Magnetic exchange interactions at proximity of a superconductor

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Abstract

Magnetic impurities coupled to superconductors give rise to a plethora of rich physics such as sub-gap states like Yu-Shiba-Rusinov states and Majorana zero modes, which constitute key mechanisms on the road towards a topological quantum computer. The interplay of spin-orbit coupling and (non-collinear) magnetism enrich the complexity and topological nature of the in-gap states hosted in proximity-induced super-conductors. However, little is known about the impact of superconductivity on the different contributions to the magnetic exchange interactions, like the bilinear isotropic exchange and the Dzyaloshinskii-Moriya interaction — and in turn the impact on the magnetic textures. In this work, we propose a method for the extraction of the tensor of exchange interactions in the superconducting regime as described in the framework of the Bogoliubov-de Gennes method. We propose Mn monolayers deposited on the Nb(110) surface as prototypical test systems based on our multi-orbital tight-binding code TITAN.

Tight-binding framework

TITAN

F. S. M. Guimarães et al., Sci. Rep. 7, 3686 (2017)
F. S. M. Guimarães et al., Phys. Rev. B 92, 220410(R) (2015)

TITAN is a powerful multi-orbital tight-binding software developed to investigate ground state, excitations and magnetic properties. We recently included a superconducting module, it's non-superconducting Hamiltonian is

$$H^{\mu\nu}_{ij,\sigma\eta} = H^{0\mu\nu}_{ij}\sigma^0 + \boldsymbol{\sigma}\cdot\hat{e}_i B^{[xc]\mu\nu}_i \delta_{ij} + \boldsymbol{\sigma}\cdot\mathbf{B}^{[soc]\mu\nu}_i \delta_{ij}$$

Were $\hat{e}_i$ is the direction of the magnetic moment at site i. The adequate parameters for the Hamiltonian can be obtained from first principles.

To render the Hamiltonian superconducting we added a BCS term and used a mean-field approximation

$$H^{MF}_S = \sum_{ij,\sigma\eta,\mu\nu} H^{\mu\nu}_{ij,\sigma\eta} c^\dagger_{i\mu\sigma} c_{j\nu\eta} - \sum_{ij,\mu}\left(\Delta^{\mu *}_{ij} c_{j\mu\downarrow} c_{i\mu\uparrow} + \Delta^{\mu}_{ij} c^\dagger_{i\mu\uparrow} c^\dagger_{j\mu\downarrow}\right)$$

Where the gap parameter is defined as

$$\Delta^{\mu}_{ij} = \lambda^{\mu\mu}_{ij}\langle c_{j\mu\downarrow} c_{i\mu\uparrow}\rangle, \quad \Delta^{\mu *}_{ij} = \lambda^{\mu\mu}_{ij}\langle c^\dagger_{i\mu\uparrow} c^\dagger_{j\mu\downarrow}\rangle$$

To diagonalize the Hamiltonian we perform a Bogoliuvob-Valatin transformation, from particle to particle-antiparticle space

$$c_{i\mu\sigma} = \sum_n{}' u^n_{i\sigma}\gamma_n + v^{n*}_{i\sigma}\gamma^\dagger_n, \quad c^\dagger_{i\mu\sigma} = \sum_n{}' u^{n*}_{i\sigma}\gamma^\dagger_n + v^n_{i\sigma}\gamma_n$$

This leads to the Bogoliubov-de Gennes (BdG) equations

$$\sum_{j\mu} H^{ij,\mu\nu}_{BdG}\phi_{j\mu} = E_n \phi_{i\nu}$$

The Hamiltonian in these equations is

$$H^{ij,\mu\nu}_{BdG} = \begin{pmatrix} H^{\mu\nu}_{ij,\uparrow\uparrow} - E_F & H^{\mu\nu}_{ij,\uparrow\downarrow} & 0 & -\Delta_{ij}\delta_{\mu\nu} \\ H^{\mu\nu}_{ij,\downarrow\uparrow} & H^{\mu\nu}_{ij,\downarrow\downarrow} - E_F & \Delta_{ji}\delta_{\mu\nu} & 0 \\ 0 & \Delta^*_{ij}\delta_{\mu\nu} & -H^{\mu\nu *}_{ij,\uparrow\uparrow} + E_F & -H^{\mu\nu *}_{ij,\uparrow\downarrow} \\ -\Delta^*_{ji}\delta_{\mu\nu} & 0 & -H^{\mu\nu *}_{ij,\downarrow\uparrow} & -H^{\mu\nu *}_{ij,\downarrow\downarrow} + E_F \end{pmatrix}$$

There is a inherent electron-hole block structure in this matrix that we can use for simplicity, namely

$$H^{ij,\mu\nu}_{BdG} = \begin{pmatrix} H^{ee} & H^{eh} \\ H^{he} & H^{hh} \end{pmatrix}$$

From here we can get the retarded Green function via

$$G_{BdG}(E + i\eta) = (E - H_{BdG} + i\eta)^{-1}$$

We also divide this matrix in blocks as with the BdG Hamiltonian

$$G_{BdG} = \begin{pmatrix} G^{ee} & G^{eh} \\ G^{he} & G^{hh} \end{pmatrix}$$

Magnetic exchanges in BdG

The Heisenberg model is commonly used in quantum mechanics to look at the properties of magnetic materials. The base is the Hamiltonian

$$E = -\frac{1}{2}\sum_{ij} \hat{e}_i \mathcal{J}_{ij} \hat{e}_j$$

Where $\mathcal{J}_{ij}$ is the tensor of magnetic exchanges. Which can be separated into isotropic, traceless anisotropic symmetric, and antisymmetric terms

$$E = -\frac{1}{2}\sum_{ij} J_{ij}\hat{e}_i\cdot\hat{e}_j - \frac{1}{2}\sum_{ij}\hat{e}_i\cdot J^s_{ij}\cdot\hat{e}_j - \frac{1}{2}\sum_{ij} D_{ij}\cdot(\hat{e}_i\times\hat{e}_j)$$

We can obtain $\mathcal{J}_{ij}$ via the infinitesimal rotations method*. Were we tilt the magnetic moments at two sites i and j, and we calculate the energy change derived from it. This is represented by

$$\mathcal{J}_{ij} = \frac{\partial^2 E}{\partial\hat{e}_i\partial\hat{e}_j}$$

The same idea applied with Green functions yields the equation

$$\partial^2 E = -\frac{1}{2\pi}\mathrm{Im\ Tr}\int_{-\infty}^{E_F} d\epsilon\,\delta V_i G_{ij}(\epsilon)\delta V_j G_{ji}(\epsilon)$$

For our case, with the BdG Hamiltonian and the infinitesimal rotations method we obtain

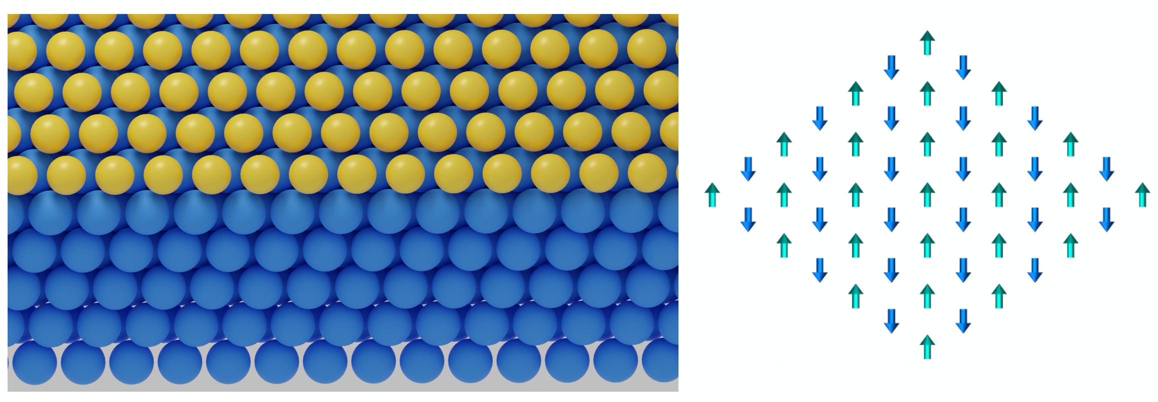
$$\partial^2 E_{ij} = -\frac{1}{2\pi}\mathrm{ImTr}_{Ls}\int_{-\infty}^{\epsilon_F} d\epsilon\,\left[\delta V^e_i G^{ee}_{ij}(\epsilon)\delta V^e_j G^{ee}_{ji}(\epsilon) + \delta V^e_i G^{eh}_{ij}(\epsilon)\delta V^h_j G^{he}_{ji}(\epsilon)\right]$$

For the non-superconducting case we recover the original equation.

* A.I. Liechtenstein et al., J. Magn. Magn. Mater., 67 (1), 65-74 (1987)

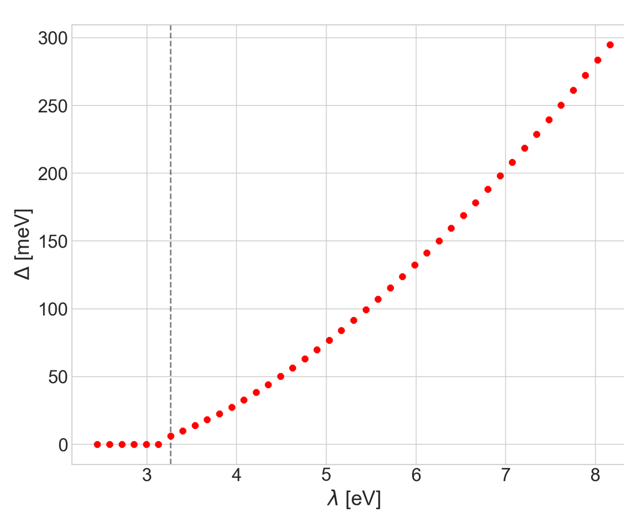
Superconducting gap parameter

We chose to explore a system of a 5-atom superconducting Nb (110) slab with a magnetic monolayer of Mn (110) on top. This system has been studied recently and its magnetic ground state found to be row-wise antiferromagnetic*.



For clean Nb (110) surfaces the superconducting gap from experiments is [Δ] $\Delta = 1.53$ meV at $T = 1.3$ K. In ab-initio calculations the values of $\lambda^{\mu\mu}_{ij}$ used to match the experimental Δ go from 1.11 eV[†] to 1.17 eV[æ].

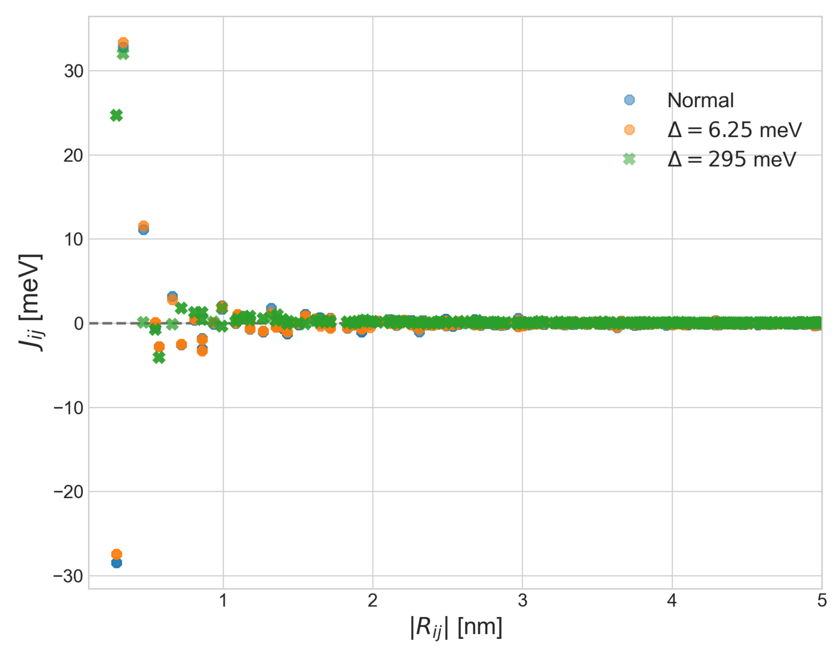
Since $\lambda^{\mu\mu}_{ij}$ is directly related to the magnitude of Δ we took a grid with several values of $\lambda^{\mu\mu}_{ij}$ to obtain superconducting gaps of different sizes, which would allow us to asses the impact of the superconducting state on the magnetic exchange interactions.



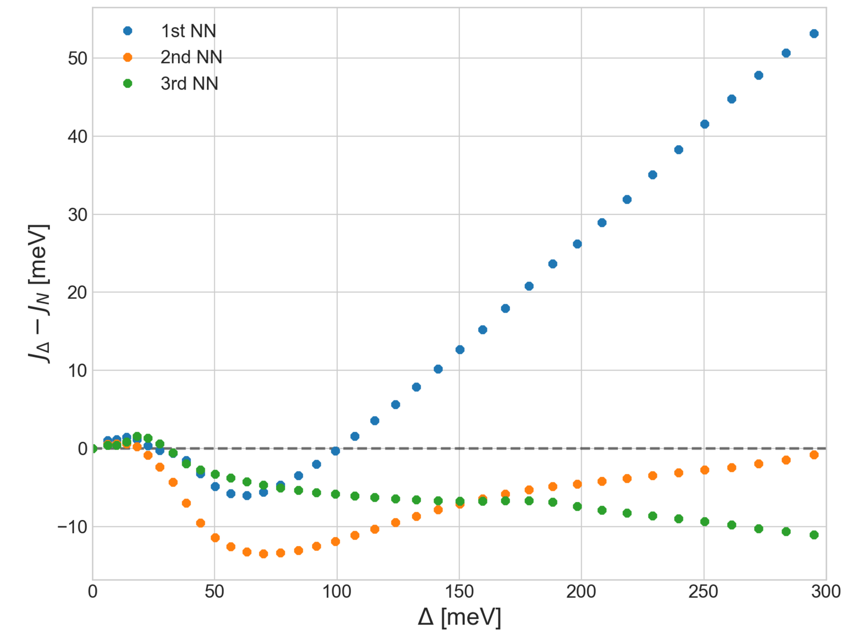
* R. Lo Conte et al, Phys. Rev. B 105, L100406 (2022)
Δ A. B. Odobesko et al. Phys. Rev. B 99, 115437 (2019)
† P. Rüßmann and S. Blügel, Phys. Rev. B 105, 125143 (2022)
æ T. G. Saunderson et al., Phys. Rev. B 101, 064510 (2020)

Impact on the magnetic state

When we check the isotropic part of the tensor of magnetic exchanges for the normal against the superconducting regime with the lowest gap parameter ($\Delta = 6.25$ meV), we notice minimal changes. However the magnetic ground state stays the same; namely, row-wise antiferromagnetic. For large values (e.g. $\Delta = 295$ meV) the ground state changes to a ferromagnetic alignment



We can see this clearly when we analyse the behaviour of the isotropic part of $\mathcal{J}_{ij}$ for the first three nearest-neighbours



Conclusions

TITAN successfully simulates multi-orbital superconducting systems with realistic superconducting gaps, coming from realistic parameters. We recover the experimental magnetic ground state and show that there is a phase transition from antiferro- to ferromagnetic alignment when the size of the superconducting gap increases.

Outlook

TITAN provides already the possibility of calculating dynamical magnetic responses in the non-superconducting regime. In the future we will extend this capabilities to conduct investigations of these quantities on superconductors interfaced with magnetic materials. Another future direction in our sight heads towards investigations on magnetic nanostructures (chains, islands, skyrmions) and superconductors with realistic superconducting gaps. We will analyse the mutual impact of superconductivity and magnetism.

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