Materials for quantum computing : Magnetic impurities embedded in superconductors from first principles

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Introduction

Due to the physical limits of classical processor architectures, future progress in scientific computing is expected to come from the realization of **quantum computers**, that requires to overcome challenges of decoherence and dephasing of the qubits. Materials that combine **magnetism**, **spin-orbit** interaction and conventional s-wave **superconductivity** are a suitable platform to study Majorana zero modes (MZM) [1], that can be used as building blocks for fault-tolerant topological qubits. In general, magnetic impurities in superconductors lead to localized **Yu-Shiba-Rusinov** (YSR) states bound to the impurities [2]. Understanding their interplay with MZMs is crucial to achieve topological quantum computers in the future.

In our work, we implemented the **Bogoliubov-de Gennes** (BdG) formalism in the **juKKR** Korringa-Kohn-Rostoker Green function impurity code [3] to allow material-specific description of defects perfectly embedded in superconductors from first principles. We apply it to magnetic **transition metal adatoms** placed on a superconducting Nb(110) surface to observe the emergence of YSR states, and discuss the influence of the impurity-substrate distance on the energy of the YSR states.

The KKR-BdG Method

The Korringa-Kohn-Rostoker (KKR) method

- In the KKR method, we define the Green's function as the resolvent of the Hamiltonian, which can be formulated as [4] :

$$\mathcal{G}(\boldsymbol{r}+\boldsymbol{R}^n,\boldsymbol{r}'+\boldsymbol{R}^{n'};E)=\underbrace{\delta_{nn'}\sqrt{E}\sum_L H_L^n(\boldsymbol{r}_>;E)R_L^n(\boldsymbol{r}_<;E)}_{\text{single site}}+\underbrace{\sum_{LL'}R_L^n(\boldsymbol{r};E)G_{LL'}^{nn'}(E)R_{L'}^{n'}(\boldsymbol{r}';E)}_{\text{multiple scattering}}$$

Structure constants

The Bogoliubov-de Gennes (BdG) formalism

- Superconductivity can be described using the BdG equations. These can be formulated in the effective single particle picture of density functional theory [5]:

$$H_{\mathrm{BdG}}=\begin{pmatrix}-\nabla^2-E_{\mathrm{F}}+V^{\mathrm{eff}}(\vec{x}) & \Delta^{\mathrm{eff}}(\vec{x})\\ \Delta^{\mathrm{eff}\,*}(\vec{x}) & \nabla^2+E_{\mathrm{F}}-V^{\mathrm{eff}\,*}(\vec{x})\end{pmatrix}$$

- The normal and anomalous densities $\rho(\vec{x})$ and $\chi(\vec{x})$ can be calculated from the correspoding Green's function :

$$\rho(\vec{x})=-\frac{1}{\pi}\int_{-\infty}^{\infty}d\epsilon f(\epsilon)\sum_L Im[G_{LL}^{ee}(\epsilon,\vec{x},\vec{x}')]-\frac{1}{\pi}\int_{-\infty}^{\infty}d\epsilon[1-f(\epsilon)]\sum_L Im[G_{LL}^{hh}(\epsilon,\vec{x},\vec{x}')]$$
$$\chi(\vec{x})=-\frac{1}{4\pi}\int_{-\infty}^{\infty}d\epsilon[1-2f(\epsilon)]\sum_L Im[G_{LL}^{eh}(\epsilon,\vec{x},\vec{x}')]-\frac{1}{4\pi}\int_{-\infty}^{\infty}d\epsilon[1-2f(\epsilon)]\sum_L Im[G_{LL}^{he}(\epsilon,\vec{x},\vec{x}')]$$

- The potentials are then defined as :

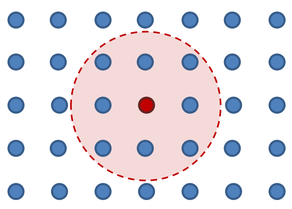
$$V^{\mathrm{eff}}(\vec{x})=V^{\mathrm{ext}}(\vec{x})+\int\frac{\rho(\vec{x'})}{|\vec{x}-\vec{x'}|}\mathrm{d}^3x'+\frac{\delta E_{\mathrm{xc}}^0[\rho]}{\delta\rho(\vec{x})}$$

$$\Delta^{\mathrm{eff}}(\vec{x})=\underbrace{\lambda}_{\text{Coupling matrix}}\cdot\underbrace{\chi(\vec{x})}_{\text{Superconducting order parameter}}$$

Impurities within the KKR-Green function method

- The Green's function $\mathcal{G}$ of a perturbed system which Hamiltonian is $\mathcal{H}=\mathcal{H}_0+\Delta\mathcal{V}$ can be obtained from the Green's function $\mathcal{G}_0$ of the unperturbed system through the Dyson equation [4] :

$$\mathcal{G}_{LL'}^{nn'}(E)=\mathcal{G}_{LL'}^{0,nn'}(E)+\sum_{n''L''}\mathcal{G}_{LL''}^{0,nn''}\Delta t_{L''}^{n''}\mathcal{G}_{L''L'}^{n''n'}$$



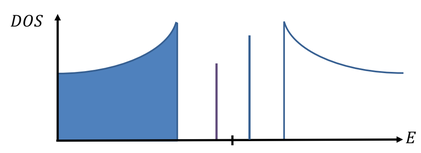
Due to the screening from the electrons of neighbouring atoms, The new Green's function only has to be calculated in a small area around the imputity.

YSR states

YSR states formation

- Magnetic impurities embedded in a superconductor provides a scattering potential that locally breaks the Cooper pairs :

- This give rise to sharp peaks in the superconducting gap of opposite spin and energy :

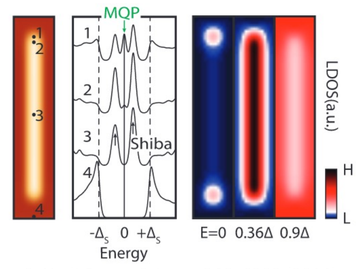


In the single band model, the energy of the YSR states is given by [2] :

$$\varepsilon_b=\pm\Delta\frac{1-(\pi\nu_0JS)^2}{1+(\pi\nu_0JS)^2}$$

From YSR states to Majorana Zero Modes

- Interacting YSR states can lead to Majorana Zero Modes, by engineering specific structures such as magnetic atoms chain on superconducting surface



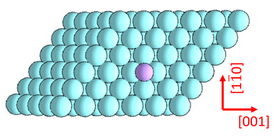
S. Nadj-Perge, Science **346,** 6209 (2014)

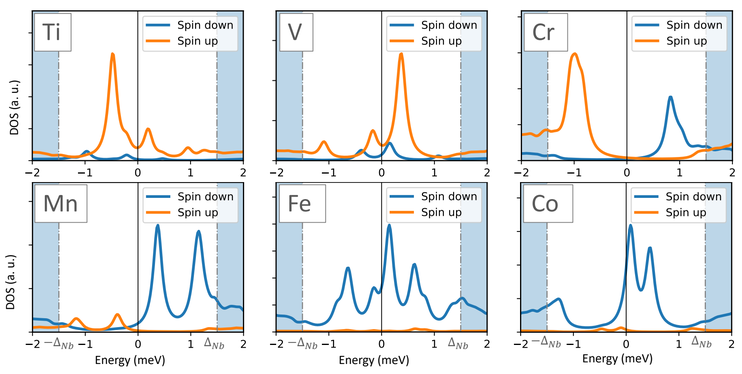
At some given chain length, the quasiparticle interferences trapped inside the chain create a zero bias peak located at the chain's ends. This state is topologically protected by the superconducting gap, providing robustness suitable for creating fault-tolerant qubits.

Results

- **DOS of single 3d adatoms on a Nb(110) surface :**

21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn



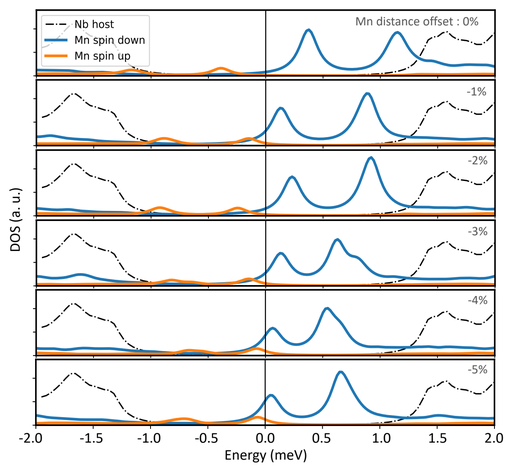


Specific YSR states patterns arise from the different magnetic impurities, depending on the orbital's interactions with the Nb crystal field.

A switch of majority spin channel is observed at half filling of the d shell.

- **DOS of single Mn adatom at different distances from Nb(110) surface :**

The closer the Mn adatom gets to the surface, the smaller the energy of the YSR states, due to the weakening of the adatom's magnetic moment. The relaxation of the adatom on the SC surface is crucial to get accurate YSR states energies.



Outlook :

- Apply to 4f-elements
- Apply to dimers/chains/nanostructures

References

[1] Nadj-Perge et al., Science **346**, 6209 (2014).
[2] L. Yu, Acta Physica Sinica **21**, 75 (1965); H. Shiba, Prog. Theor. Phys. **40**, 435 (1968); A. I. Rusinov, Sov. J. Exp. Theor. Phys. **29**, 1101 (1969).
[3] https://iffgit.fz-juelich.de/kkr/jukkr
[4] N. Papanikolaou, R. Zeller and P.H. Dederichs, J. Phys. : Condens. Matter **14,** 2799-2823 (2002)
[5] G. Csire, B. Újfalussy, J. Cserti, and B. Győrffy, Phys. Rev. B **91**, 165142 (2015)

Acknowledgements

This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – Cluster of Excellence Matter and Light for Quantum Computing (ML4Q) EXC 2004/1 – 390534769. Computing time was granted by the JARA Vergabegremium and provided on the JARA Partition part of the supercomputer CLAIX at RWTH Aachen University (project "jara0191").