Electronic structure and inelastic transport through a single magnetic adatom

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Recent works [1-7] show that inelastic electron scanning tunnelling microscope (STM) probes the elementary spin excitations of a single and a few magnetic atoms in a thin insulating layer as well as the interactions between spins in individual atomic-scale magnetic structures. The experimental data have been successfully explained in terms of a phenomenological model in which both, the tunnel process and the electronic structure of the magnetic atom, are described with spin operators [8]. Here we provide a microscopic understanding of these phenomenological spin-models. This is done in two steps.

We study the energy spectra of a magnetic atom embedded in an insulating layer. Configuration interaction (CI) method is used as a computational tool to study the system. In our approach, only electrons belonging to the incomplete d-shell of the magnetic ion (Mn^{2+}, Fe^{2+}), are considered. Effects of the surrounding atoms are accounted for by a point charge model, which permits to simulate different environments and strengths of this interaction. The model also includes Coulomb repulsion and spin orbit coupling. The combination of spin orbit and crystal field is crucial to derive the single ion magnetic anisotropy observed experimentally. The spectra of the magnetic atoms as a function of the intensity and direction of the magnetic field compare well with the simpler phenomenological single ion spin models.

Within this approach, inelastic spin assisted transport is described with a generalized Anderson model, while current is calculated up to second order in the tunnelling Hamiltonian (cotunnelling) [9]. For that matter, we derive an effective cotunnelling Hamiltonian using degenerate second order perturbation theory. This permits us to derive an expression for the inelastic current based upon a theory without effective spins. Thus, our theory provides a complete microscopic understanding of the origin of the spin assisted tunnelling spectroscopy.

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Fig. 1 Schematic upper view of a CuN surface. The magnetic ion forming the last contact point of the STM tip (green circles) is positioned over a Cu atom (yellow circles).

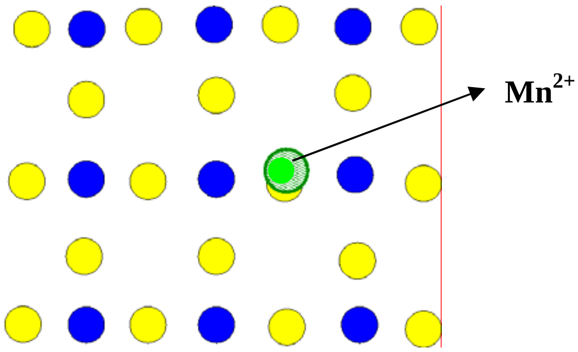

Fig. 2 Typical low energy spectrum of the Mn^{2+} ion in a tetragonal environment. Magnetic field is applied along the long axis (z-axis). Symbols correspond to the energy spectrum obtained with the spin model with vales fitted to the CI calculation at B=0.