

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:

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

λ - spin-orbit coupling constant

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

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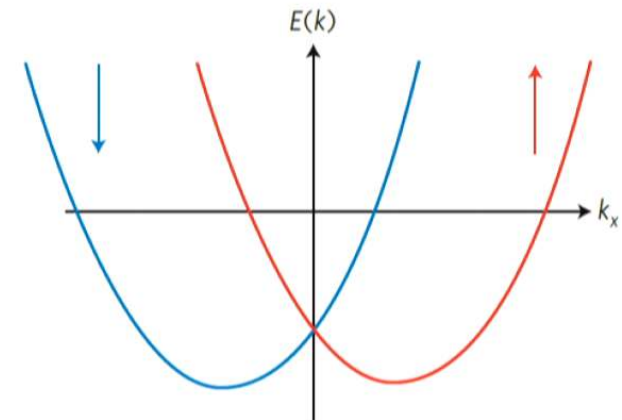
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- Main effect in atoms:
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- In solids \rightarrow Rashba effect (Rashba SO)

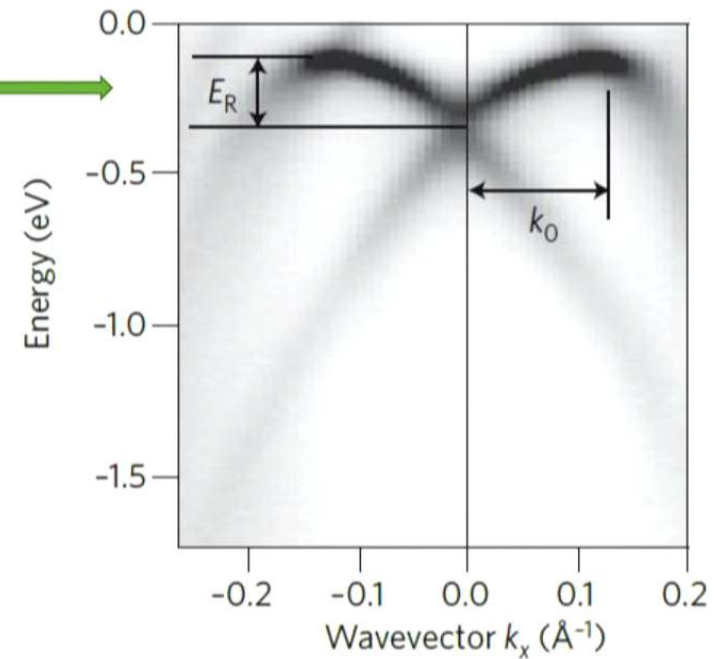
$$\hat{H}_R = \lambda(\boldsymbol{\sigma} \times \mathbf{p}) \cdot \mathbf{z}$$

momentum-dependent splitting of spin bands
plays key role in topological phenomena



Measuring the Rashba spin-orbit

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



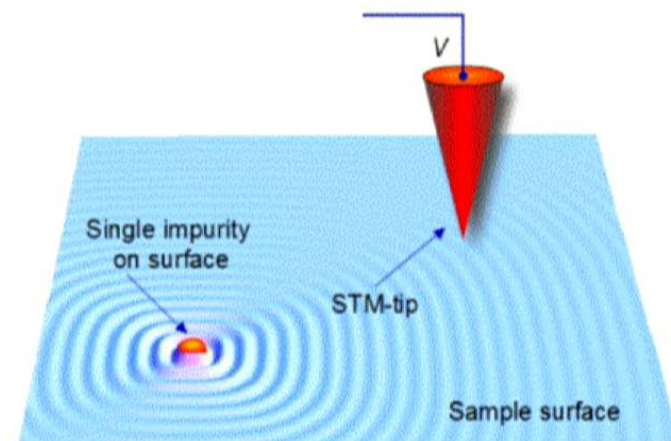
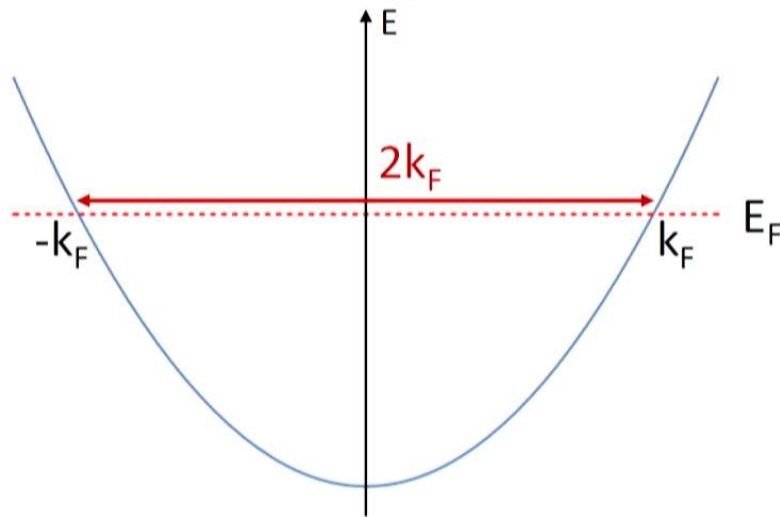
A. Manchon et al., Nature Materials 14, 871 (2015)

Friedel oscillations

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

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

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

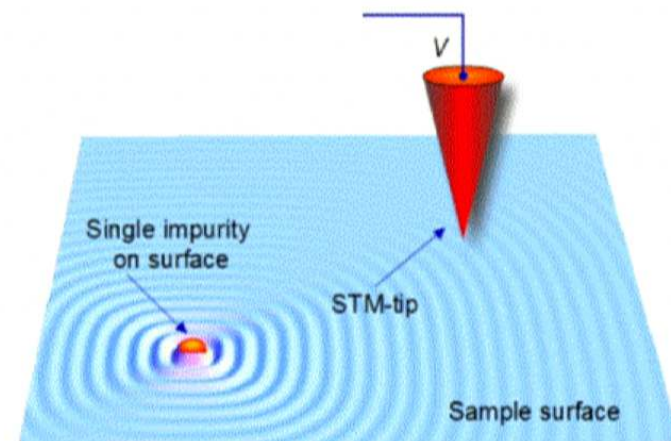
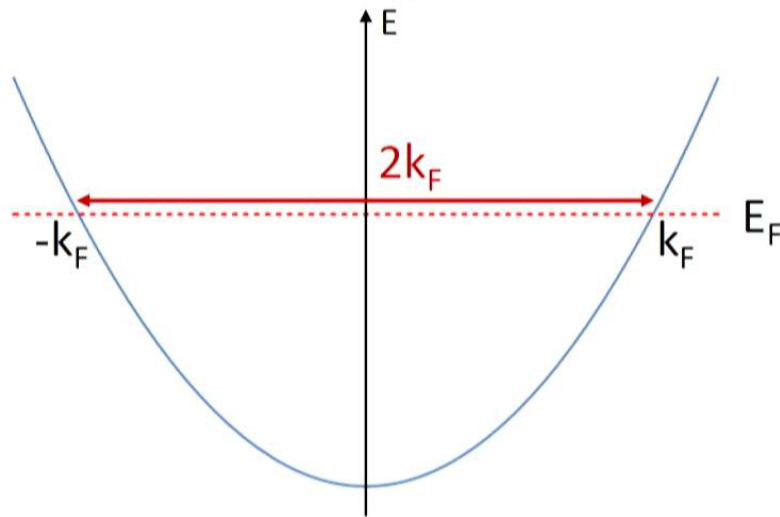


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Superconductivity

- Cooper pairs
 - Spin number: singlet ($S = 0$) and triplet ($S = 1$)
 - Orbital number: $L = 0, 1, 2, \dots$
 - 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** \times asymmetric **spin part**:
s-wave ($L = 0, S = 0$), d-wave ($L = 2, S = 0$), etc
 - asymmetric **orbital part** \times symmetric **spin part**:
p-wave ($L = 1, S = 1$), f-wave ($L = 3, S = 1$), etc

Superconductivity

- s-wave ($\mathbf{L} = 0, S = 0$)

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

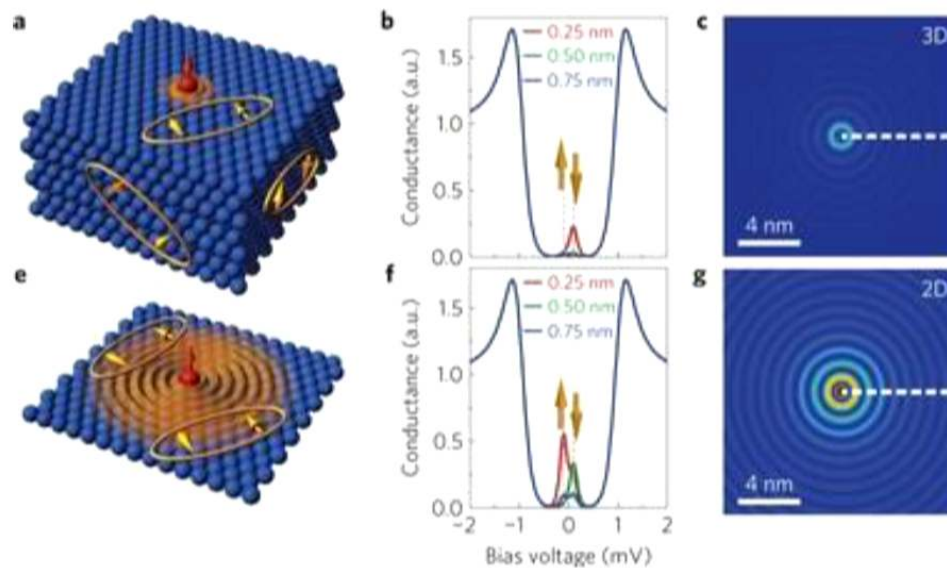
$$\mathcal{H}_{SC} = \begin{pmatrix} \xi_p \boldsymbol{\sigma}_0 & \Delta_s \boldsymbol{\sigma}_0 \\ \Delta_s \boldsymbol{\sigma}_0 & -\xi_p \boldsymbol{\sigma}_0 \end{pmatrix} \quad \xi_p = \frac{p^2}{2m} - \varepsilon_F$$

$\boldsymbol{\sigma}_0$ 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

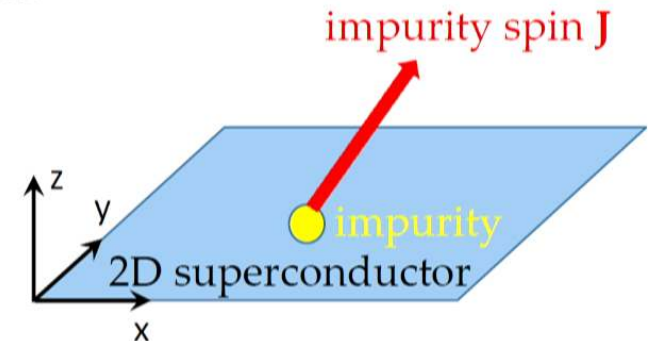
Model and motivation

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

$$\mathcal{H} = \underbrace{\begin{pmatrix} \xi_p \sigma_0 & \Delta_s \sigma_0 \\ \Delta_s \sigma_0 & -\xi_p \sigma_0 \end{pmatrix}}_{\mathcal{H}_{SC}} + \underbrace{\begin{pmatrix} \lambda (p_y \sigma_x - p_x \sigma_y) & 0 \\ 0 & -\lambda (p_y \sigma_x - p_x \sigma_y) \end{pmatrix}}_{\mathcal{H}_{SO}} + \underbrace{\begin{pmatrix} \mathbf{J} \cdot \boldsymbol{\sigma} & 0 \\ 0 & \mathbf{J} \cdot \boldsymbol{\sigma} \end{pmatrix}}_{\mathcal{H}_{imp}} \delta(\mathbf{r})$$

Before: non-polarised local density of states

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



Methods: analytical

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

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

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


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

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

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 \longrightarrow energies of Shiba states
- T-matrix \longrightarrow perturbed Green's function

Methods: numerical

Definitions of local density of states

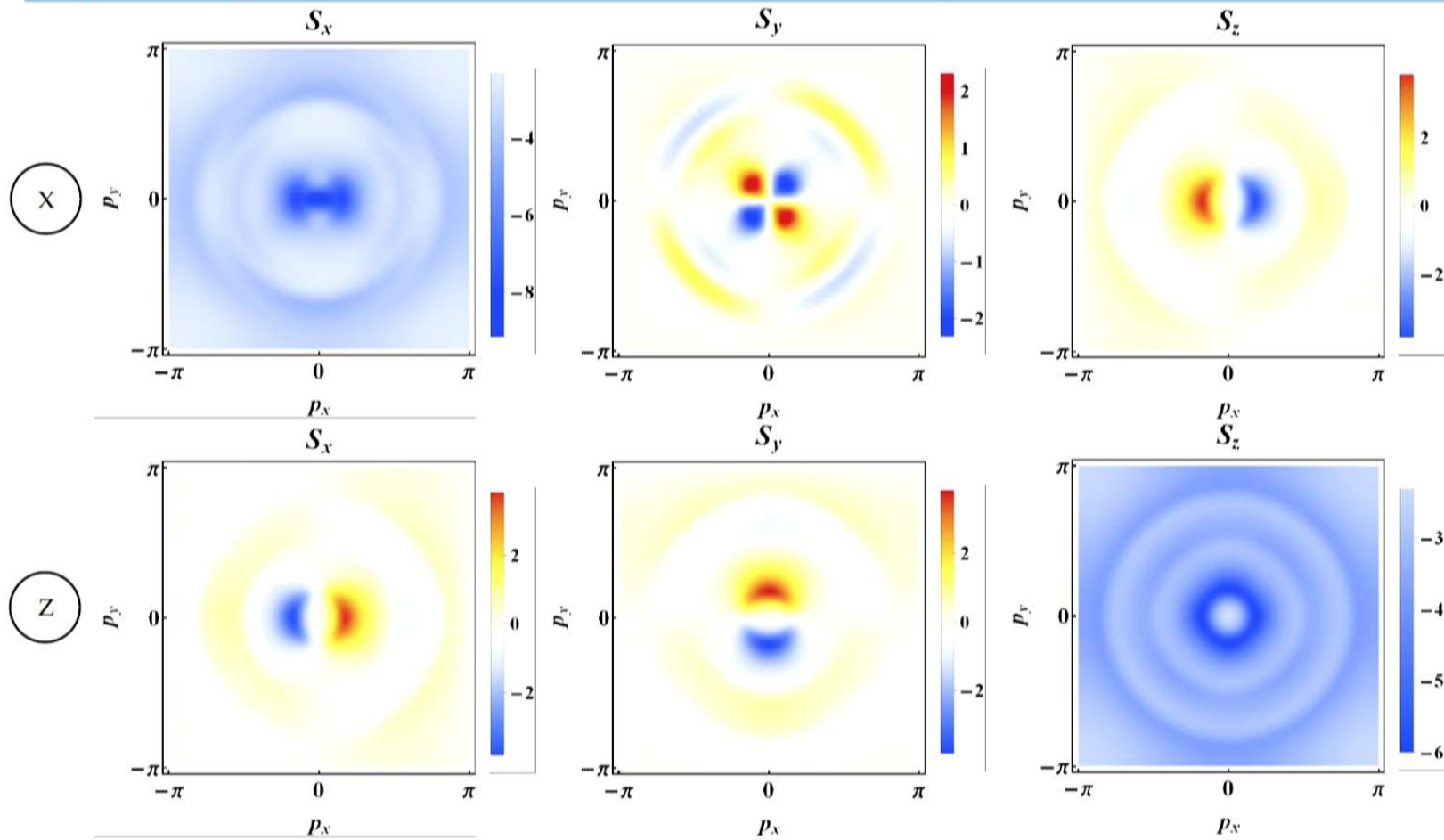
$$\begin{aligned} S_x(\mathbf{p}, E) &= -\frac{1}{2\pi i} \int \frac{d\mathbf{q}}{(2\pi)^2} [\tilde{g}_{12}(E, \mathbf{q}, \mathbf{p}) + \tilde{g}_{21}(E, \mathbf{q}, \mathbf{p})] \\ S_y(\mathbf{p}, E) &= -\frac{1}{2\pi} \int \frac{d\mathbf{q}}{(2\pi)^2} [g_{12}(E, \mathbf{q}, \mathbf{p}) - g_{21}(E, \mathbf{q}, \mathbf{p})] \\ S_z(\mathbf{p}, E) &= -\frac{1}{2\pi i} \int \frac{d\mathbf{q}}{(2\pi)^2} [\tilde{g}_{11}(E, \mathbf{q}, \mathbf{p}) - \tilde{g}_{22}(E, \mathbf{q}, \mathbf{p})] \\ \rho(\mathbf{p}, E) &= -\frac{1}{2\pi i} \int \frac{d\mathbf{q}}{(2\pi)^2} [\tilde{g}_{11}(E, \mathbf{q}, \mathbf{p}) + \tilde{g}_{22}(E, \mathbf{q}, \mathbf{p})] \end{aligned} \quad \left. \vphantom{\begin{aligned} S_x \\ S_y \\ S_z \\ \rho \end{aligned}} \right\} \text{Spin-polarised}$$

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

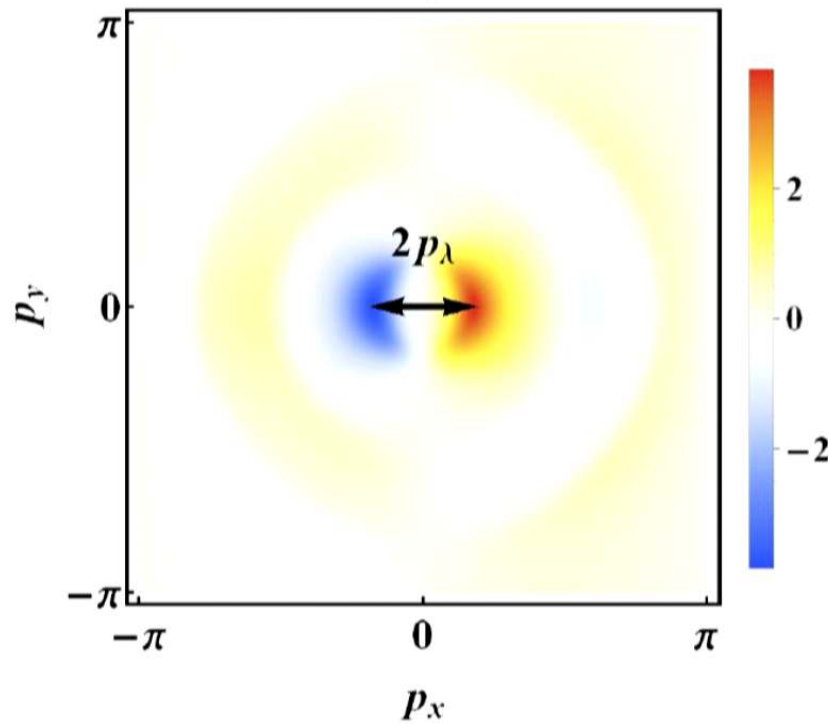
Spin-polarised local density of states



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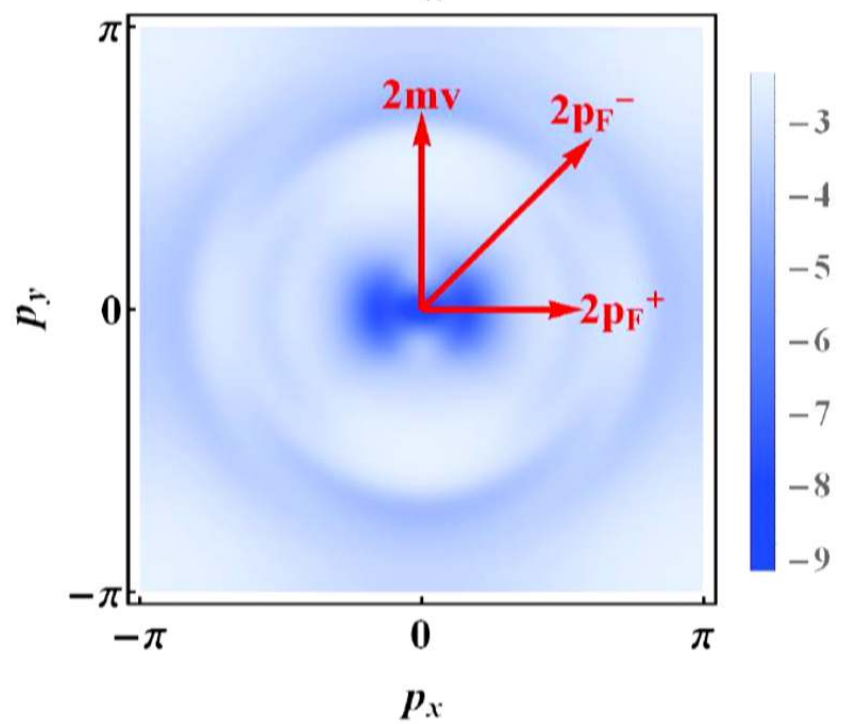
z-impurity

S_x



x-impurity

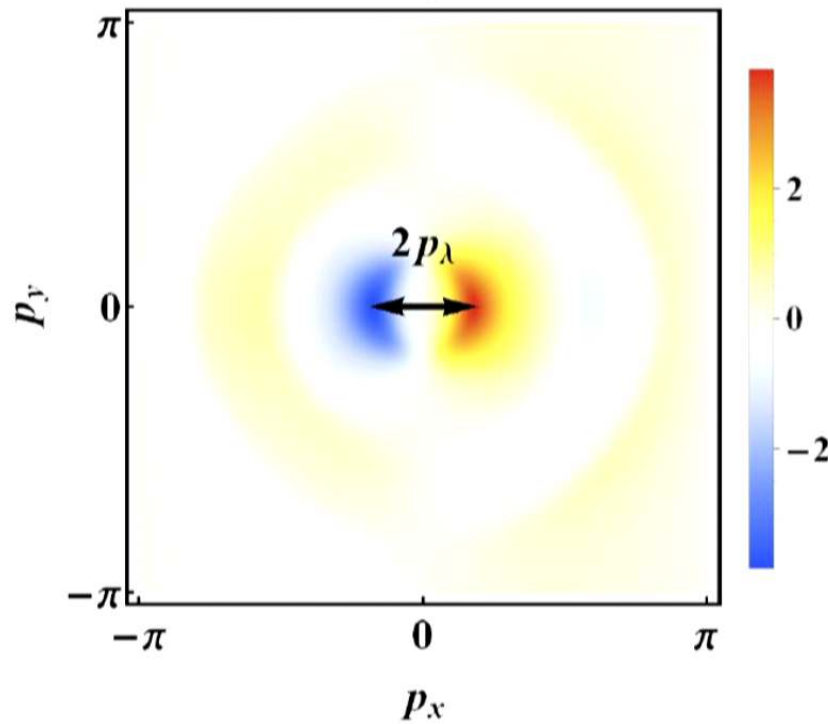
S_x



Spin-polarised local density of states

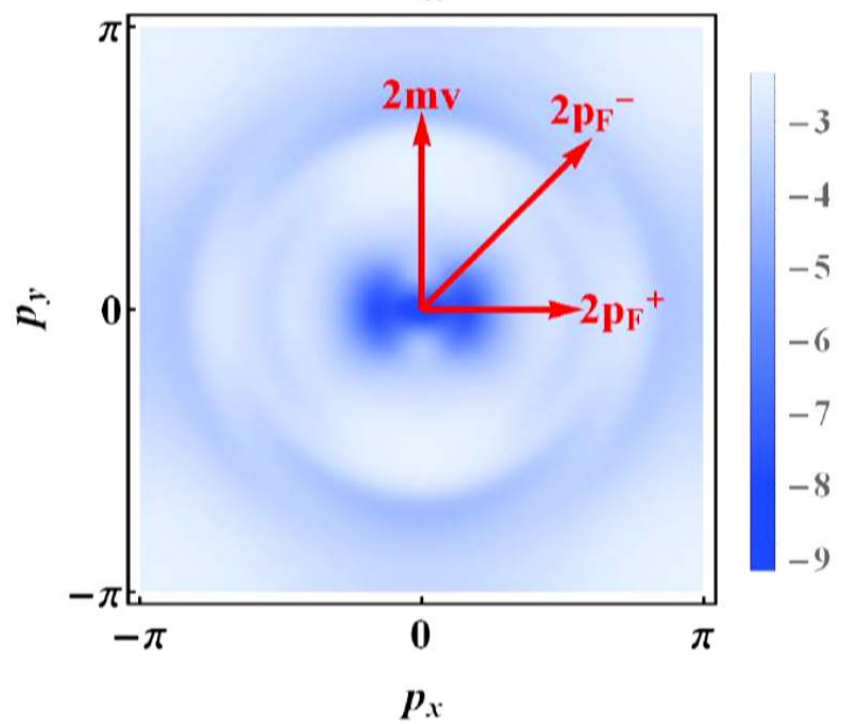
z-impurity

S_x

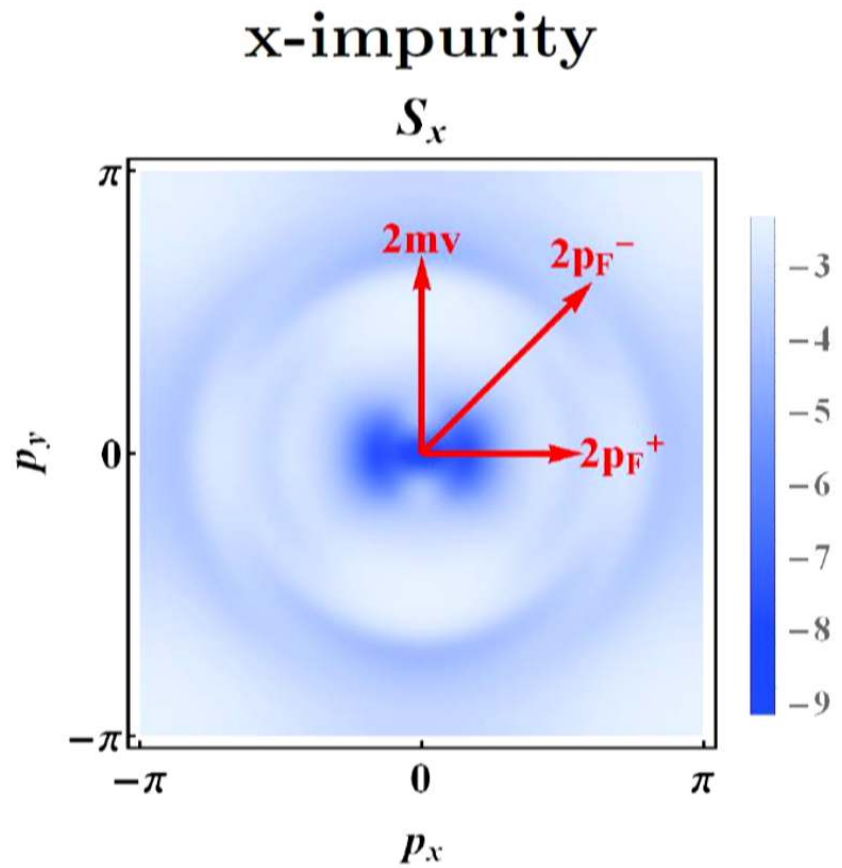
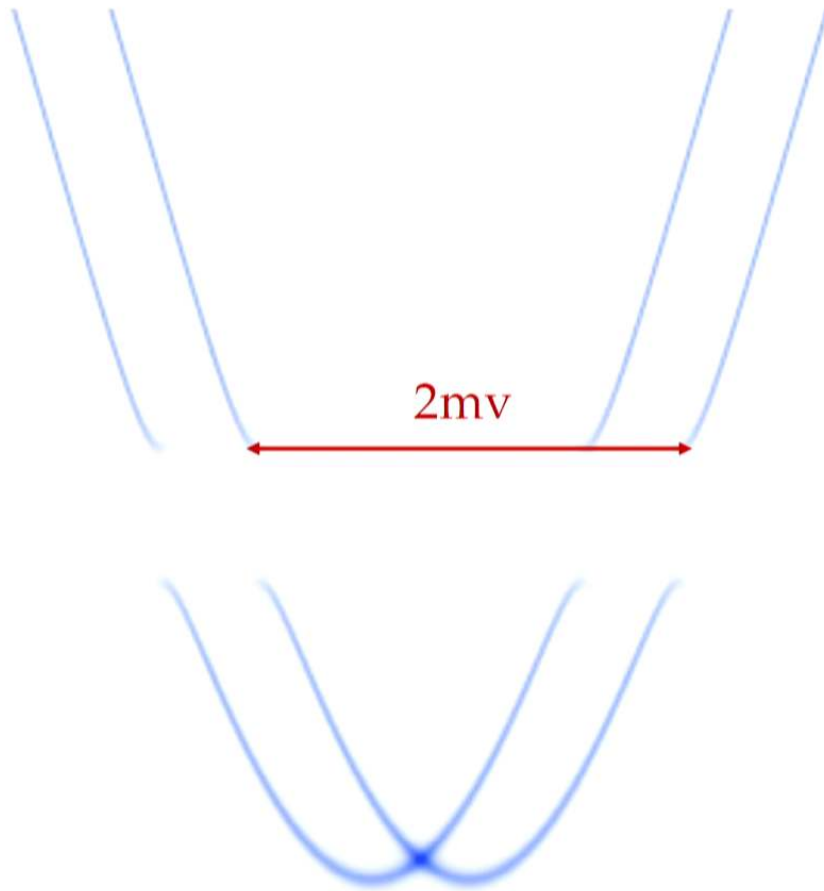


x-impurity

S_x



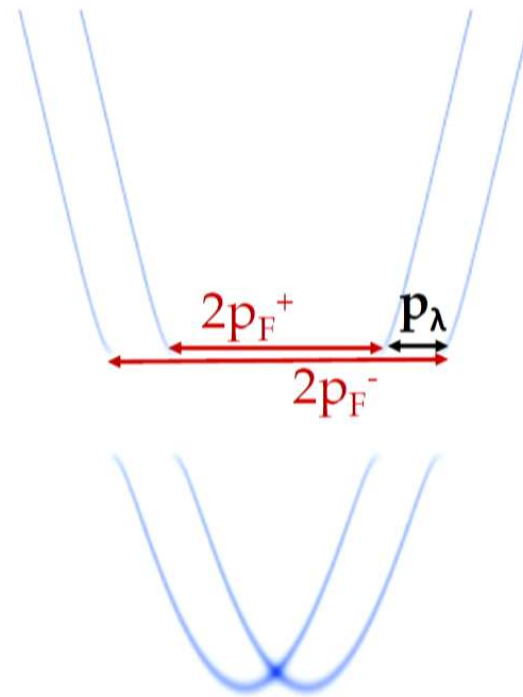
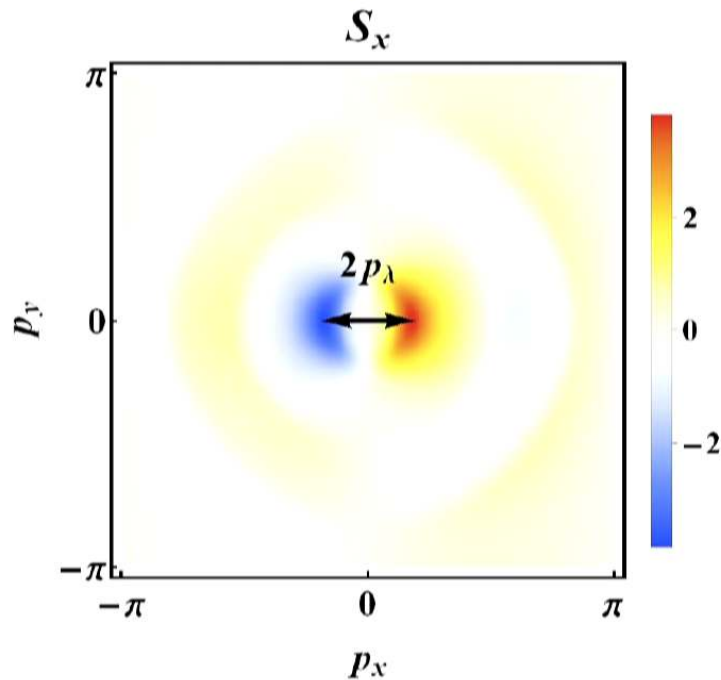
Spin-polarised LDOS: x-impurity



Spin-polarised LDOS: analytics

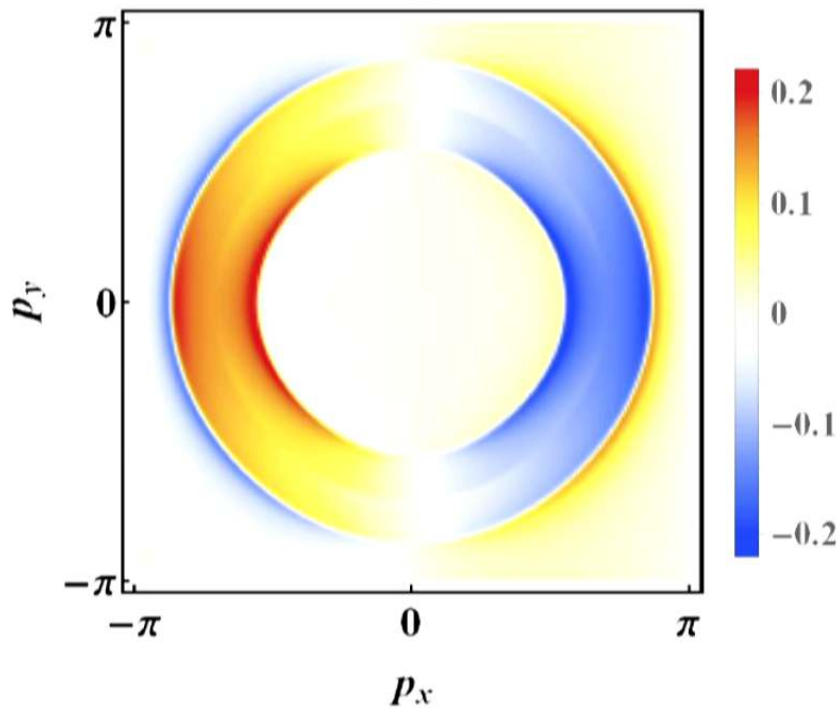
$$S_x(\mathbf{r}) = +J_z^2 \left(1 + \frac{1}{\alpha^2}\right) \frac{e^{-2p_s r}}{r} \cos \phi_r \times \left\{ \sum_{\sigma} \frac{\sigma v_{\sigma}^2}{p_F^{\sigma}} \cos(2p_F^{\sigma} r - \theta) + 2v^2 \frac{v_F^2}{v^2 p_F} \sin p_{\lambda} r \right\}$$

z-impurity

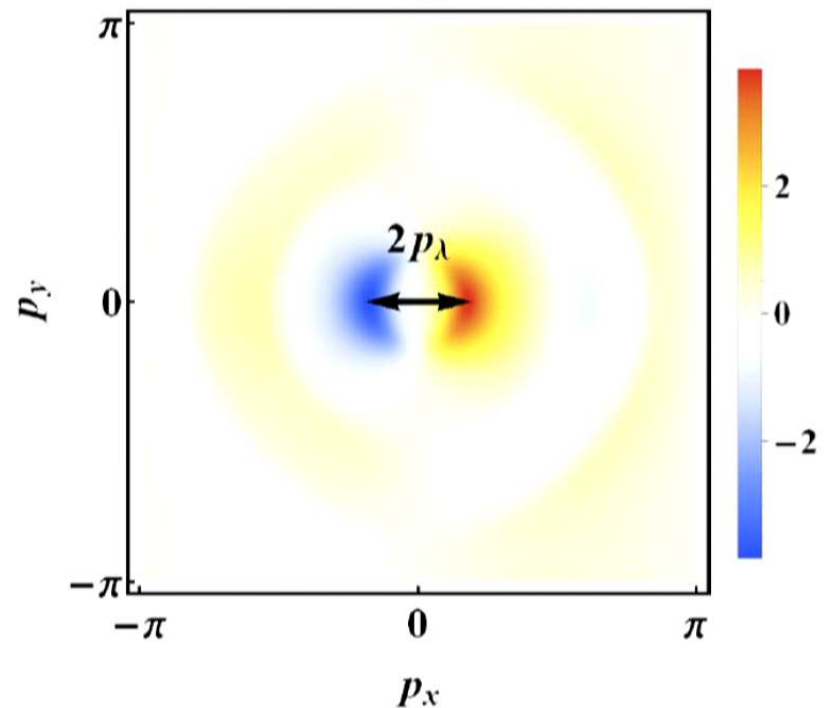


Comparison to the metallic phase

Metallic phase
z-impurity
 S_x

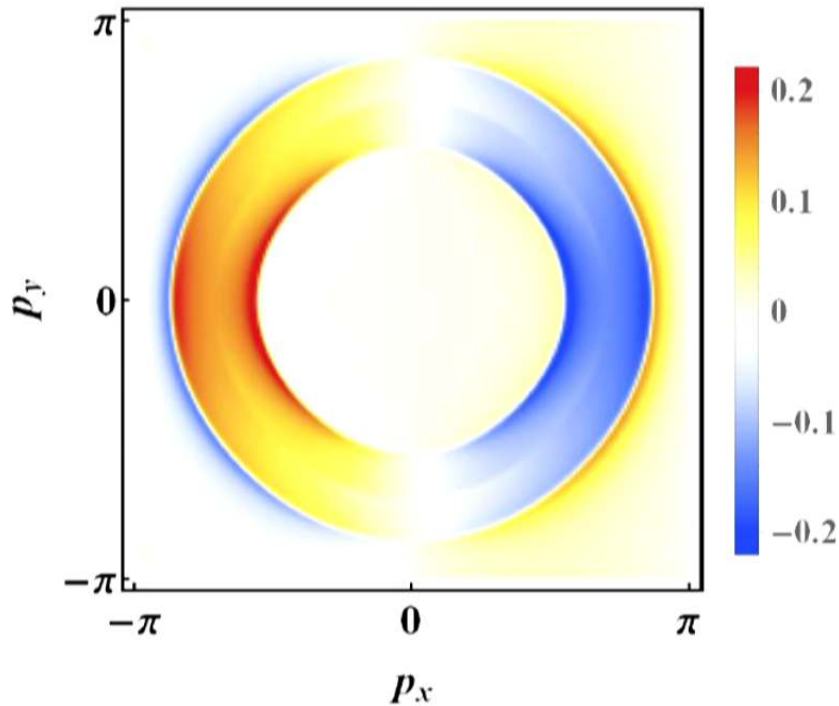


Superconducting phase
z-impurity
 S_x

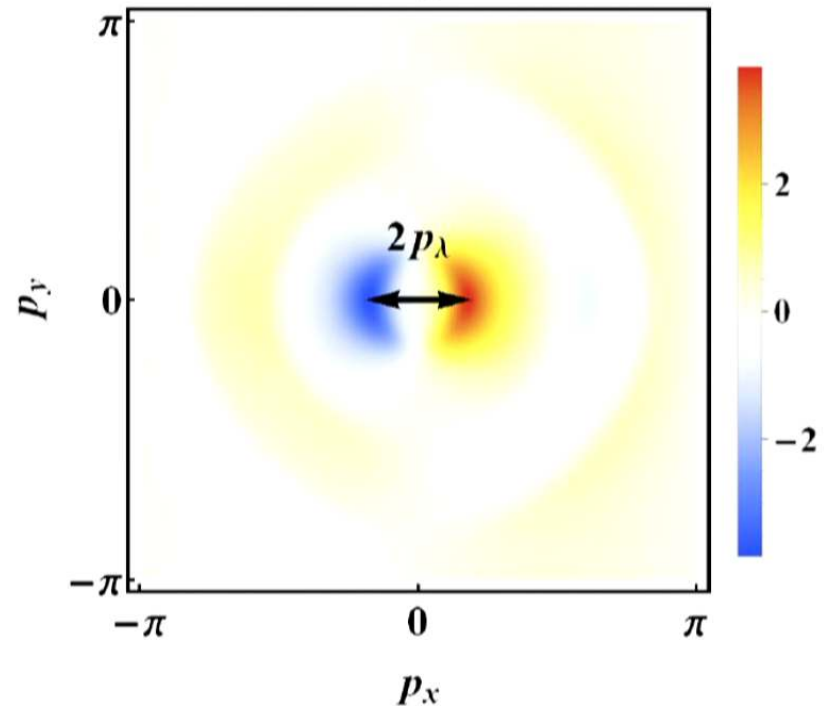


Comparison to the metallic phase

Metallic phase
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Superconducting phase
z-impurity
 S_x



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)