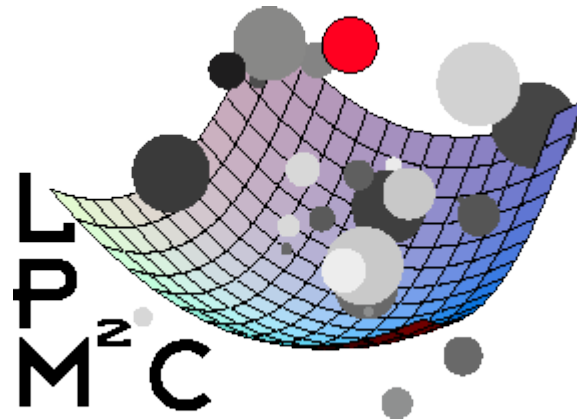


From single impurity to Kondo clusters: Determining the spin exchange interaction by STM

Pascal SIMON

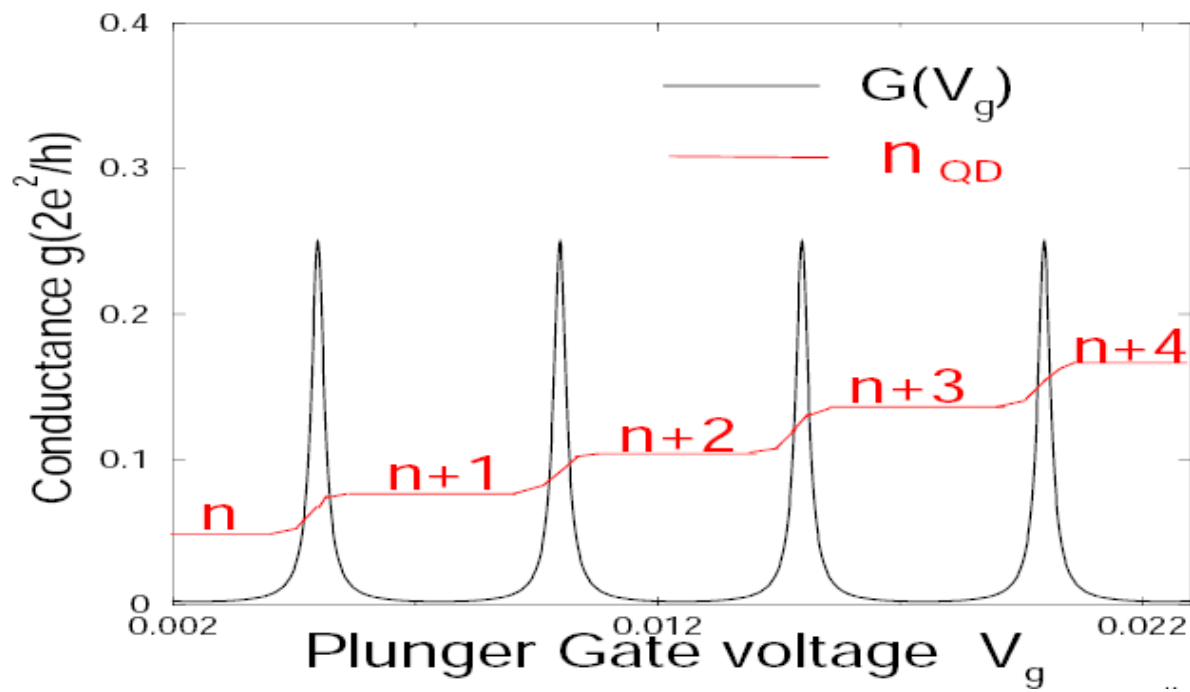
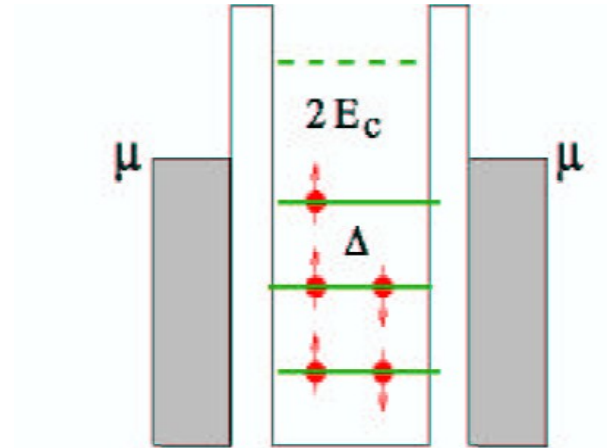
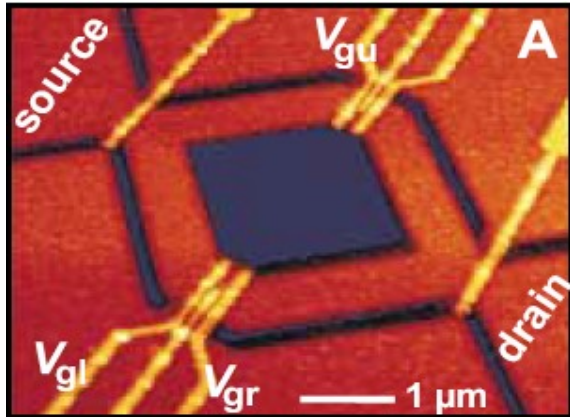


OUTLINE

- I. SPECTROSCOPY OF SINGLE MAGNETIC IMPURITIES
- II. SPECTROSCOPY OF TWO IMPURITIES SYSTEMS
- III. TOWARD KONDO CLUSTERS
- IV. CONCLUSION

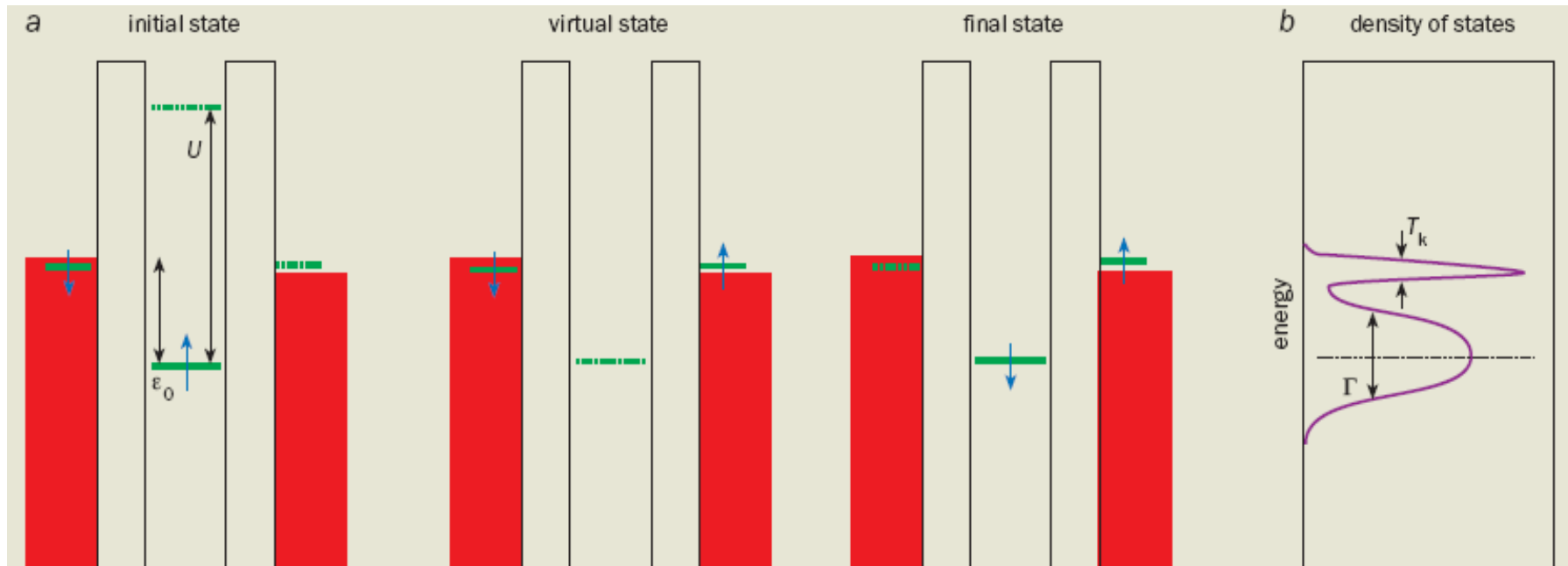
I. Spectroscopy of single magnetic impurities

Quantum dots

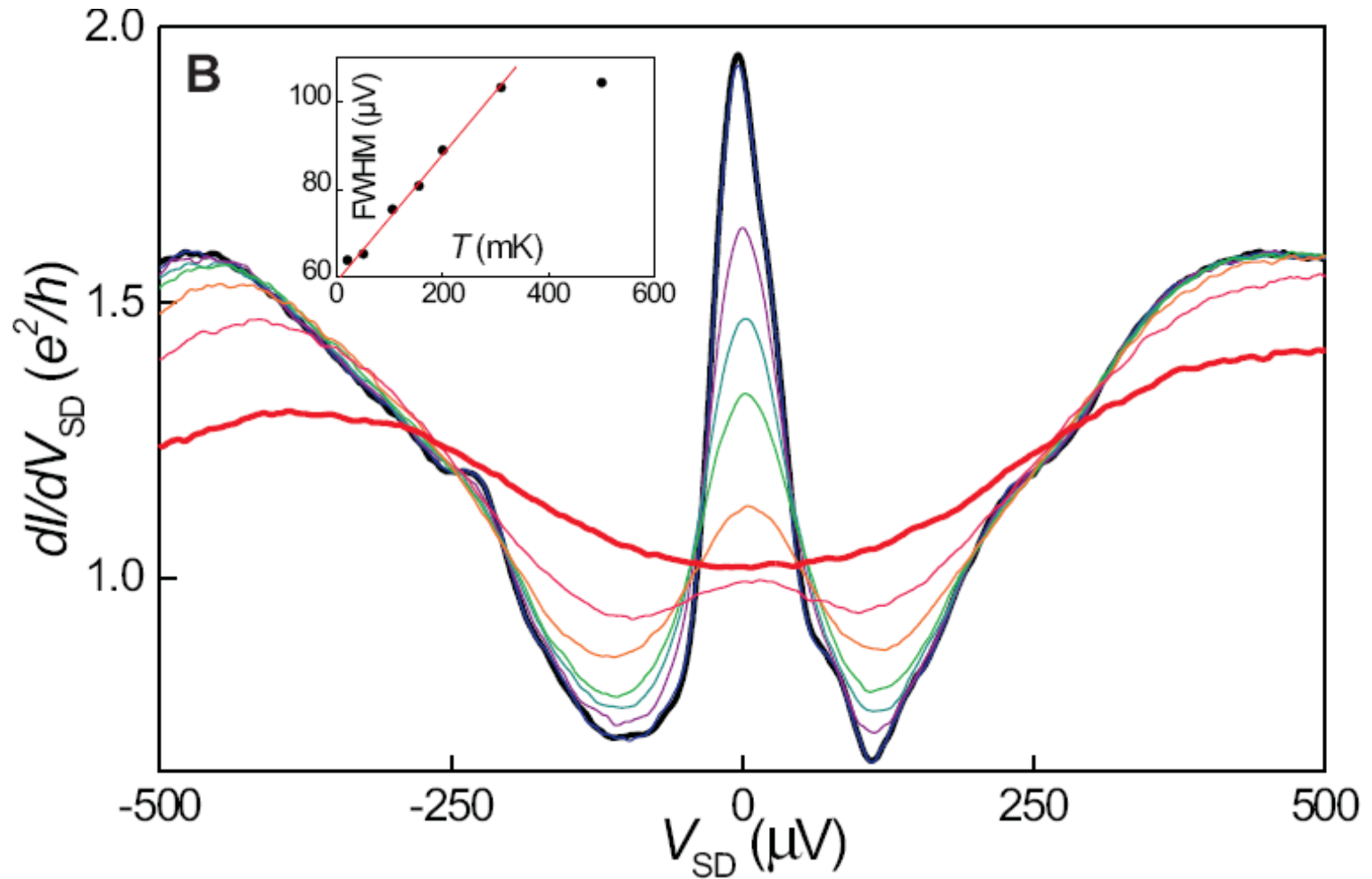


Kondo effect in quantum dots

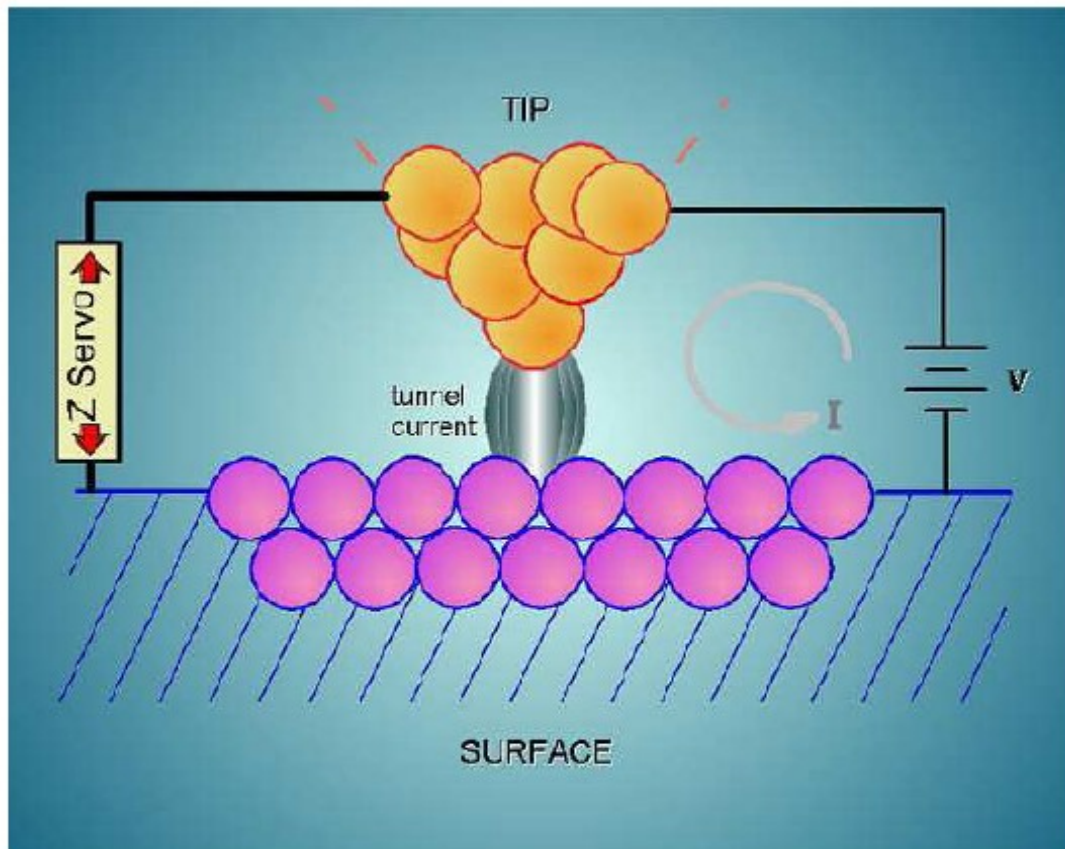
Cotunneling regime: Virtual charge fluctuations



Spectroscopic analysis of the Kondo resonance

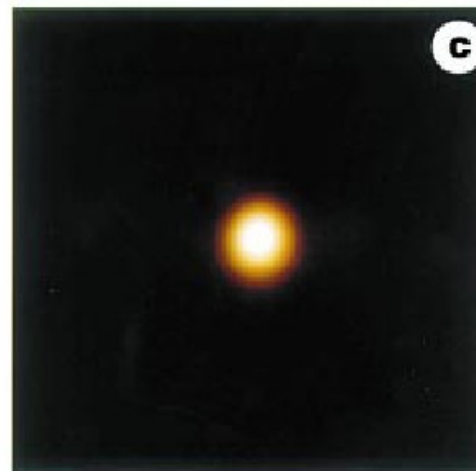
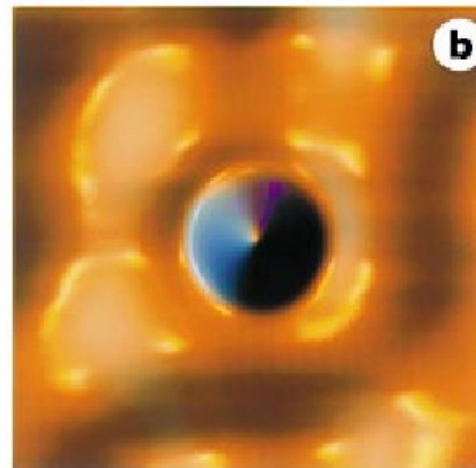
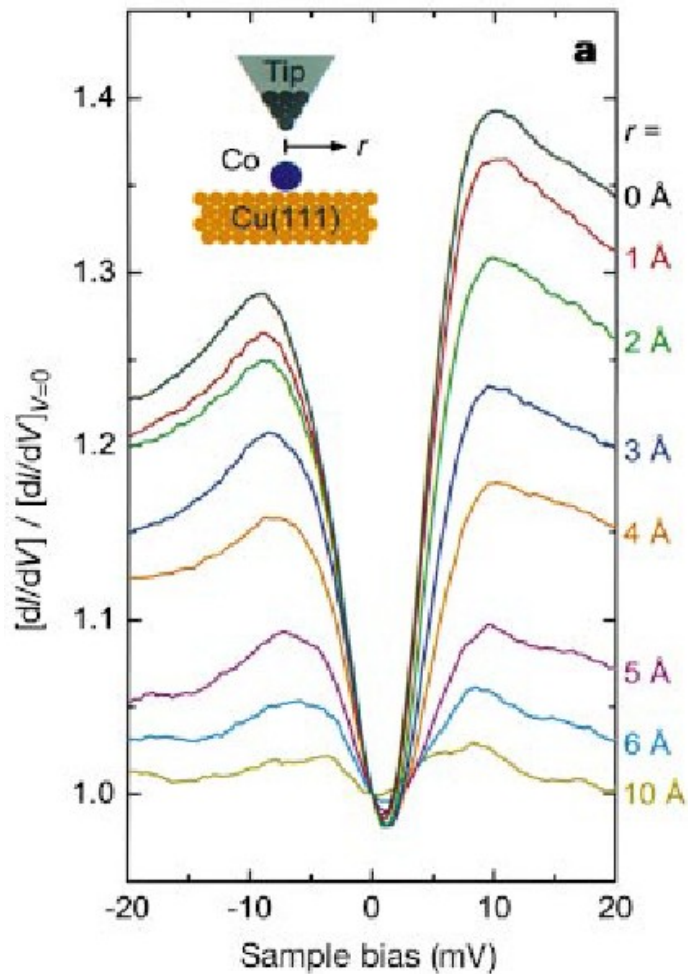


STM Principle

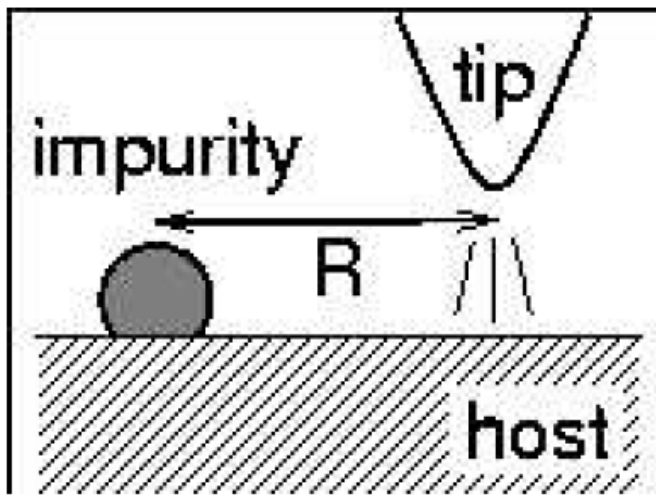


$$dI/dV \propto \rho_s(E_F + eV)$$

Spectrum around a magnetic impurity



Spectroscopic analysis



$$\Delta\rho_R(\epsilon) = \frac{1}{\pi} \text{Im} \delta G_R(\epsilon - i0^+)$$

where

$$\delta G_R(\epsilon) = G_{R,0}^{(0)}(\epsilon) t(\epsilon) G_{0,R}^{(0)}(\epsilon)$$

$t(\epsilon) = V^2 G_d(\epsilon)$ is the impurity T-matrix and $G_{R,0}^{(0)}$ the bare propagator.

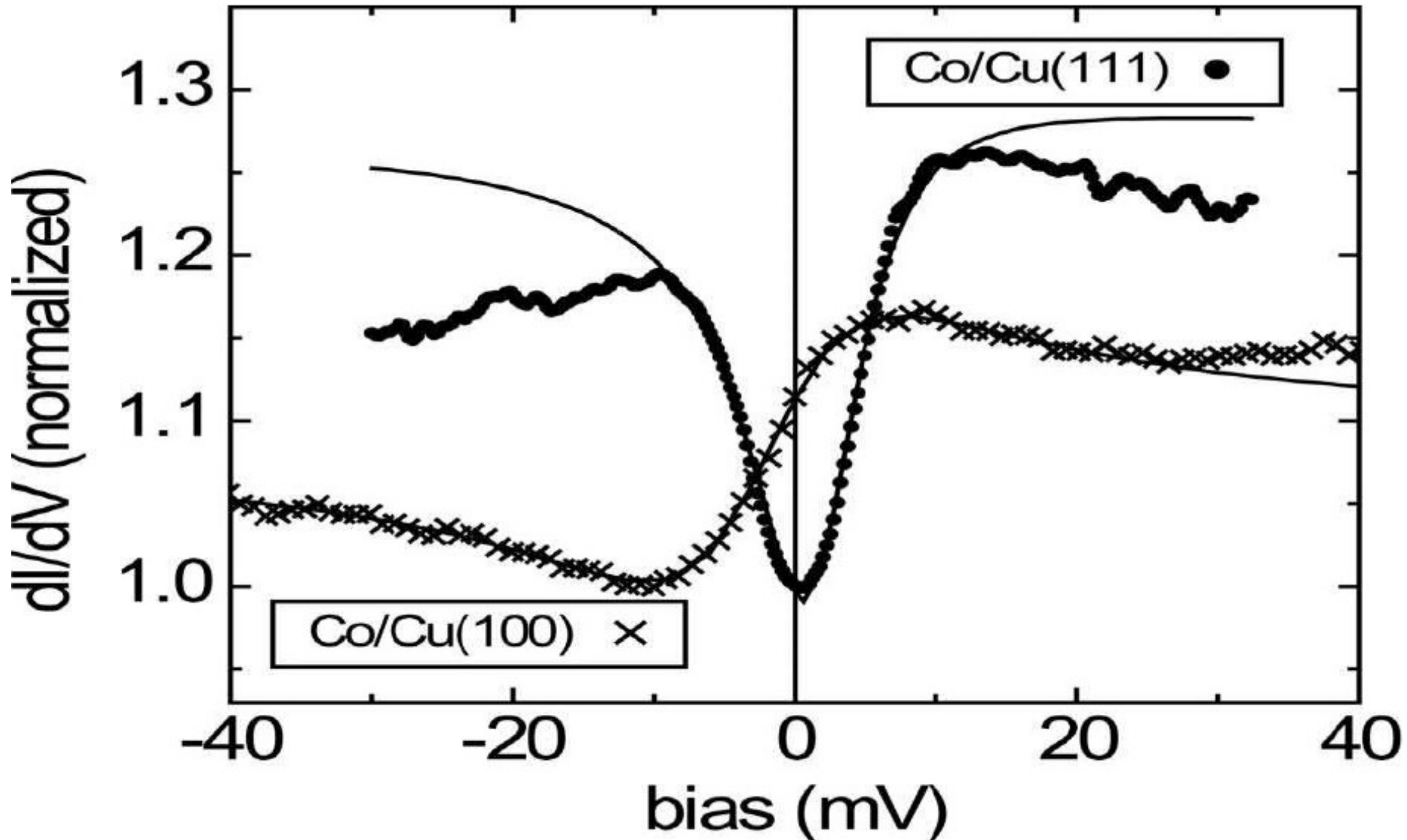
$$\Delta\rho_R(\epsilon) = \frac{1}{\pi} [\text{Im} G_R^{(0)}(\epsilon)]^2 [(q_R^2 - 1) \text{Im} t(\epsilon) + 2q_R \text{Re} t(\epsilon)]$$

and $q_R = \text{Re} G_R^0(\epsilon) / \text{Im} G_R^0(\epsilon)$

For a resonant level at $R = 0$, $\rho_R(\epsilon) = \rho_0 \frac{(x+q)^2}{(x^2+1)}$ with $x = (\epsilon - \epsilon_d) / \Gamma$

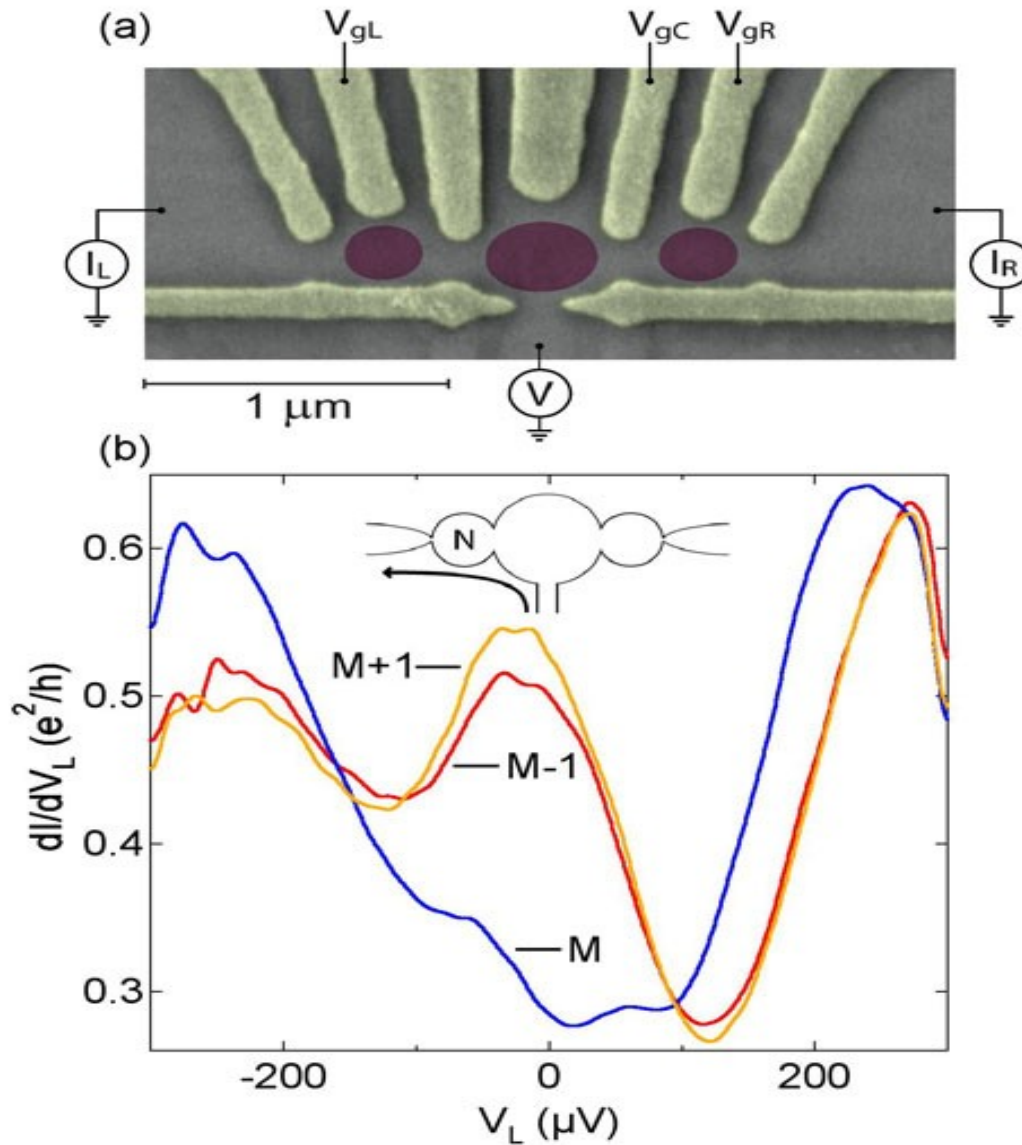
A general expression can be also cast for a magnetic Kondo impurity able to fit the experimental results

Different spectral shapes



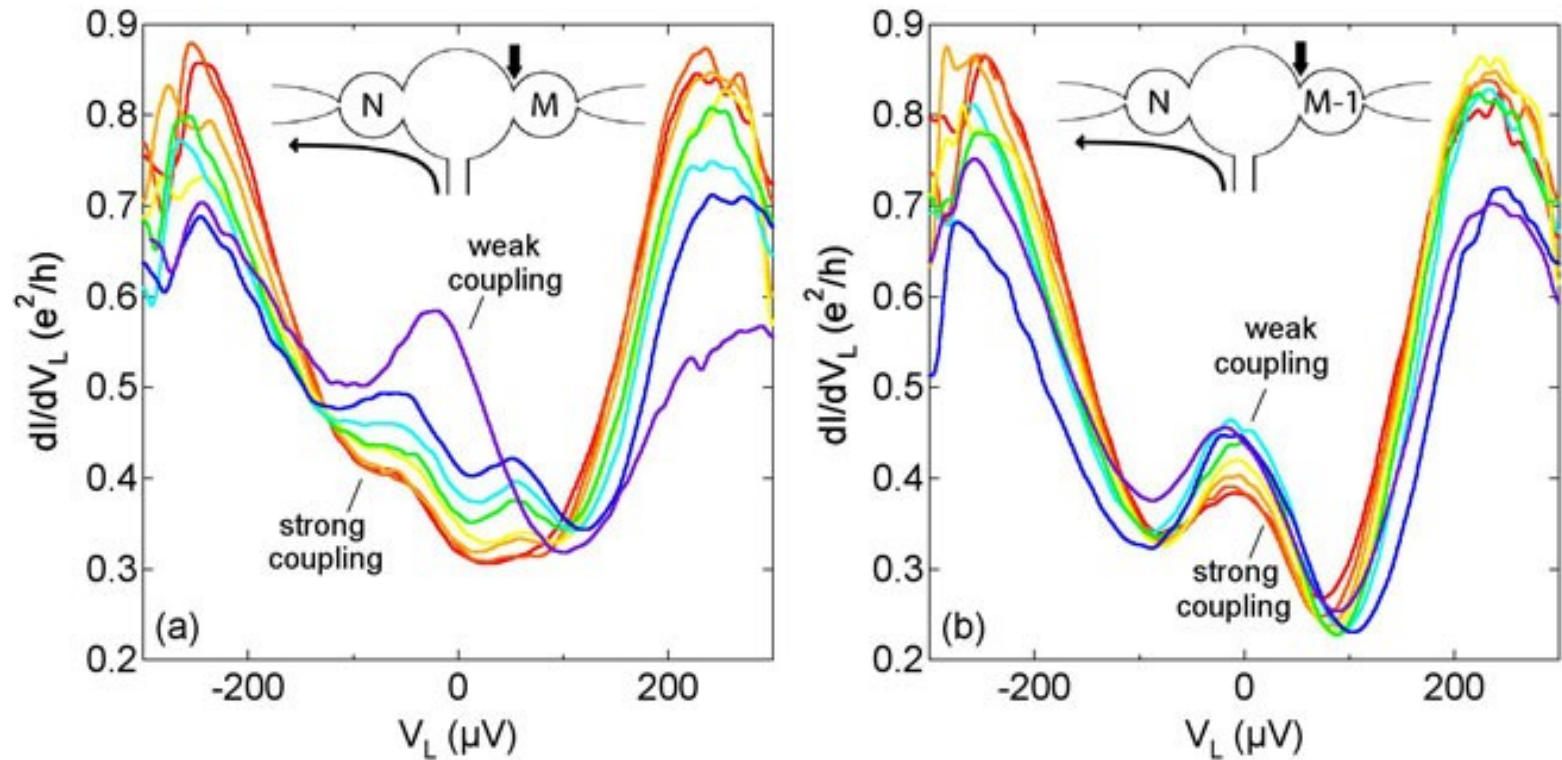
II. Spectroscopy of two impurities systems

Experimental results with quantum dots



[Craig et al., Science 2004](#)

Experimental Analysis



[N. Craig et al., Science 304, 565 \(2004\)](#)

A theoretical Description

$$\mathcal{H} = \mathcal{H}_C + J_1 \vec{S}_1 \cdot \vec{\sigma}_1 + J_2 \vec{S}_2 \cdot \vec{\sigma}_2 + I \vec{S}_1 \cdot \vec{S}_2.$$

Asymmetrical two impurity system: three energy scales: T_K^1, T_K^2, I

If $I < 0, |I| \gg \max(T_K^1, T_K^2)$

Formation of a **triplet state**: Two stage screening



Peak in the DOS at $T=0$

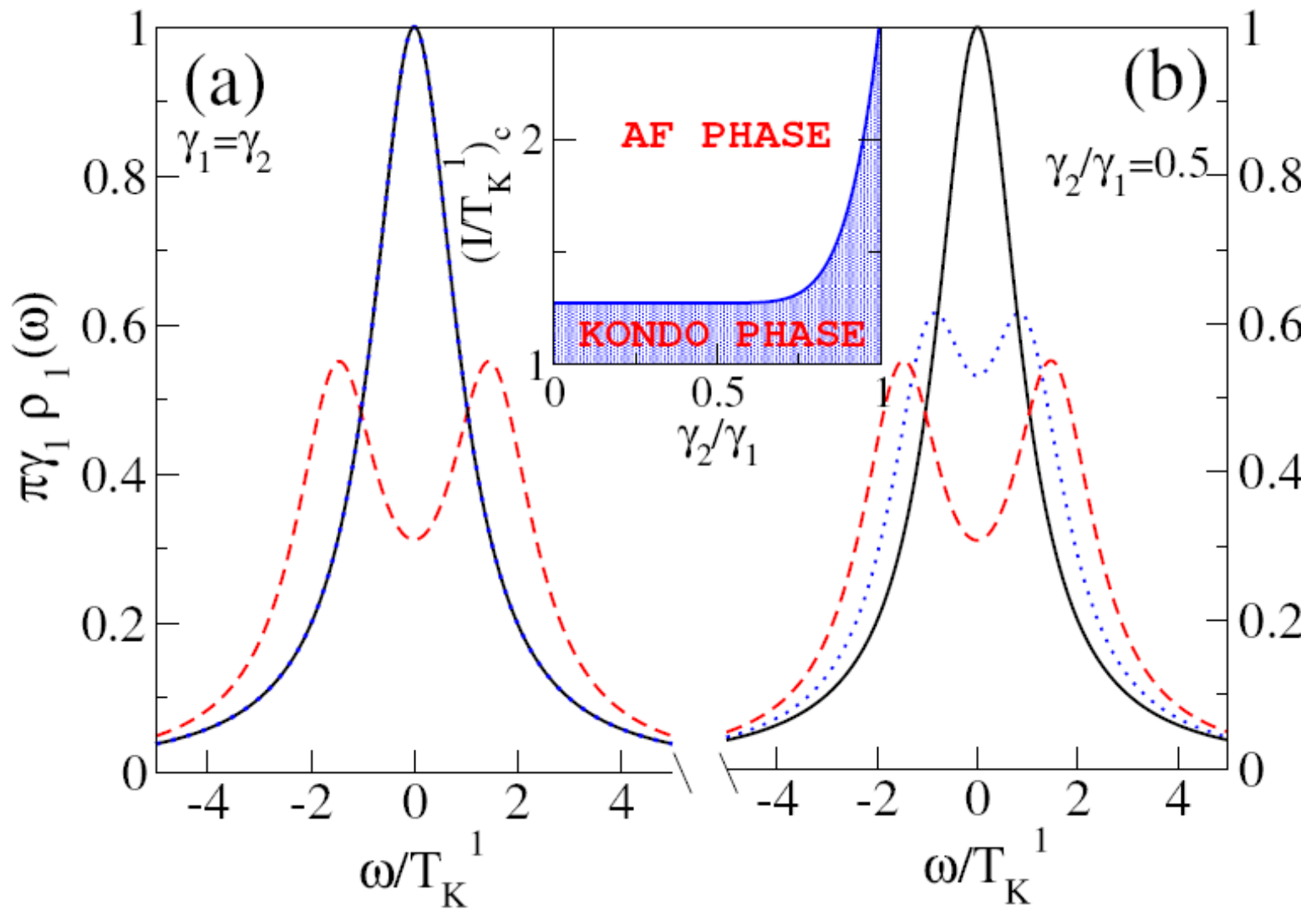
If $|I| < \max(T_K^1, T_K^2)$

Independent screening of each impurity

If $I > 0, |I| \gg \max(T_K^1, T_K^2)$

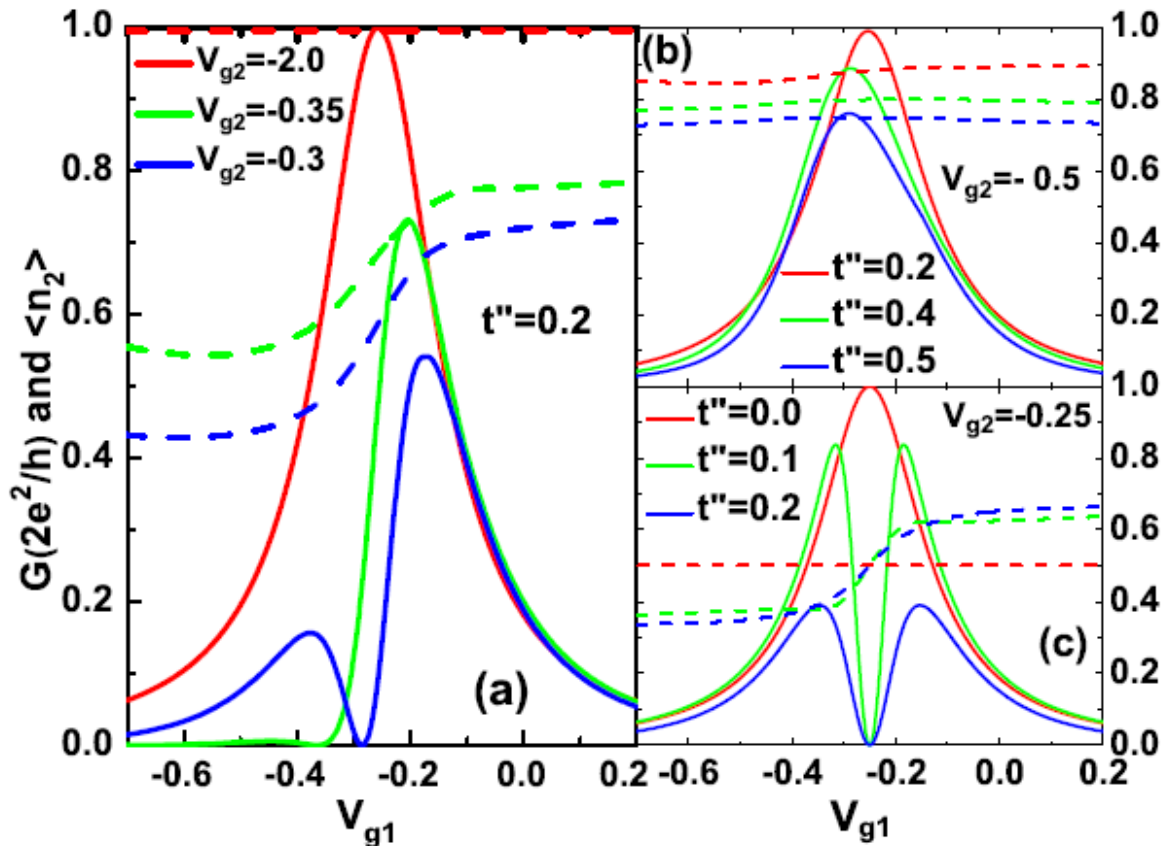
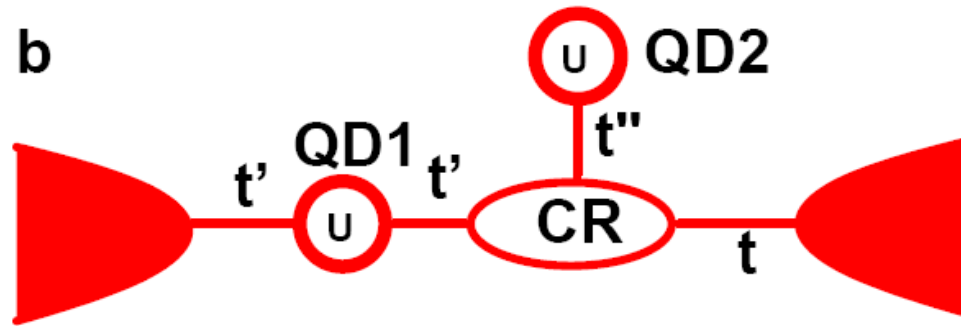
Formation of a **singlet**: Conductance $G=0$ at $T=0$

Spectroscopy using the slave boson mean field theory for $I > 0$



An alternative description

A circuit model:



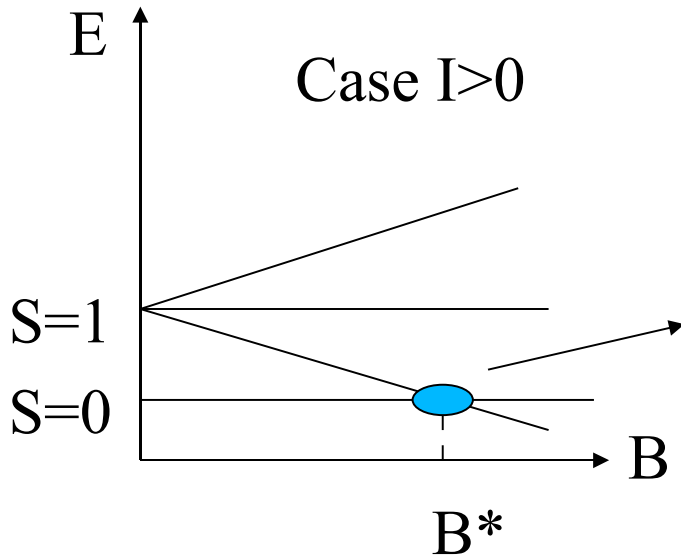
Dagotto et al.,

PRL 2006

Effect of a magnetic field

$$\mathcal{H} = \mathcal{H}_C + J_1 \vec{S}_1 \cdot \vec{\sigma}_1 + J_2 \vec{S}_2 \cdot \vec{\sigma}_2 + I \vec{S}_1 \cdot \vec{S}_2 - \vec{B} \cdot (\vec{S}_1 + \vec{S}_2)$$

For $I > 0$, competition between I et B



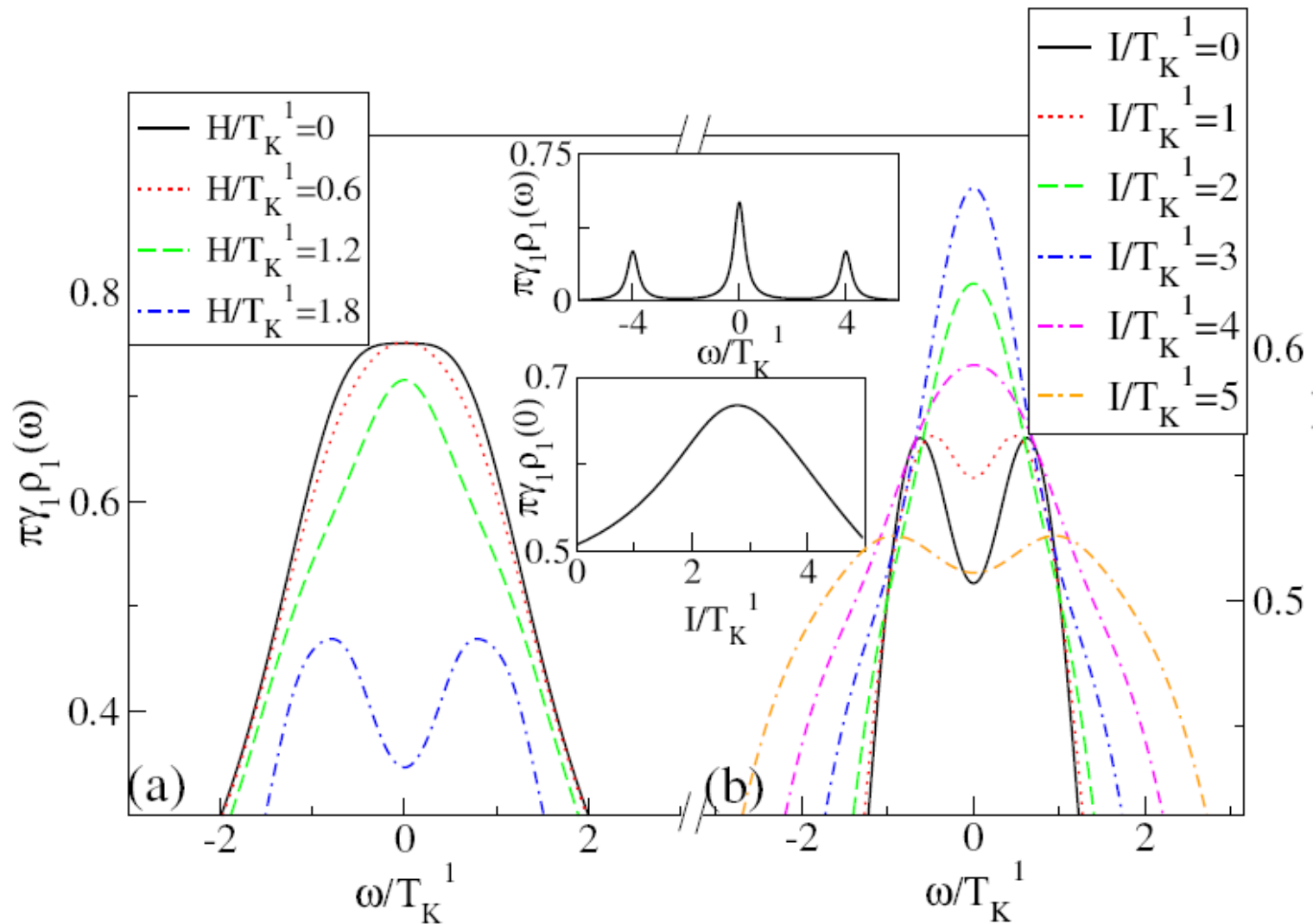
For B of order I ;

Two impurity magnetic field induced

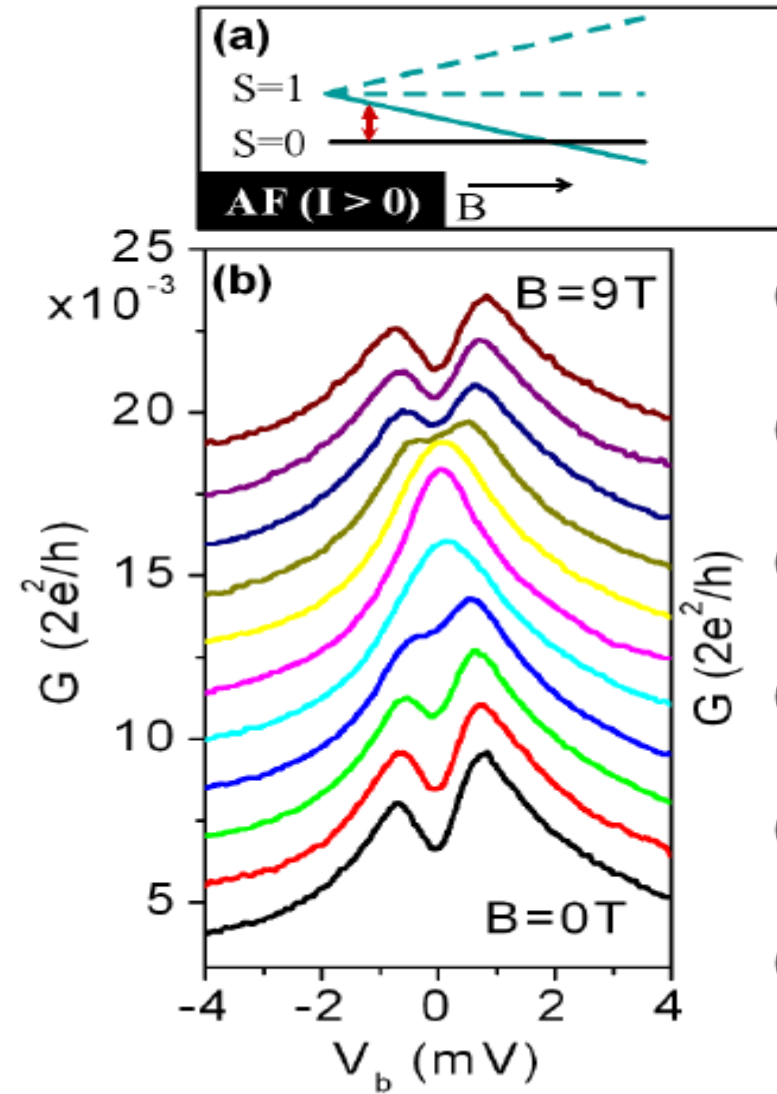
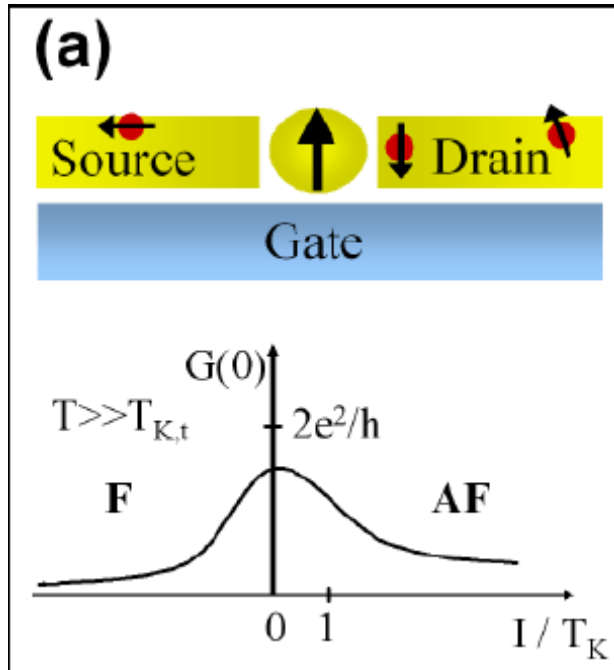
Kondo effect

$$T_K(B^*) = T_K (T_K/B)^\alpha$$

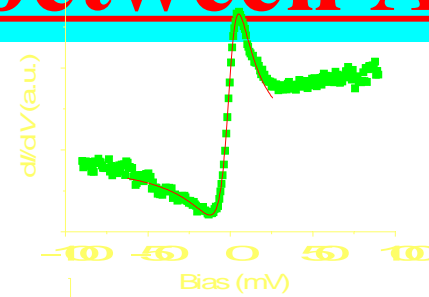
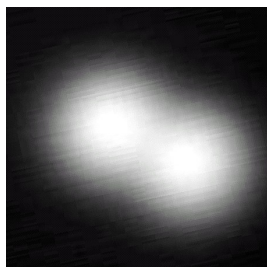
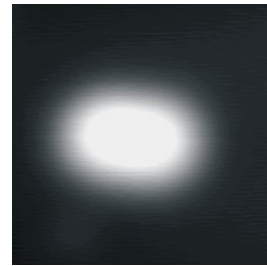
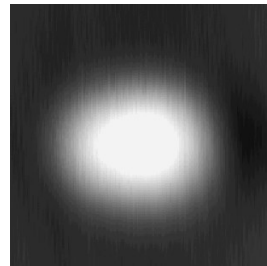
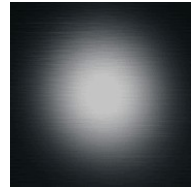
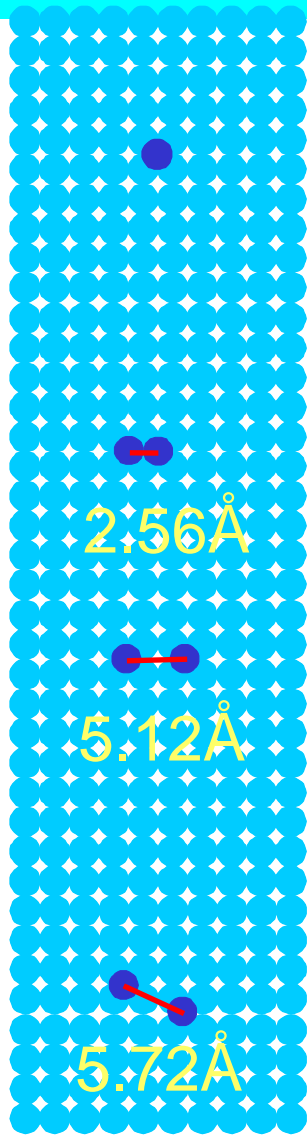
Results of the magnetic field



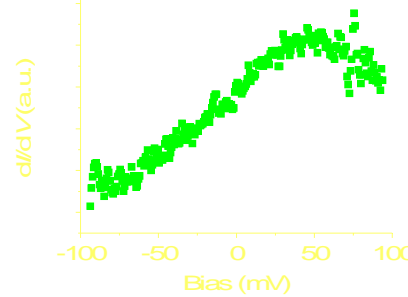
Experimental results



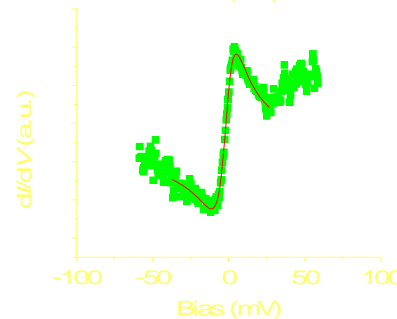
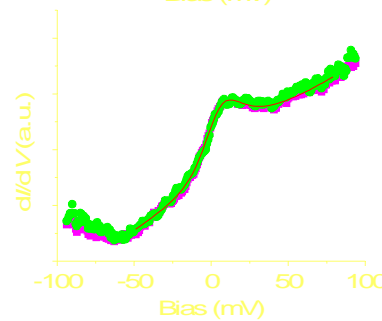
Interaction between Adatoms



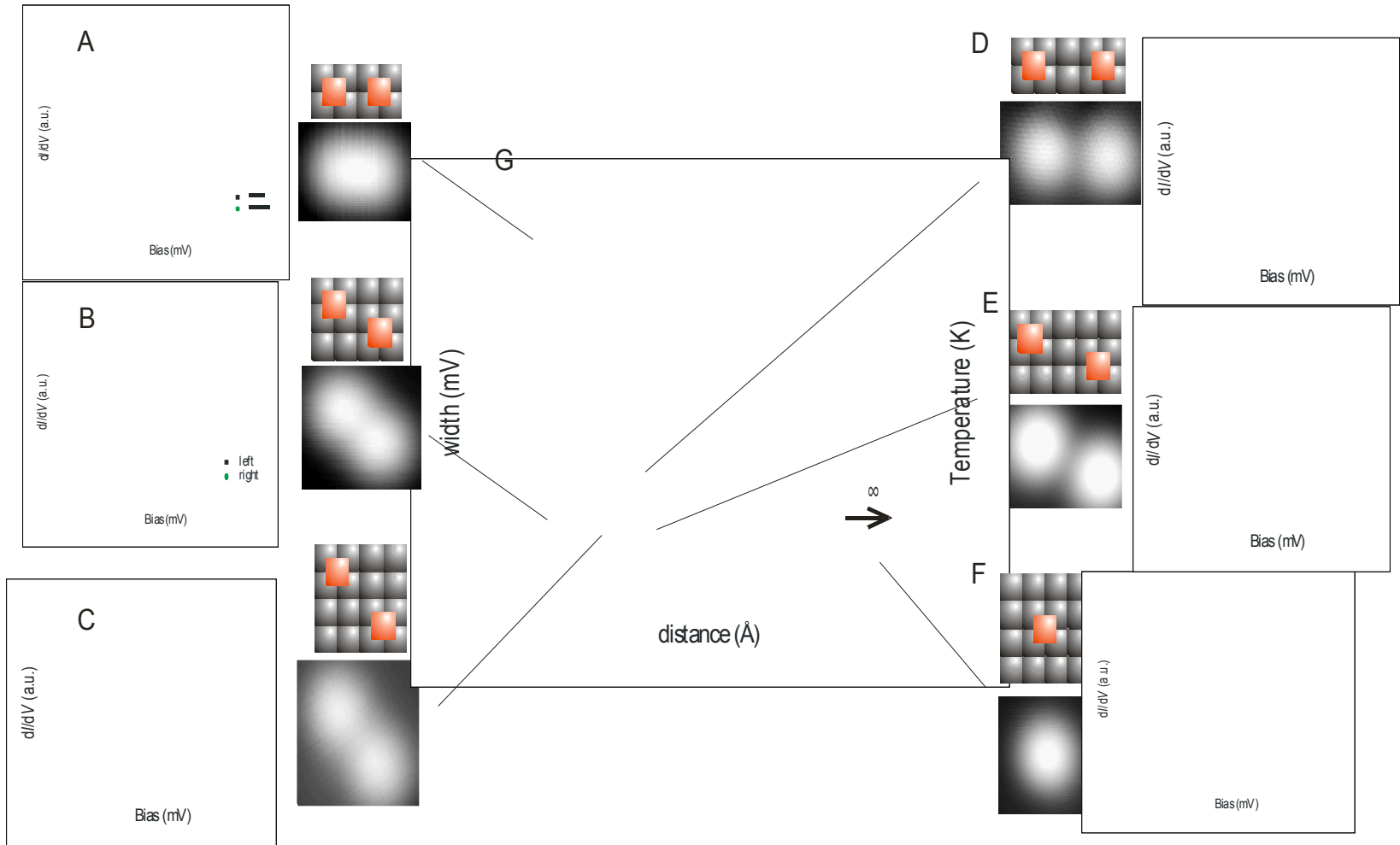
$T_K = 88\text{ K}$



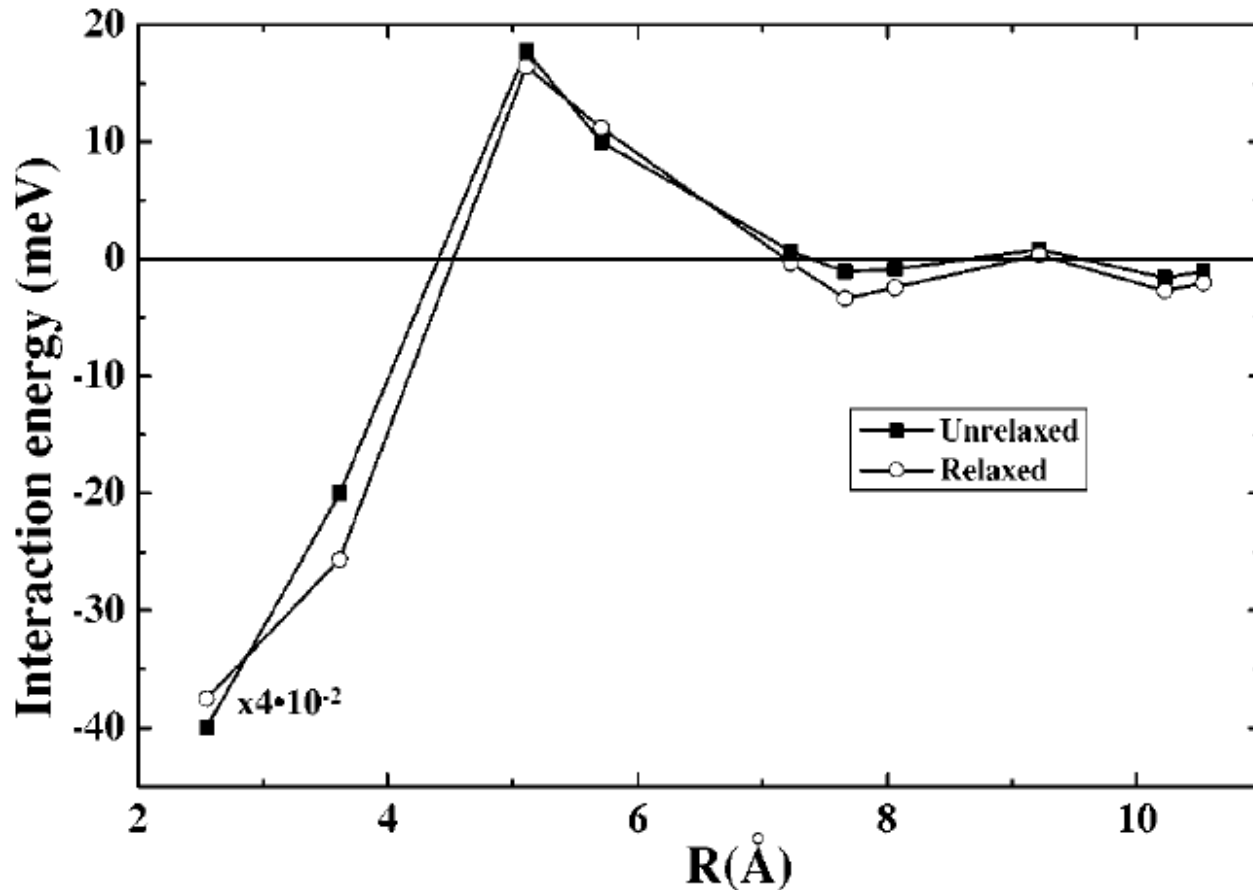
No Kondo



Spectroscopy of dimer with STM



Ab initio calculations



V. S. Stepanyuk et al. , Phys Rev. B 68, 205422 (2003)

Spectroscopy of magnetic clusters

Dyson equation:

$$\delta G(\vec{r}, \omega) \approx V^2 \sum_{i,j=1}^p G_{\vec{r}\vec{r}_i}^{(0)}(\omega) G_{ij}(\omega) G_{\vec{r}_j\vec{r}_i}^{(0)}(\omega)$$

Where p is the number of impurities

$G^{(0)}$ is the bare surface Green function


G_{ij} is the exact Cluster Green function

$$\delta\rho(\vec{R}, \omega) \propto \text{Im} \left(\int d^2\vec{r} w(\vec{r}) \delta G(\vec{R} + \vec{r}, \omega) \right)$$

$w(\vec{r})$ is a form factor depending on the spatial extension of the tip-substrate matrix elements

Approximate dimer Green function

At $d=5.12$ Ang., one expects $I > 2T_K^0$

 Splitting of the Kondo resonances due to the formation of a singlet state

The slave boson mean field theory provides:

$$G_{1,1/2} \approx \frac{1/2}{\omega - I/2 + i\Delta} \pm \frac{1/2}{\omega + I/2 + i\Delta}$$

$\Delta = \Delta(I)$ is a the width of the peaks

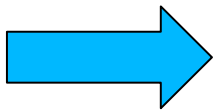
Approximate Fano line shape

Using a window function about 8 Ang. for the form factor

It generates a local d.o.s almost independent of the tip position

$$\rho(\omega) \approx a_1 f\left(\frac{\omega - I/2}{\Delta}, q\right) + a_2 f\left(\frac{\omega + I/2}{\Delta}, q\right) + c$$

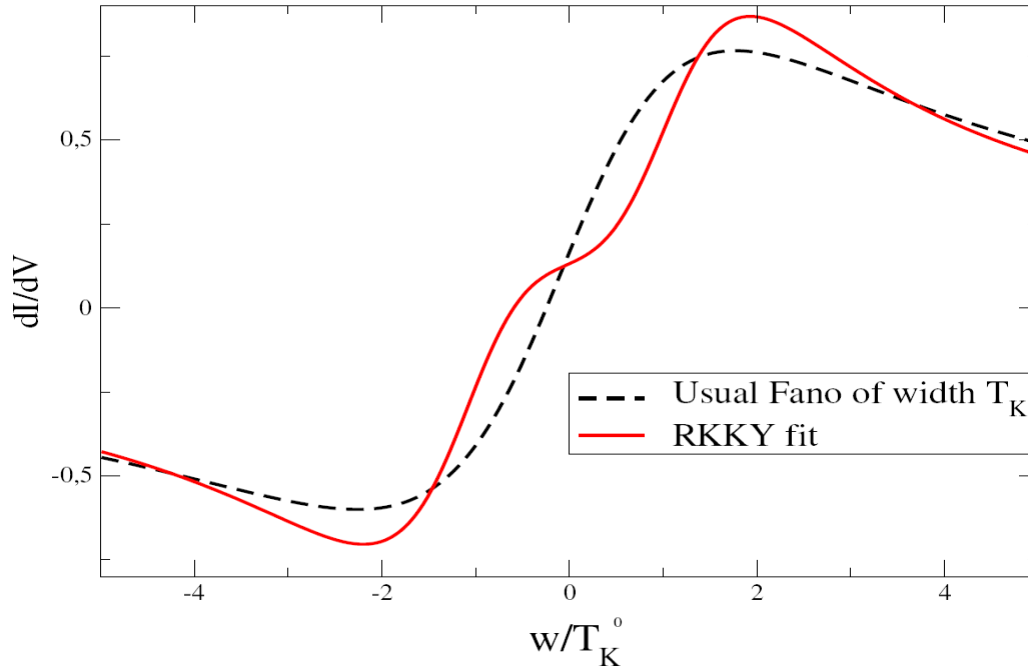
where $f(x, q) = \frac{(x+q)^2}{x^2+1}$ and $a_1 \sim a_2$



This describes a superposition of two Fano line shapes

A theoretical interpretation

For $R=5.12$ Ang. the RKKY dominates and splits the Kondo resonance



We use $I \sim 16mev$

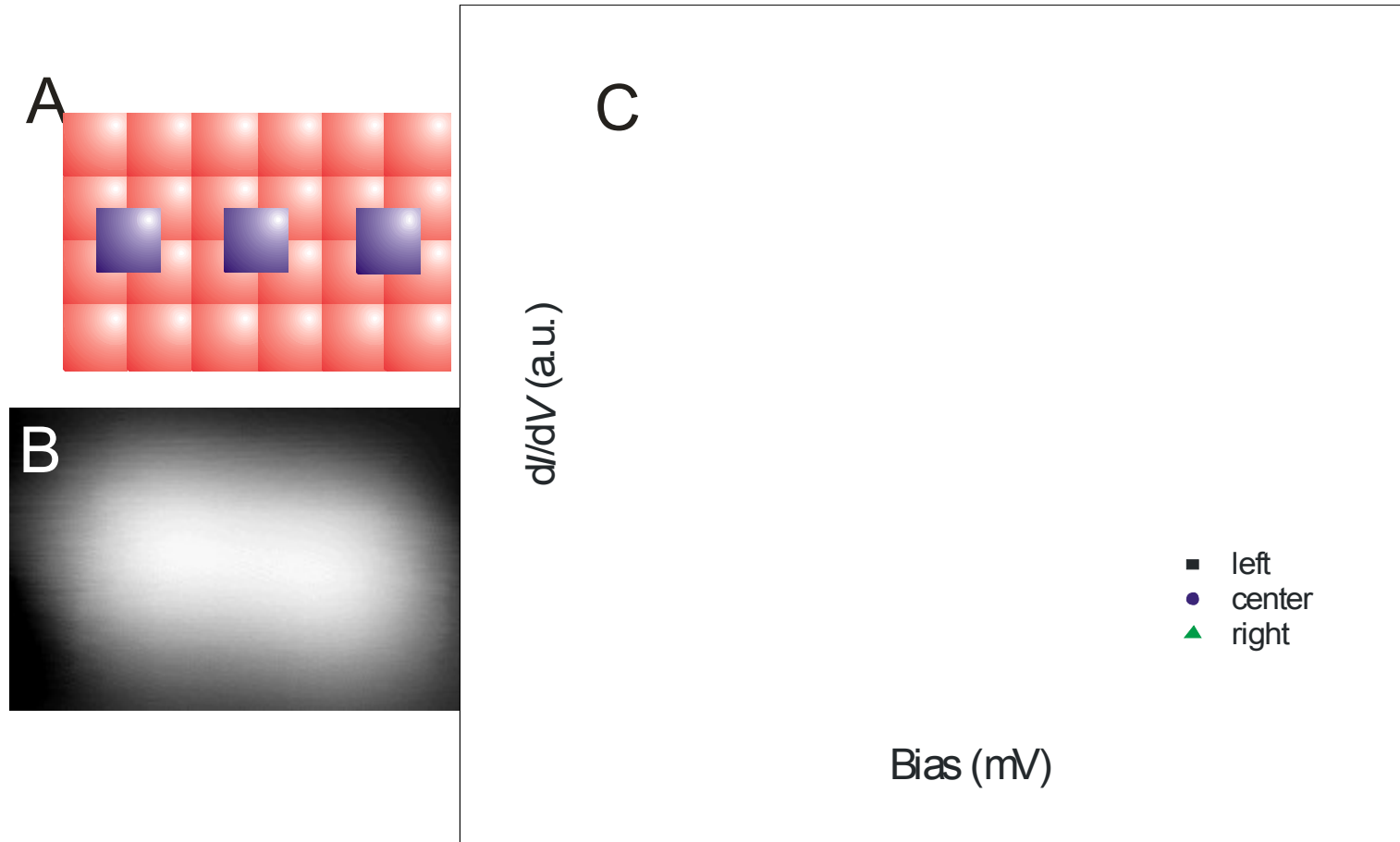
$$\Delta \sim T_K^0 \sim 8mev$$

Comparison between the double Fano resonance and a single Fano resonance of width I .

By fitting the experimental data with a double Fano resonance, one obtains I around 17mev

III. Spectroscopy of magnetic clusters

In line trimer

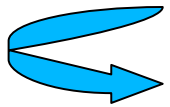


➔ Two features are present around zero bias!

Some attempts of interpretation

$$H = H_C + I\vec{S}_2 \cdot (\vec{S}_1 + \vec{S}_3) + J_K \sum_{i=1}^3 \vec{S}_i \cdot \vec{\sigma}_i$$

Ab initio calculations also predict $I \approx 17\text{meV}$ for $d=5.12$ Ang.



It suggests a correlated cluster

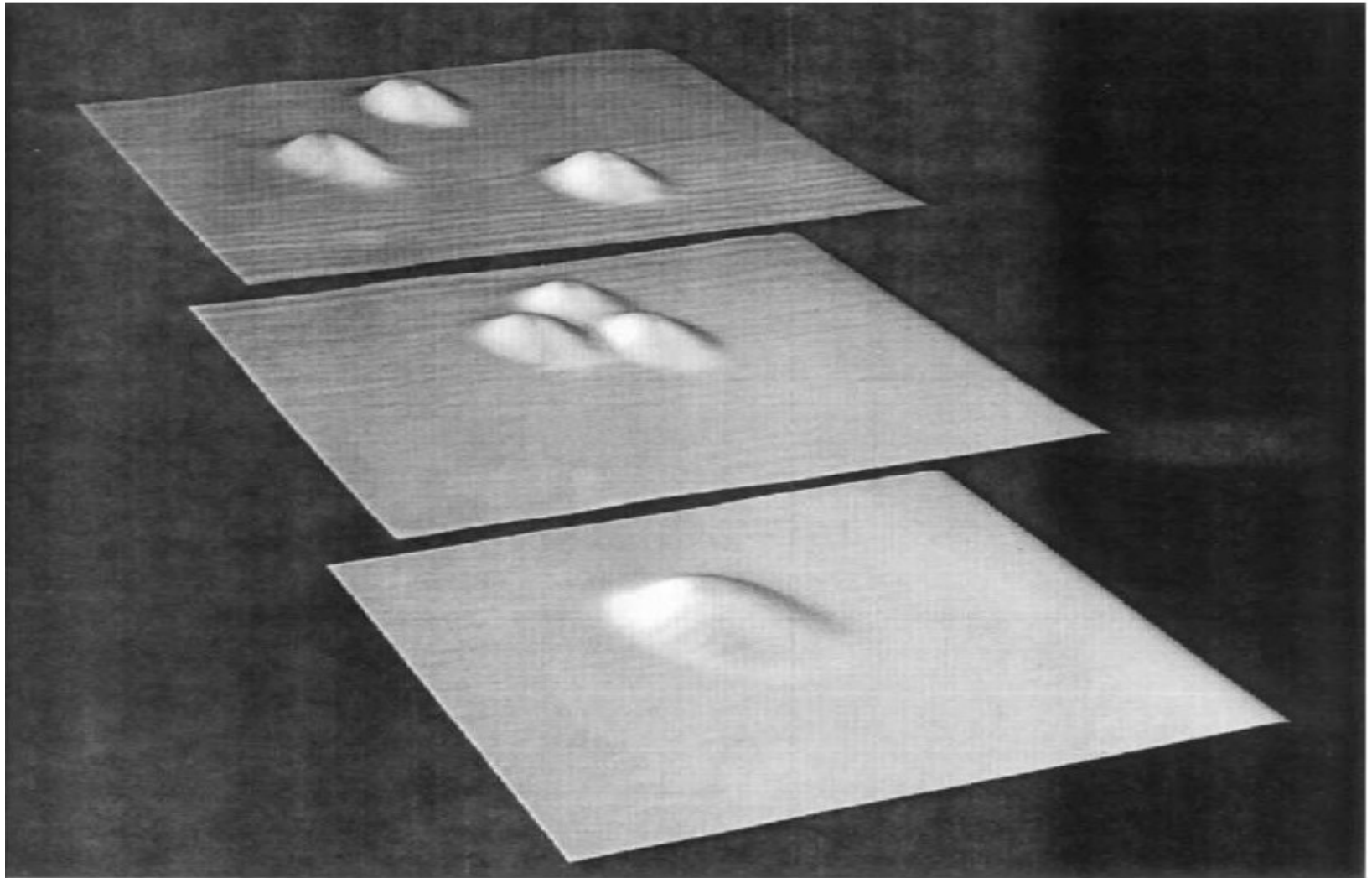
One can extend the SBMFT to this three-impurity problem:

It predicts 3 peaks in the DOS at $0, \pm I/2$



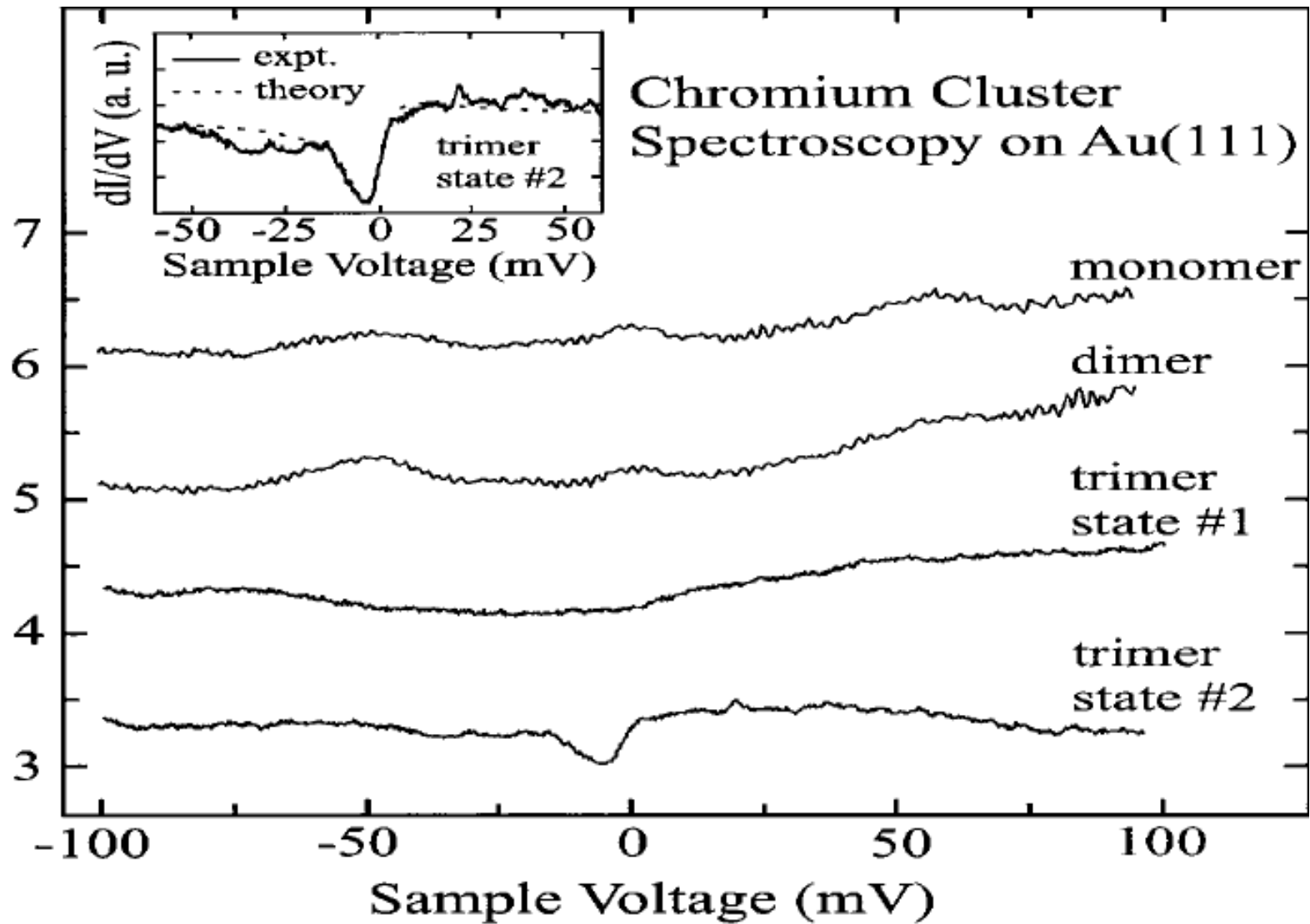
This does not describe the data!!!

Chromium trimer on Gold



[T. Jamaneala, V. Madhavan, M. Crommie, Phys. Rev. Lett. 87, 256804 \(2001\)](#)

Experimental results



Summary of main experimental results

No resonance for the monomer or dimer at $T=7\text{K}$

A resonance of width 50K appears for one trimer configuration

This resonance can be switched on and off reversibly by
the STM Tip

The most frequent configuration corresponds to no resonance

See Gergely Zarand's talk this evening for an explanation

CONCLUSION :

- Evidence of RKKY interaction by spectroscopy
 - 1) In semi-conducting quantum dots
 - 2) In adsorbed impurities on metallic surfaces
- Rich and exotic physics already in small clusters
- Right field to develop methods combining ab initio and NRG calculations

Acknowledgments

R. Lopez and Y. Oreg (quantum dots)

P. Wahl, L. Diekhoner, W. Schneider, P. Bruno, V. Stepanuk,

K. Kern and J. Merino (Cobalt clusters)

B. Lazarovits, L. Szunyoth and G. Zarànd (Cr trimers)

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