Zero-bias peak induced by a magnetic impurity in a conventional superconductor based on *first principles*

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Motivation

- Zero-bias peak (ZBP) was observed as a signature of Majorana zero mode in ferromagnetic Fe atomic chains on a superconducting substrate

  S. Nadj-Perge et al., Science **346**, 6209 (2014); R. Pawlak et al., npj Quantum Info. **2**, 16035 (2016); M. Ruby et al., PRL **115**, 197204 (2015)

- However, ZBP was not observed in Co chains on Pb

  M. Ruby et al., Nano Lett. **17**, 4473 (2017)

Methods

Fully relativistic SKKR-BdG solver including DFT band structure + SKKR impurity solver without supercell

G. Csire et al., Phys. Rev. B **91**, 165142 (2015); G. Csire et al., Phys. Rev. B **97,** 024514 (2018); B. Lazarovits et al., Phys. Rev. B **65**, 104441 (2012)

$$\mathcal{H}_{\mathrm{DBdG}} = \begin{pmatrix} \mathcal{H}_{\mathrm{D}} & \Delta_{\mathrm{eff}}(\mathbf{r},\mathbf{r}') \\ \Delta^*_{\mathrm{eff}}(\mathbf{r},\mathbf{r}') & -\mathcal{H}^*_{\mathrm{D}} \end{pmatrix}$$

$$V_{eff}(\mathrm{r}) = V_{ext}(\mathrm{r}) + \int \frac{\rho(\mathrm{r}')}{|\mathrm{r}-\mathrm{r}'|}d\mathrm{r}' + \frac{\delta \mathrm{E}_{xc}[\rho,\chi]}{\delta\rho(\mathrm{r})} \rightarrow \frac{\delta \mathrm{E}^0_{xc}[\rho]}{\delta\rho(\mathbf{r})}$$

$$\Delta^*_{eff}(\mathrm{r},\mathrm{r}') = \Delta^*_{ext}(\mathrm{r},\mathrm{r}') + \frac{\delta \mathrm{E}_{xc}[\rho,\chi]}{\delta\chi(\mathrm{r},\mathrm{r}')} \rightarrow \Lambda\chi(\mathbf{r})$$

Effective pairing potential

Suvasini, Temmerman & Győrffy, Phys. Rev. B **48** 1202 (1999)

Λ: electron-phonon coupling

χ(**r**): SC order parameter

Scattering path operator of impurity cluster to compute Green's function:

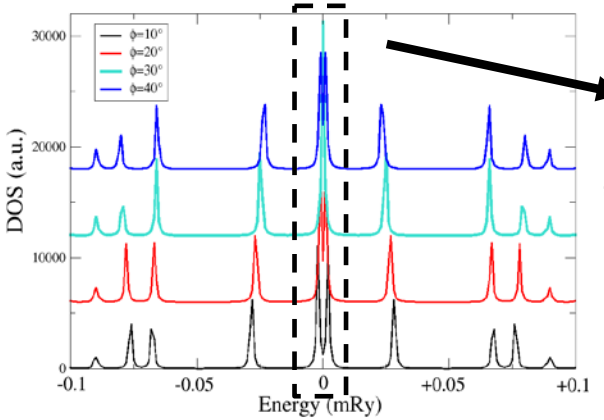
$$\boldsymbol{\tau}^{\mathrm{imp}}(\varepsilon) = \boldsymbol{\tau}^{\mathrm{host}}(\varepsilon)[\boldsymbol{I}_{N\times N} - \Delta\boldsymbol{t}^{-1}_{\mathrm{imp}}(\varepsilon)\boldsymbol{\tau}^{\mathrm{host}}(\varepsilon)]^{-1}$$

Local density of states of a Fe impurity on Pb: Yu-Shiba-Rusinov states

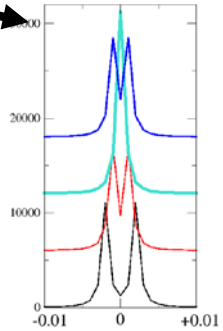
Fe magnetic moment: Rotation in **xy** plane Δ_{Pb} = 0.1 mRy (exp value)

$$\mathrm{LDOS}(\varepsilon) = -\frac{1}{\pi}\,\mathrm{Im\ Tr}\,G^{+}(\varepsilon)$$

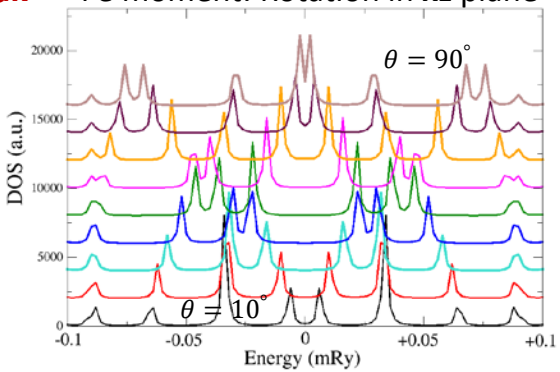
Yu, Acta Phys. Sin. (1965); Shiba, Prog. Th. Phys. (1968); Rusinov, JETP Lett. (1969)



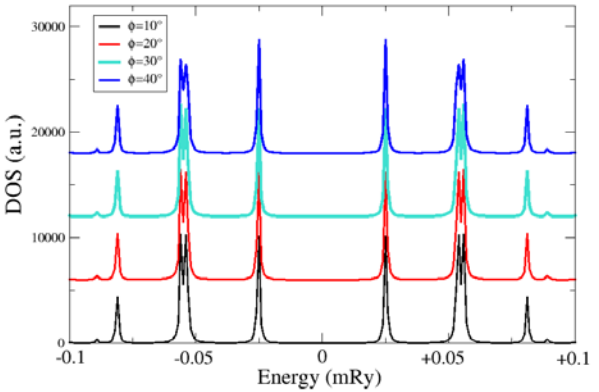
Zero-bias peak



Fe moment: Rotation in **xz** plane



Without spin-orbit coupling



Summary

- Sub-gap excitations induced by a Fe impurity on Pb are studied based on first principles using SKKR-BdG impurity solver.
- Yu-Shiba-Rusinov states appear within the Pb superconducting gap.
- With in-plane magnetic moment of the Fe impurity, a zero-bias peak (zero-energy excitation) is found. The origin of the zero-bias peak needs to be studied.

Computational support: XSEDE San Diego SC & VT ARC

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