Title: TBA

Date: Jul 19, 2016 03:30 PM

URL: http://pirsa.org/16070002

Abstract:

Spin-orbit coupling

- Orbital motion of electrons ⟹ effective magnetic fields
- Spins of electrons interact with those fields:

$$\hat{H} = \lambda \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}$$

λ - spin-orbit coupling constant

- Main effect in atoms:
  - Shifts of spectral lines
  - Splittings of spectral lines (fine structure)

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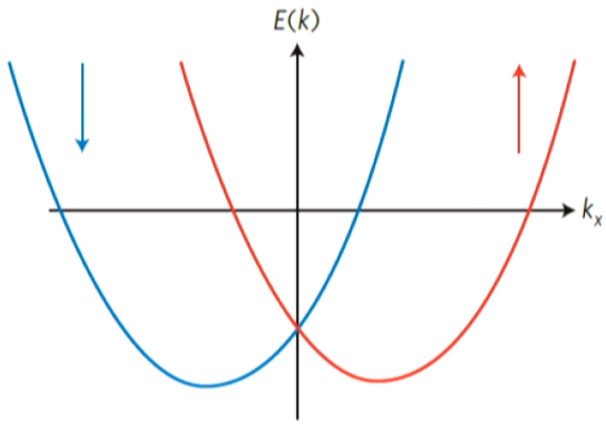


- In solids ⟹ Rashba effect (Rashba SO)

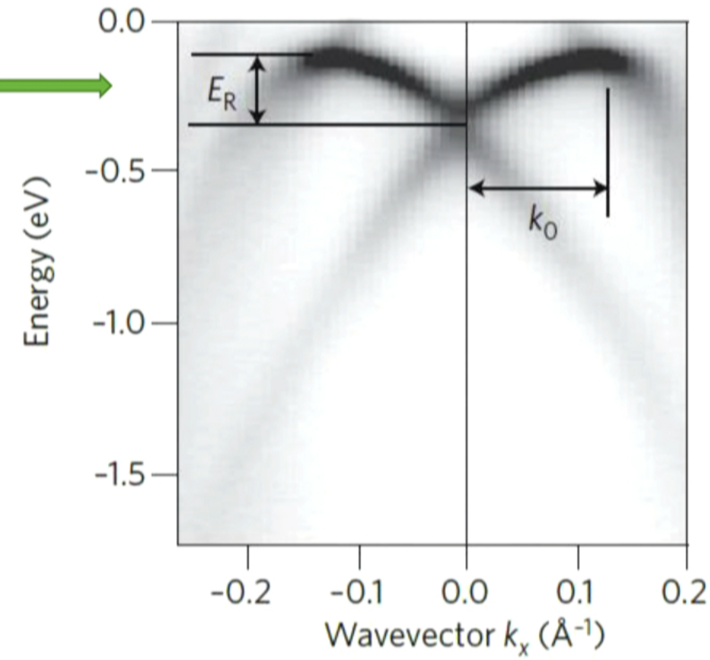
$$\hat{H}_R = \lambda(\boldsymbol{\sigma} \times \boldsymbol{p}) \cdot \boldsymbol{z}$$

momentum-dependent splitting of spin bands

plays key role in topological phenomena

Measuring the Rashba spin-orbit

- (spin-resolved) ARPES
- Magneto-transport measurements



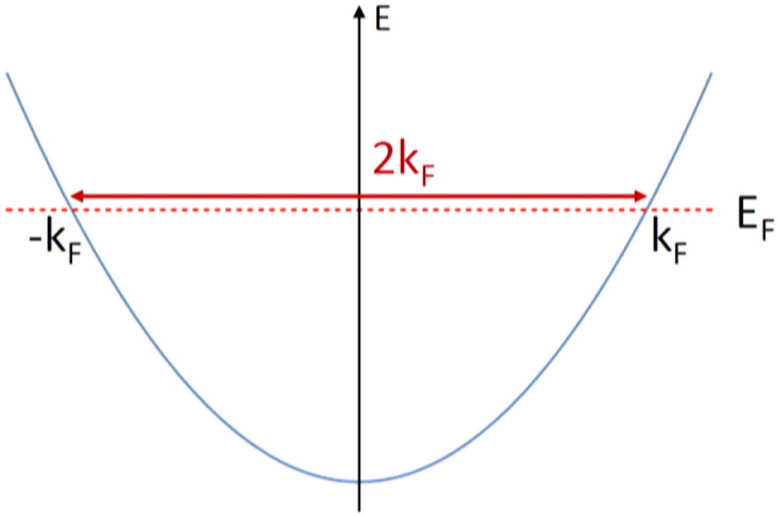
A. Manchon et al., Nature Materials 14, 871 (2015)

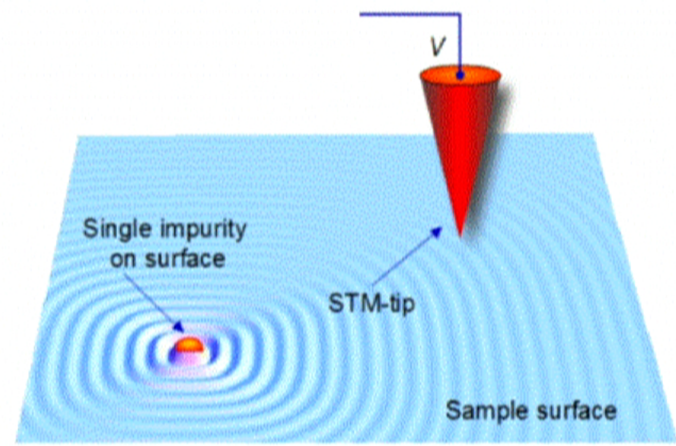
Friedel oscillations

- 3D metal + localised imp. = oscillations in local density of states

$$\delta\rho(r) \sim \frac{\cos 2k_F r}{r^3} \qquad T = \frac{\pi}{k_F}$$

- Appear in many different systems (3D, 2D, 1D, graphene, etc.)
- Observed using STM





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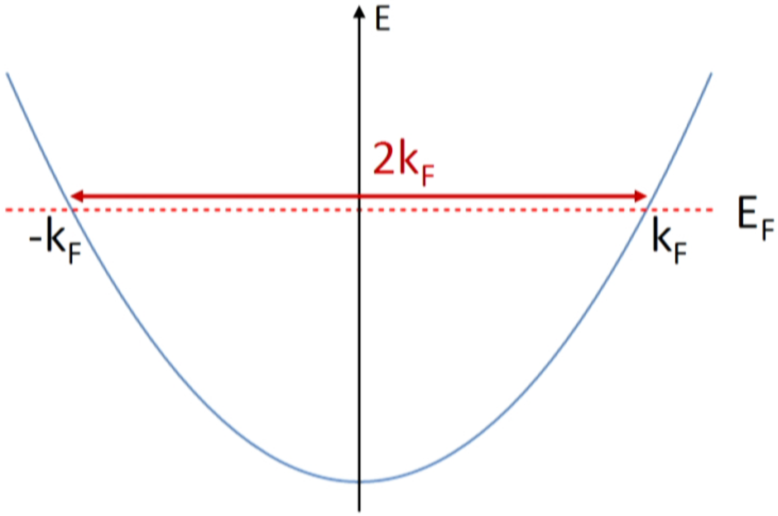

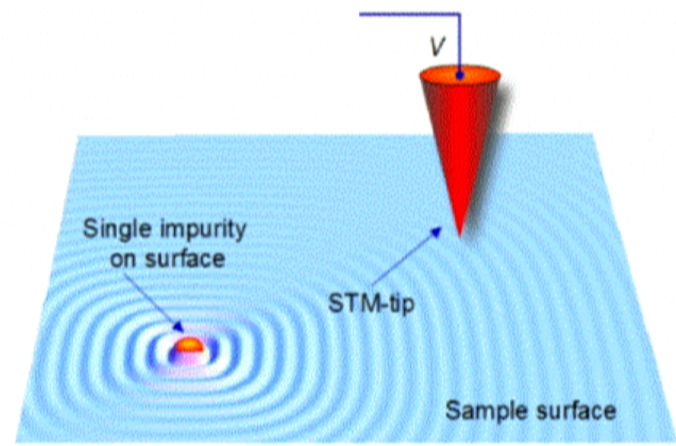

Superconductivity

- Cooper pairs

  - Spin number: singlet ($S = 0$) and triplet ($S = 1$)
  - Orbital number: $L = 0, 1, 2, \ldots$
  - Wave function of fermions must be asymmetric (Pauli principle)
    $(-1)^L (-1)^{S+1} = -1$

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- Two possibilities for the wave function of the pair:

  - symmetric orbital part × asymmetric spin part:

  s-wave ($L = 0$, $S = 0$), d-wave ($L = 2$, $S = 0$), etc

  - asymmetric orbital part × symmetric spin part:

  p-wave ($L = 1$, $S = 1$), f-wave ($L = 3$, $S = 1$), etc

Superconductivity

- s-wave (L = 0, S = 0)

- BdG Hamiltonian in Nambu basis $\left\{\psi_\uparrow, \psi_\downarrow, \psi_\downarrow^\dagger, -\psi_\uparrow^\dagger\right\}$

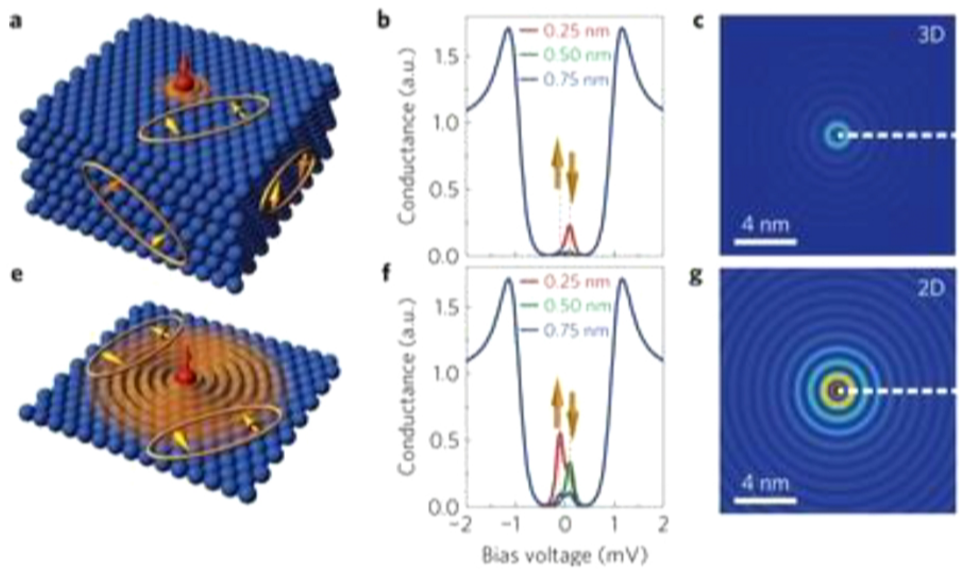
$$\mathcal{H}_{SC} = \begin{pmatrix} \xi_p \boldsymbol{\sigma}_0 & \Delta_s \boldsymbol{\sigma}_0 \\ \Delta_s \boldsymbol{\sigma}_0 & -\xi_p \boldsymbol{\sigma}_0 \end{pmatrix} \qquad \xi_p = \frac{p^2}{2m} - \varepsilon_F$$

$\boldsymbol{\sigma}_0$ acts in spin space as a 2x2 identity matrix

Δ_s is the superconducting pairing amplitude
(mean field approximation)

Shiba states

- 3D,2D superconductor + localised **magnetic** impurity = Shiba states
- Mechanism: Cooper pair breaking



$$E_{1,\bar{1}} = \pm\frac{1-\alpha^2}{1+\alpha^2}\Delta_s$$

$$\alpha = \pi\nu J \text{ and } \nu = \frac{m}{2\pi}$$

3D: A. Yazdani et al., Science 275, 1767 (1997)
2D: G. Ménard and et al., Nature Physics 11, 1013 (2015)

Determining the spin-orbit coupling

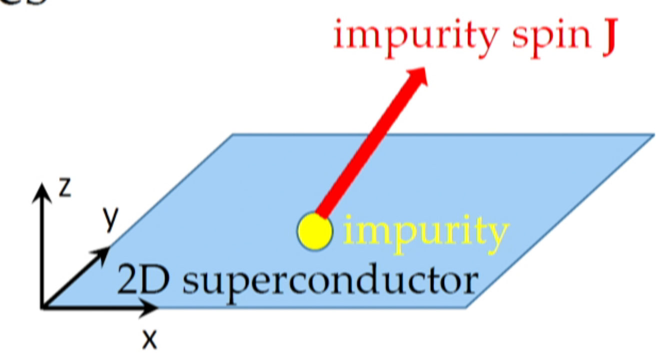
Model and motivation

Nambu basis $\left\{\psi_\uparrow, \psi_\downarrow, \psi_\downarrow^\dagger, -\psi_\uparrow^\dagger\right\}$

$$\mathcal{H} = \underbrace{\begin{pmatrix} \xi_p \boldsymbol{\sigma}_0 & \Delta_s \boldsymbol{\sigma}_0 \\ \Delta_s \boldsymbol{\sigma}_0 & -\xi_p \boldsymbol{\sigma}_0 \end{pmatrix}}_{\mathcal{H}_{SC}} + \underbrace{\begin{pmatrix} \lambda \left(p_y \boldsymbol{\sigma}_x - p_x \boldsymbol{\sigma}_y\right) & 0 \\ 0 & -\lambda \left(p_y \boldsymbol{\sigma}_x - p_x \boldsymbol{\sigma}_y\right) \end{pmatrix}}_{\mathcal{H}_{SO}} + \underbrace{\begin{pmatrix} \boldsymbol{J} \cdot \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{J} \cdot \boldsymbol{\sigma} \end{pmatrix} \delta(\boldsymbol{r})}_{\mathcal{H}_{imp}}$$

Before: non-polarised local density of states

What can we learn from **spin-polarised** local density of states?



Methods: analytical

Schrödinger equation: $[H_{SC} + H_{SO} + V\delta(\boldsymbol{r})]\,\Phi(\boldsymbol{r}) = E\Phi(\boldsymbol{r})$

Green's function: $G_0 = (E + i0 - H_{SC} - H_{SO})^{-1}$

Shiba state energies: $[\mathbb{I}_4 - VG_0(E, \boldsymbol{r} = \boldsymbol{0})]\,\Phi(\boldsymbol{0}) = 0$

↓

E, $\Phi(\mathbf{0})$

↓

Shiba wave functions: $\Phi(\boldsymbol{r}) = G_0(E, \boldsymbol{r})V\Phi(\boldsymbol{0})$

Methods: numerical

- Definition on a square lattice: $\xi_p = \mu - 2t(\cos p_x + \cos p_y)$

μ – chemical potential, t – hopping parameter

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- T-matrix definition and properties

$$T(E) = \left[1 - V \int \frac{d^2\mathbf{p}}{(2\pi)^2} G_0(E, \mathbf{p})\right]^{-1} V.$$

  - Poles of the T-matrix ⟹ energies of Shiba states
  - T-matrix ⟹ perturbed Green's function

Methods: numerical

Definitions of local density of states

$$S_x(\boldsymbol{p},E) = -\frac{1}{2\pi i}\int \frac{d\mathbf{q}}{(2\pi)^2}[\tilde{g}_{12}(E,\mathbf{q},\mathbf{p})+\tilde{g}_{21}(E,\mathbf{q},\mathbf{p})]$$

$$S_y(\boldsymbol{p},E) = -\frac{1}{2\pi}\int \frac{d\mathbf{q}}{(2\pi)^2}[g_{12}(E,\mathbf{q},\mathbf{p})-g_{21}(E,\mathbf{q},\mathbf{p})]$$

$$S_z(\boldsymbol{p},E) = -\frac{1}{2\pi i}\int \frac{d\mathbf{q}}{(2\pi)^2}[\tilde{g}_{11}(E,\mathbf{q},\mathbf{p})-\tilde{g}_{22}(E,\mathbf{q},\mathbf{p})]$$

Spin-polarised

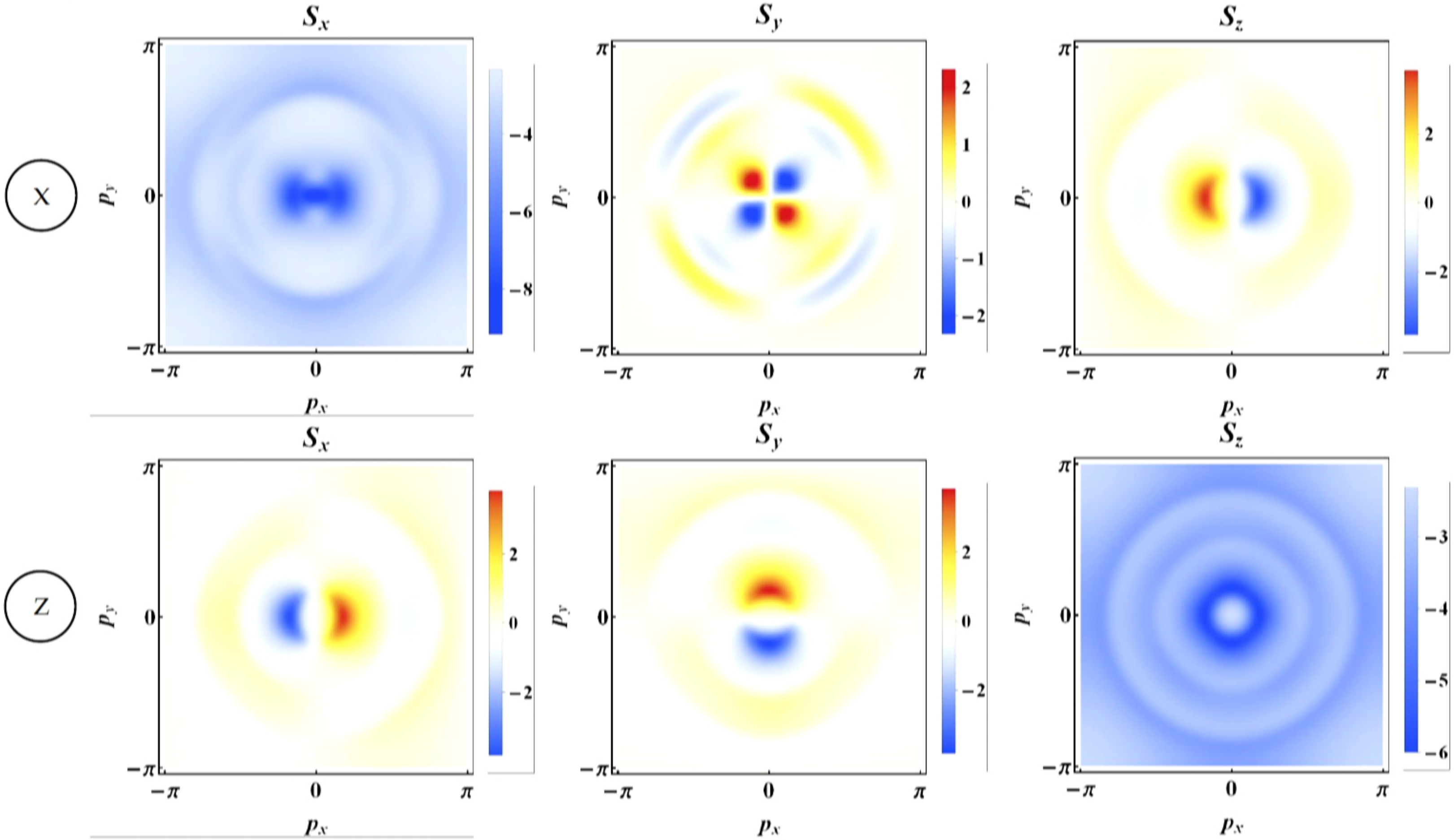
$$\rho(\boldsymbol{p},E) = -\frac{1}{2\pi i}\int \frac{d\mathbf{q}}{(2\pi)^2}[\tilde{g}_{11}(E,\mathbf{q},\mathbf{p})+\tilde{g}_{22}(E,\mathbf{q},\mathbf{p})]$$

where

$$g/\tilde{g}(E,\mathbf{q},\mathbf{p}) = G_0(E,\mathbf{q})T(E)G_0(E,\mathbf{p}+\mathbf{q}) \pm G_0^*(E,\mathbf{p}+\mathbf{q})T^*(E)G_0^*(E,\mathbf{q})$$

G_0 is the unperturbed Green's function

Spin-polarised local density of states



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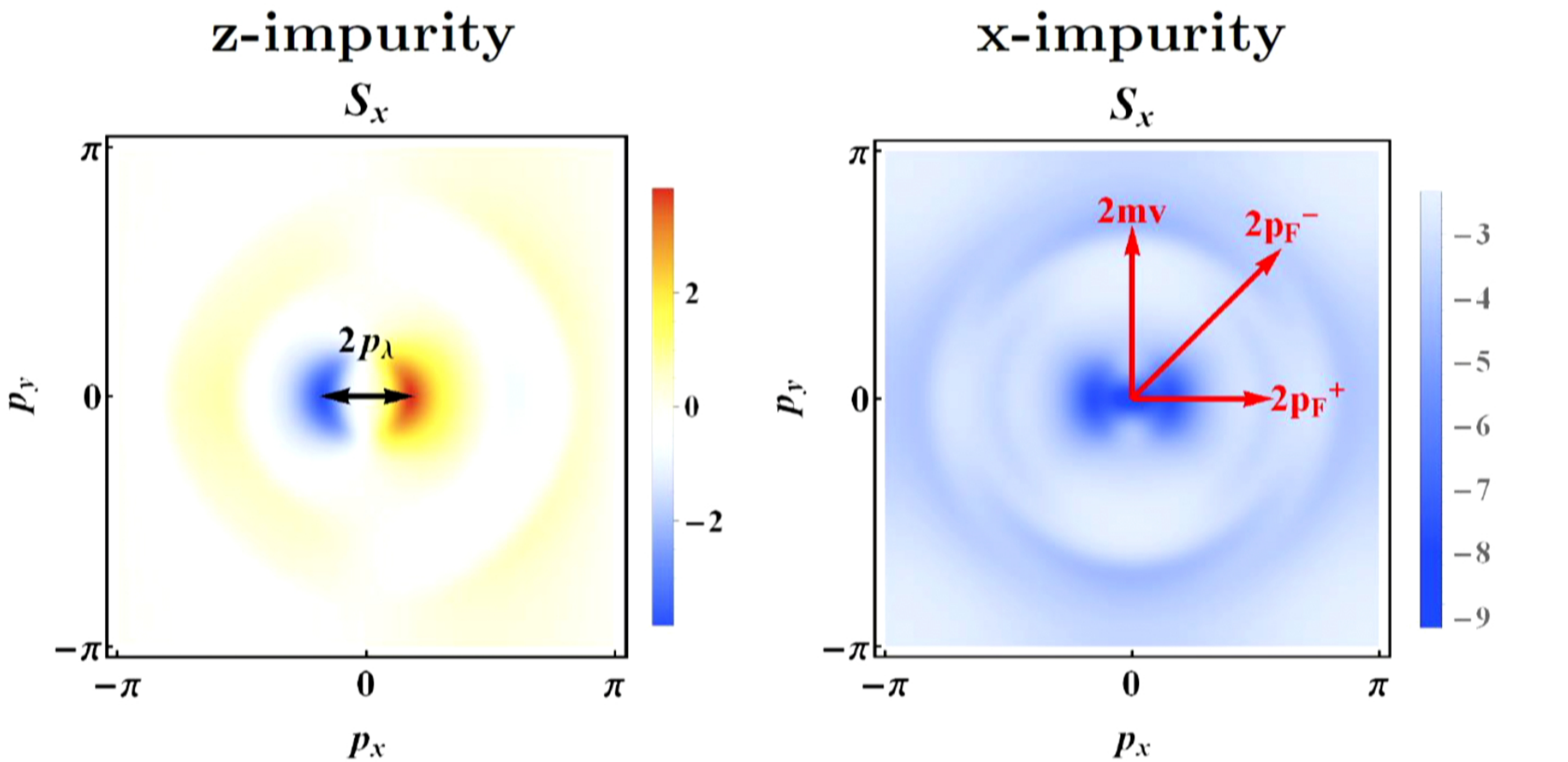

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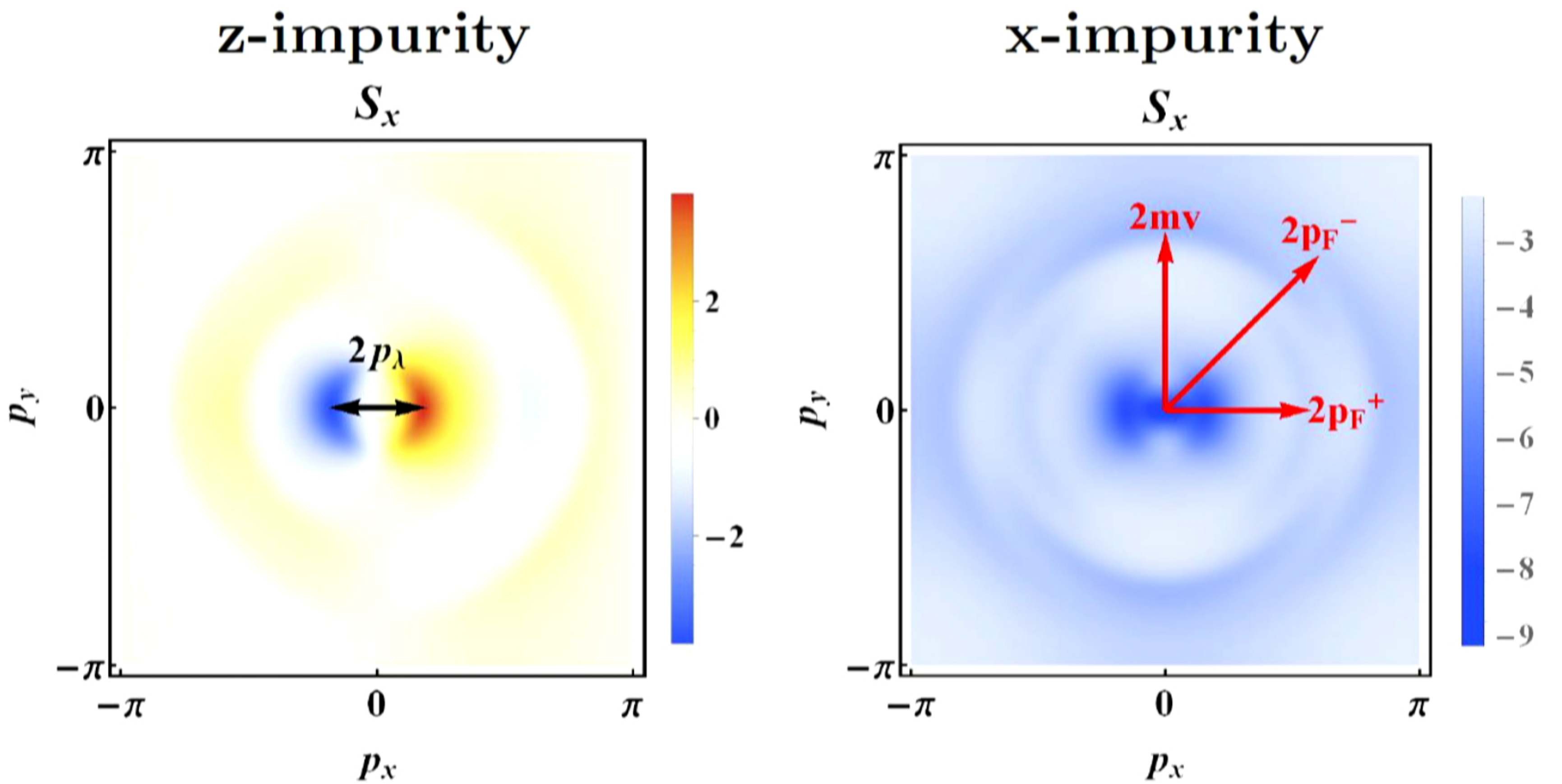
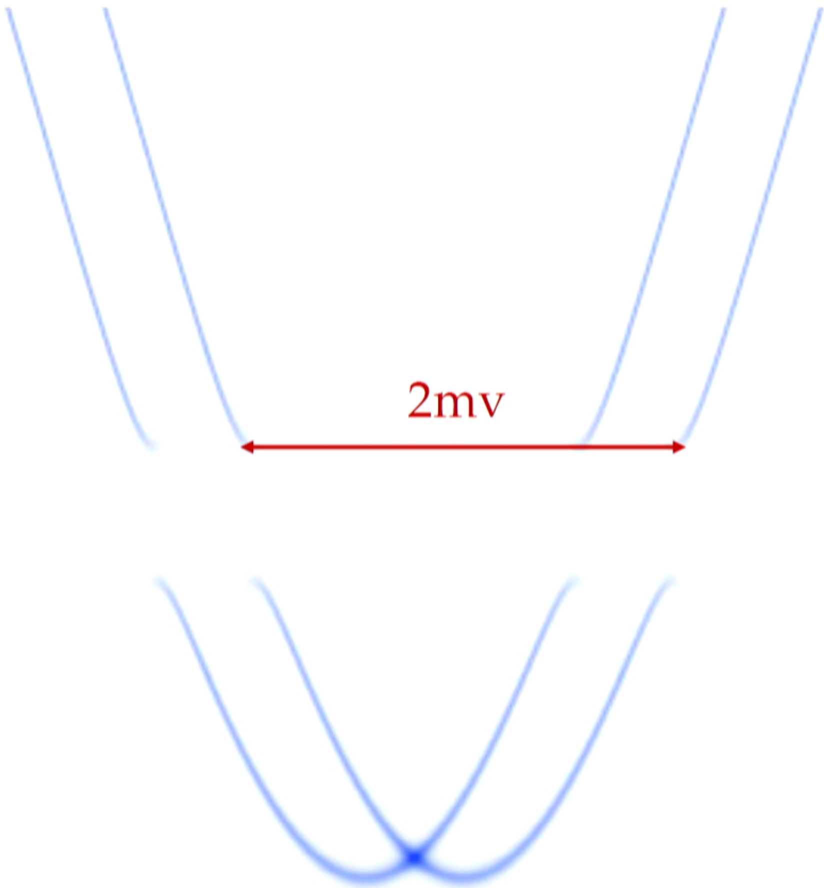
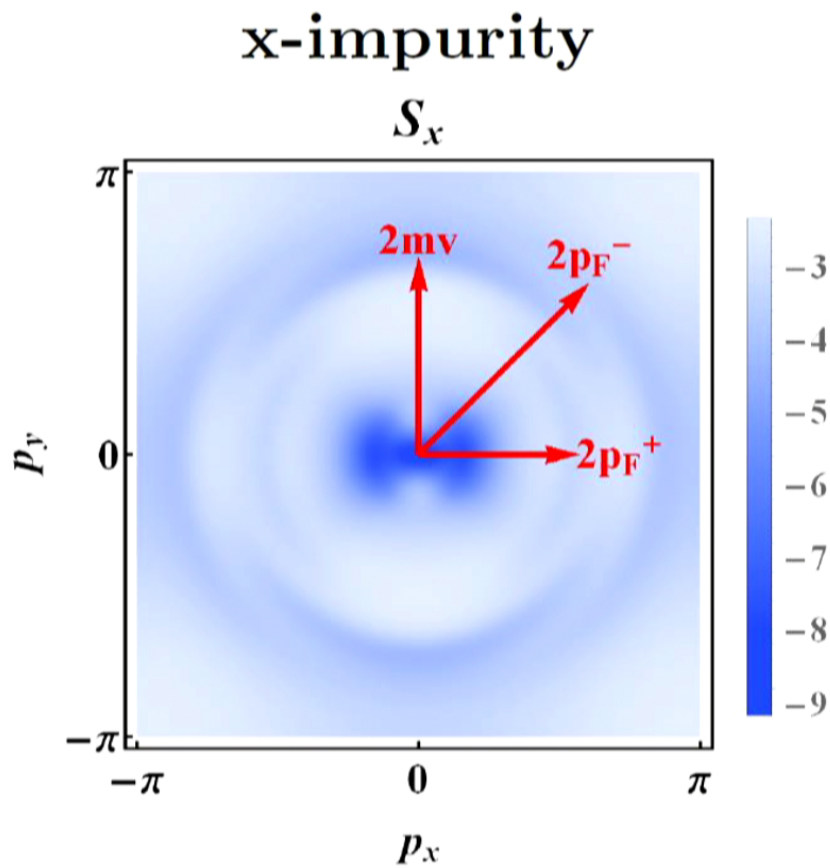


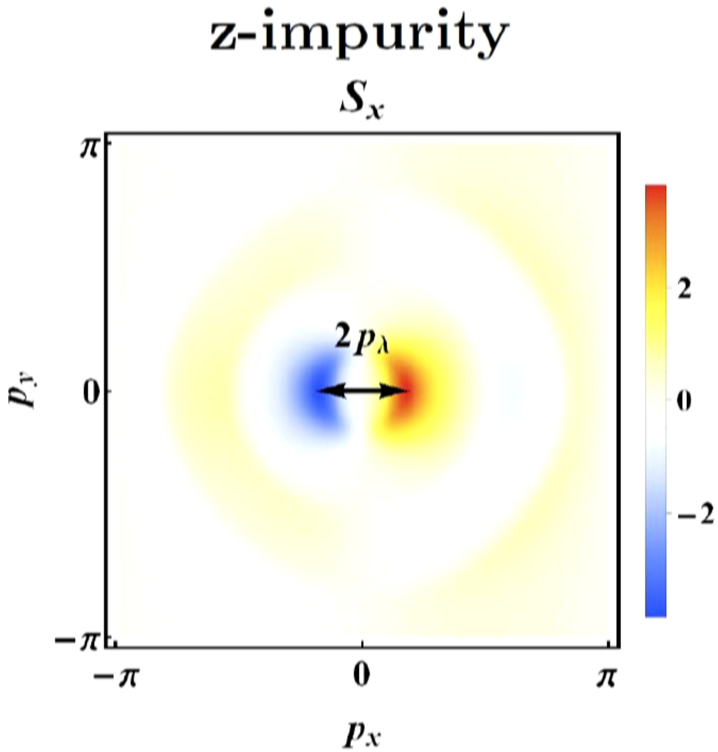
Spin-polarised LDOS: x-impurity

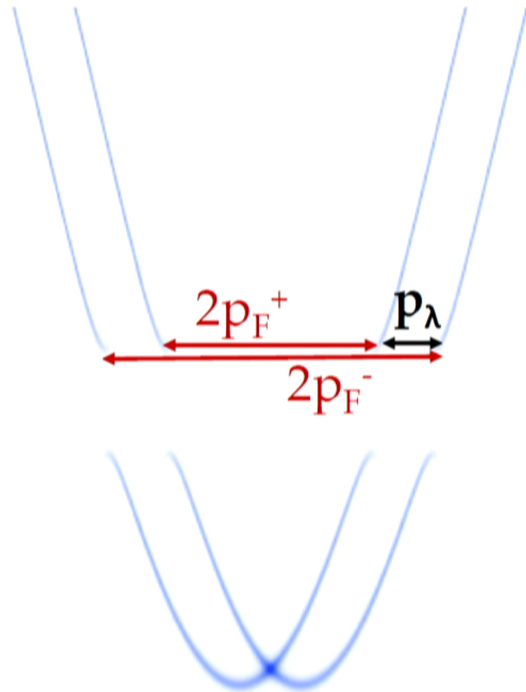




Spin-polarised LDOS: analytics

$$S_x(\boldsymbol{r}) = +J_z^2\left(1+\frac{1}{\alpha^2}\right)\frac{e^{-2p_s r}}{r}\cos\phi_{\boldsymbol{r}} \times \left\{\sum_\sigma \frac{\sigma\nu_\sigma^2}{p_F^\sigma}\underline{\cos\left(2p_F^\sigma r-\theta\right)} + 2\nu^2\frac{v_F^2}{v^2 p_F}\underline{\sin p_\lambda r}\right\}$$

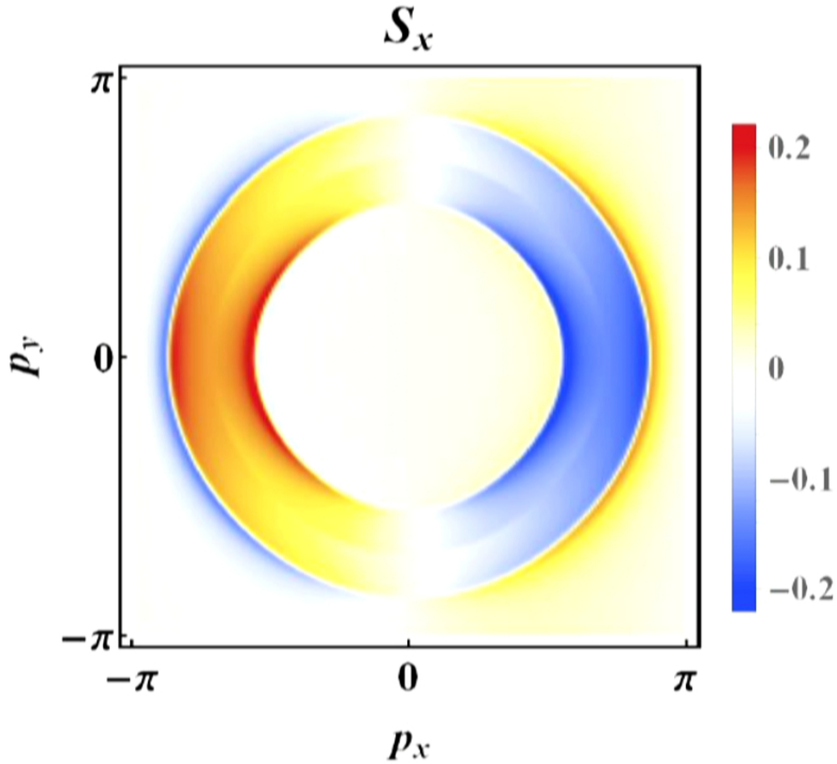




Comparison to the metallic phase

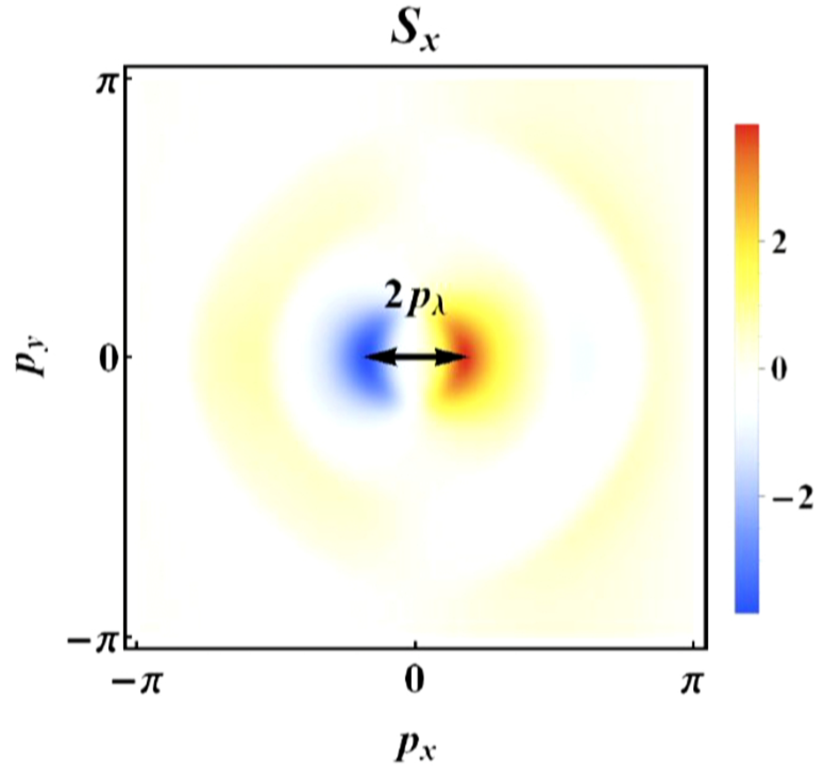
Metallic phase

z-impurity



Superconducting phase

z-impurity



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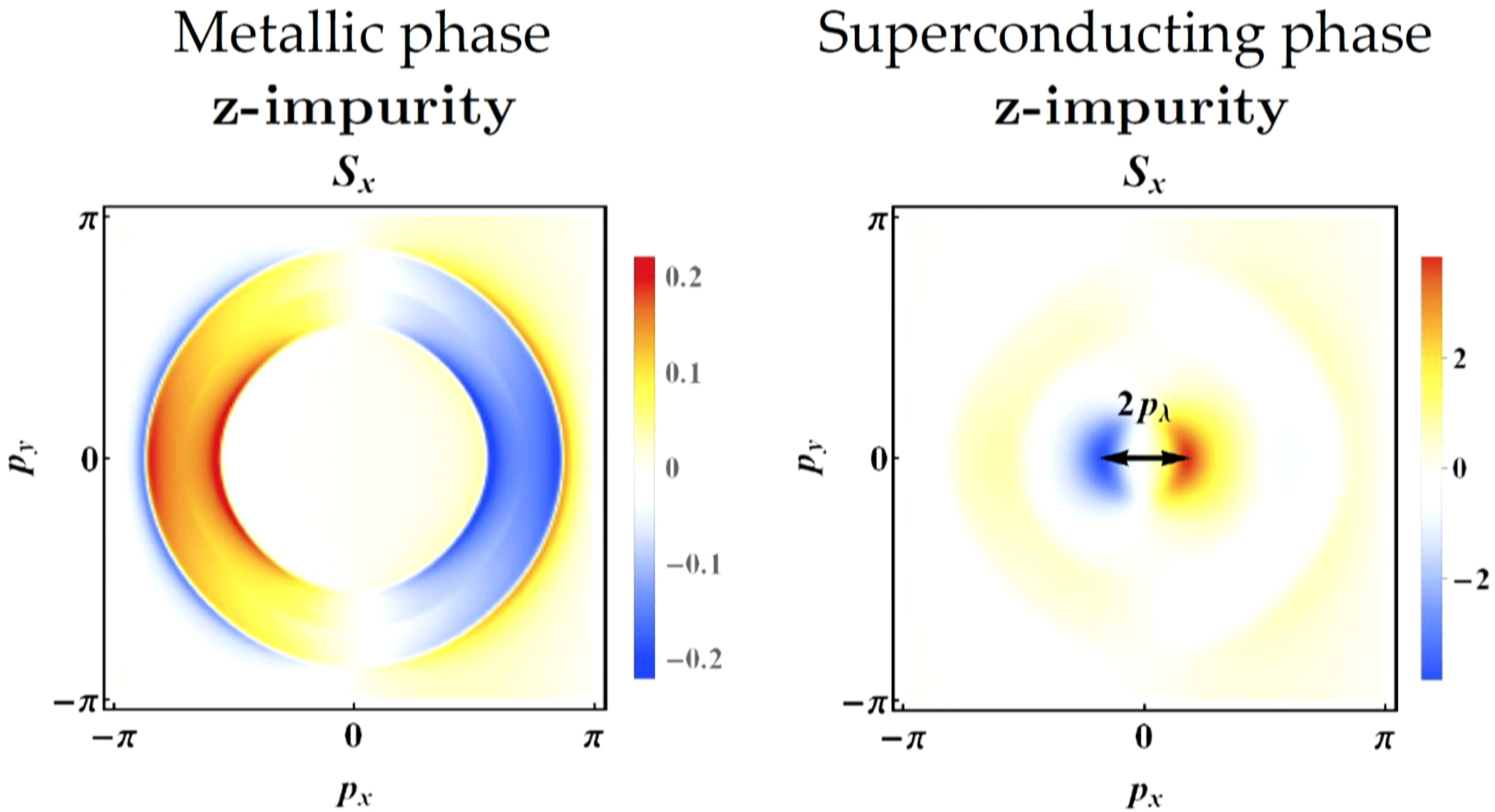

Conclusions

- Spin-polarised local density of states gives a direct access to the spin-orbit coupling constant
- We suggest to use the spin-polarised STM, which becomes more and more accessible (Weizmann, Princeton, etc)