Theory of Electron Spin Resonance in Scanning Tunneling Microscopy

Tutor: Juan Carlos Cuevas
Departamento de Física Teórica de la Materia Condensada (juancarlos.cuevas@uam.es)

Electron spin resonance (ESR), also known as electron paramagnetic resonance (EPR), and nuclear magnetic resonance (NMR) are two broadly used characterization and imaging techniques, employed from medical and bio applications to chemical characterization of paramagnetic complexes [1]. Recently, in an important breakthrough in Nanoscience, it has been demonstrated that it is possible to combine ESR spectroscopy with scanning tunneling microscopy (STM) [2-5]. With this combination it is now possible to investigate atomic-scale magnetic systems with an unprecedented energy resolution (nano-eV scale). However, while numerous experimental groups have succeeded in implementing this STM-ESR technique, the physical mechanism behind it is still under debate [6]. The goal of this master thesis project is to develop a complete and consistent theory of electron spin resonance spectroscopy in the context of STM experiments probing single magnetic impurities on surfaces.

For this purpose, the master student will learn and apply a variety of theoretical techniques ranging from nonequilibrium Green's function techniques to describe the electronic transport in STM experiments, to master equations to describe the dynamics (including relaxation and decoherence) of atomic-scale systems under a microwave drive. This theory project will be carried out in close collaboration with one of the leading experimental groups in the field, namely with group of "Atomic-scale Phenomena" led by Christian Ast in the Max Planck Institute for Solid State Research in Stuttgart (Germany).

[1] A. Abragam, B. Bleaney, *Electron Paramagnetic Resonance of Transition Ions*, Oxford University Press, Oxford, 1970.
[2] S. Baumann, W. Paul, T. Choi, C.P. Lutz, A. Ardavan, A.J. Heinrich, *Electron paramagnetic resonance of individual atoms on a surface*, Science **350**, 417-420 (2015).
[3] F.D. Natterer, K. Yang, W. Paul, P. Willke, T. Choi, T. Greber, A.J. Heinrich, C.P. Lutz, *Reading and writing single-atom magnets*, Nature **543**, 226-228 (2017).
[4] T. Choi, W. Paul, S. Rolf-Pissarczyk, A.J. Macdonald, F.D. Natterer, K. Yang, P. Willke, C.P. Lutz, A.J. Heinrich, *Atomic-scale sensing of the magnetic dipolar field from single atoms*, Nature Nanotechnology **12**, 420-424 (2017).
[5] K. Yang, W. Paul, S.-H. Phark, P. Willke, Y. Bae, T. Choi, T. Esat, A. Ardavan, A.J. Heinrich, C.P. Lutz, *Coherent spin manipulation of individual atoms on a surface*, Science **366**, 509-512 (2019).
[6] F. Delgado and N. Lorente, *A theoretical review on the single-impurity electron spin resonance on surfaces*, Progress in Surface Science **96**, 100625 (2021).

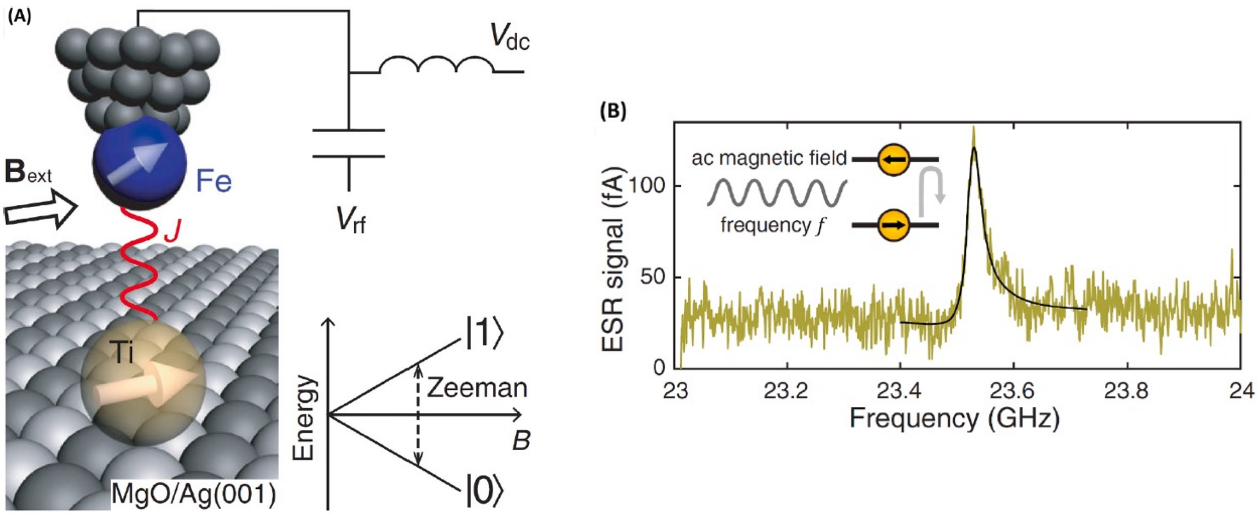

Figure 1: (A) Experimental setup of the STM-ESR. (B) Example of an ESR spectrum. Adapted from Ref. [6].