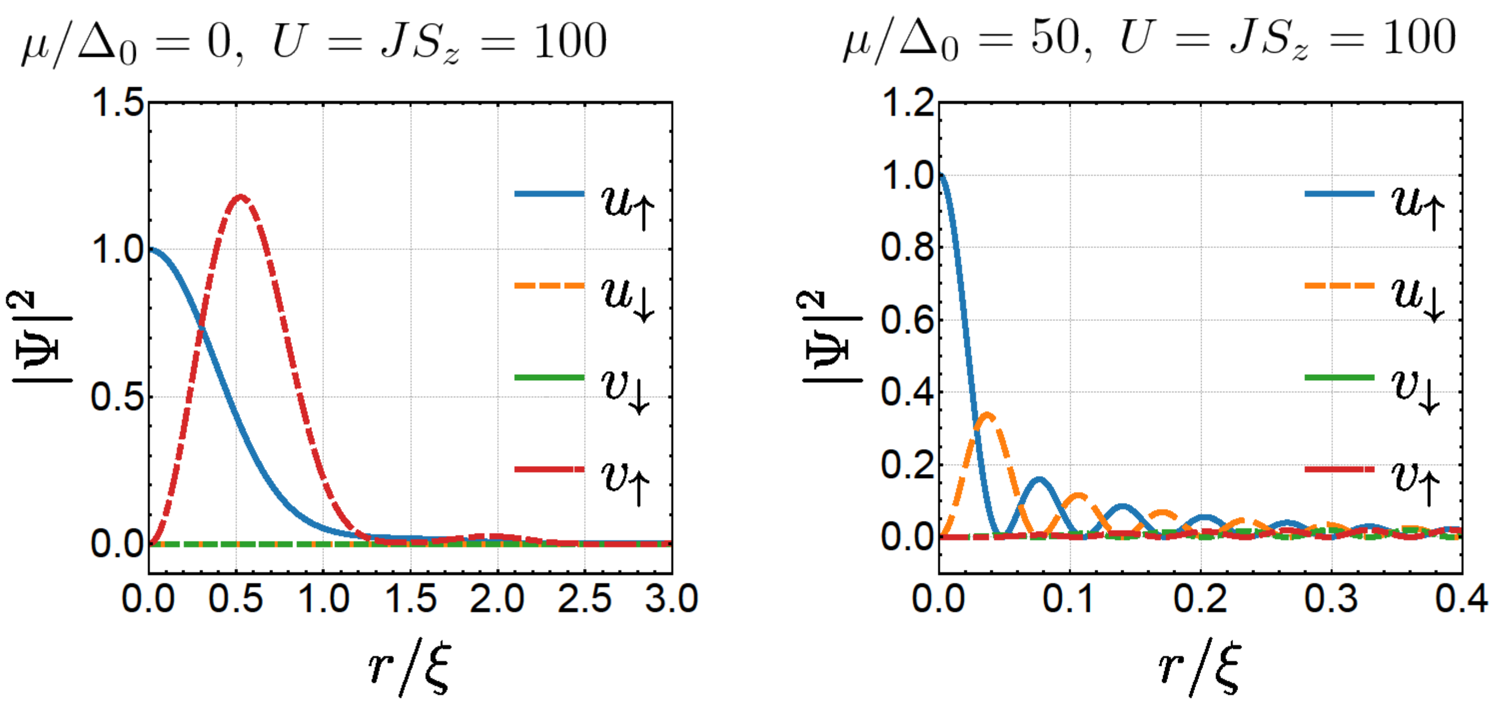
Further differences will be found if we look at wave functions.

# Wave function

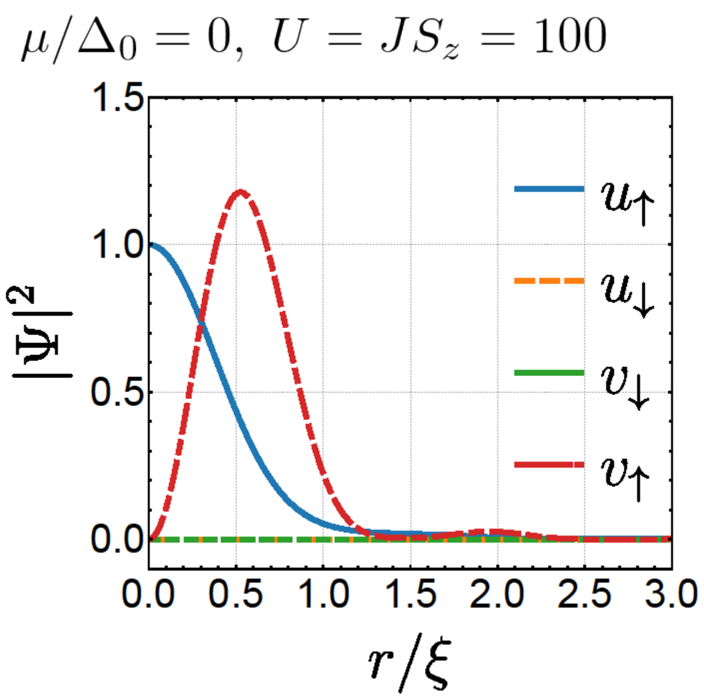
Solve the Bogoliubov-de Gennes equation: Pientka *et al*. (2013)

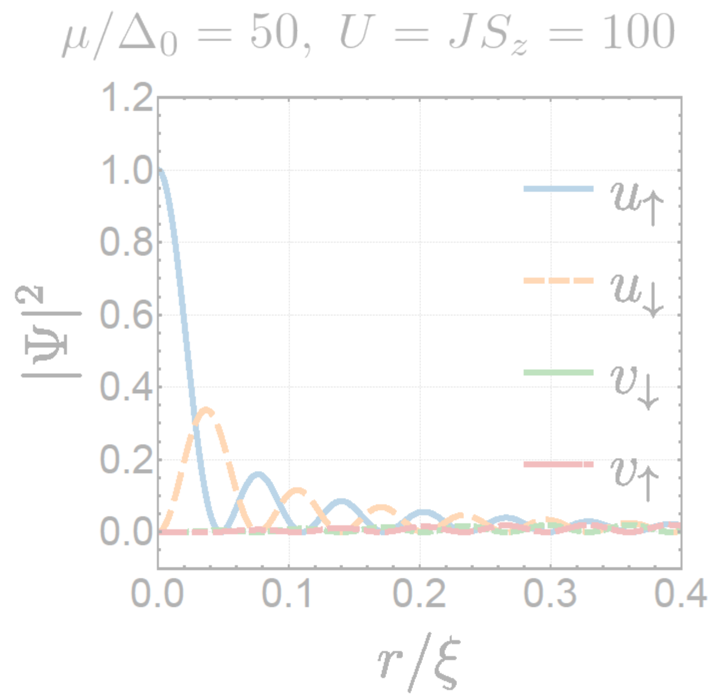
$$(H_0 + H_{\rm imp})\chi(\boldsymbol{r}) = E\chi(\boldsymbol{r})$$

$$H_{\rm imp} = V\delta(\boldsymbol{r}) = (U\tau^z\sigma^0 - J\tau^0\boldsymbol{S}\cdot\boldsymbol{\sigma})\delta(\boldsymbol{r})$$



# Wave function



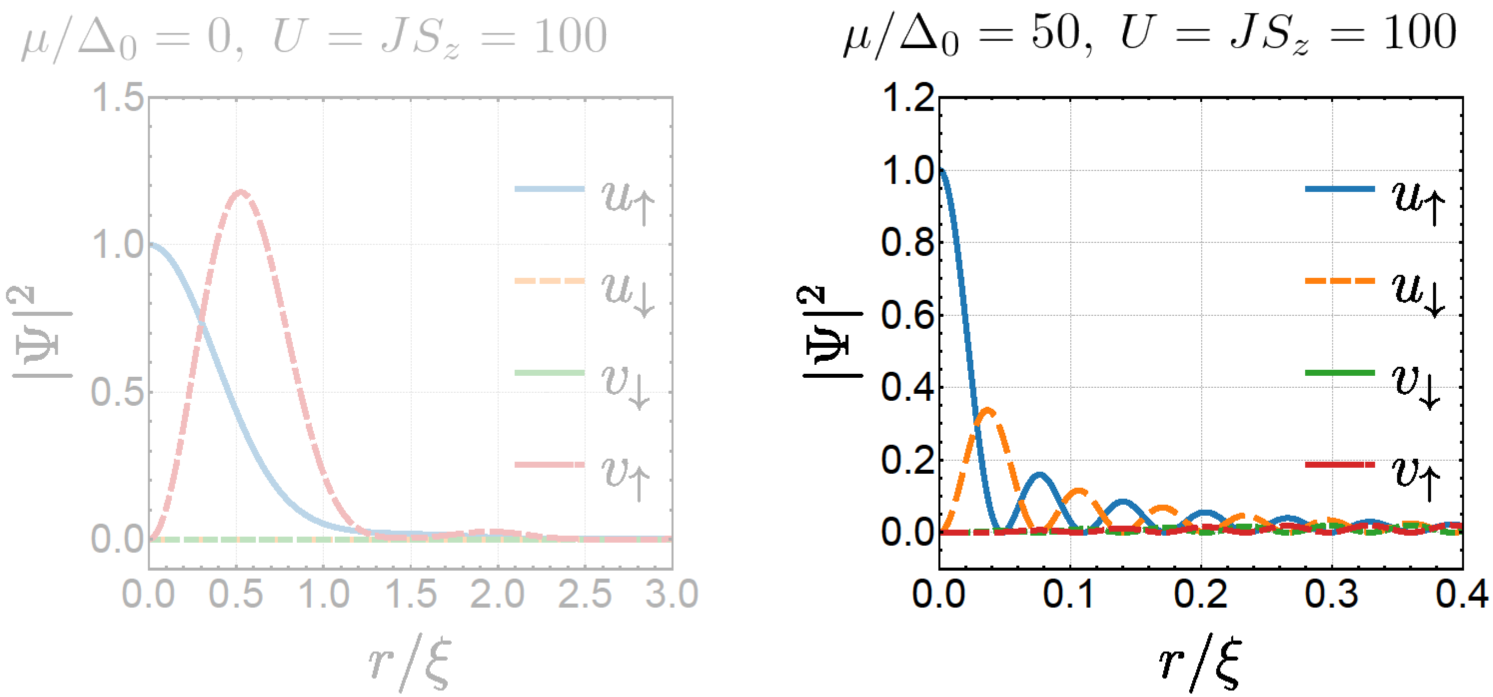

$$\chi_z^+(\boldsymbol{r}) \simeq (K_0(r/\xi), 0; 0, -ie^{-i\phi}e^{i\theta}K_1(r/\xi))^T$$

$$\chi_z^-(\boldsymbol{r}) \simeq (ie^{i\phi}e^{-i\theta}K_1(r/\xi), 0; 0, K_0(r/\xi))^T$$

Only spin-up components

$K_n(r/\xi) \approx e^{-r/\xi}\sqrt{\pi\xi/(2r)}$ : modified Bessel function $\quad r \gtrsim \xi$

# Wave function



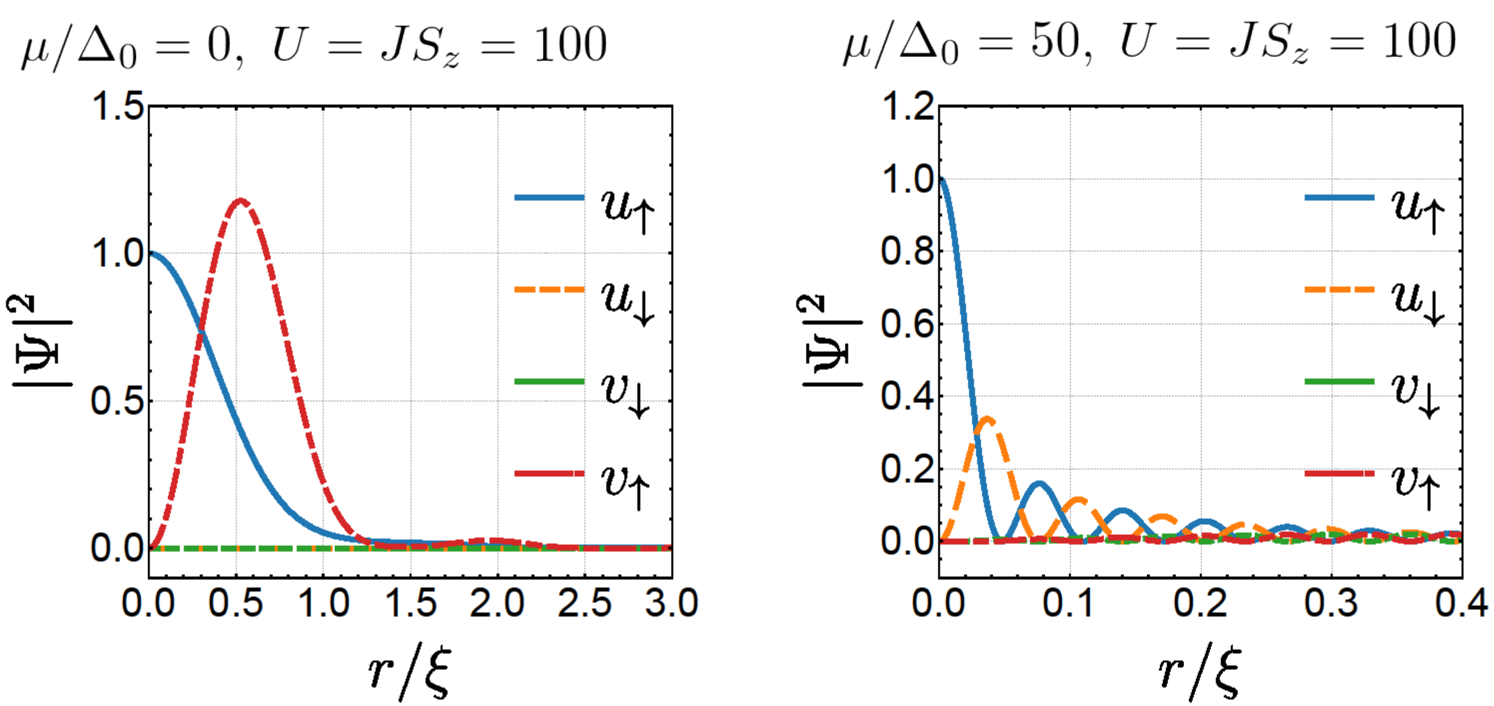

Only electron components

$$\chi_z^+(\boldsymbol{r}) \simeq (F_0(r), i\mathrm{sgn}(\mu)e^{i\theta}F_1(r); 0, 0)^T$$

$$\chi_z^-(\boldsymbol{r}) \simeq (0, 0; i\mathrm{sgn}(\mu)e^{-i\theta}F_1(r), F_0(r))^T$$

$$\begin{pmatrix} F_0(r) = \xi\sqrt{2\pi k_F/r}e^{-r/\xi}\cos(k_F r - \pi/4) \\ F_1(r) = -\xi\sqrt{2\pi k_F/r}e^{-r/\xi}\cos(k_F r + \pi/4) \end{pmatrix}$$

# Wave function




Two length scales:

- Coherence length $\xi = v/\Delta_0$ (decay)
- Fermi wavelength $\lambda_F = 2\pi/k_F$ (oscillations)

# Local density of states (LDOS)

STM measurement $N(E, \boldsymbol{r}) = N_\uparrow(E, \boldsymbol{r}) + N_\downarrow(E, \boldsymbol{r})$

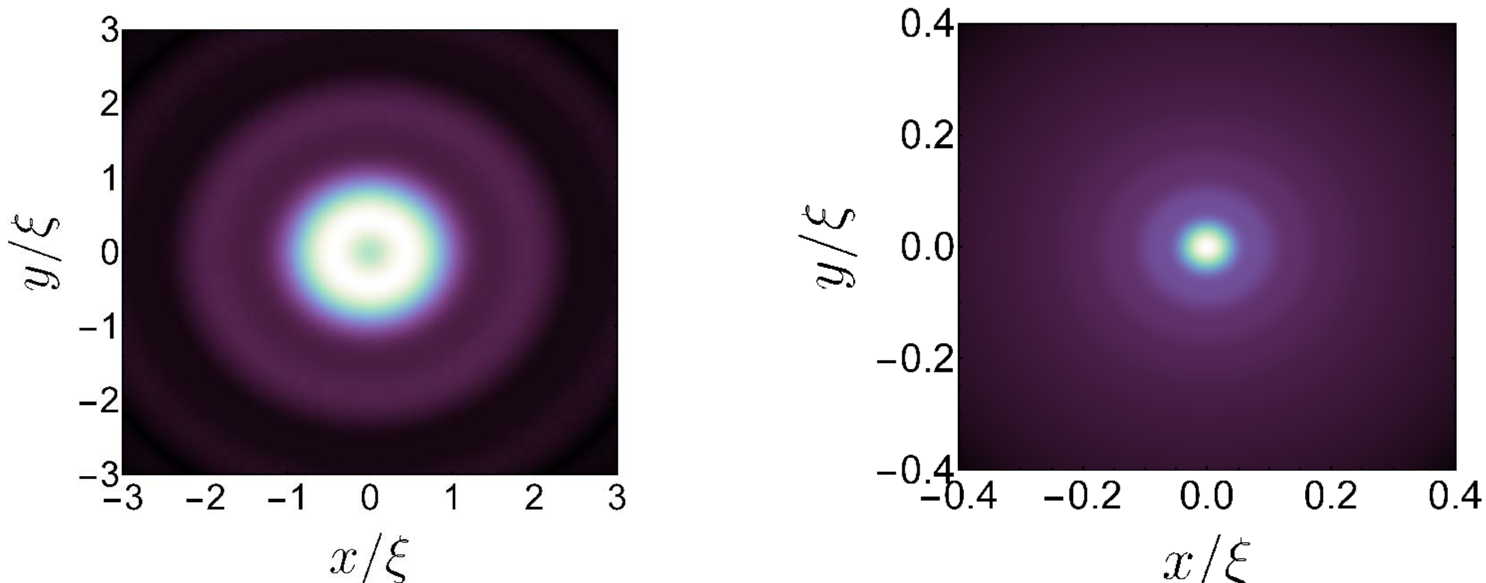
$$N_\sigma(E, \boldsymbol{r}) = \sum_n [|u_{n,\sigma}|^2 \delta(E - E_n) + |v_{n,\sigma}|^2 \delta(E + E_n)]$$

$$\chi = (u_\uparrow, u_\downarrow; v_\downarrow, -v_\uparrow)^T$$

Spin-averaged LDOS

- Oscillation for large doping

$\mu/\Delta_0 = 0,\ U = JS_z = 100$ $\mu/\Delta_0 = 50,\ U = JS_z = 100$



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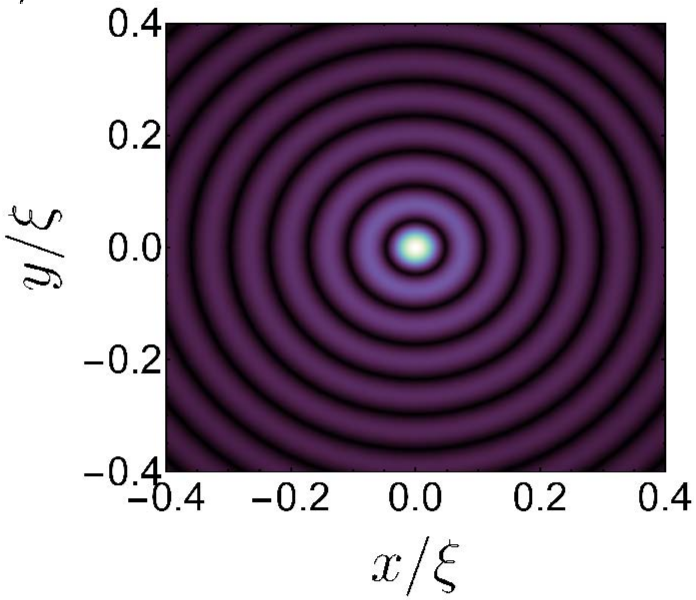
$$\chi = (u_{\uparrow}, u_{\downarrow}; v_{\downarrow}, -v_{\uparrow})^T$$

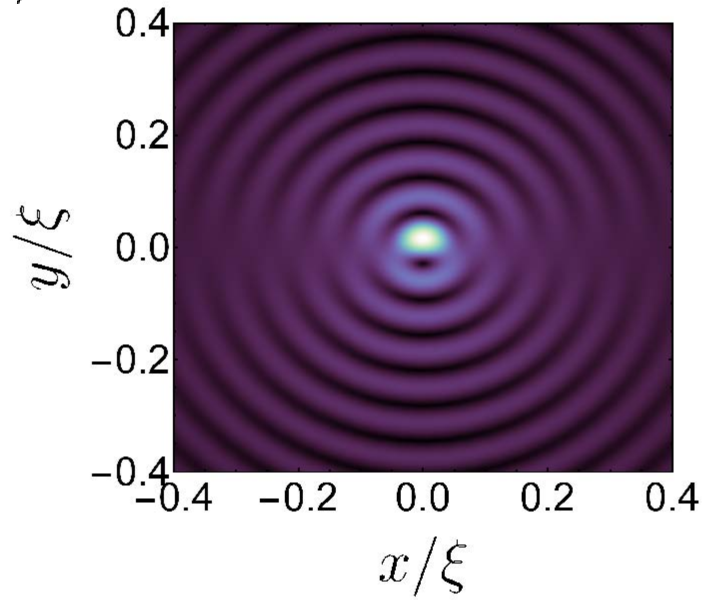
Spin-resolved LDOS

- At large doping:

$S_z \neq 0$



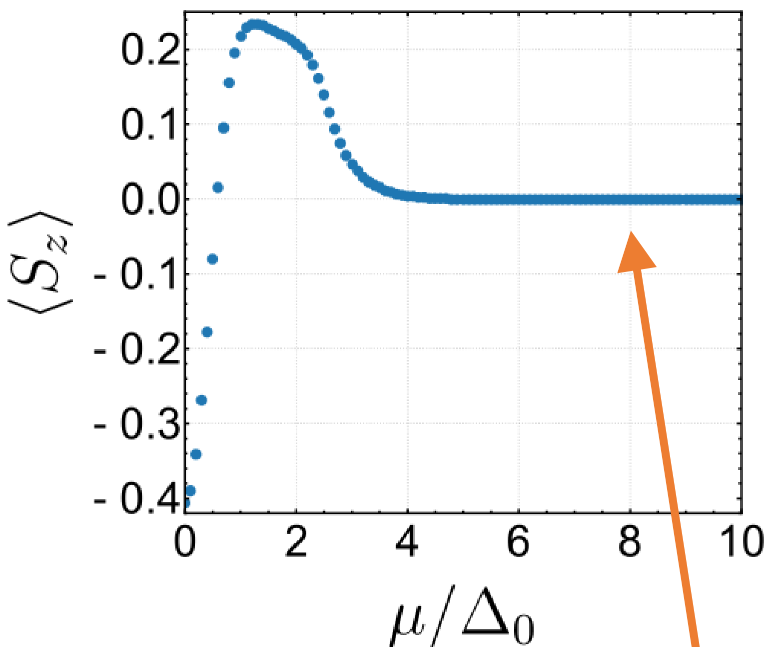

$S_x \neq 0$

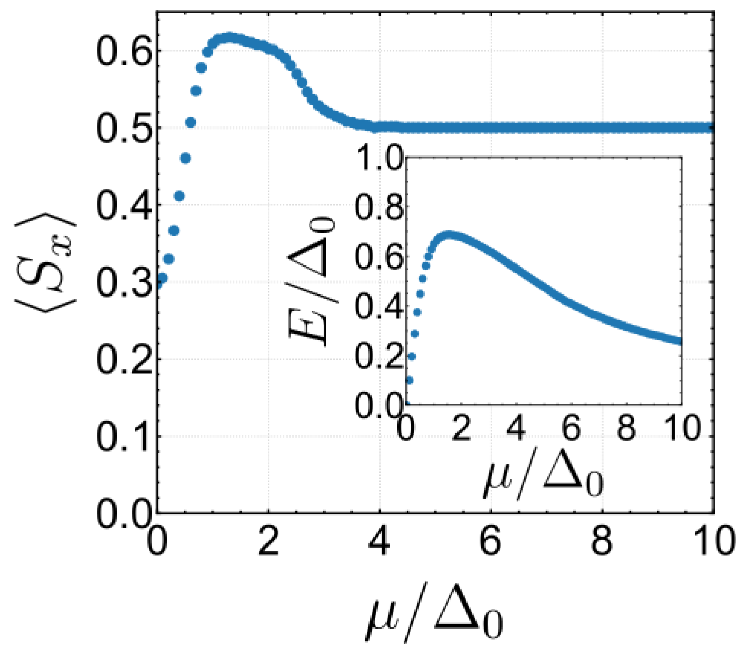


# Spin accumulation

Response to external magnetic field $\boldsymbol{S} = \frac{1}{2}\boldsymbol{\sigma}\tau_0$

$S_z \neq 0$ $\quad$ $S_x \neq 0$




Insensitive to external magnetic field

$U = JS = 100$

# Difference from Majorana zero modes

| | **Impurity bound states** | **Majorana zero modes** |
|---|---|---|
| Localized at … | Impurity | Vortex (magnetic flux) |
| Locked at zero energy? | No | Yes |
| Appear in pairs? | Yes, but may be degenerate. | No |
| Oscillation of LDOS? | | |
| (spin-averaged) | Yes/No (depending on $\mu$) | No |
| (spin-resolved) | Yes | Yes |
| Energy shift under ***B*** field? | Yes/No (***B*** field direction) | No |

# Summary

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- Differences in measureable quantities.
- Clues for experimental detection of Majorana zero modes.