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# Lectures: Condensed Matter II

1 – Electronic Transport in  
Quantum dots

2 – Kondo effect: Intro/theory.

3 – Kondo effect in nanostructures

Luis Dias – UT/ORNL

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# Lecture 3: Outline

- Quantum Dots: brief review.
  - Kondo effect: Review.
  - Kondo effect in quantum dots.
  - Kondo effect in Single Molecule Transistors.
  - Kondo effect in Surfaces (STM, “quantum mirage”).
  - Kondo effect in carbon nanotubes.
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# “More is Different”



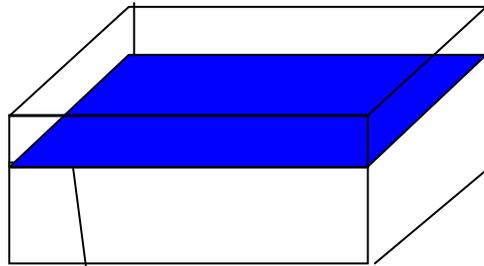
“ The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of simple extrapolation of the properties of a few particles.

Instead, at each level of complexity entirely new properties appear and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other.“

Phillip W. Anderson, “More is Different”,  
*Science* **177** 393 (1972)

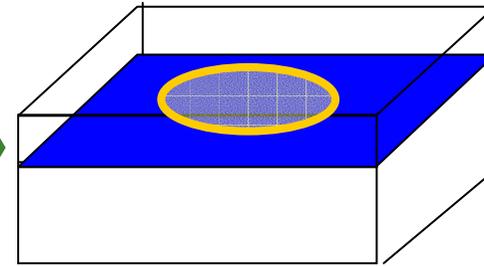
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# Can you make “atoms” out of atoms?

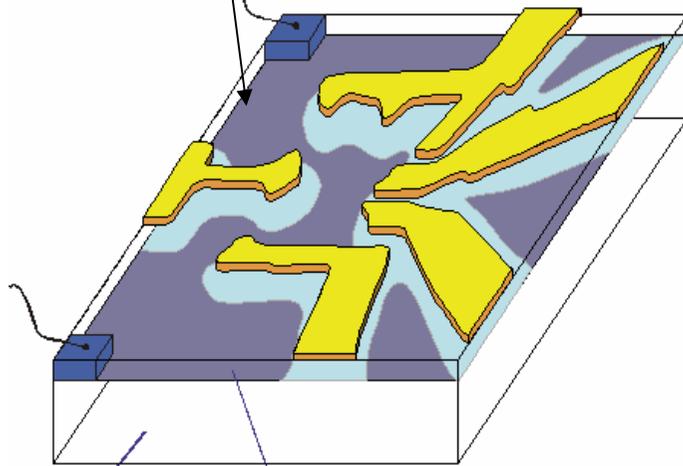


2D Electron gas

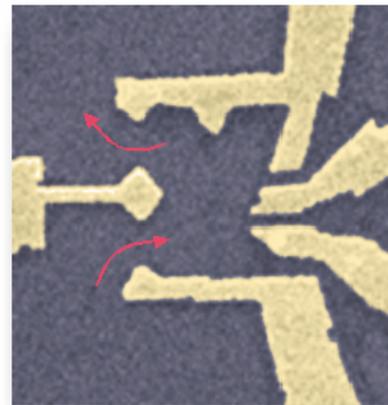
Electrostatically confine electrons within a small (nanometer-size) region.



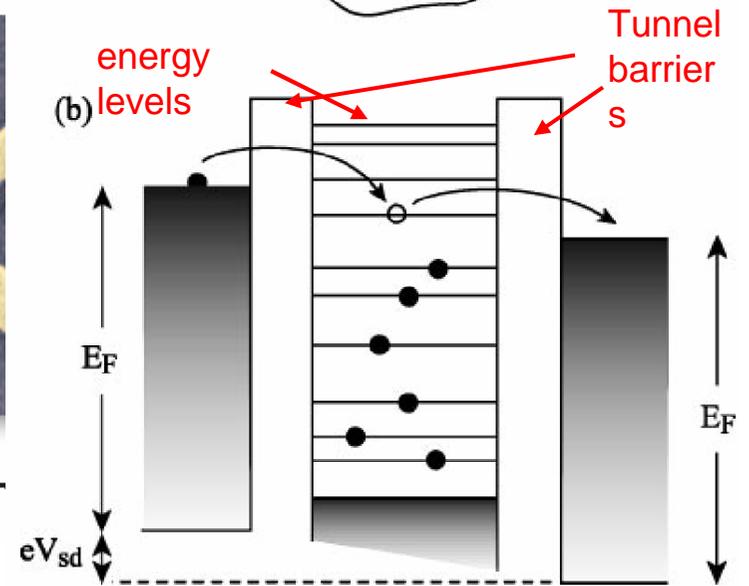
“Quantum dot”



GaAs  $\text{Al}_x\text{Ga}_{1-x}\text{As}$

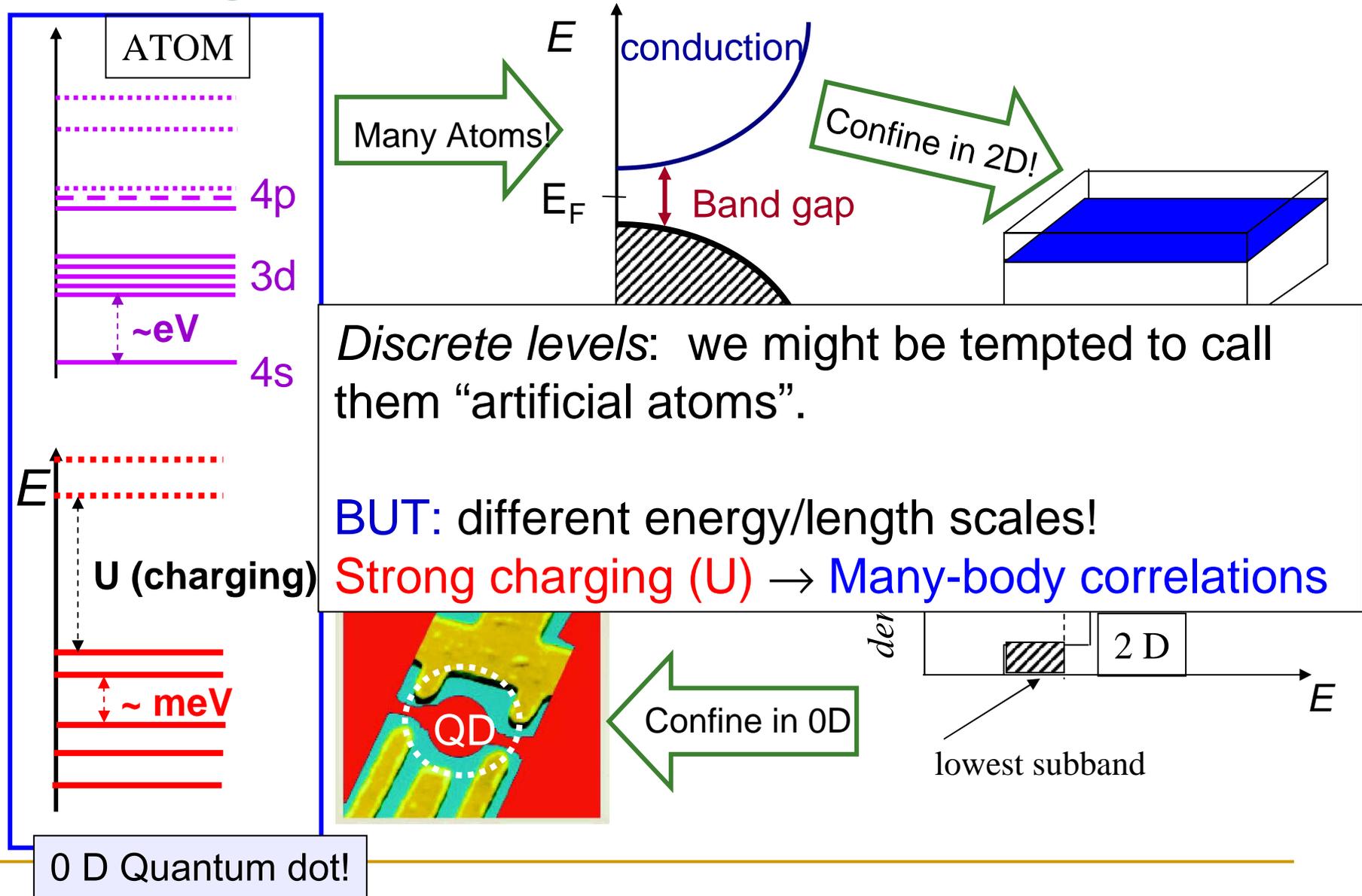


$1\mu\text{m}$



from Charlie Marcus' Lab website ([marcuslab.harvard.edu](http://marcuslab.harvard.edu))

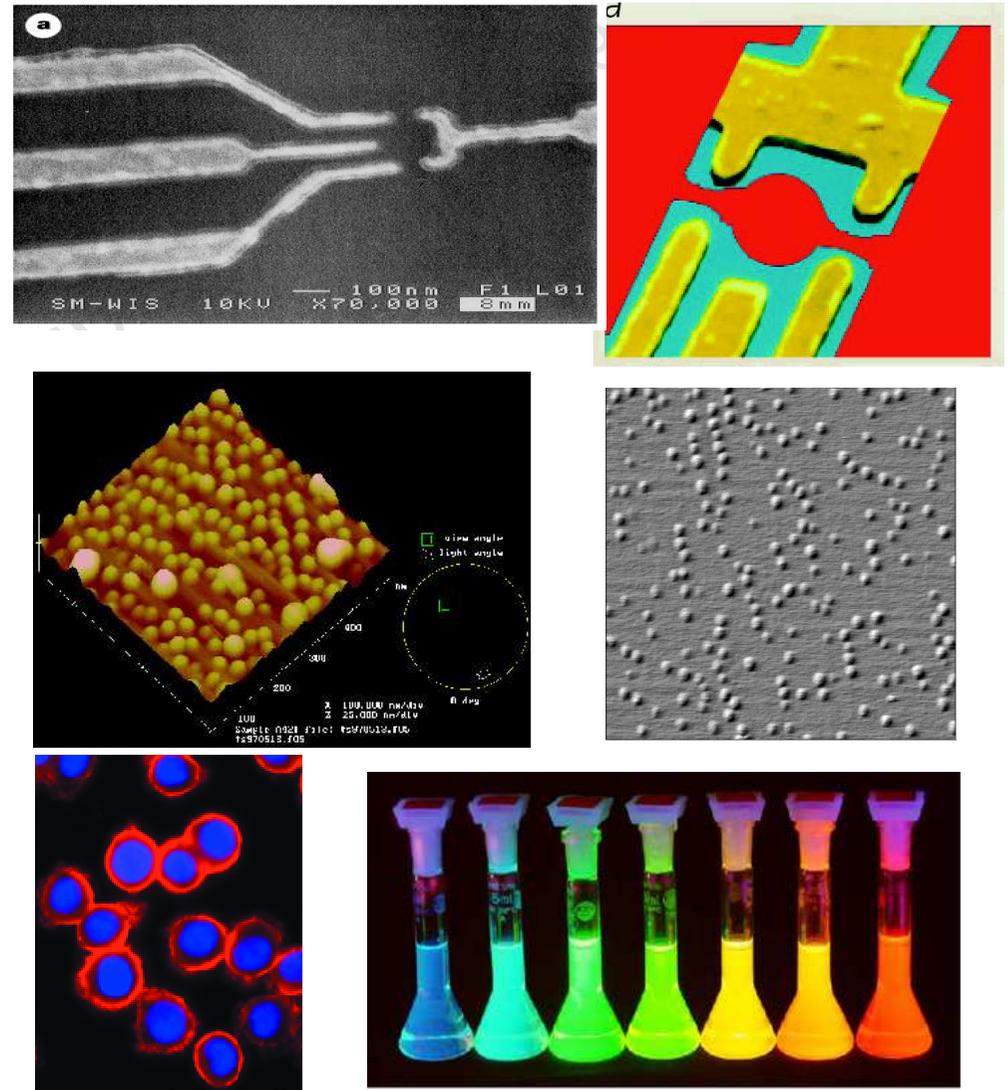
# Making “artificial atoms”(?) out of atoms



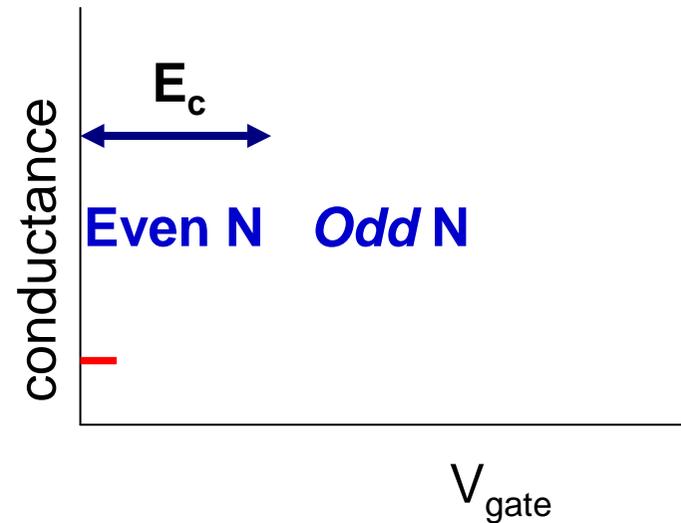
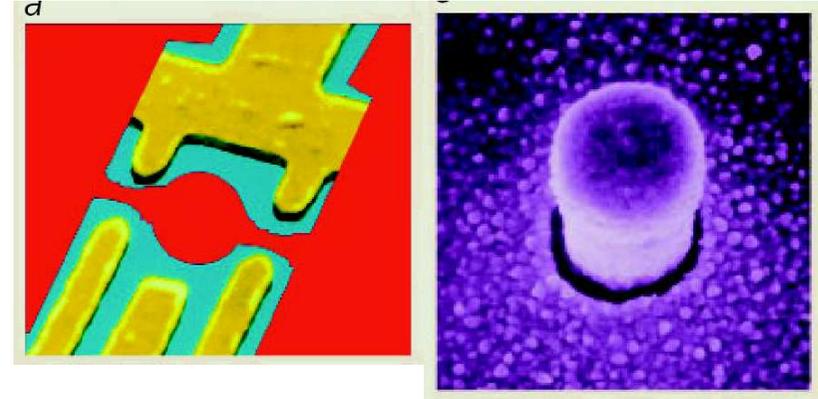
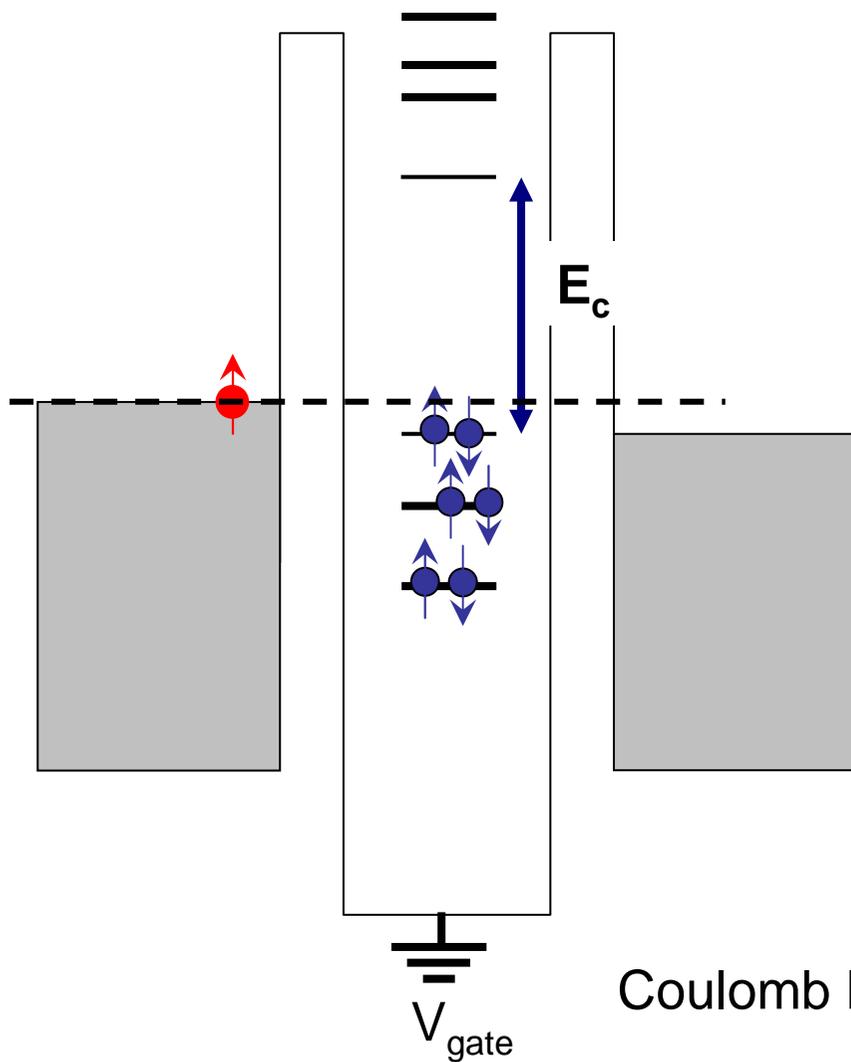
# What are *Quantum Dots*?

## Semiconductor Quantum Dots:

- Devices in which electrons are **confined** in nanometer size volumes.
- Sometimes referred to as “artificial atoms”.
- “Quantum dot” is a generic label: **lithographic QDs**, self-assembled QDs, colloidal QDs have different properties.

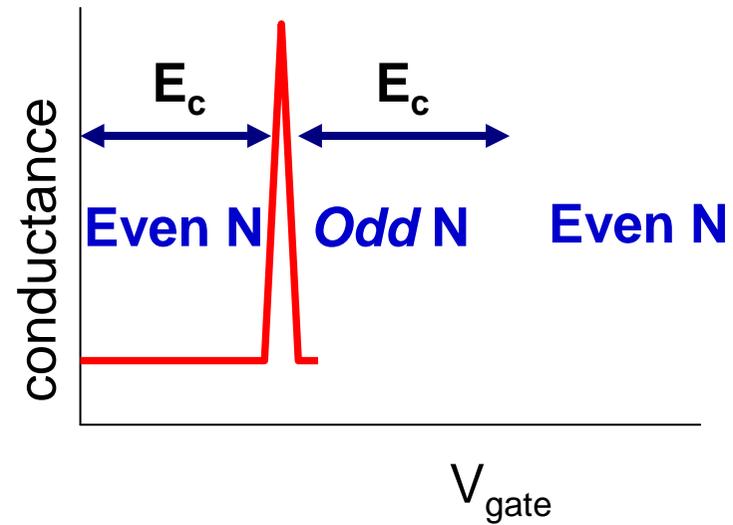
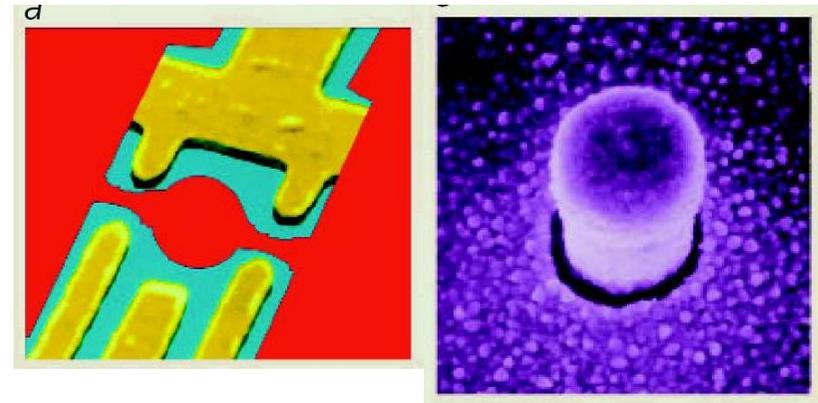
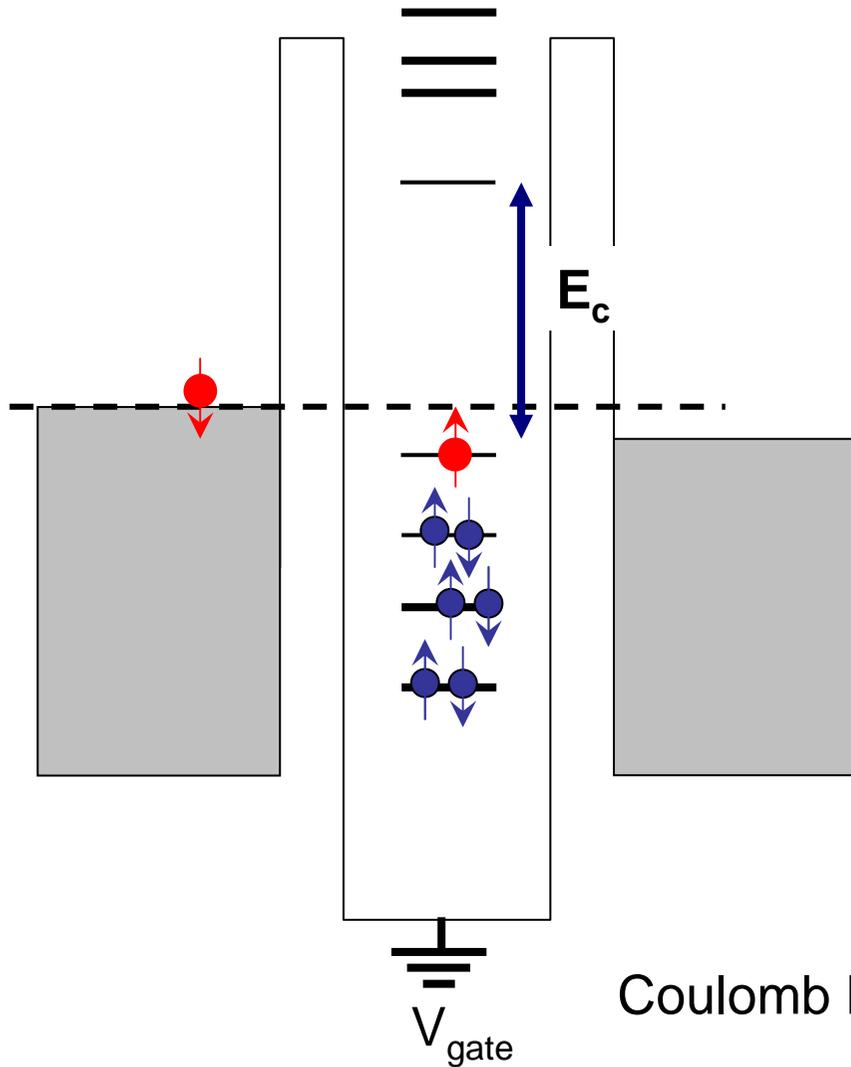


# Coulomb Blockade in Quantum Dots



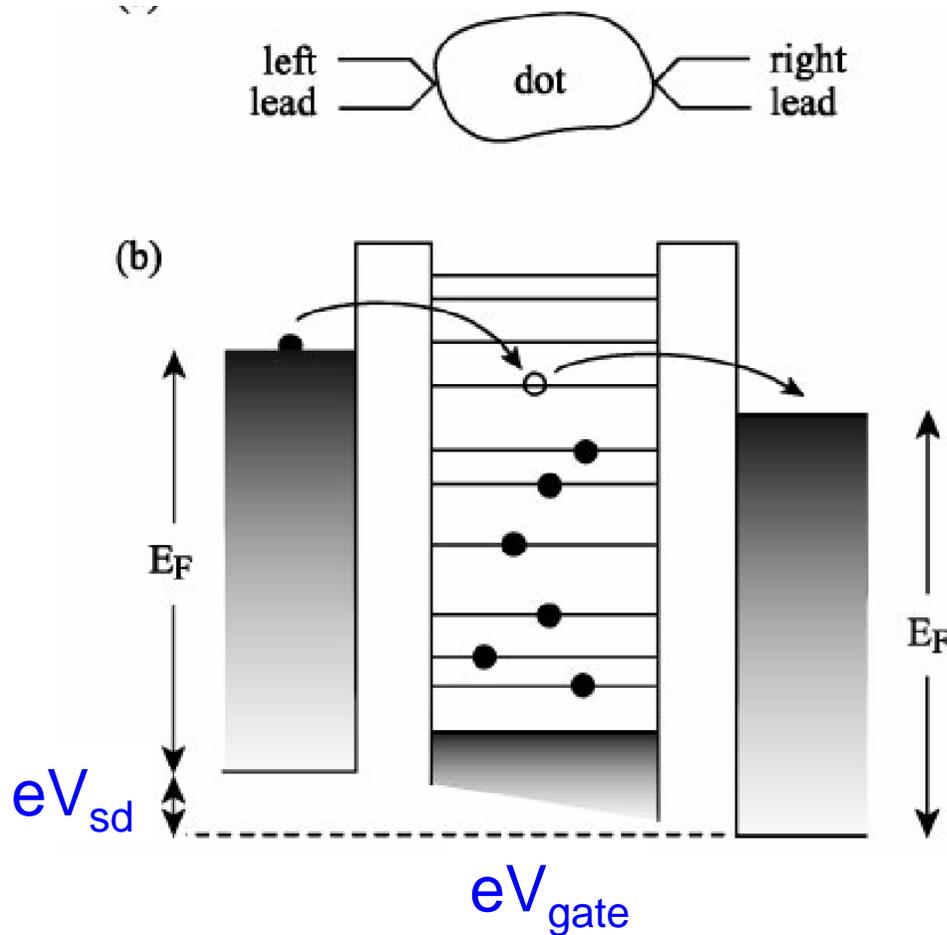
Coulomb Blockade in Quantum Dots

# Coulomb Blockade in Quantum Dots

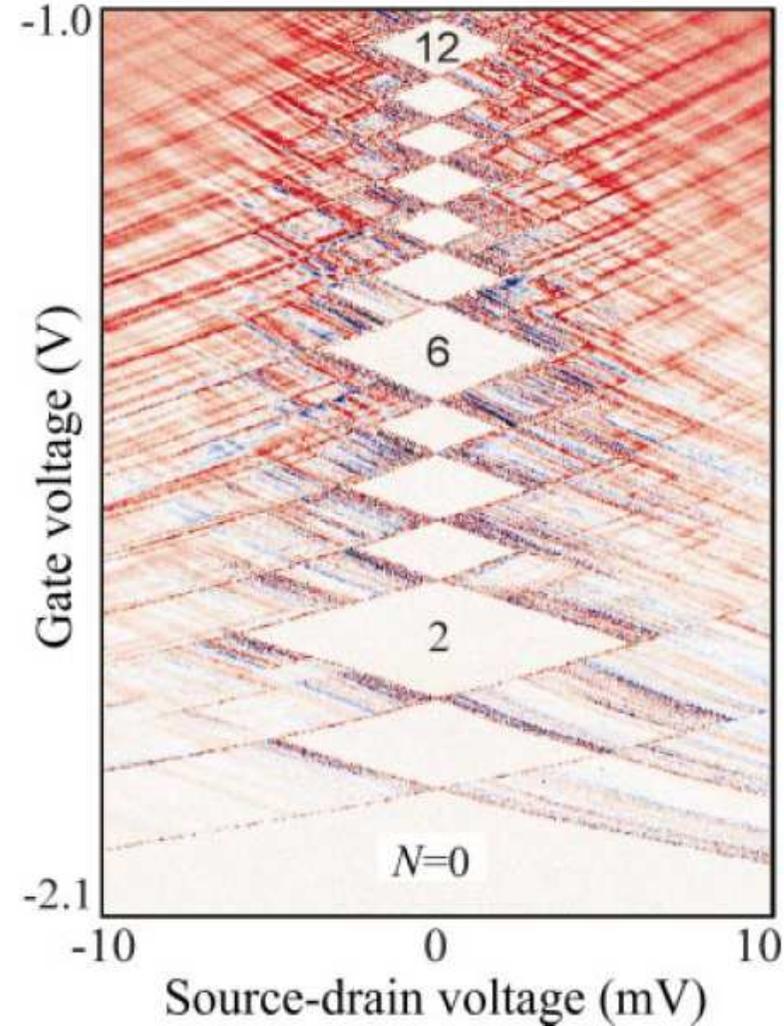


Coulomb Blockade in Quantum Dots

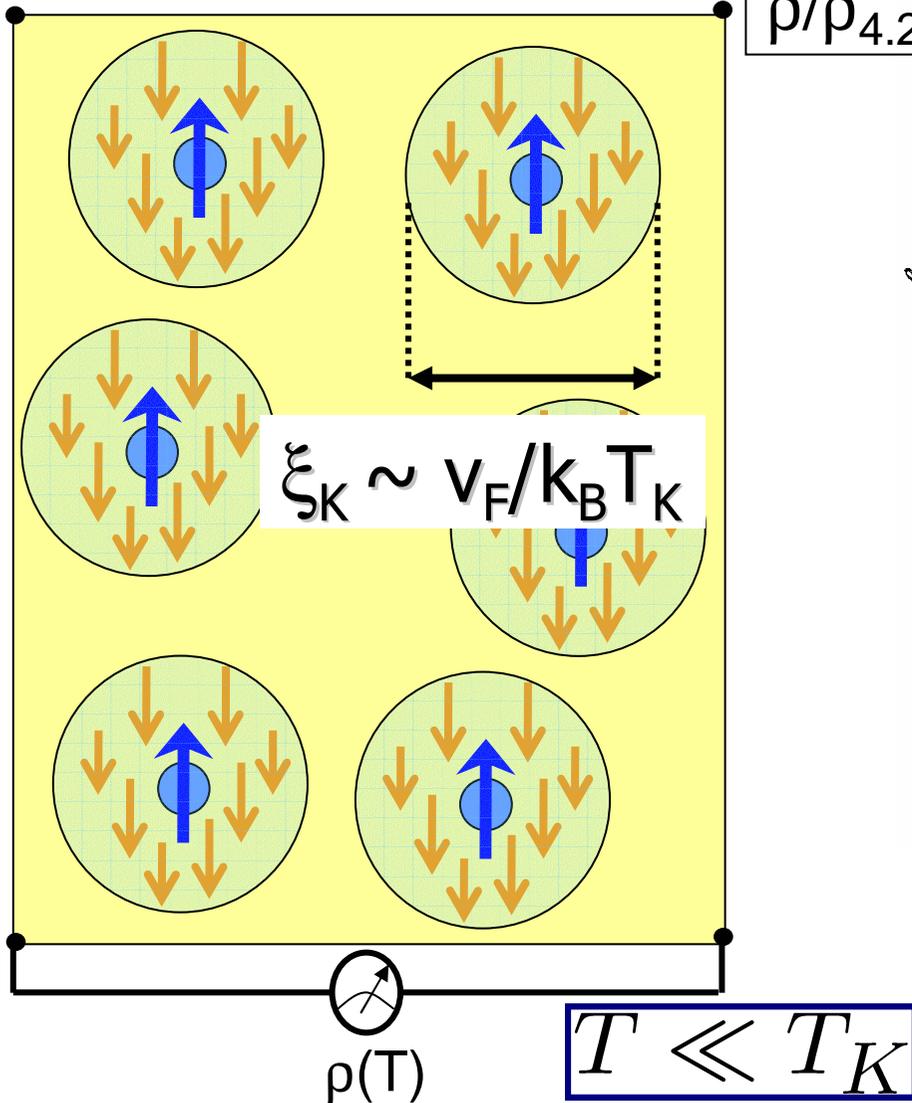
# “Coulomb Diamonds” (Stability Diagram)



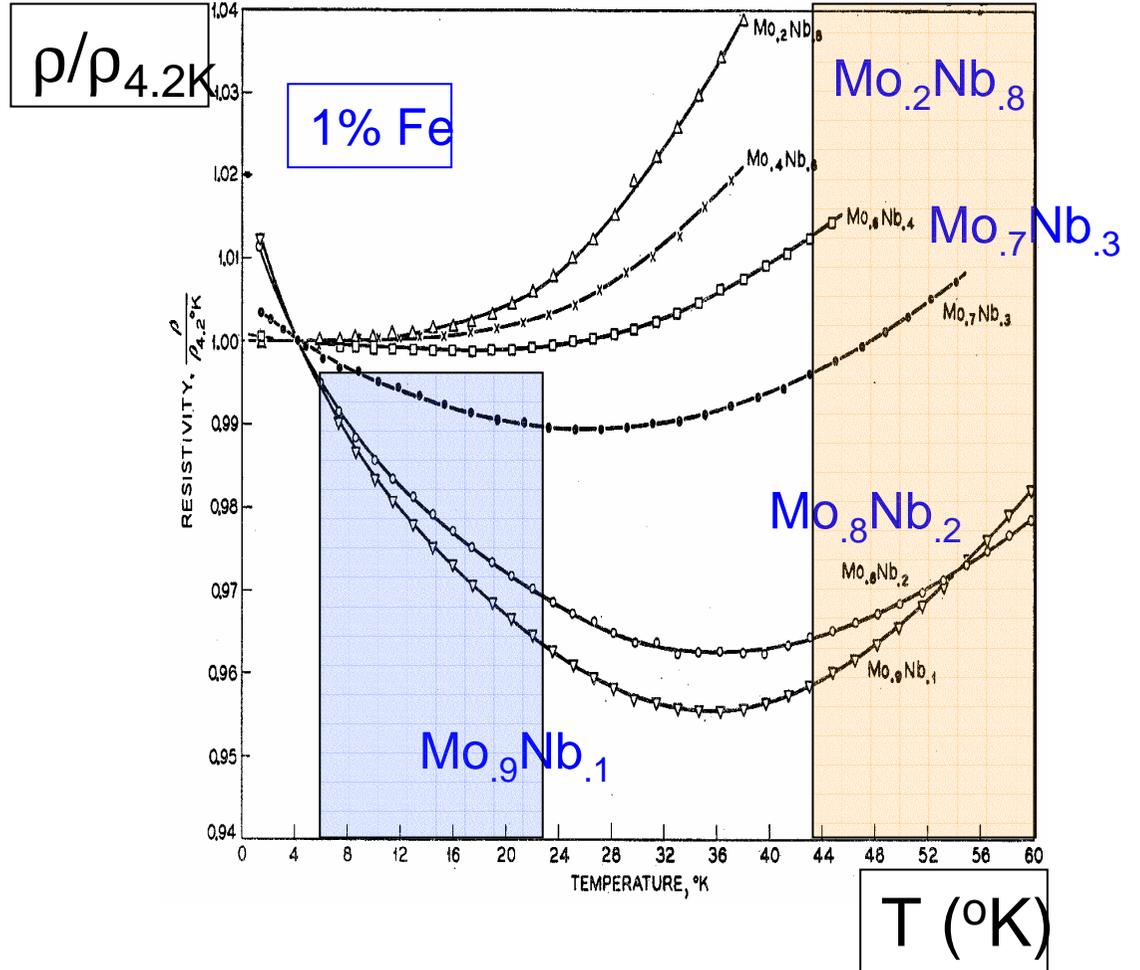
Coulomb Blockade in Quantum Dots



# Kondo effect



M.P. Sarachik *et al* Phys. Rev. **135** A1041 (1964).

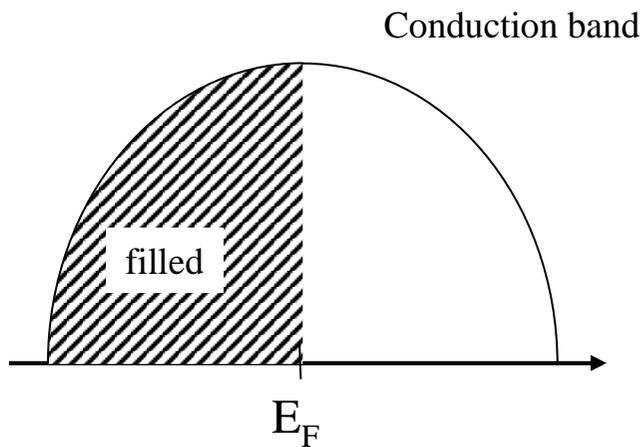


Resistivity increases with decreasing  $T$  (Kondo effect): the Kondo effect

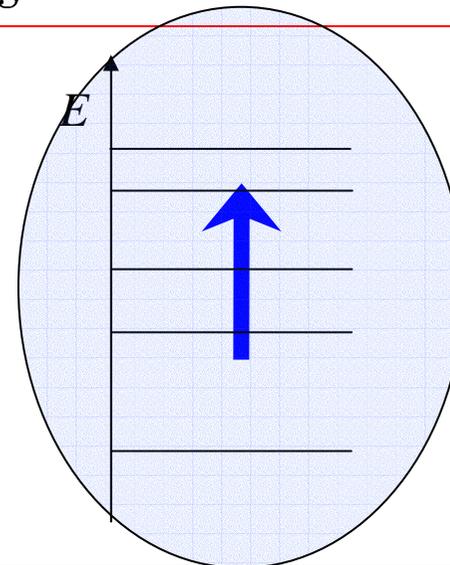
# Kondo problem: s-d Hamiltonian

- Kondo problem: s-wave coupling with spin impurity (s-d model):

$$H_K = \sum_{\mathbf{k}s} \epsilon_{\mathbf{k}s} \hat{n}_{\mathbf{k}s} + J \sum_{\mathbf{k}s; \mathbf{k}'s'} c_{\mathbf{k}s}^\dagger (\mathbf{S} \cdot \vec{\sigma})_{ss'} c_{\mathbf{k}'s'}$$



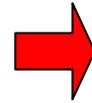
**Metal (non magnetic, s-band)**



**Magnetic impurity (unfilled d-level)**

# Kondo's explanation for $T_{\min}$ (1964)

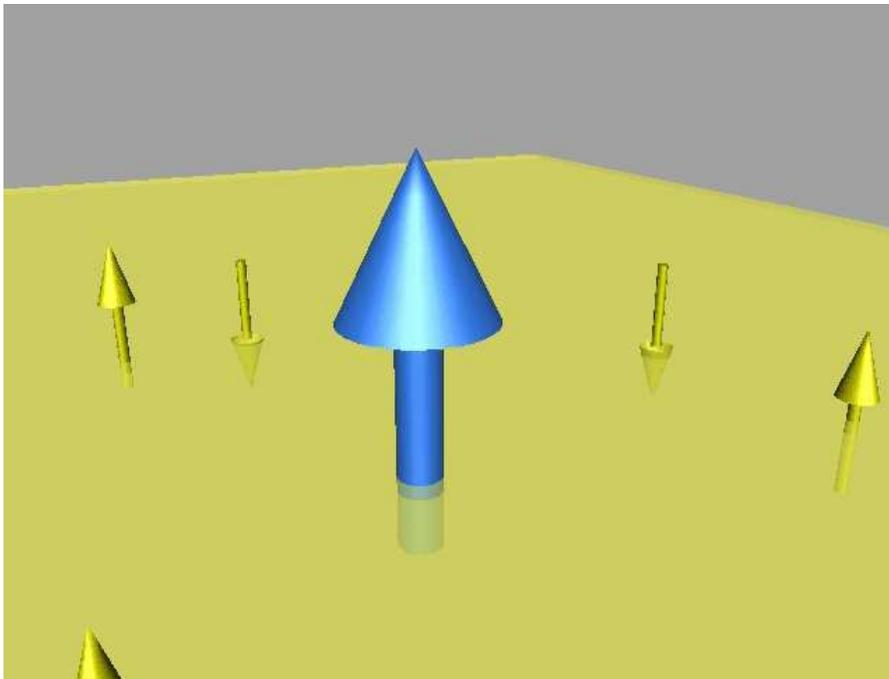
- Perturbation theory in  $J^3$ :
  - Kondo calculated the conductivity in the linear response regime



$$R_{\text{imp}}^{\text{spin}} \propto J^2 \left[ 1 - 4J\rho_0 \log\left(\frac{k_B T}{D}\right) \right]$$

$$R_{\text{tot}}(T) = aT^5 - c_{\text{imp}} R_{\text{imp}} \log\left(\frac{k_B T}{D}\right)$$

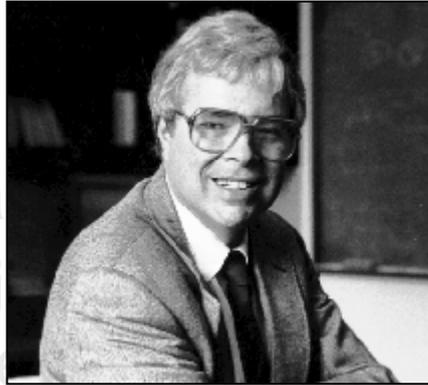
$$T_{\min} = \left( \frac{R_{\text{imp}} D}{5ak_B} \right)^{1/5} c_{\text{imp}}^{1/5}$$



- Only one free parameter: the Kondo temperature  $T_K$ 
  - Temperature at which the perturbative expansion **diverges.**  $k_B T_K \sim D e^{-1/2J\rho_0}$

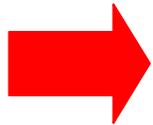
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## A little bit of Kondo history:



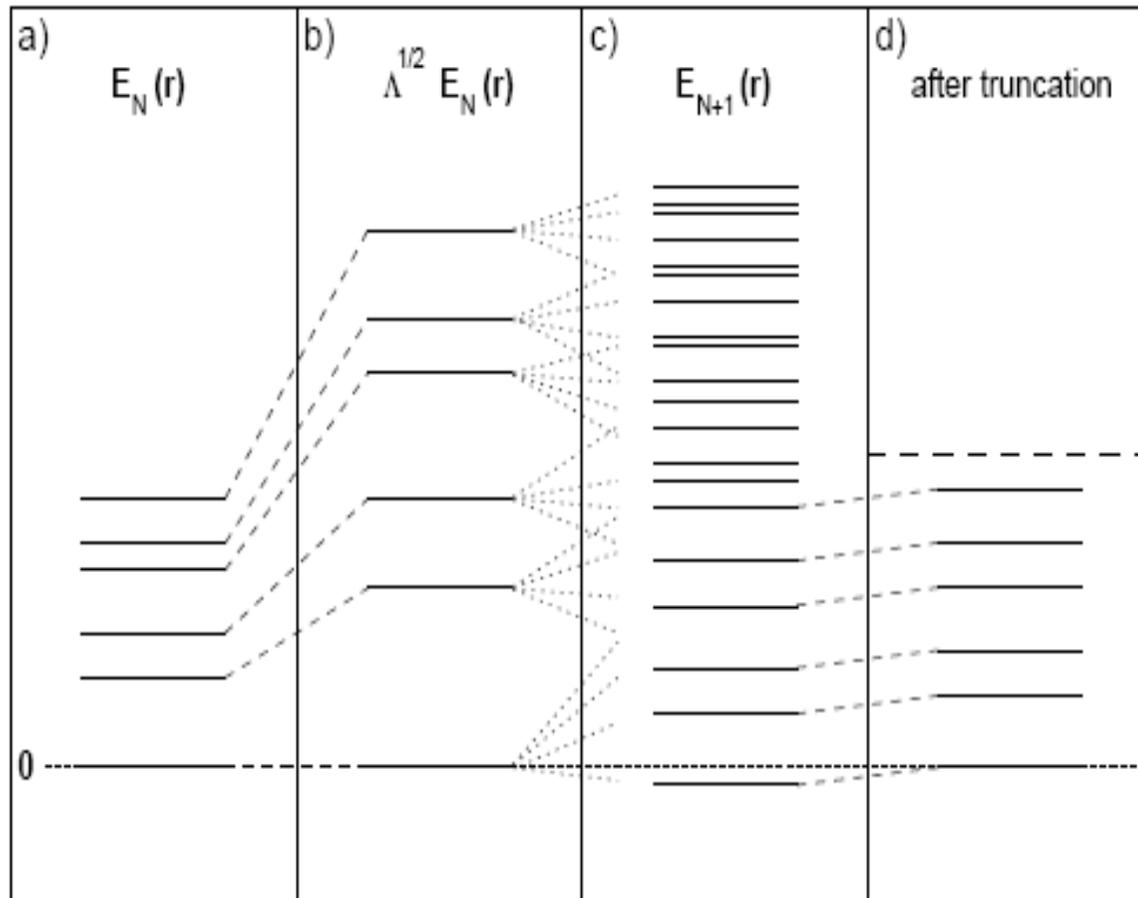
Kenneth G. Wilson – Physics Nobel Prize in 1982  
"for his theory for critical phenomena in connection  
with phase transitions"

- Early '30s : Resistance in some metals
- Early '50s : theoretical impurities in metals  
"Virtual Bound States"
- 1961: Anderson in metals
- 1964: s-d model and Kondo solution (PT)
- 1970: Anderson "Poor's law scaling"
- ➔ 1974-75: Wilson's Numerical Renormalization Group (non PT)
- 1980 : Andrei and Wiegmann's exact solution

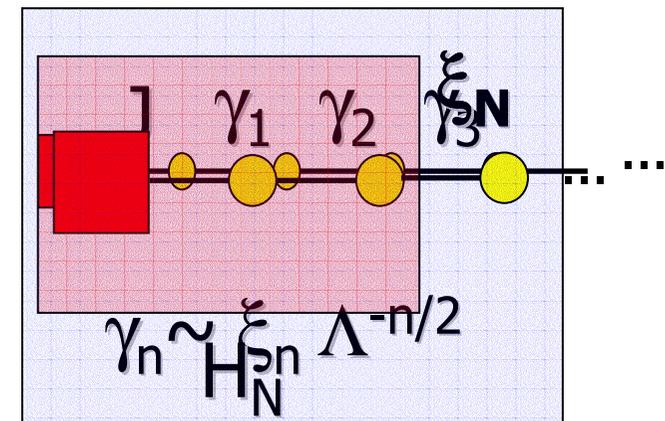


# Renormalization Procedure

$$H_{N+1} = \sqrt{\Lambda} H_N + \xi_N \sum_{\sigma} f_{N+1\sigma}^{\dagger} f_{N\sigma} + f_{N\sigma}^{\dagger} f_{N+1\sigma}$$

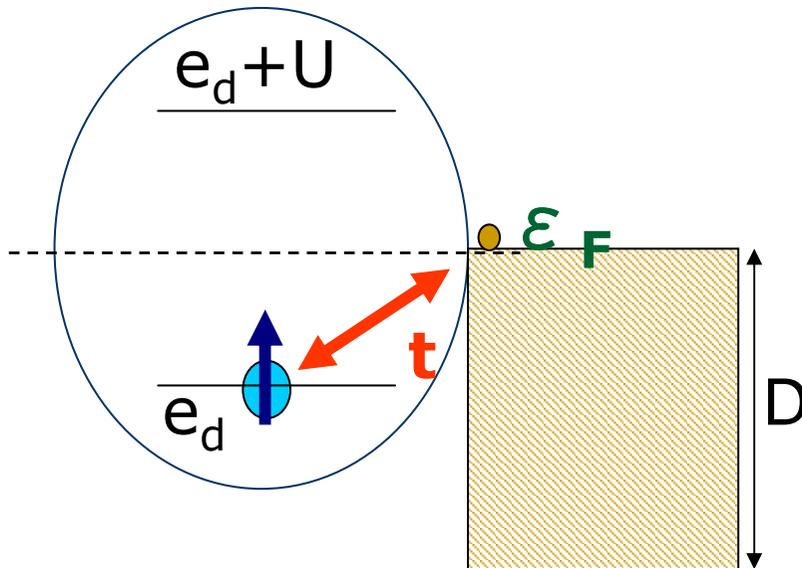


- Iterative numerical solution.
- Renormalize by  $\Lambda^{1/2}$ .
- Keep low energy states.



$H_{N+1}$

# Anderson Model



$$\begin{aligned}
 H = & \epsilon_d \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \\
 & + \sum_k \epsilon_k \hat{n}_{k\sigma} \\
 & + t \sum_k c_{d\sigma}^\dagger c_{k\sigma} + \text{h.c.}
 \end{aligned}$$

with

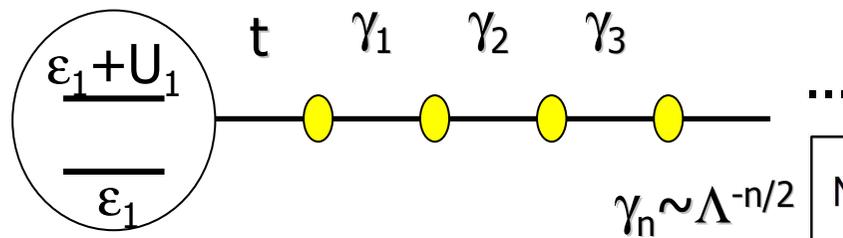
$$\begin{aligned}
 \hat{n}_{d\sigma} &= c_{d\sigma}^\dagger c_{d\sigma} \\
 \hat{n}_{k\sigma} &= c_{k\sigma}^\dagger c_{k\sigma}
 \end{aligned}$$

“Quantum dot language”

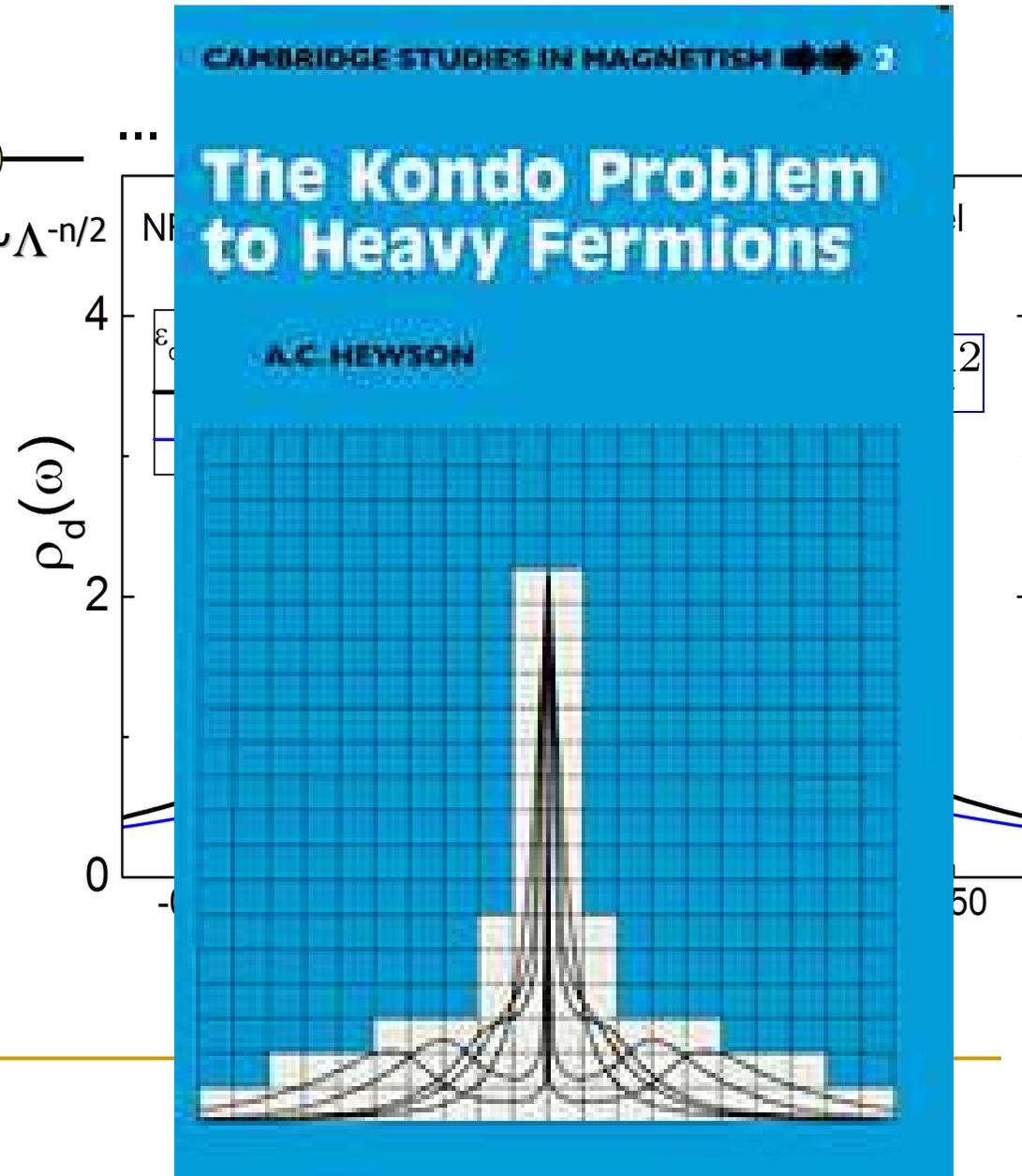
- $e_d$ : energy level
- $U$ : Coulomb repulsion
- $e_F$ : Fermi energy in the metal
- $t$ : Hybridization
- $D$ : bandwidth

- $e_d$ : position of the level ( $V_g$ )
- $U$ : Charging energy
- $e_F$ : Fermi energy in the leads
- $t$ : dot-lead tunneling
- $D$ : bandwidth

# NRG on Anderson model: LDOS



- Single particle peaks at  $\varepsilon_d$  and  $\varepsilon_d + U$ .
- *Many body* peak at the Fermi energy: **Kondo resonance** (width  $\sim T_K$ ).
- NRG: good resolution at low  $\omega$  (log discretization).



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# History of Kondo Phenomena

- Observed in the '30s
- Explained in the '60s
- Numerically Calculated in the '70s (NRG)
- Exactly solved in the '80s (Bethe-Ansatz)

**So, what's new about it?**

## **Kondo correlations observed in many different set ups:**

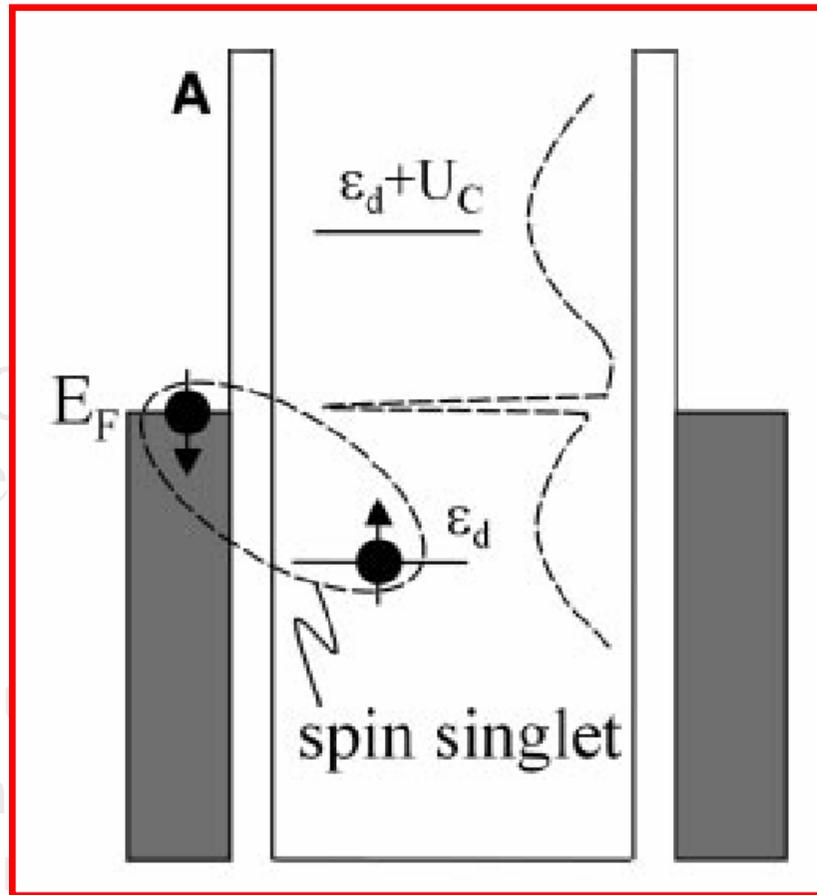
- Transport in quantum dots, quantum wires, etc
  - STM measurements of magnetic structures on metallic surfaces (e.g., single atoms, molecules. "Quantum mirage")
  - ...
-

# History of Kondo Phenomena

- Observed in the '30s
  - Explained in the '60s
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  - Exactly solved in the '80s
- So, what's new?

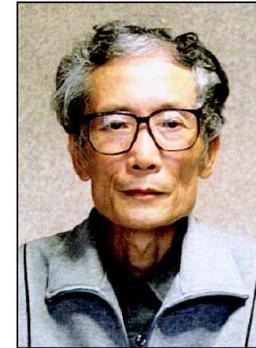
## Kondo correlations observed

- Transport in quantum dots, q
- STM measurements of magn surfaces (e.g., single atoms,
- ...



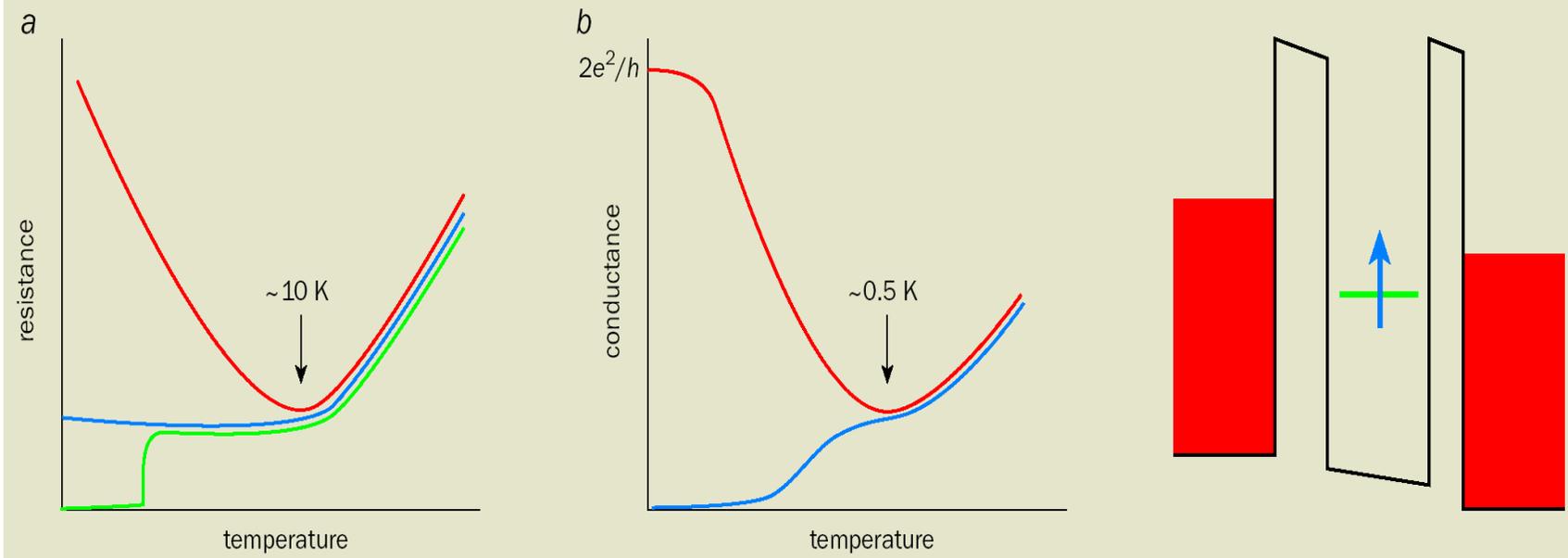
# Kondo Effect in Quantum Dots

## Revival of the Kondo effect



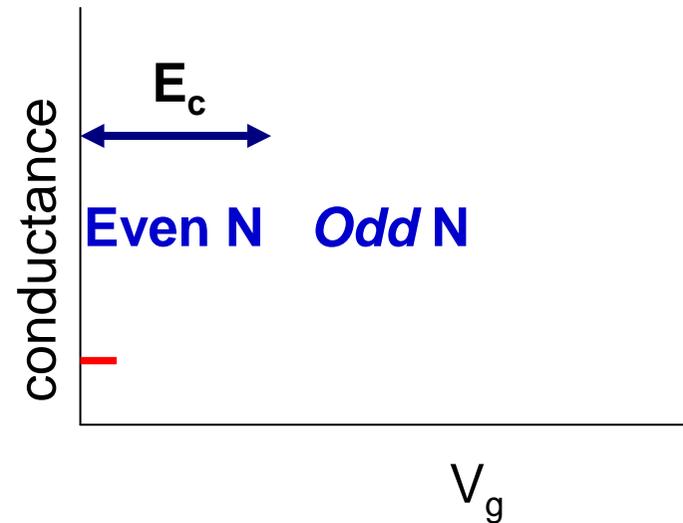
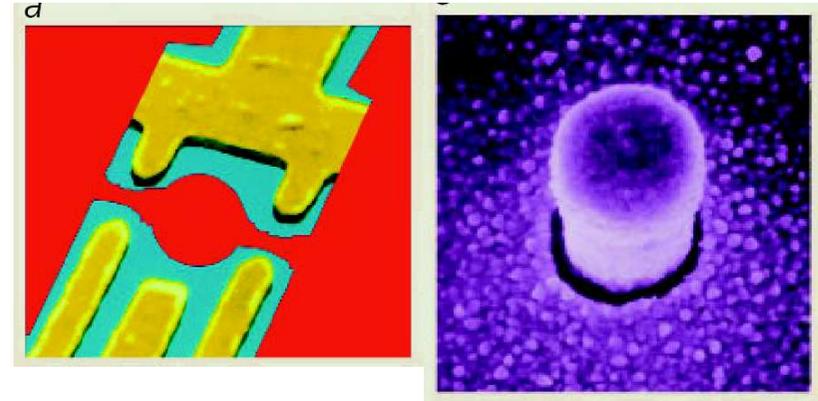
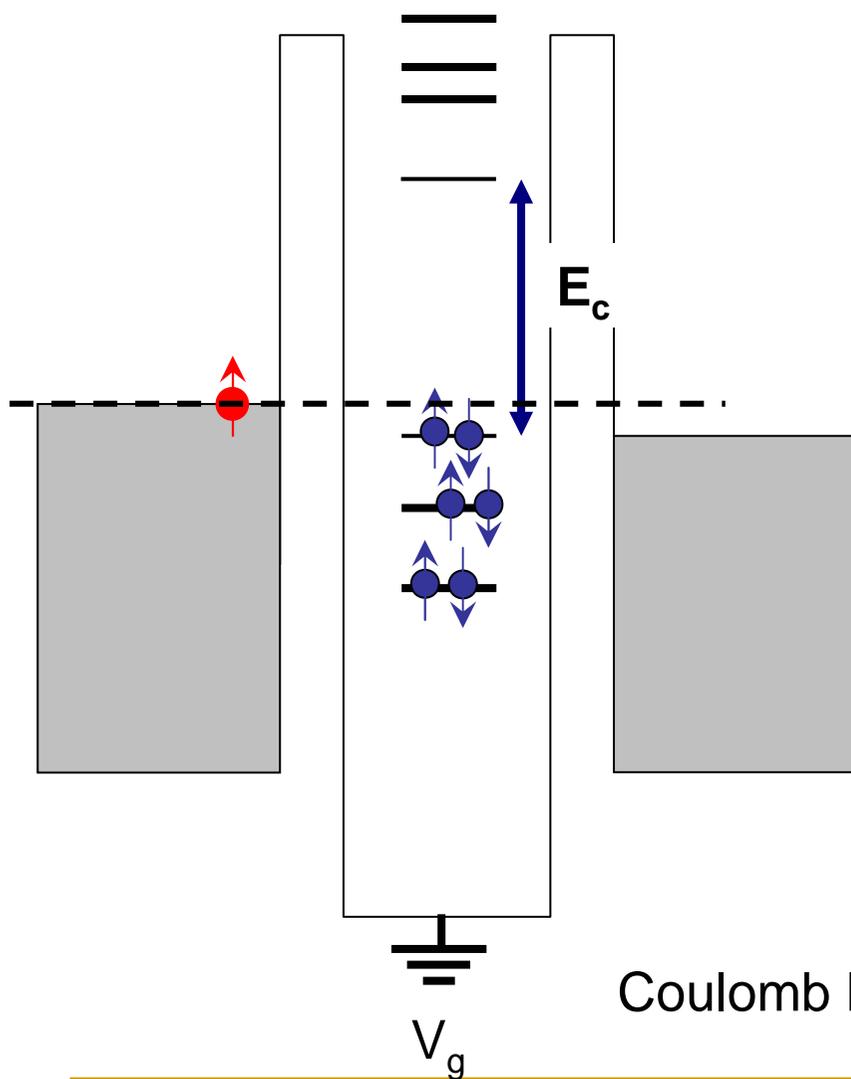
Leo Kouwenhoven and Leonid Glazman

### 1 The Kondo effect in metals and in quantum dots



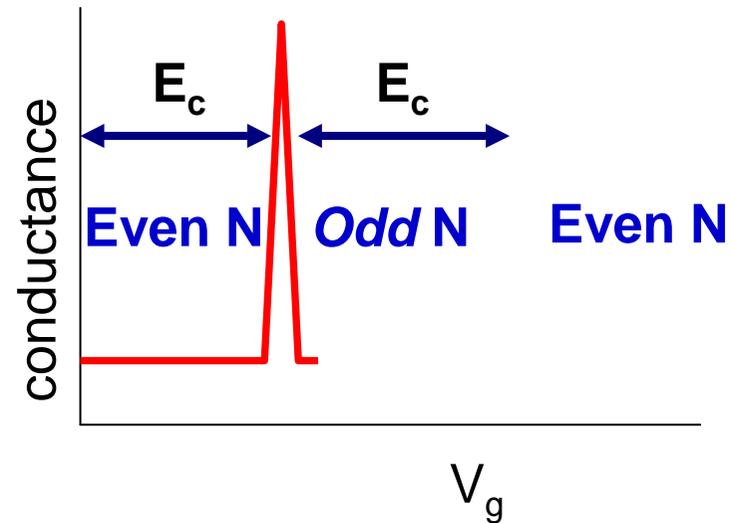
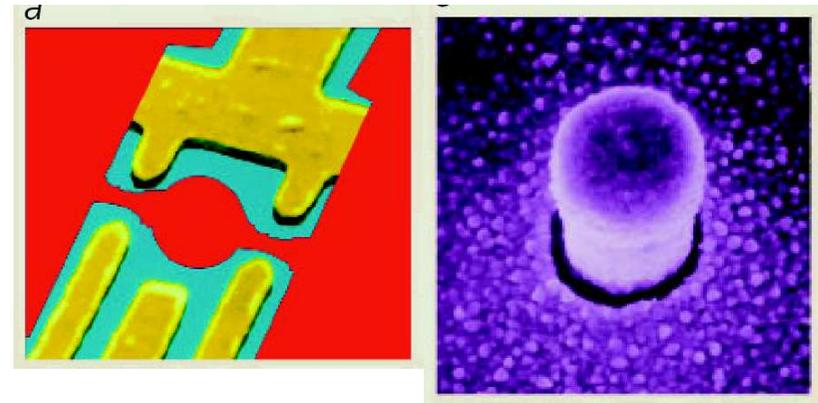
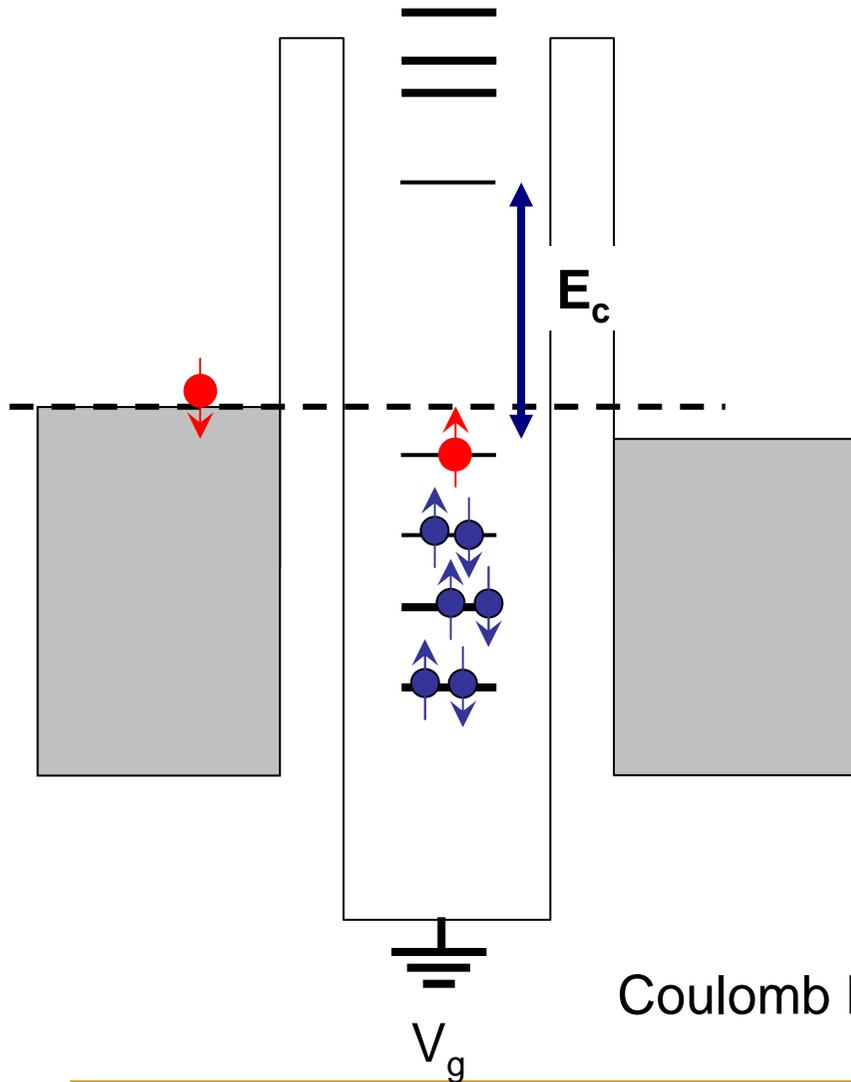
Kouwenhoven and Glazman *Physics World* – Jan. 2001.

# Coulomb Blockade in Quantum Dots



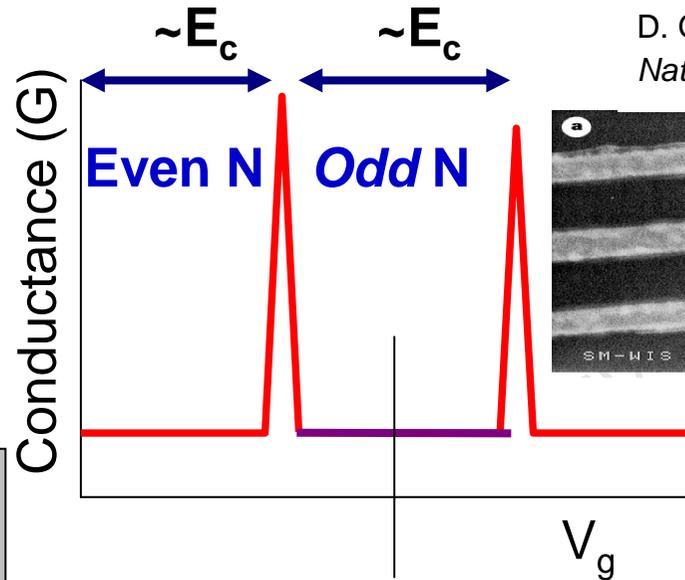
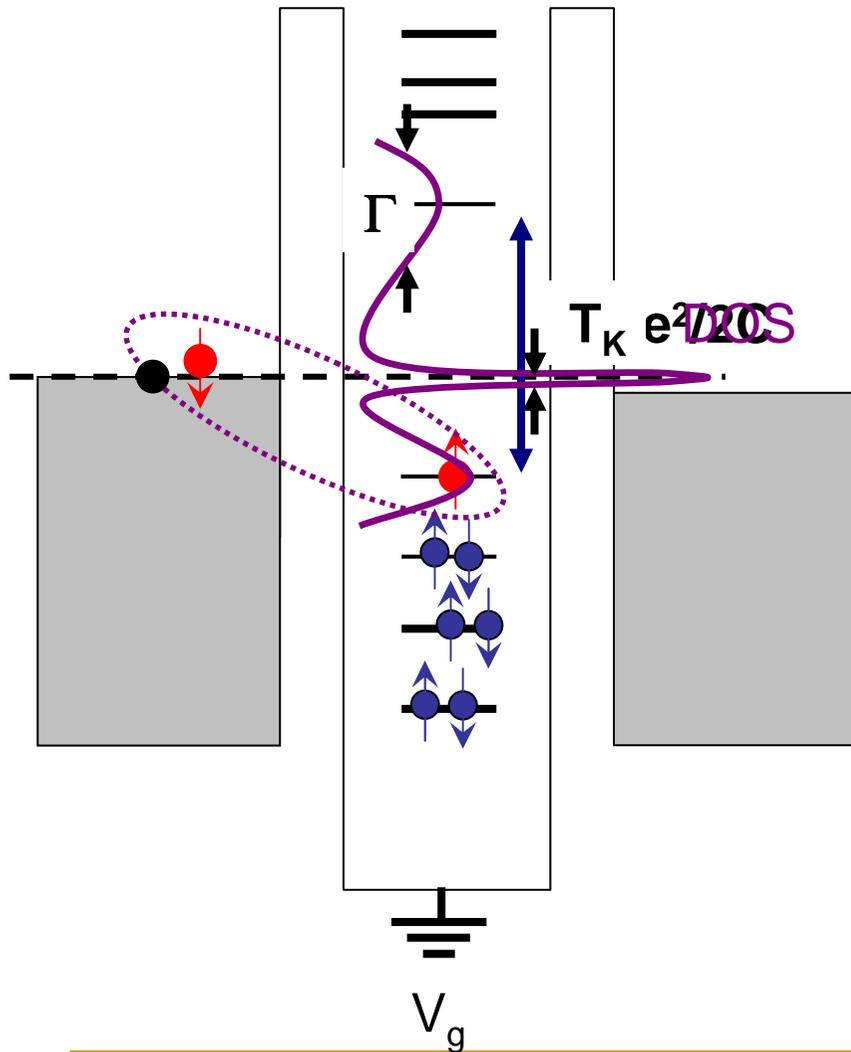
Coulomb Blockade in Quantum Dots

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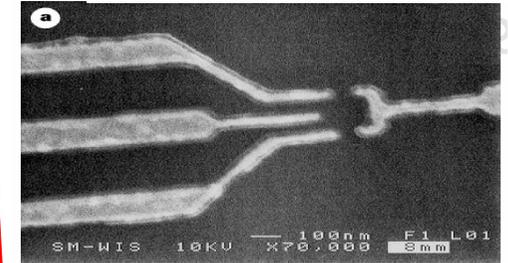


Coulomb Blockade in Quantum Dots

# Kondo Effect in Quantum Dots



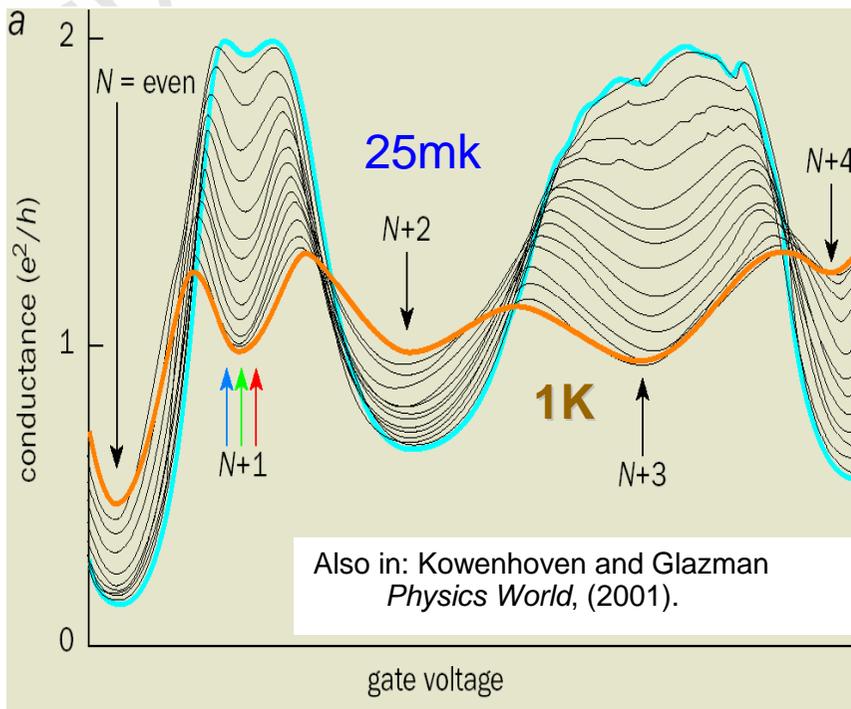
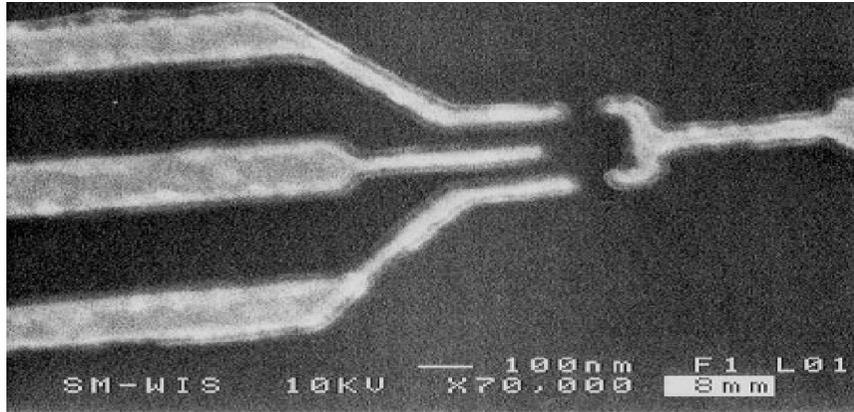
D. Goldhaber-Gordon et al  
*Nature* **391** 156 (1998)



- $T > T_K$ : Coulomb blockade (**low G**)
- $T < T_K$ : Kondo singlet formation
- **Kondo resonance** at  $E_F$  (width  $T_K$ ).
- New conduction channel at  $E_F$ :  
**Zero-bias enhancement of G**

# Kondo effect in Quantum Dots

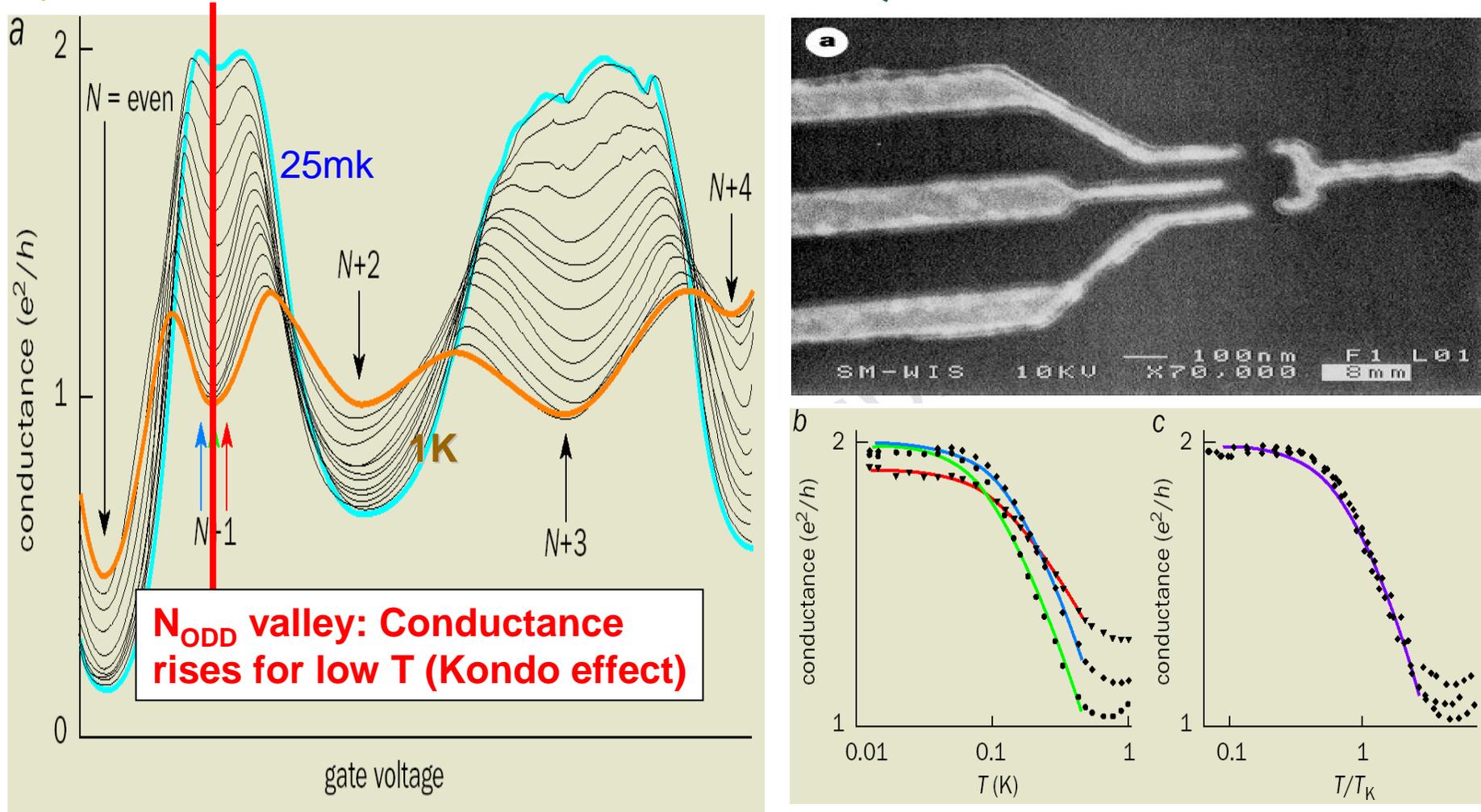
D. Goldhaber-Gordon et al. Nature **391** 156 (1998)



Semiconductor Quantum Dots:

- Allow for systematic and *controllable* investigations of the Kondo effect.
- QD in  $N_{\text{odd}}$  Coulomb Blockade valley: realization of the Kondo regime of the Anderson impurity problem.

# Kondo Effect in CB-QDs



Kondo Temperature  $T_K$ : only scaling parameter ( $\sim 0.5\text{K}$ , depends on  $V_g$ )

Kowenhoven and Glazman *Physics World* – Jan. 2001.

From: Goldhaber-Gordon *et al. Nature* **391** 156 (1998)

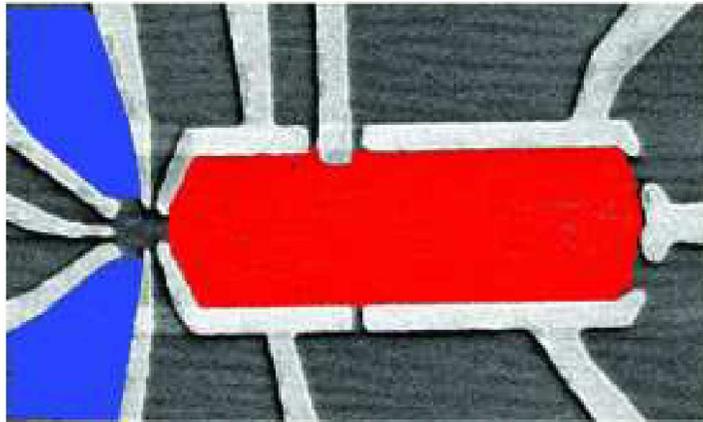
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## Examples of “fundamental” physics (in the “More is Different” sense) we can learn from quantum dots:

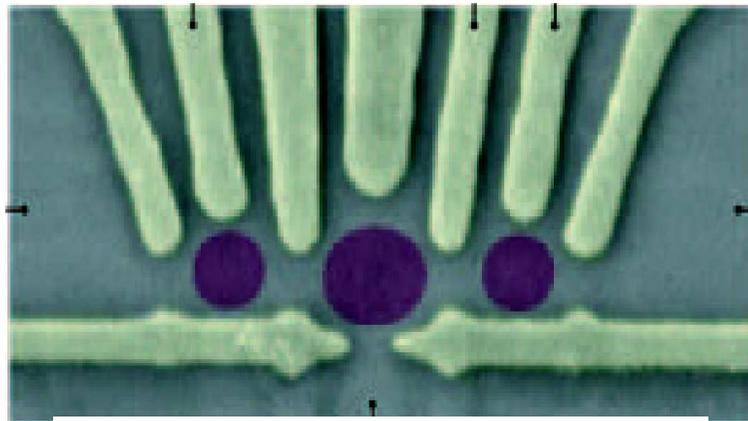
- *Strongly correlated effects*: Charging effects due to electron-electron interactions are dominant in QDs.
  - *Quantum effects* (spin, tunneling, discrete energy levels, interference) probed in a very controllable way.
  - **Quantum Many-body physics**:
    - **Kondo effect**, Quantum phase transitions, ...
-

# Kondo Effect in *Double* QDs

“Side dot” configuration

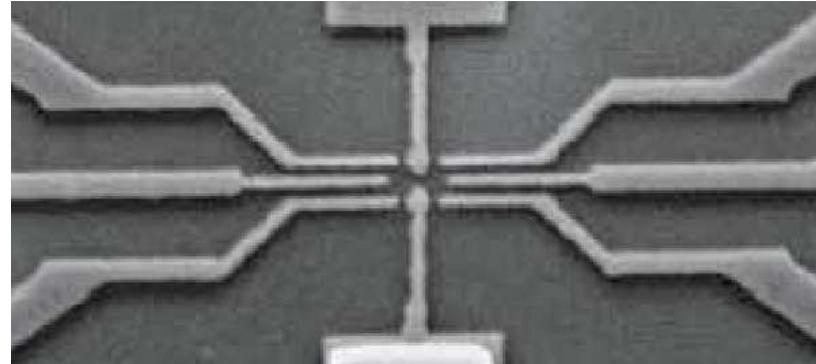


R. Potok *et al.* *Nature* 446 167 (2007).



Craig *et al.*, *Science* 304 565 (2004)

“Parallel” configuration

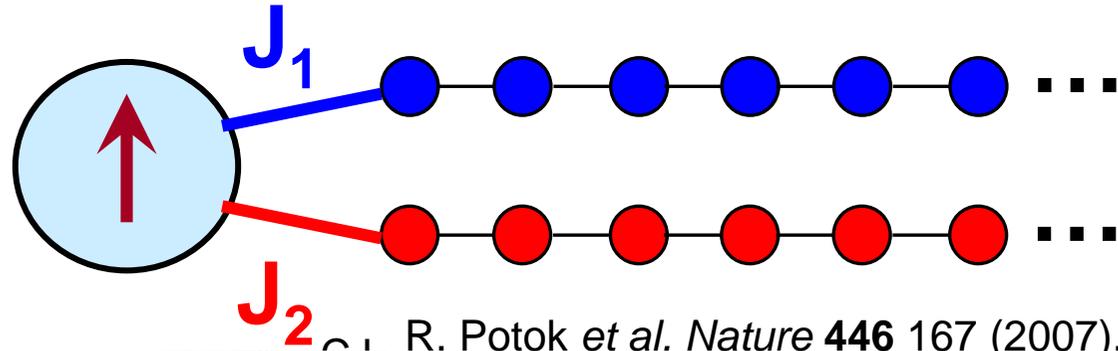


Chen, Chang, Melloch, *PRL* 92 176801 (2004)

- Tunability of **intradot** and **interdot** parameters (couplings, gate voltage).
- Prospects for experimental probe of many-body phenomena, e.g:
  - SU(4) Kondo, RKKY interactions,...
  - Non-Fermi liquid physics (2-ch Kondo)
  - **Quantum phase transitions.**

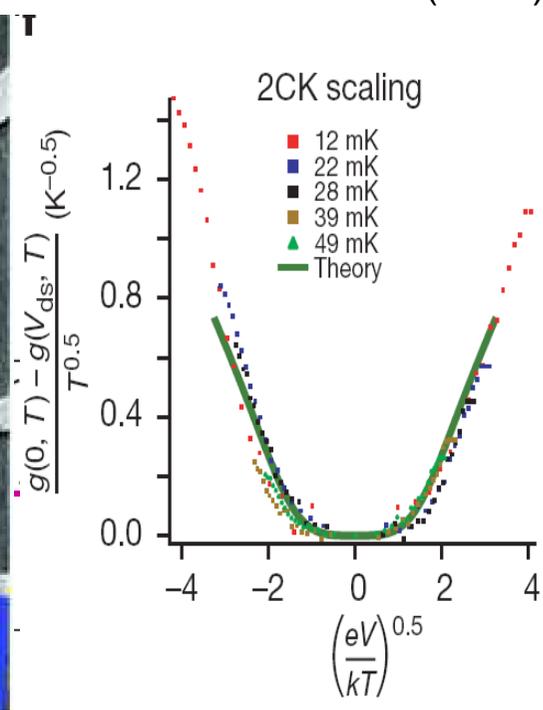
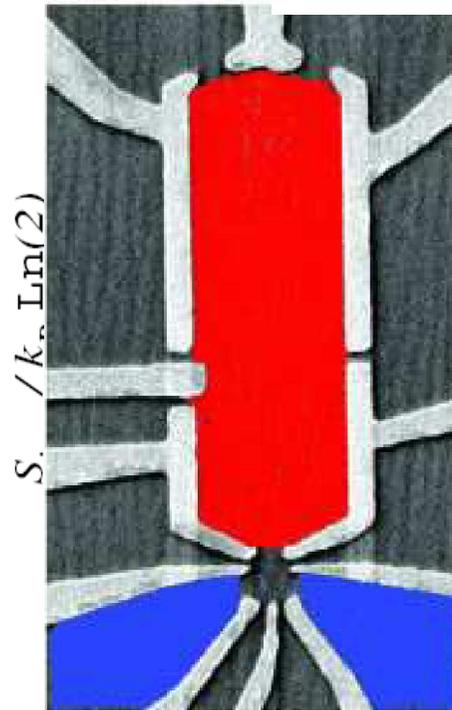
# Two-channel Kondo effect.

- Spin 1/2 coupled to two **independent** bands: 2-channel Kondo model ("overscreened").

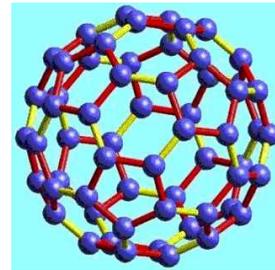
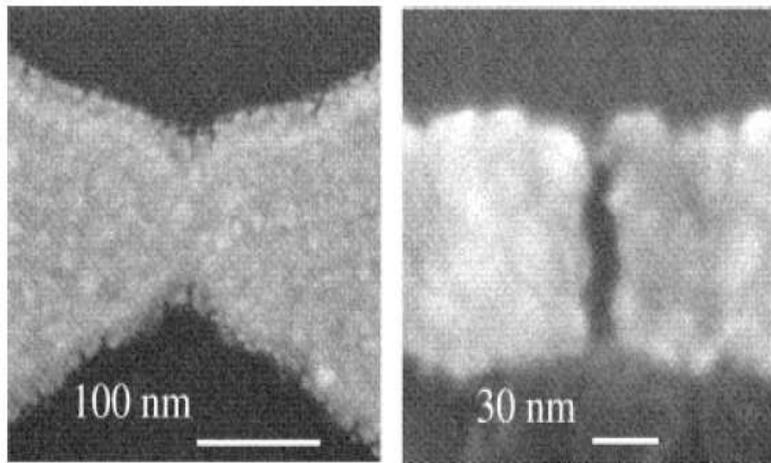


R. Potok et al. Nature 446 167 (2007).

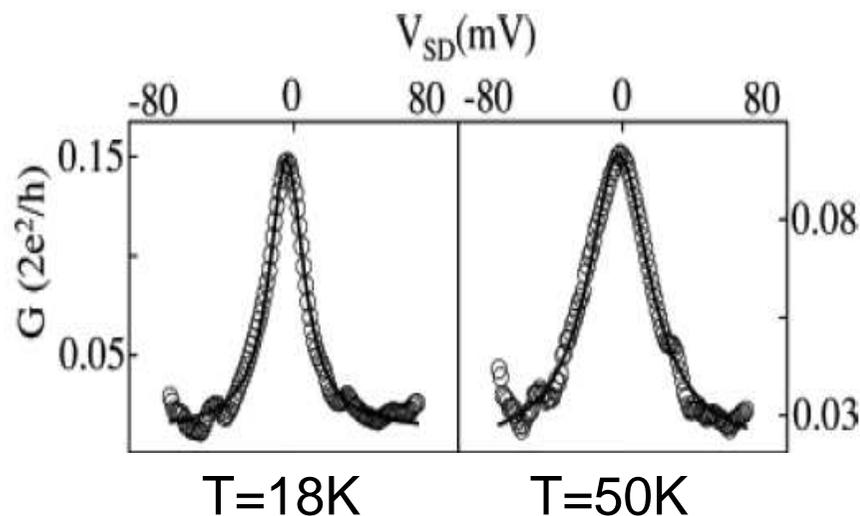
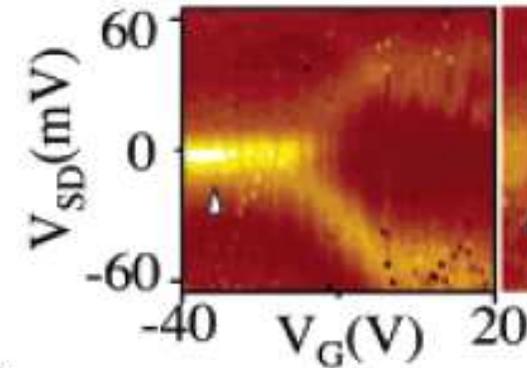
- Non Fermi liquid (NFL) behavior for  $J_1 = J_2$ .
- Impurity entropy (NFL):  
 $S_{\text{imp}} = k_B \log(\sqrt{2})$   
 (NRG, Bethe ansatz).
- Recent expts in q dots.



# Kondo effect in Single Molecule Transistors



$C_{60}$

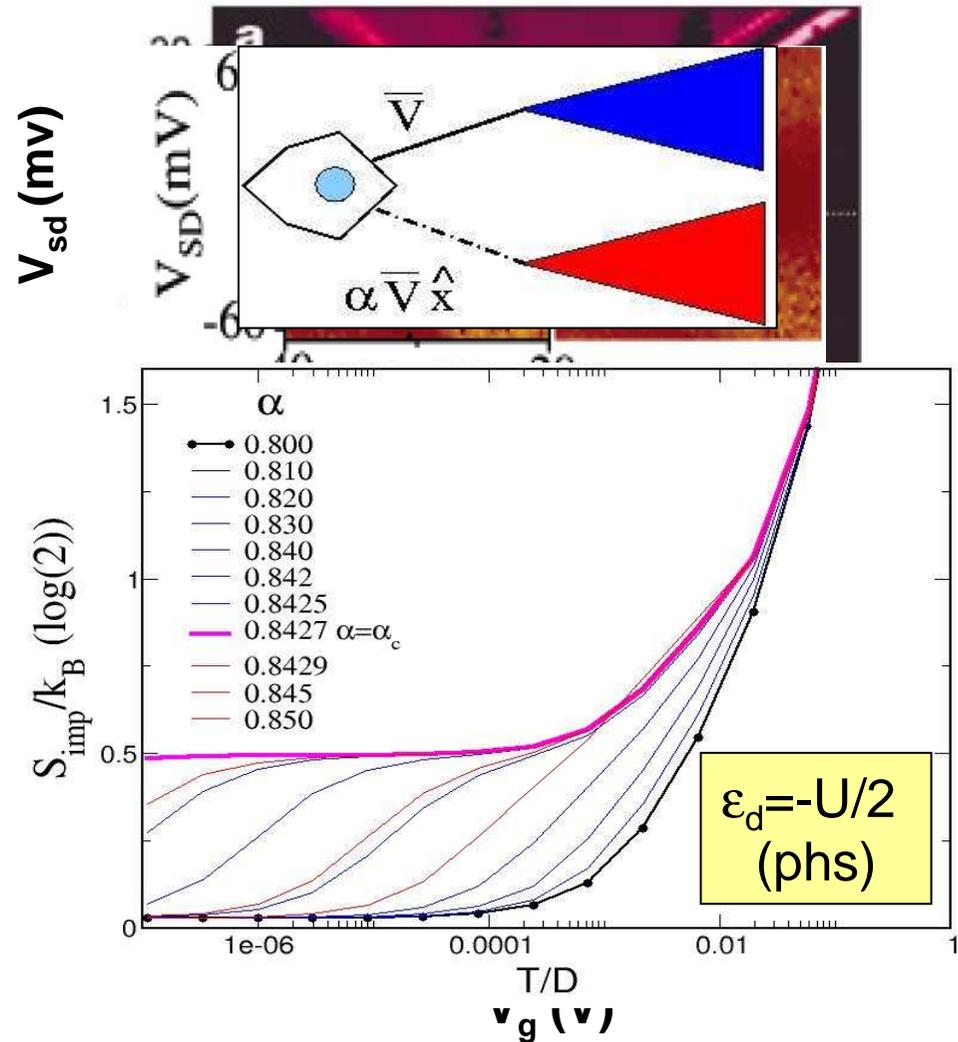
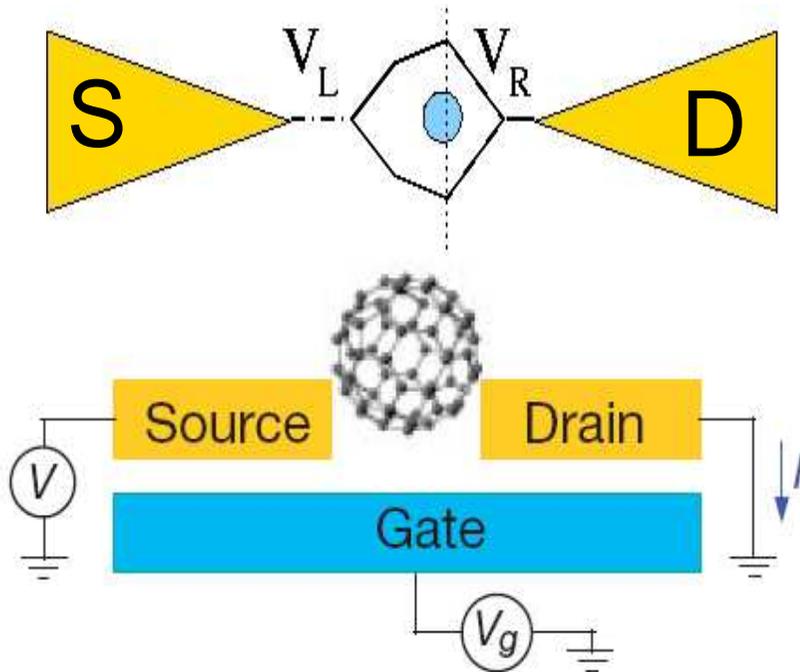


- Single molecule transistors:  $C_{60}$  molecules “caught” between electrodes (break junction).
- Zero-bias peak as a function of gate voltage: correct Kondo scaling.
- Correct behavior vs. Bias.
- $T_K > 50K$ .

Yu, Natelson, *NanoLett.* **4** 79 (2004).

# Transport in molecular junctions.

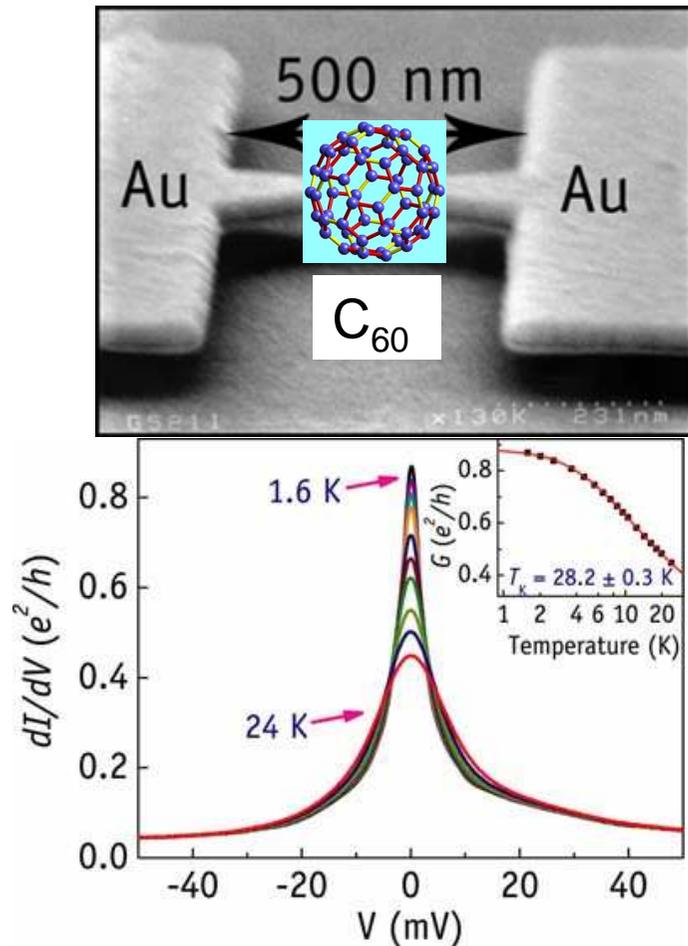
- Coulomb blockade effects .
- Features consistent with vibrational modes in  $dI/dV$ .
- Kondo signatures.



Park et al. *Nature* **407** 57 (2000)

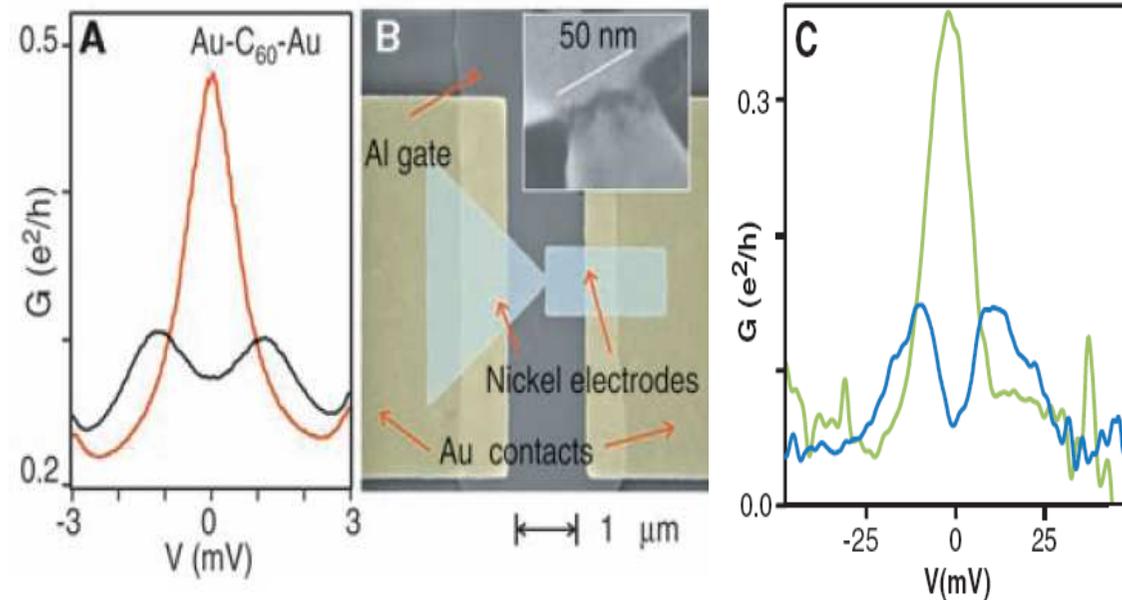
Connection of vibrational modes with 2-channel Kondo:  
 LDS, E. Dagotto – PRB **79** 155302 (2009); arXiv:0902.3225.

# Kondo effect in Single Molecule Transistors



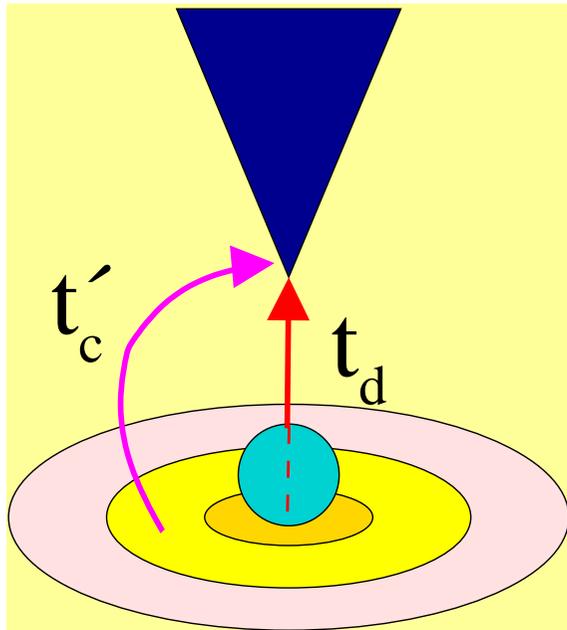
From Dan Ralph's webpage:  
<http://people.ccmr.cornell.edu/~ralph/>

Pasupathy et al., *Science* **306** 86 (2004)



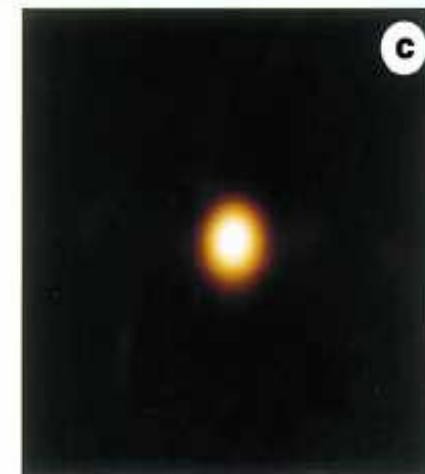
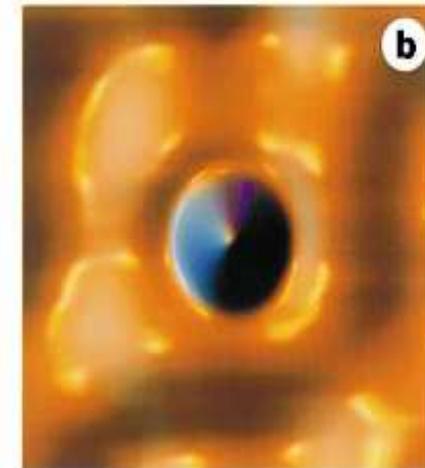
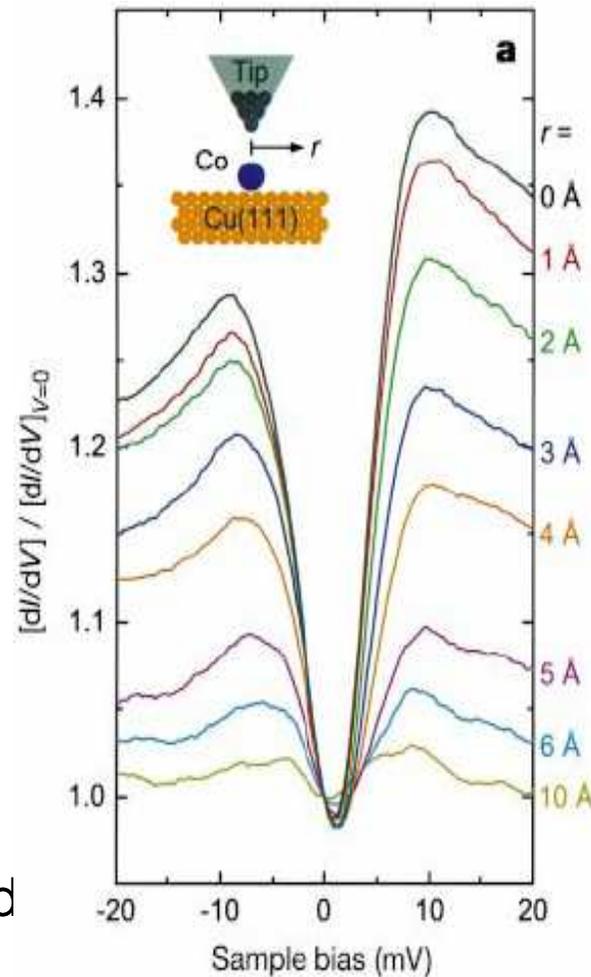
- Similar expts (D. Ralph's group).
- Suppression of the Kondo resonance in the presence of a **magnetic field** (top left, black curve,  $B=10$ T) and **magnetic leads** (top right, parallel [green] and antiparallel [blue] magnetizations).

# Kondo effect in surfaces (STM images).

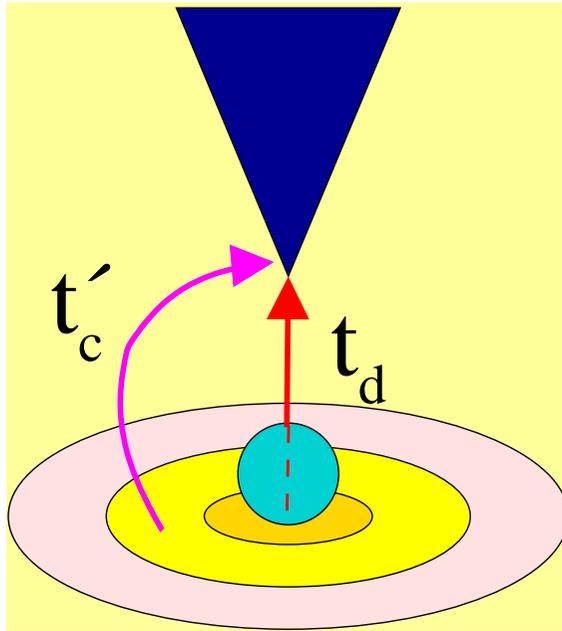


- Magnetic (Co, Fe) atoms on metallic *surfaces*! Right ingredients for Kondo.
- In this case, Kondo is marked by a *dip* at zero-bias conductance ( $dI/dV$  at  $V=0$ ).

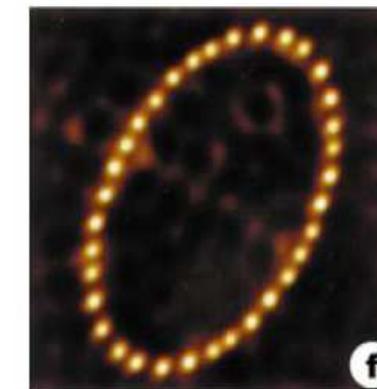
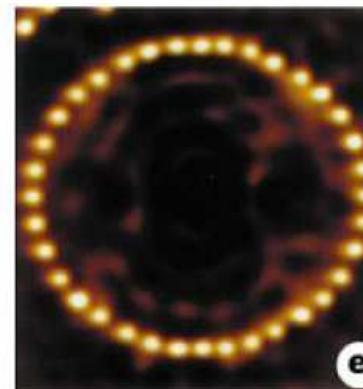
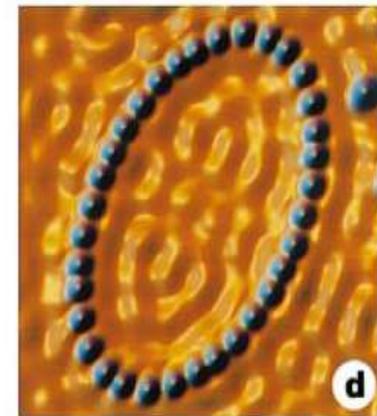
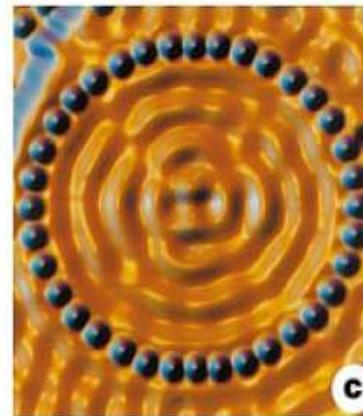
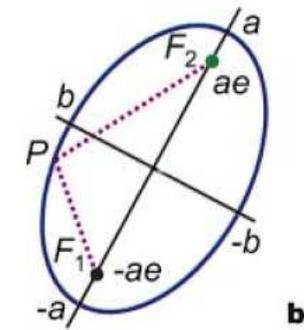
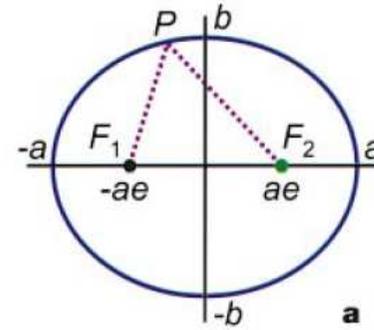
Manoharan et al., *Nature* **403** 512 (2000).



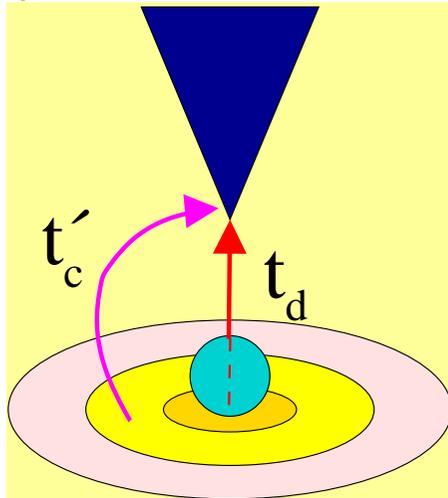
# Kondo effect surfaces: STM measurements.



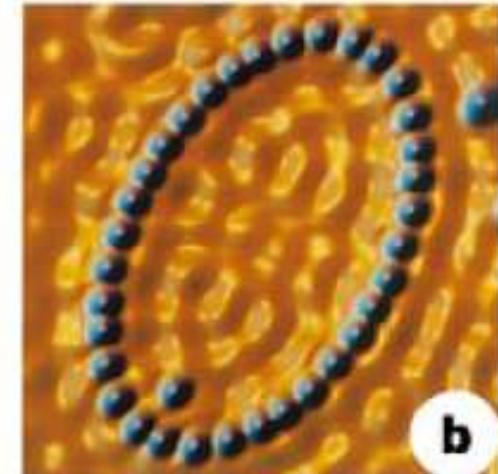
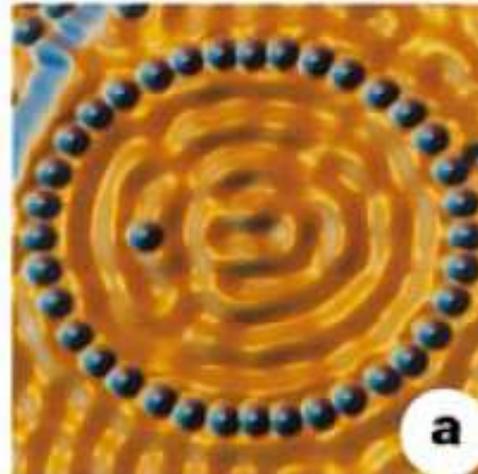
- STM atomic manipulation: can build local structures (“quantum corrals”).
- Elliptical shape: **imaging** (top) and  **$dI/dV$**  measurements (bottom).
- Cobalt atoms on Cu(111) shown.



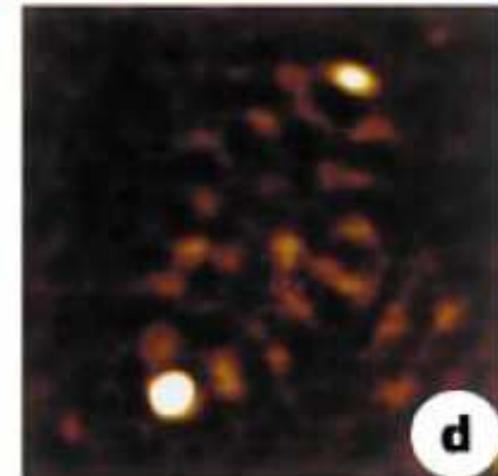
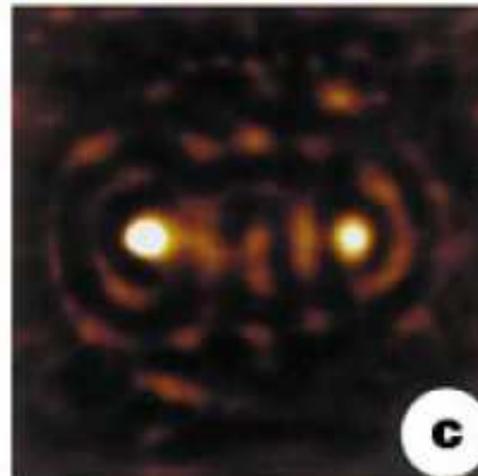
# Kondo effect surfaces: STM measurements.



Manoharan et al., *Nature* **403** 512 (2000).



- One extra atom placed in one foci: a **peak in the  $dI/dV$**  appears in the other focus although **NO ATOM** is there! (“quantum mirage”).
- Theory: “focusing” of Kondo-scattered surface electrons\*.

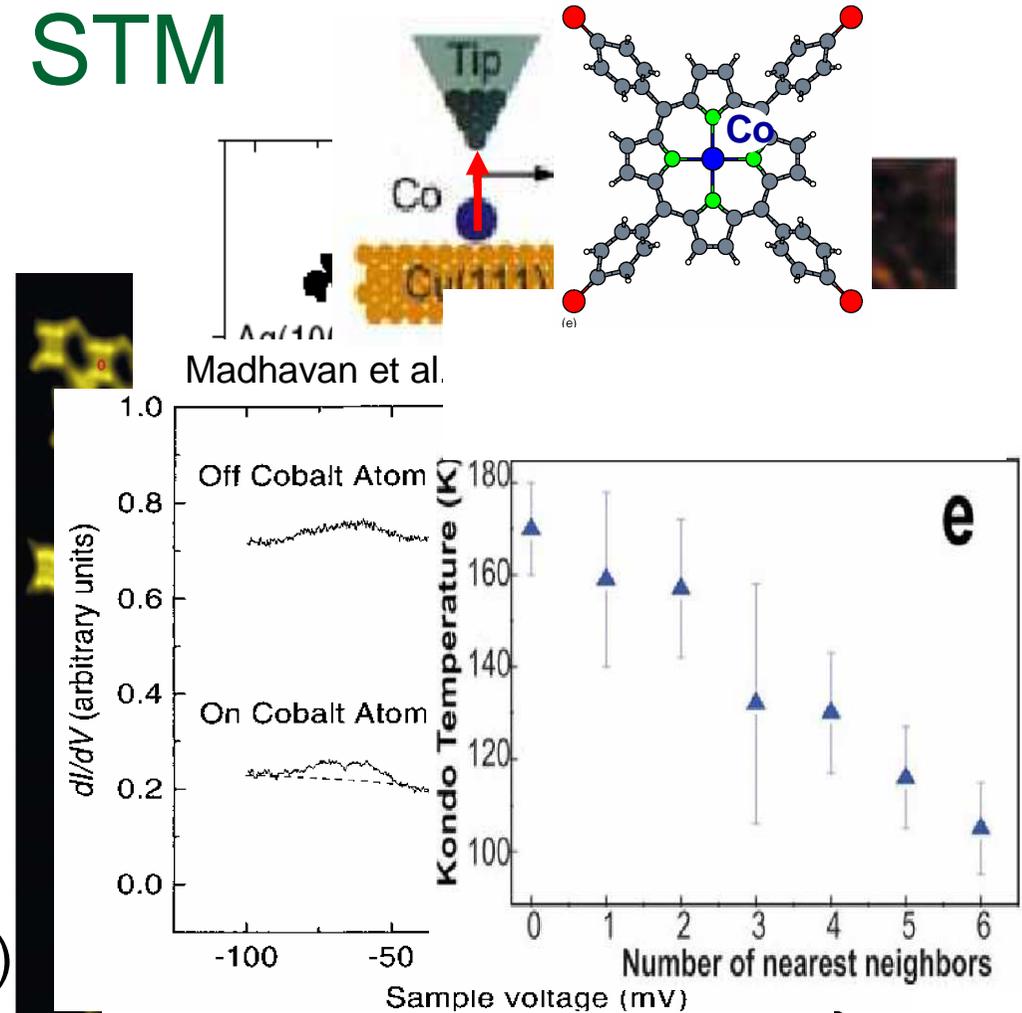


\*Schiller and Agam, *PRL* **86** 484 (2001)..

# Magnetic impurities on metallic surfaces: Kondo + STM

Kondo/Fano phenomenology quite generic:

- Early experiments: Co on Au(111)
- Co on Cu(111): “Quantum mirage”
- Co on different surfaces: Cu(100), Ag(111), Ag(100),...
- Magnetic *molecules* on Cu(111)  
Control of the Kondo temperature by atomic manipulation.

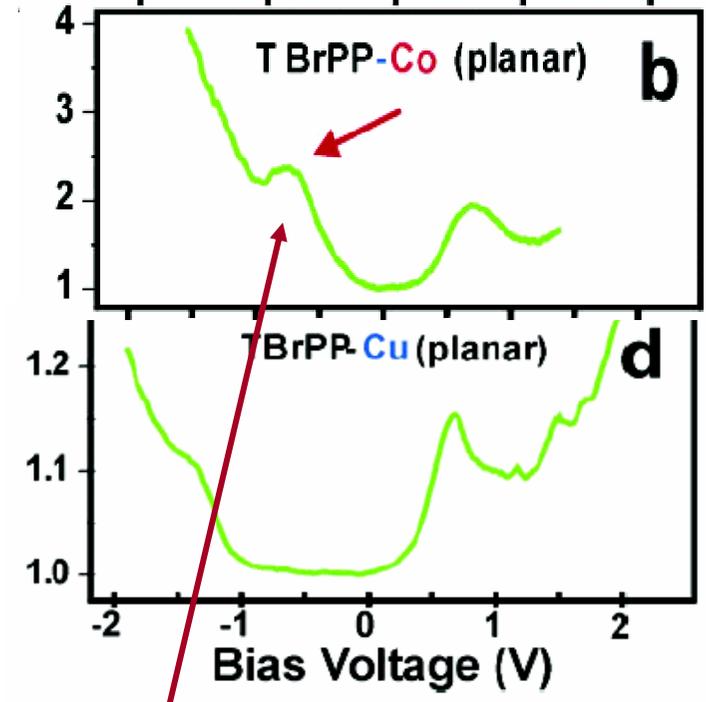
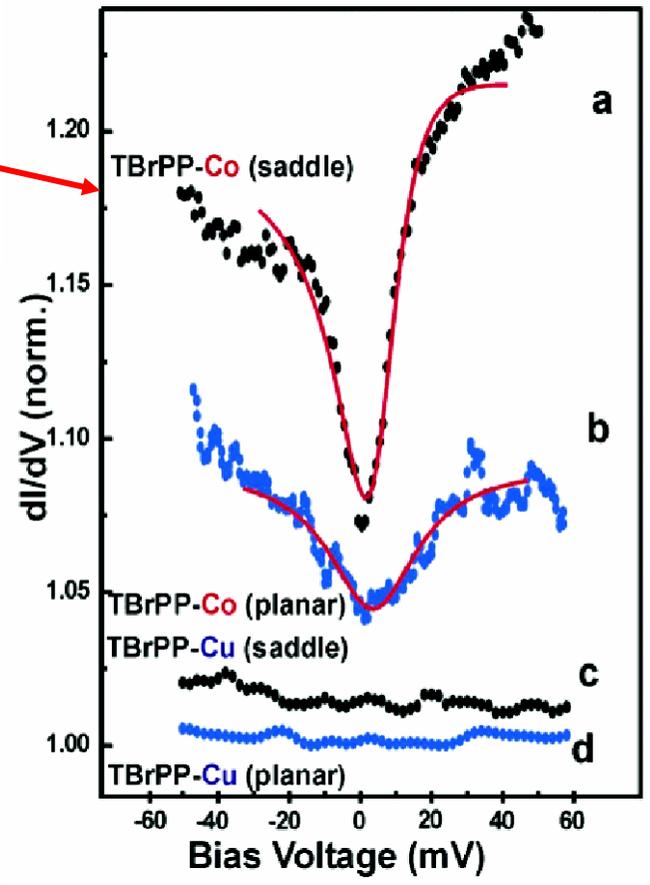
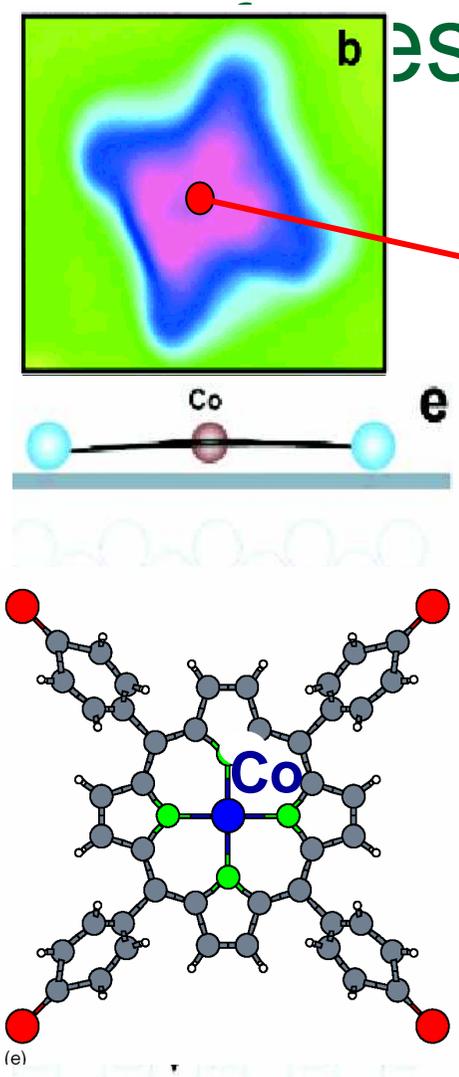


# Kondo: Magnetic molecules on

## STM measurements

V. Iancu, A. Deshpande, Saw W. Hla

Nano Lett. 6, 929 (2006)



Co  $d_{3z^2-1}$  level (at  $\sim -0.7$  eV)

Zero-bias dip: Kondo effect.  $T_K \sim 130-170$  K

# First-principles calculations (GW): hints for a microscopic model.

Model: Anderson-like Hamiltonian

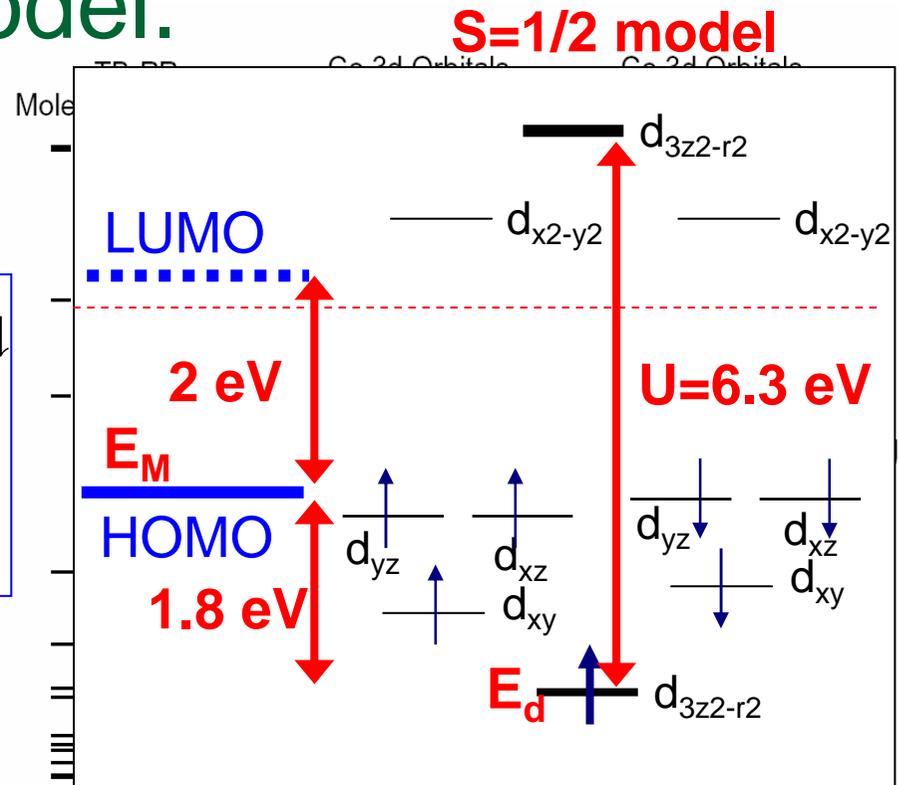
$$H = H_{\text{Molecule}} + H_{\text{Mol-Surface}}$$

$$H_{\text{Molecule}} = \sum_{\sigma} E_d \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{\sigma} E_M \hat{n}_{M\sigma}$$

**OK!**

$$H_{\text{Mol-Surf}} = \sum_{\mathbf{k}, \sigma} V_{d\mathbf{k}} c_{d\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \sum_{M\mathbf{k}, \sigma} V_{M\mathbf{k}} c_{M\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \text{h.c.}$$

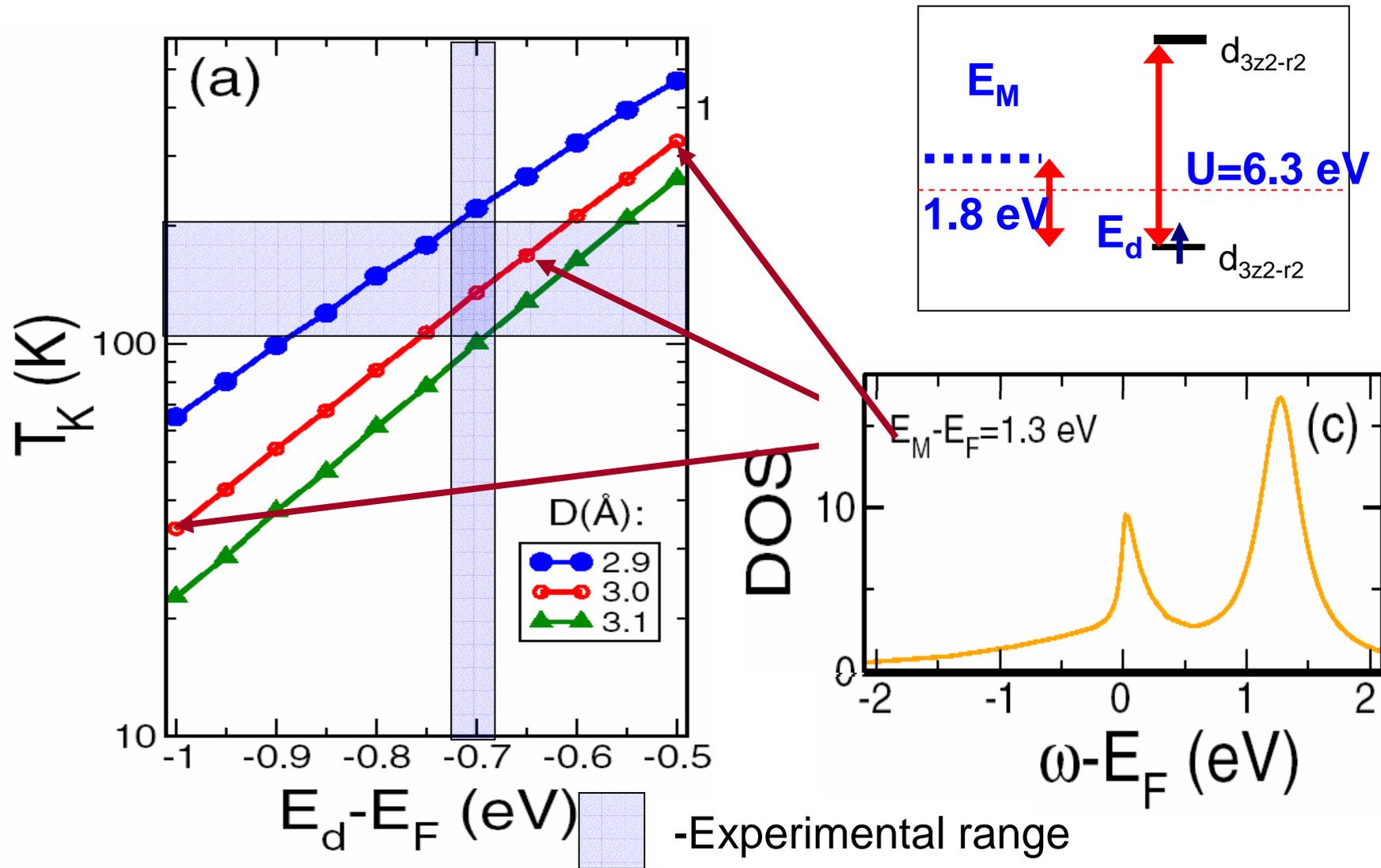
$$V_{d(M)\mathbf{k}} = \langle \phi_{d(M)} | \hat{H} | \psi_{\mathbf{k}} \rangle$$



GW: Molecular levels "Co-like" levels

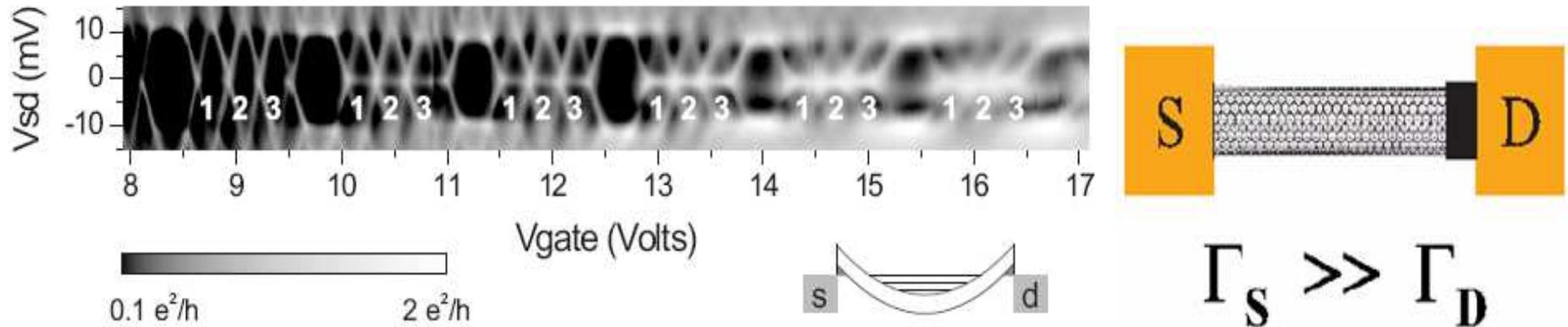
← Not easy to calculate with GW!

# NRG calculations (Kondo temperature).



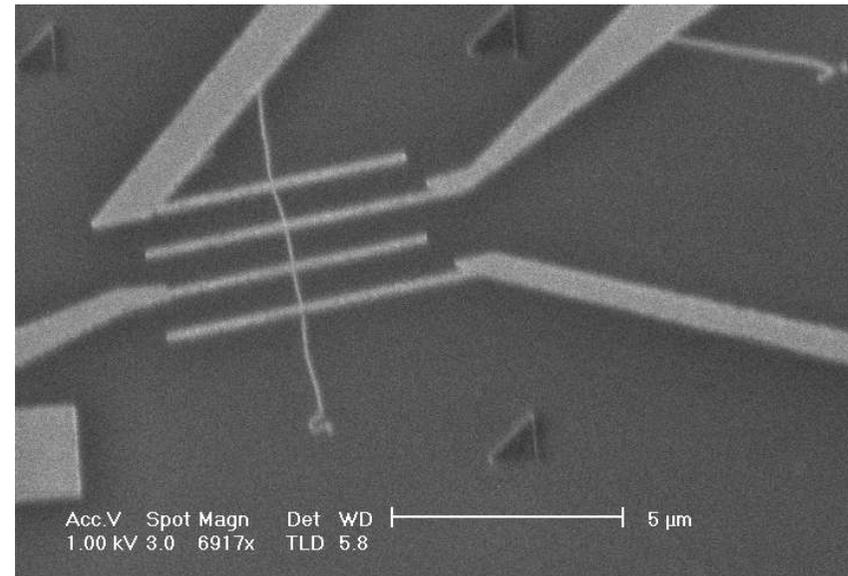
LDS, M Tiago, S Ulloa, F Reboredo E. Dagotto *PRB* **80** 155443 (2009).

# Kondo effect In Carbon nanotubes.



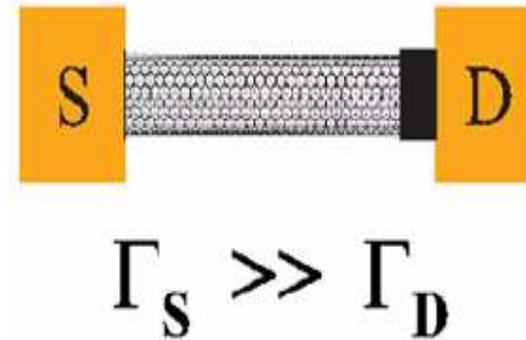
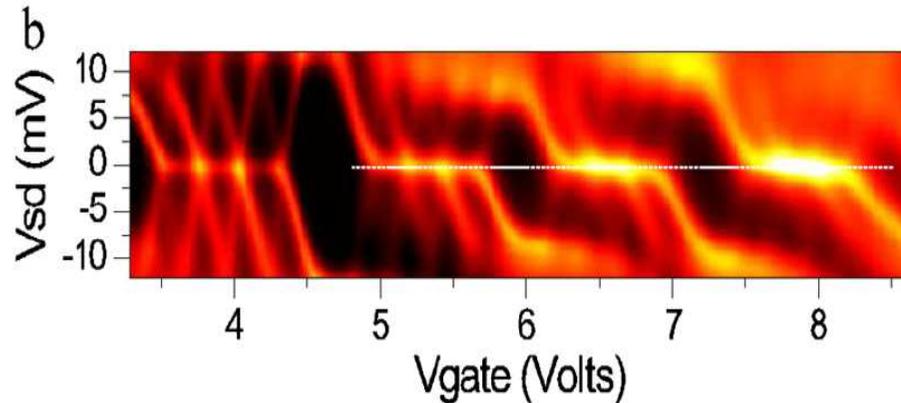
Makarovski, Zhukov, Liu, Filkenstein *PRB* **75** 241407R (2007).

- Carbon nanotubes deposited on top of metallic electrodes.
- Quantum dots defined *within* the carbon nanotubes.
- More structure than in quantum dots: “shell structure” due to *orbital* degeneracy.

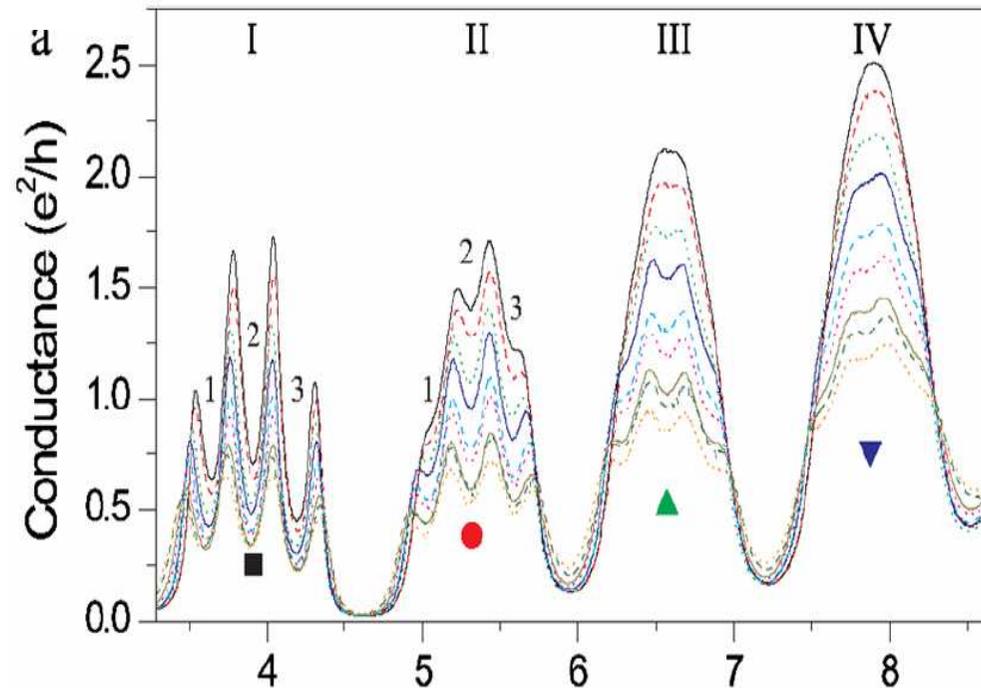


Gleb Filkenstein's webpage: <http://www.phy.duke.edu/~gleb/>

# Kondo effect In Carbon nanotubes.



- Temperature behavior is Kondo-like.
- Interesting *merging of the four shells* at high  $V_g$  (“SU(4)” Kondo instead of the usual SU(2) Kondo).
- NRG calculations\* support that picture.

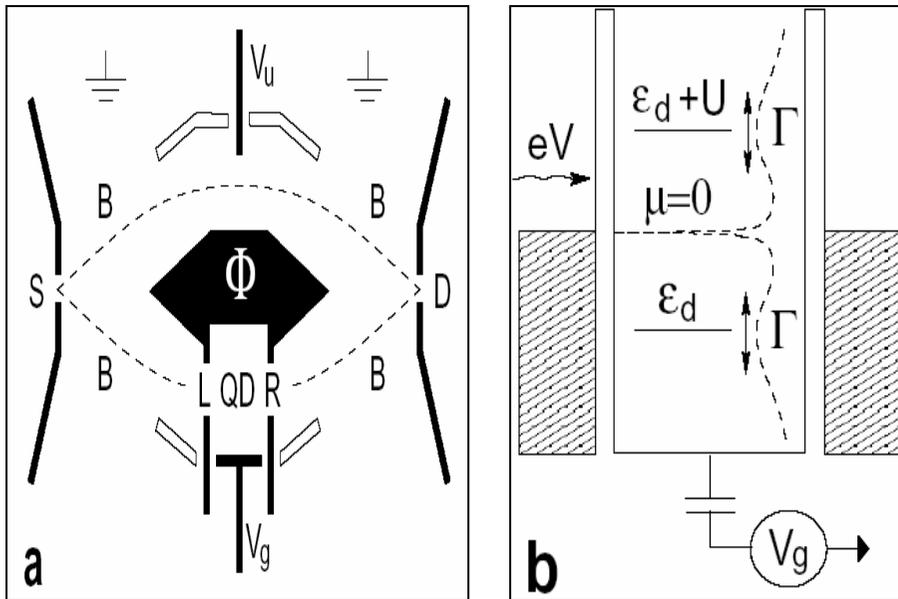


Makarovski, Liu, Filkenstein *PRL* **99** 066801 (2007).

\* Anders, Logan, Galpin, Filkenstein *PRL* **100** 086809 (2008).

# More “Theory-Experiment ballgame”

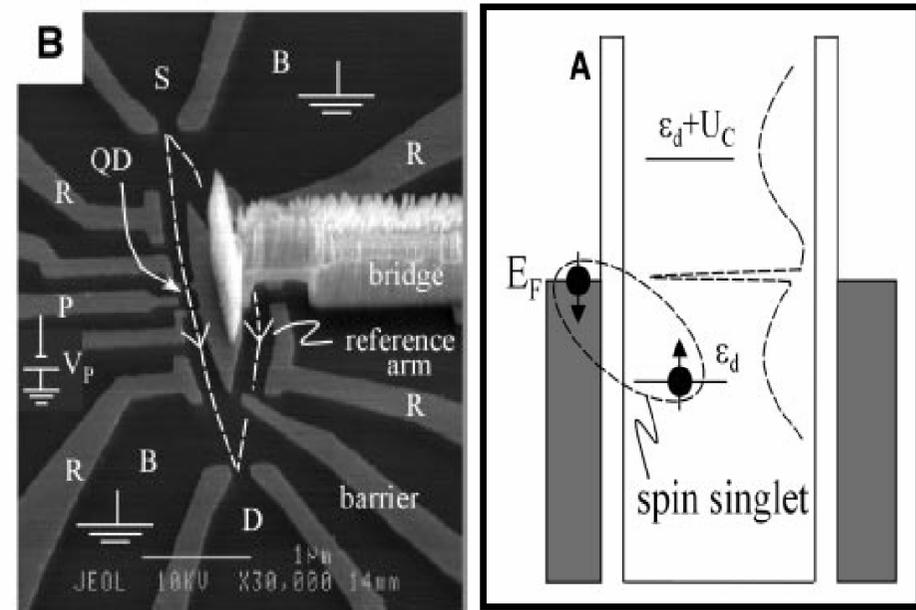
## Transmission Phase Shift of a Quantum Dot with Kondo Correlations



### Theory

(Gerland et al.  
PRL **84** 3710 (2000))

## Phase Evolution in a Kondo-Correlated System

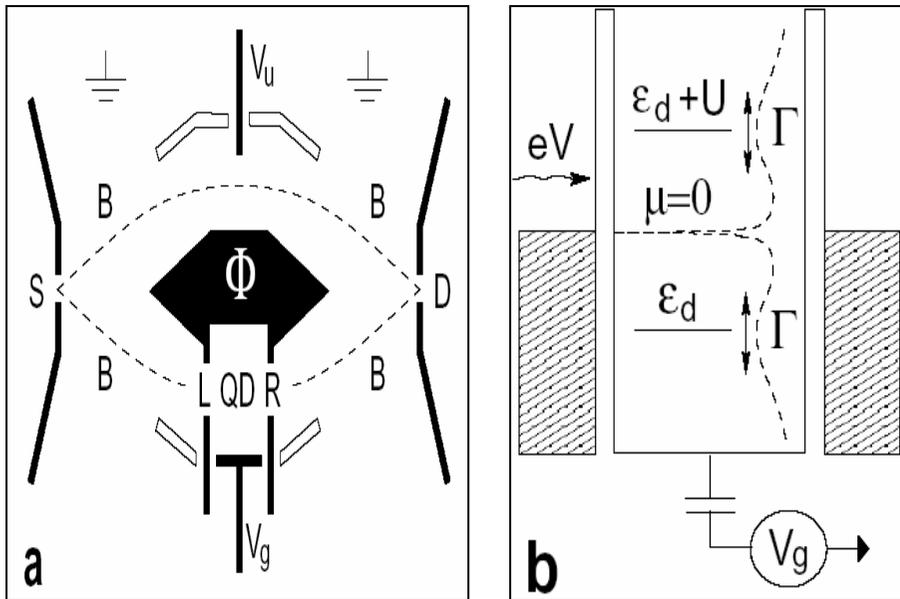


### Experiment

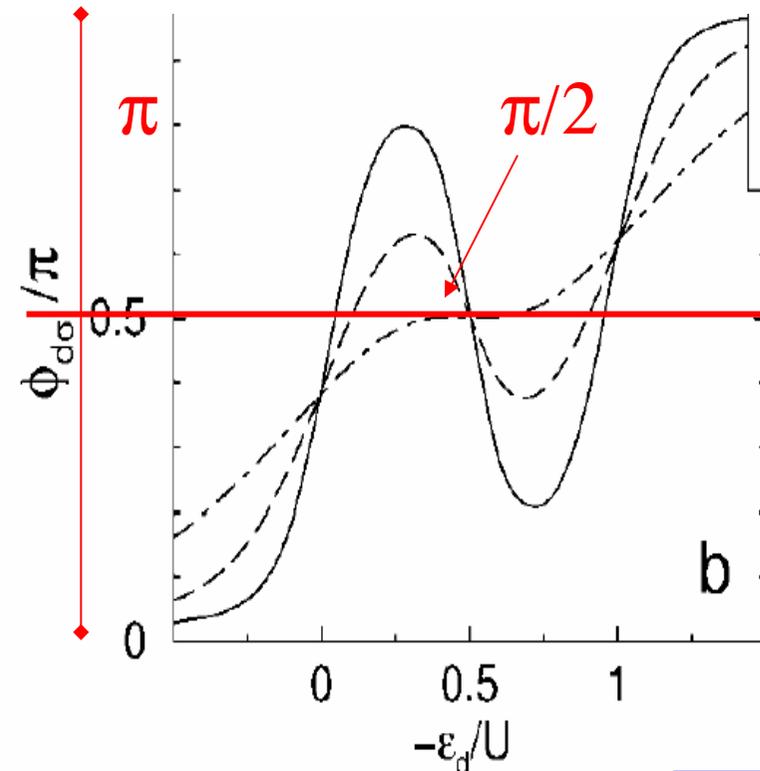
(Ji, Heiblum et al.  
*Science* **290** 779 (2000))

# More “Theory-Experiment ballgame”

## Transmission Phase Shift of a Quantum Dot with Kondo Correlations



**Theory**  
(Gerland et al.  
PRL **84** 3710 (2000))

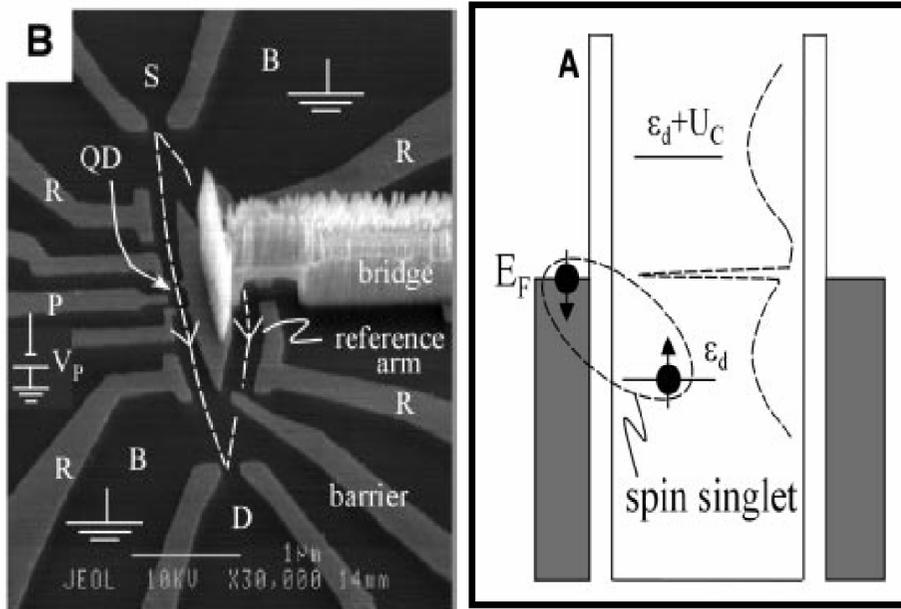


(c) For arbitrary temperatures ( $\lesssim \Gamma$ ), the only approach which gives reliable results for  $G_{d\sigma}(E)$  for all  $\Gamma, U, \epsilon_d$  is the *numerical renormalization group* (NRG)

**Theory** (Gerland et al. PRL **84** 3710 (2000))

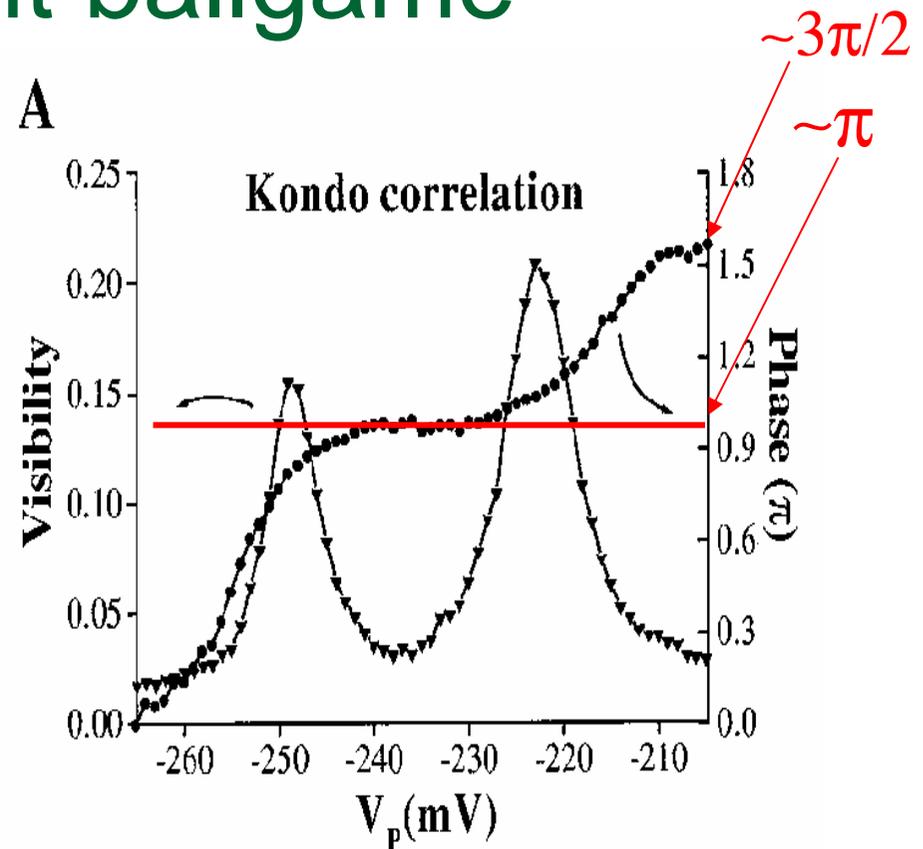
# Theory-Experiment ballgame

## Phase Evolution in a Kondo-Correlated System



### Experiment

(Ji, Heiblum et al.  
*Science* **290** 779 (2000))



Experiment (Ji et al. *Science* **290** 779 (2000))

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# Summary: Lectures on strongly correlated phenomena in nanostructures.

- *Lecture 1:* Quantum Dots.
  - *Lecture 2:* Kondo effect/NRG.
  - *Lecture 3:* Kondo effect in nanostructures.
  - **Nanostructures display an array of strongly correlated phenomena:** (Kondo and 2ch Kondo effects (= non-Fermi-liquid behavior), interplay of spin and vibrational effects... quantum phase transitions, SU(4) Kondo effect).
  - Opportunity: *controlled* studies of all these features.
    - *Thanks for your attention.*
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