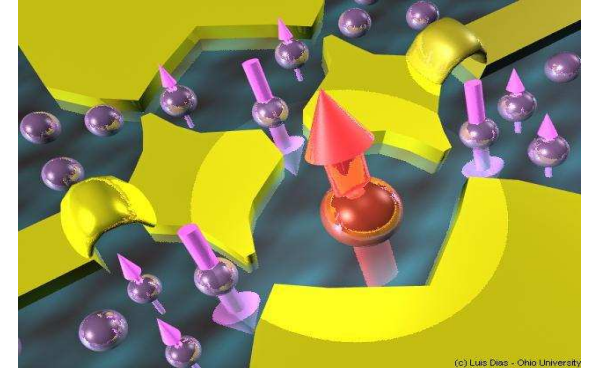


1998: O encontro de "Kondo" com "Nano"

Luis Gregório Dias da Silva



Depto. de Física dos Materiais e Mecânica - DFMT

Instituto de Física, Universidade de São Paulo - IFUSP



Mapa do Seminário

◆ 15 anos do Efeito Kondo em nanoestruturas.

- Review: Efeito Kondo em metais com impurezas.
- 1998: “Revival of the Kondo effect”: pontos quânticos e átomos em superfícies.

◆ E hoje? Alguns desenvolvimentos recentes.

- Efeito Kondo com Férmions de Dirac.
- Ação combinada com outros efeitos quânticos (graus de liberdade orbitais, efeito Zeeman, etc.): transições de fase quânticas e “filtros de spin”.

1998: "The Kondo year"

- Meu primeiro "Kontato":

1o semestre de 1998

Modelo de Anderson e Modelo de Kondo 2

Historicamente, os modelos de Kondo e Anderson apareceram com o objetivo de se estudar a formação de momentos magnéticos em metais e como esses momentos magnéticos interagem com os elétrons de condução.

E. Miranda, Notas de aula, curso de Muitos Corpos. (1o. semestre 1998)

1998: "The Kondo year"

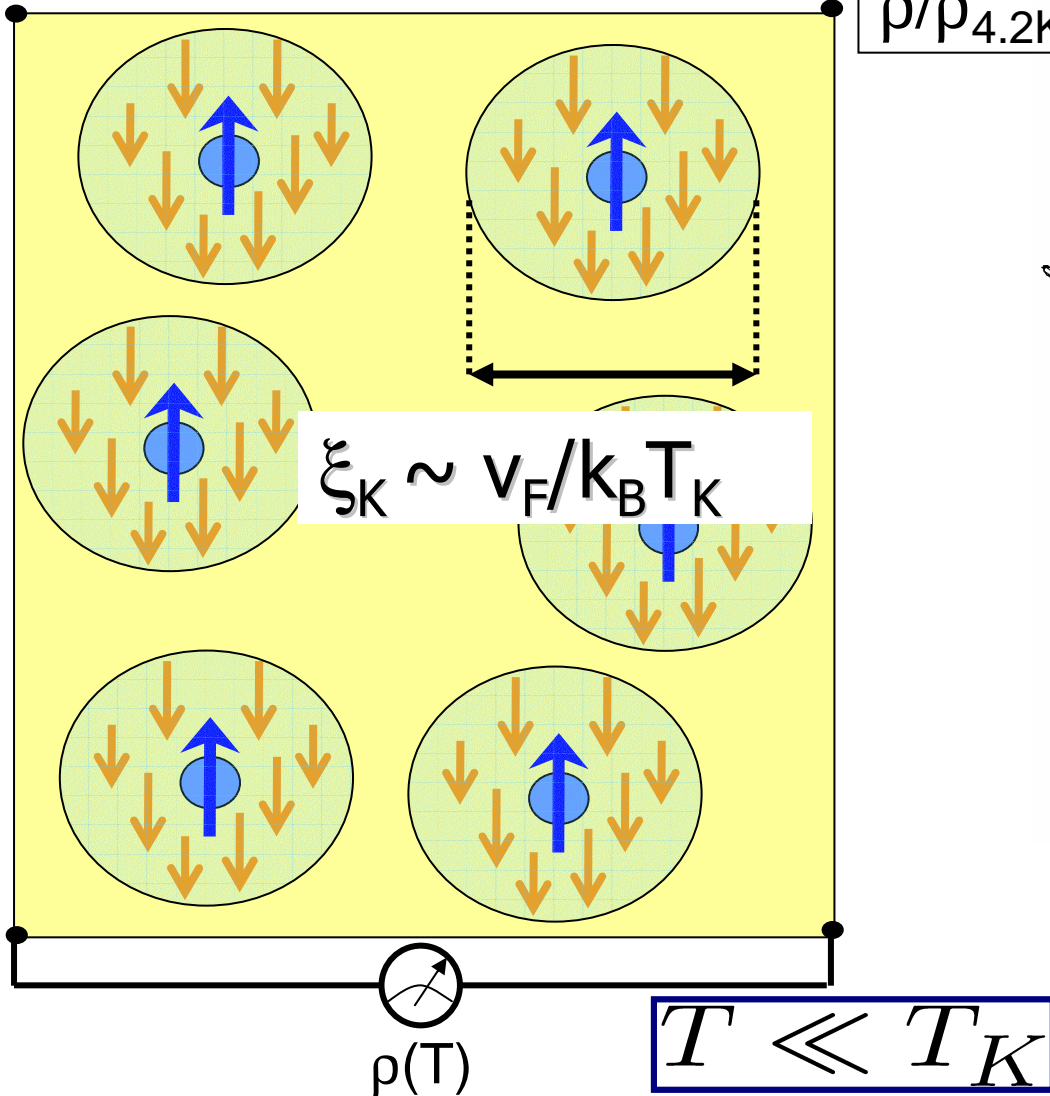
- Meu primeiro "Kontato":

1o semestre de 1998

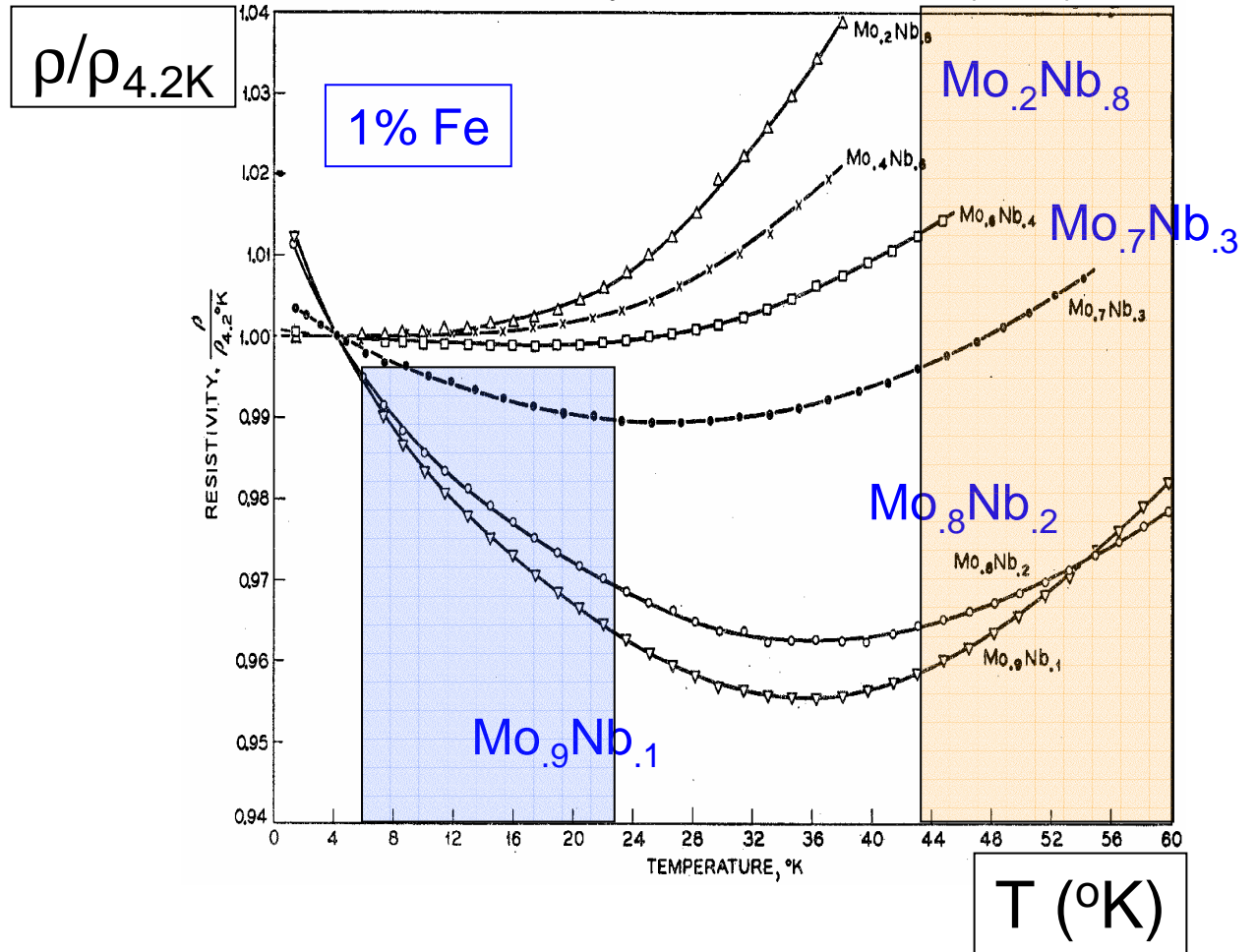
Uma das principais conclusões que se tiram dessa análise é o fato de que o estado fundamental do sistema é um singlete ($S=0$), apesar de haver um momento localizado a altas temperaturas. Os elétrons de condução "blindam" efetivamente o momento local e formam com ele um estado de $S=0$. Esse processo de blindagem do momento local é conhecido como efeito Kondo.

E. Miranda, Notas de aula, curso de Muitos Corpos. (1o. semestre 1998)

Kondo effect



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



Resistivity increases with temperature: the Kondo effect
 Decreases simple (normal) effect

Brief History of Kondo Phenomena

- First Observations: 1930's
- Kondo's Explanation for the resistance minimum: 1964
- Anderson's Poor Man's scaling: 1970
- Wilson's NRG: early 1970's (RMP 1975).
- Nozières Fermi liquid picture: 1974
- Bethe Ansatz solution: Andrei, Wiegmann: 1980
(Andrei, Furuya, Lowenstein, "Solution of the Kondo Problem" RMP 1983)

Numerical Renormalization Group (NRG):



Kenneth G. Wilson –
Physics Nobel Prize
in 1982

"for his theory for
critical phenomena in
connection
with phase
transitions"

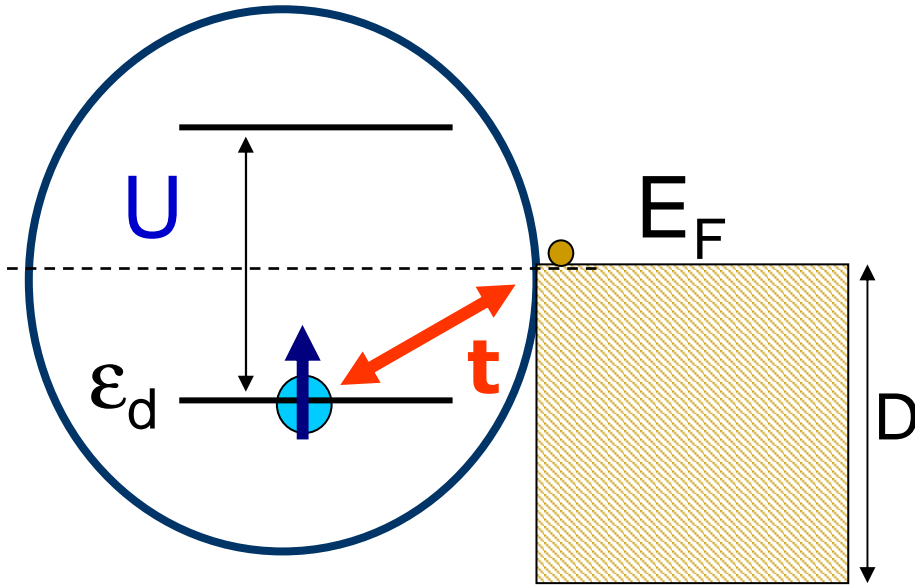
- Developed by Ken Wilson in the 70's.
- Designed to address the “Kondo problem” (magnetic impurities in metals): infrared divergencies in perturbative expansions.

Key elements in the NRG procedure:

1. **Logarithmic separation** of energy scales → Mapping into a tight binding chain.
2. **“Selective sampling”** of the Hilbert space: keep some states, discard others.
3. **Iterative numerical solution**: RG “flow” unveils low-energy physics.

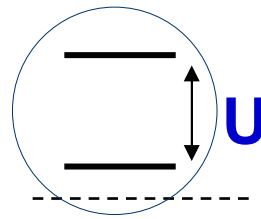
Anderson Model

Single level impurity (=atom) with local Coulomb repulsion coupled to a metal



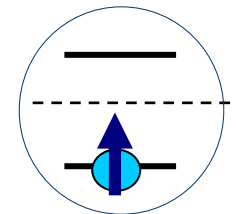
$$H = \epsilon_d \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_k \epsilon_k \hat{n}_{k\sigma} + t \sum_k c_{d\sigma}^\dagger c_{k\sigma} + \text{h.c.}$$

- ϵ_d : energy of the level
- U: Coulomb energy
- E_F : Fermi energy in the metal
- t: Hybridization with the metallic electrons
- D: metallic half-bandwidth



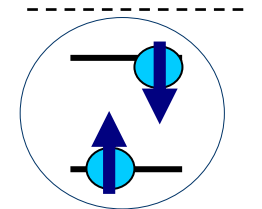
$$\langle \hat{n}_{d\sigma} \rangle \approx 0$$

$$\langle H_d \rangle \approx 0$$



$$\langle \hat{n}_{d\sigma} \rangle \approx 1$$

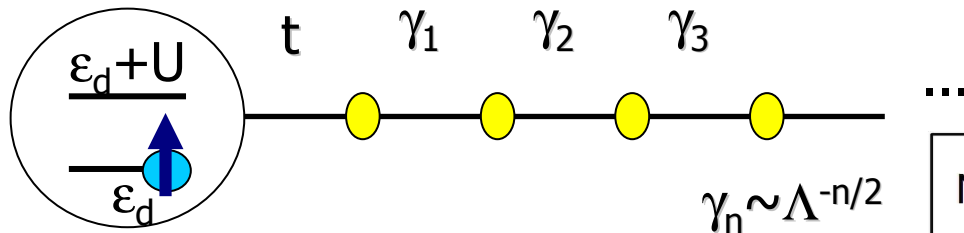
$$\langle H_d \rangle \approx \epsilon_d$$



$$\langle \hat{n}_{d\sigma} \rangle \approx 2$$

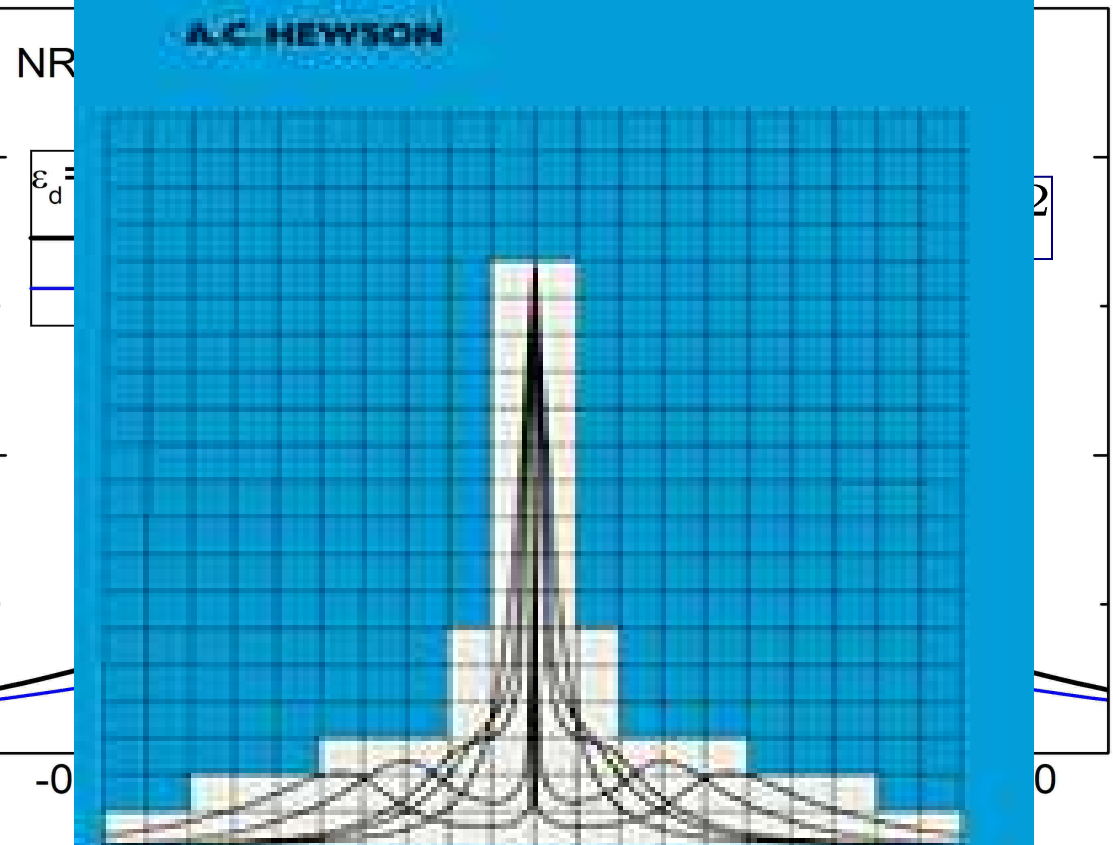
$$\langle H_d \rangle \approx 2\epsilon_d + U$$

NRG: Anderson model



- Poles in the Green's function (GF):
 - Single-particle peaks at ϵ_d and $\epsilon_d + U$.
 - *Many-body* peak at the Fermi energy: **Kondo resonance** (width $\sim T_K$).
- NRG: good resolution at low ω

$$T_K \sim \sqrt{\frac{U\Gamma}{2}} e^{-\pi|\epsilon_d+U|\epsilon_d/2U\Gamma}$$



Brief History of Kondo Phenomena

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- Bethe Ansatz solution: Andrei, Wiegmann: 1980
(Andrei, Furuya, Lowenstein, "Solution of the Kondo Problem" RMP 1983)

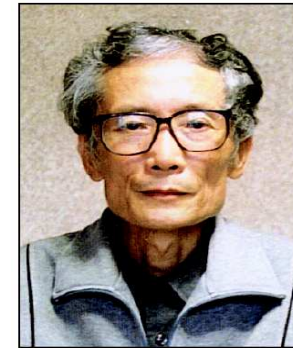
So, what's new about it?

Kondo correlations observed in many different set ups:

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

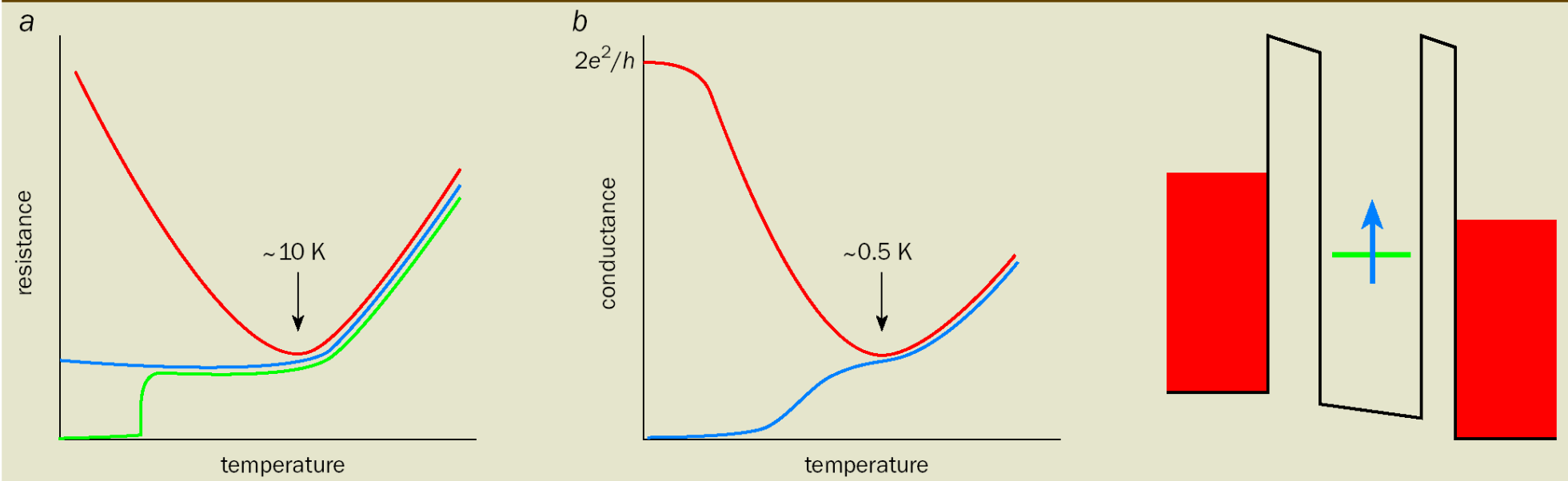
Kondo Effect in Quantum Dots

Revival of the Kondo effect



Leo Kouwenhoven and Leonid Glazman

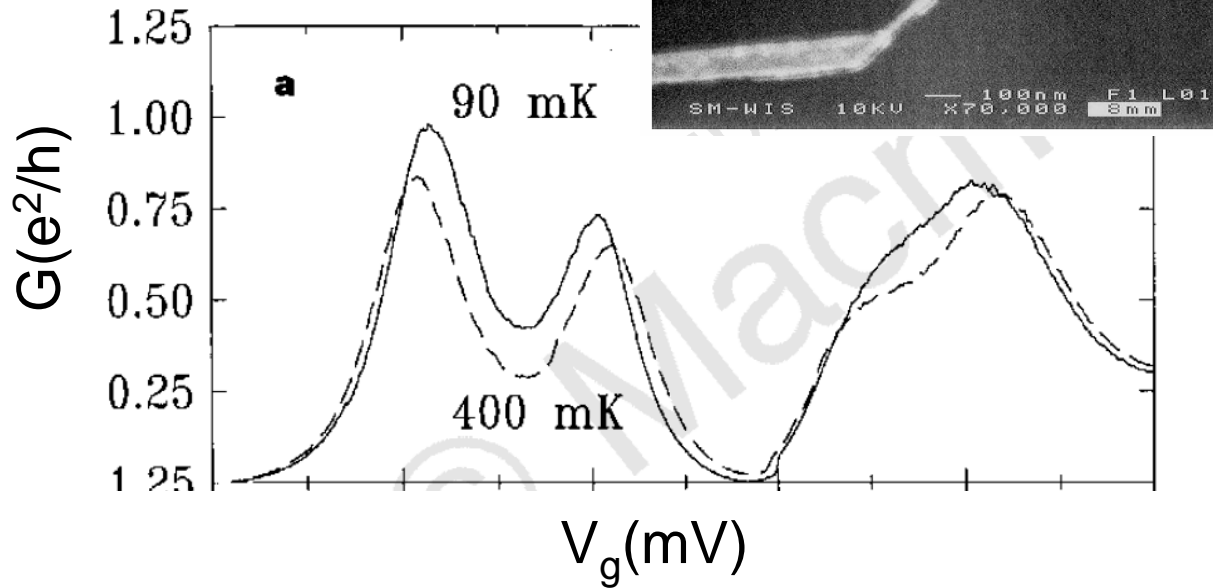
1 The Kondo effect in metals and in quantum dots



1998: “The Kondo year”

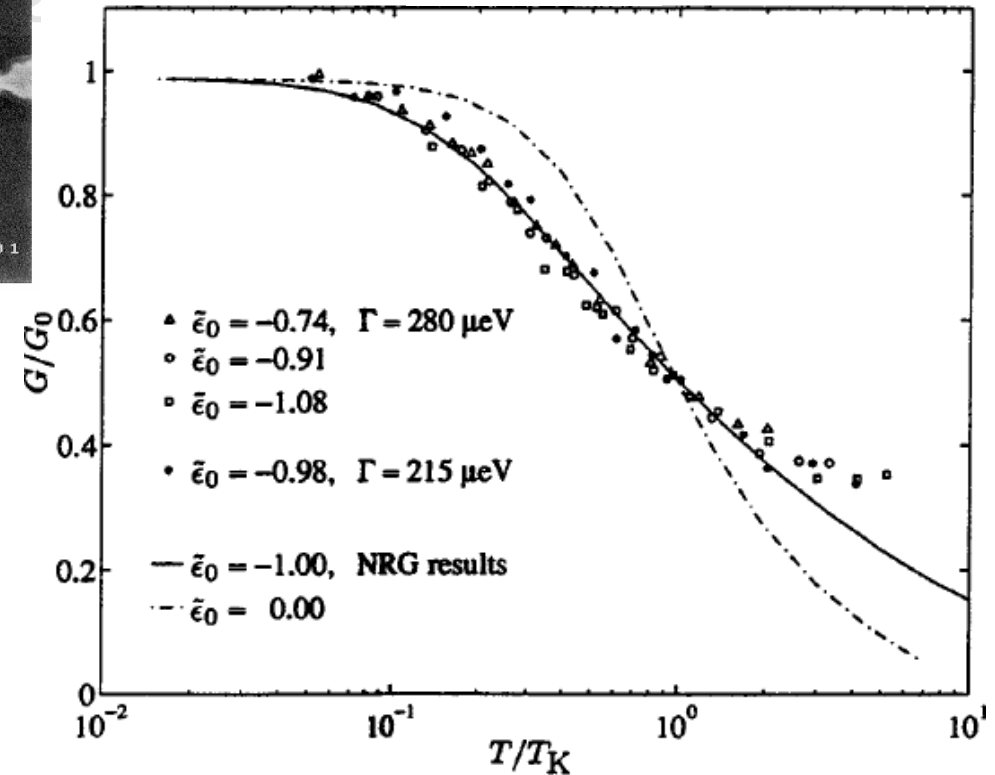
- Zero-bias conductance in semiconductor quantum dots:

January 1998



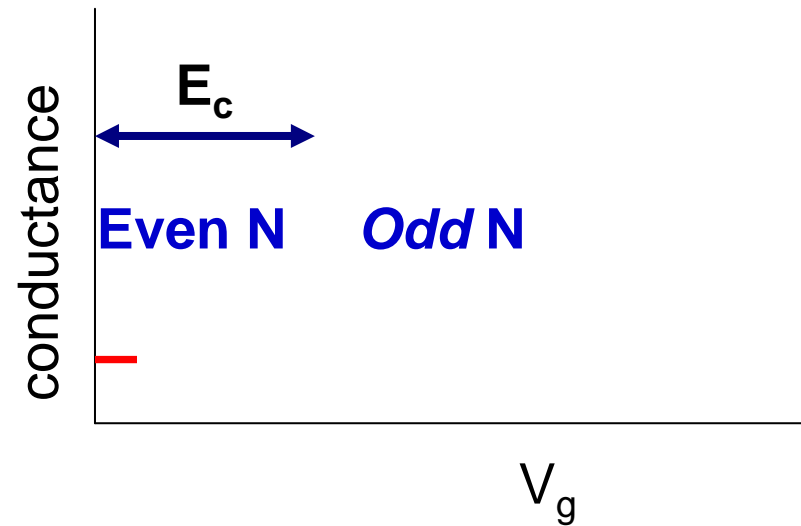
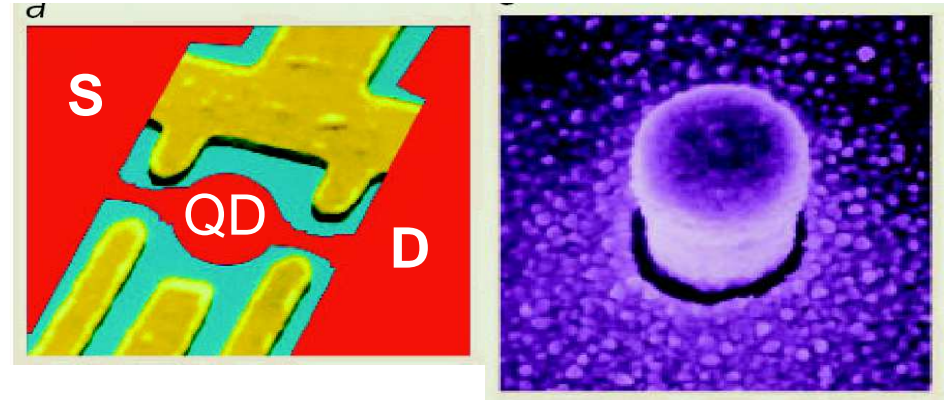
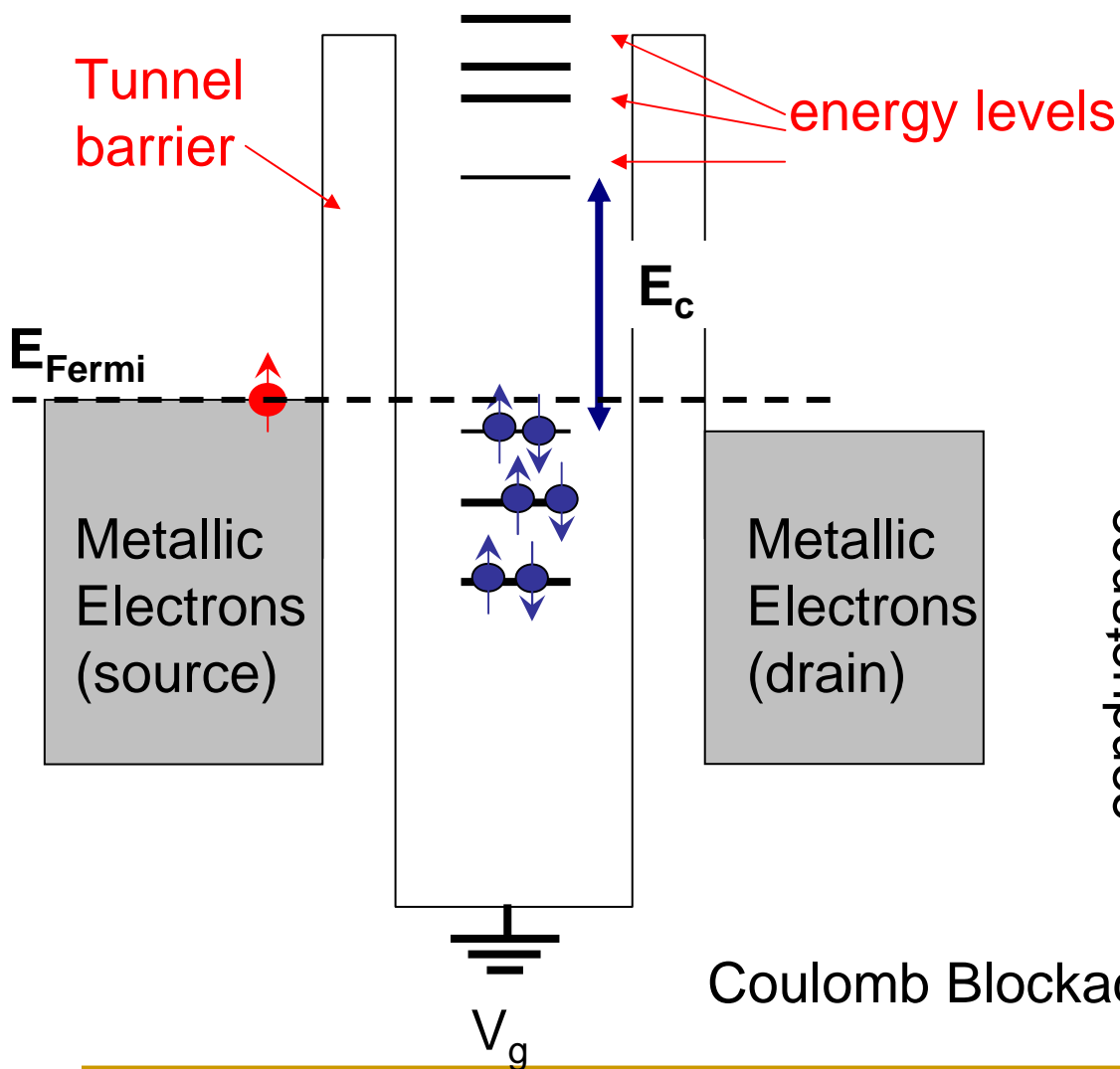
D. Goldhaber-Gordon et al. *Nature* **391** 156 (1998)

July 1998



D. Goldhaber-Gordon et al. *PRL* **81** 5225 (1998)

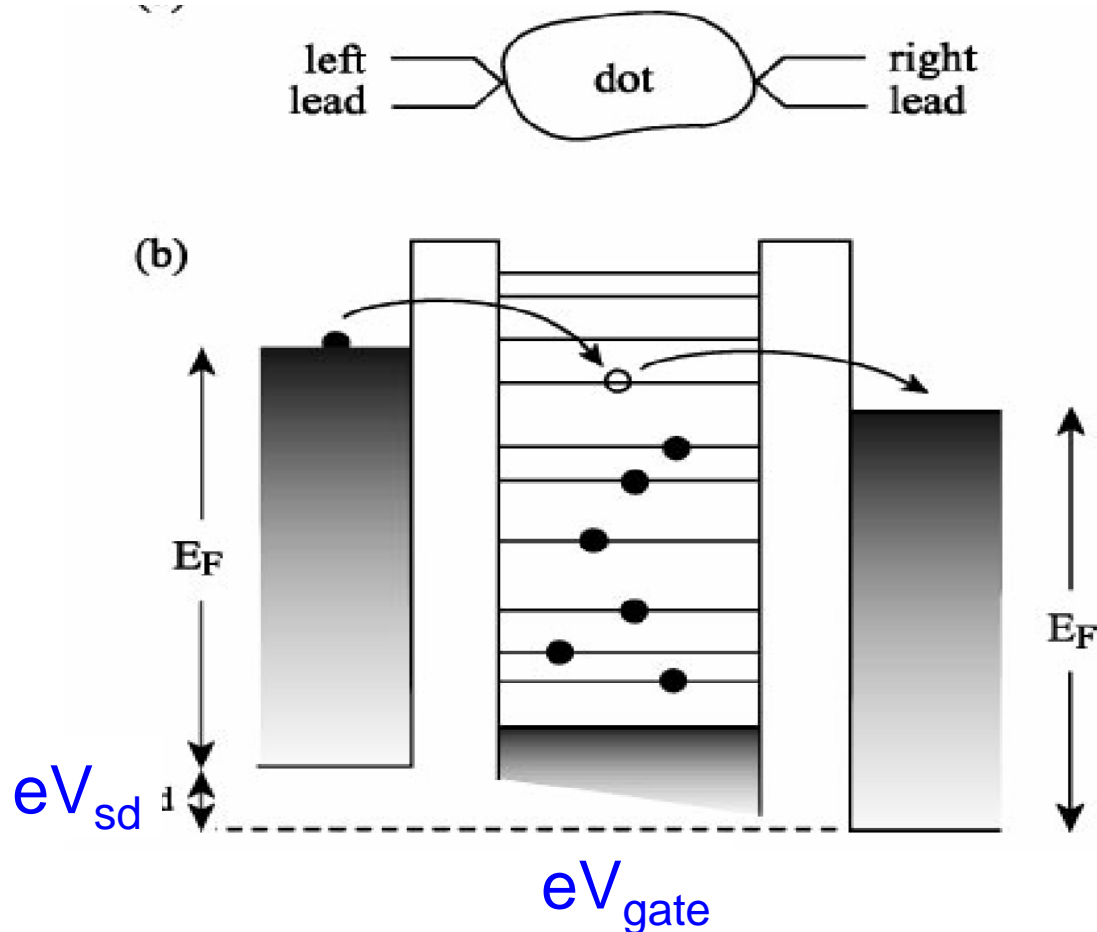
Coulomb Blockade in Quantum Dots



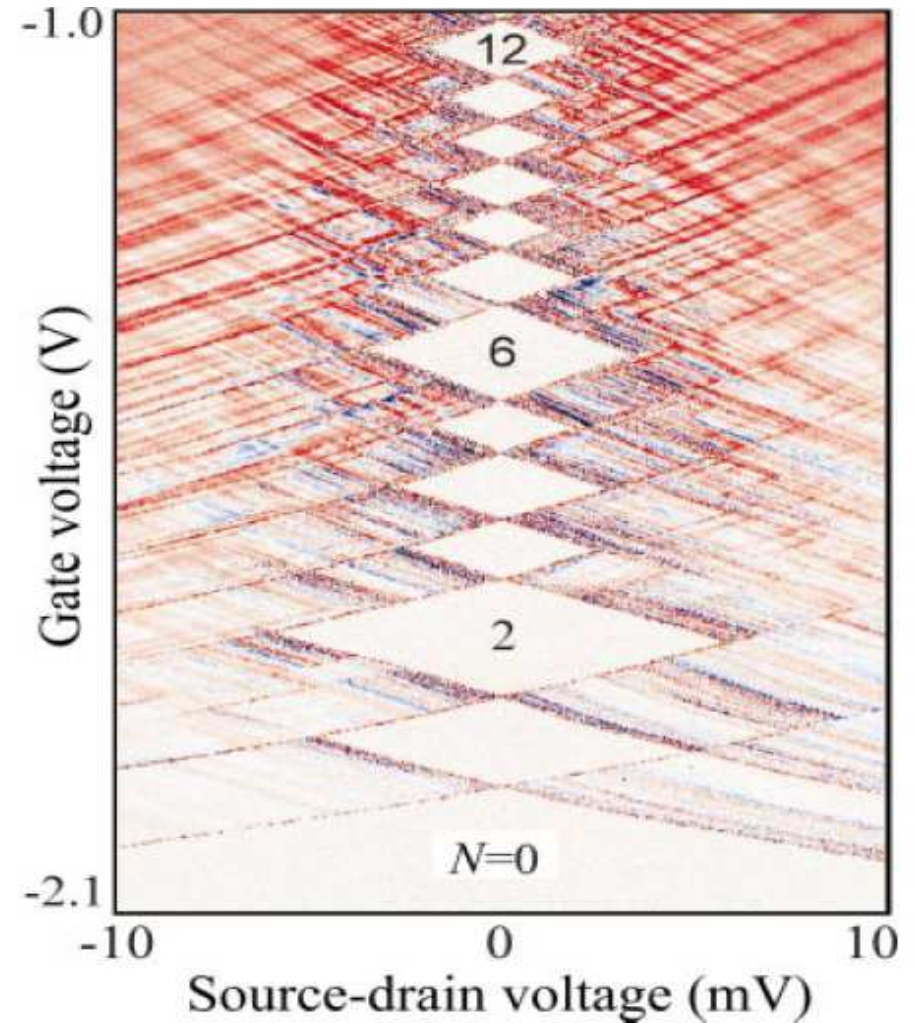
Coulomb Blockade in Quantum Dots

“Coulomb Diamonds” (Stability Diagram)

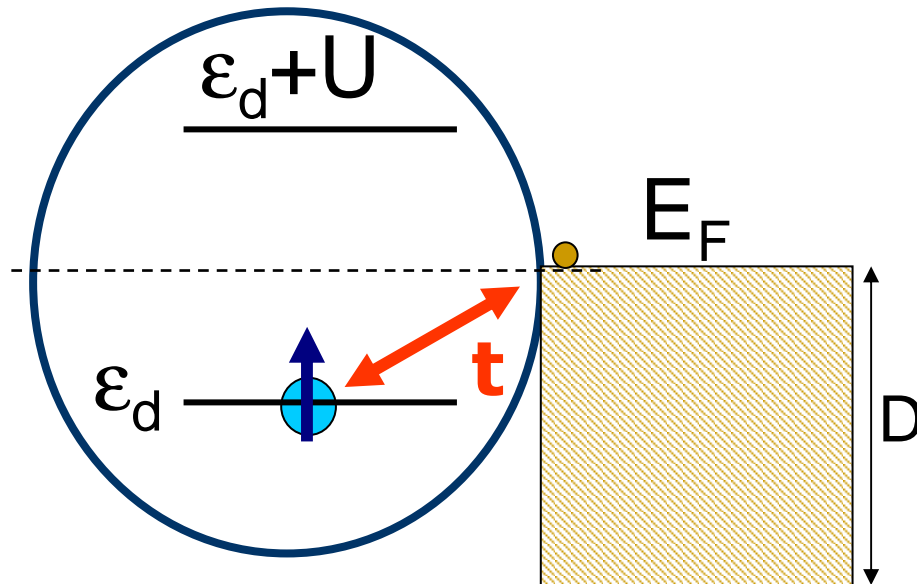
L. P. Kouwenhoven et al. *Science* **278** 1788 (1996).



Coulomb Blockade in Quantum Dots



Anderson model for quantum dots



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

with

$$\hat{n}_{d\sigma} = c_{d\sigma}^\dagger c_{d\sigma}$$

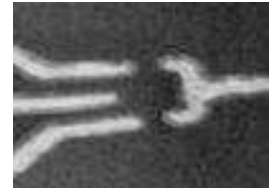
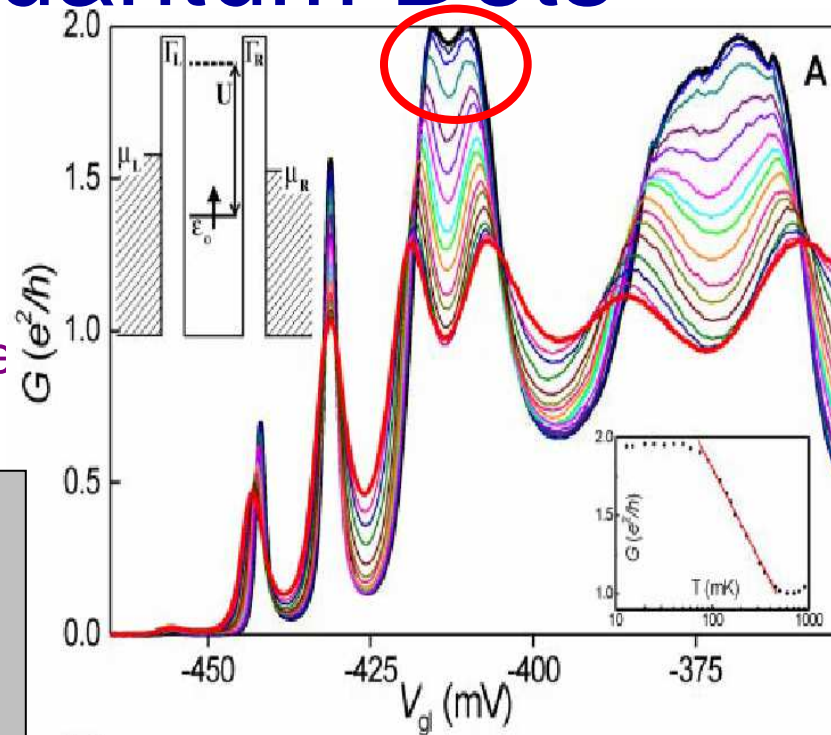
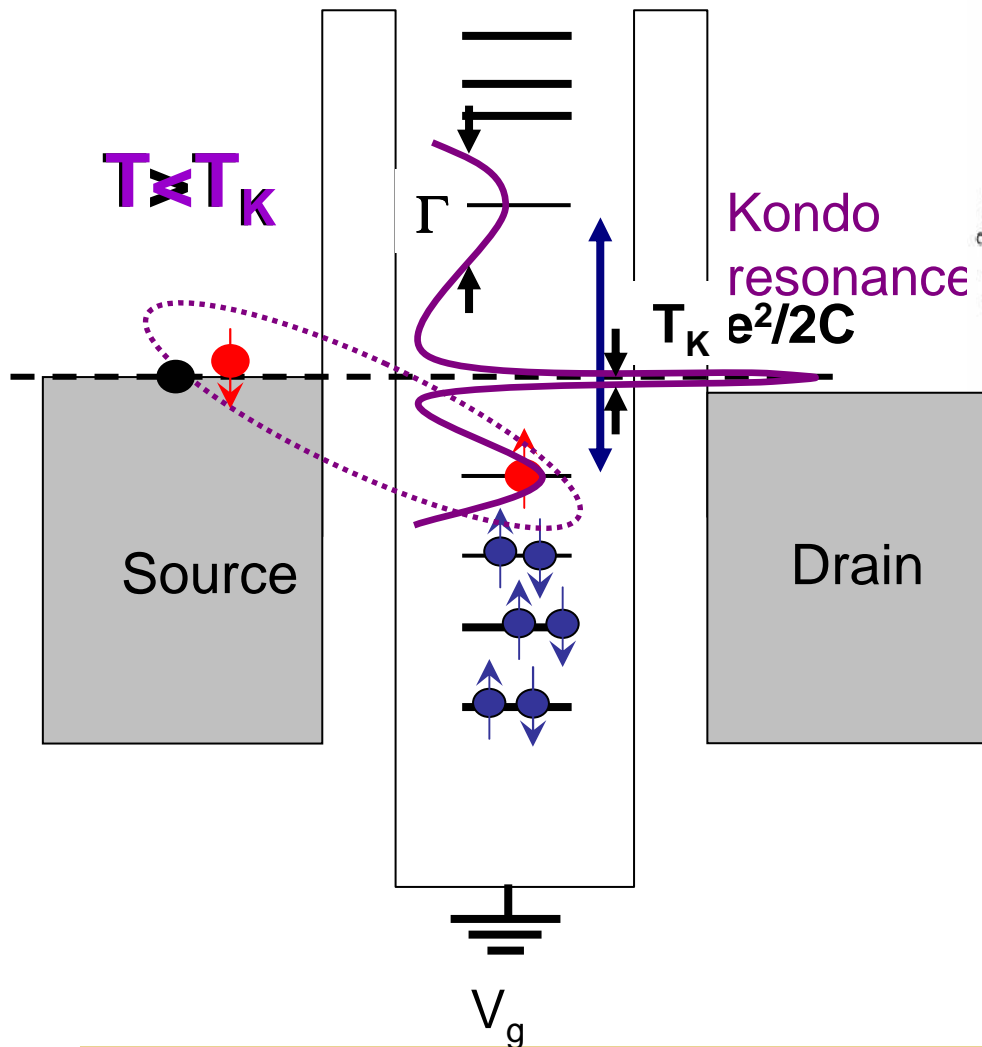
$$\hat{n}_{k\sigma} = c_{k\sigma}^\dagger c_{k\sigma}$$

“Quantum dot language”

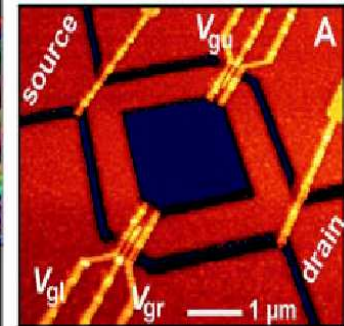
- ϵ_d : energy of the level
- U : Coulomb energy
- E_F : Fermi energy in the metal
- t : Hybridization w/ metal
- D : metallic half-bandwidth

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

Kondo Effect in Quantum Dots



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



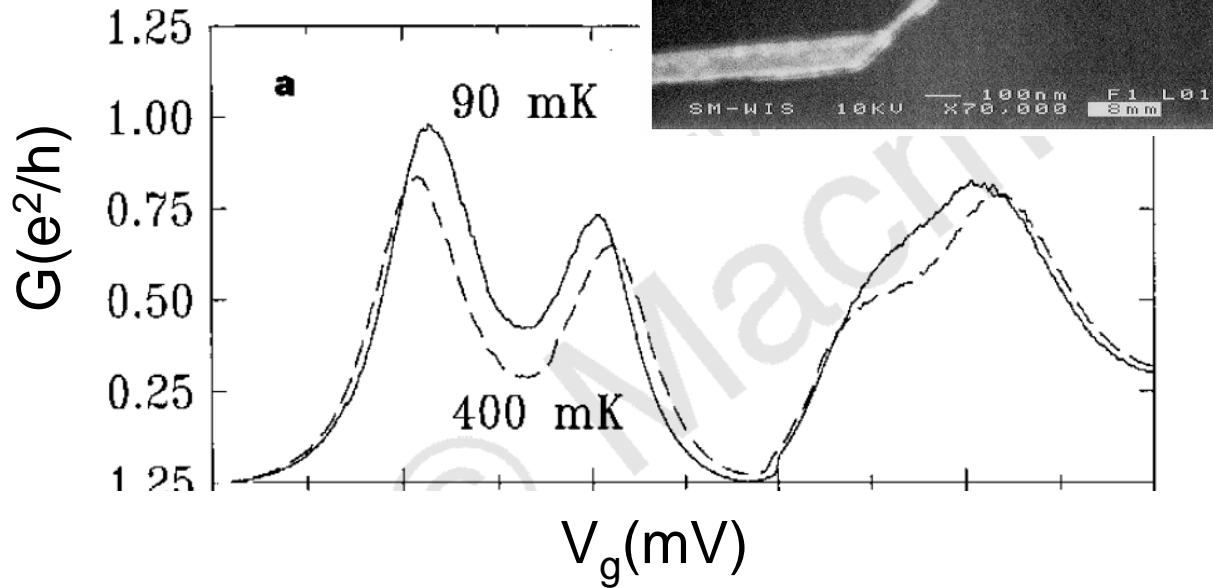
van der Wiel et al.,
Science **289** 2105
(2000).

- $T > T_K$: 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 ($\rightarrow 2e^2/h$!)

1998: “The Kondo year”

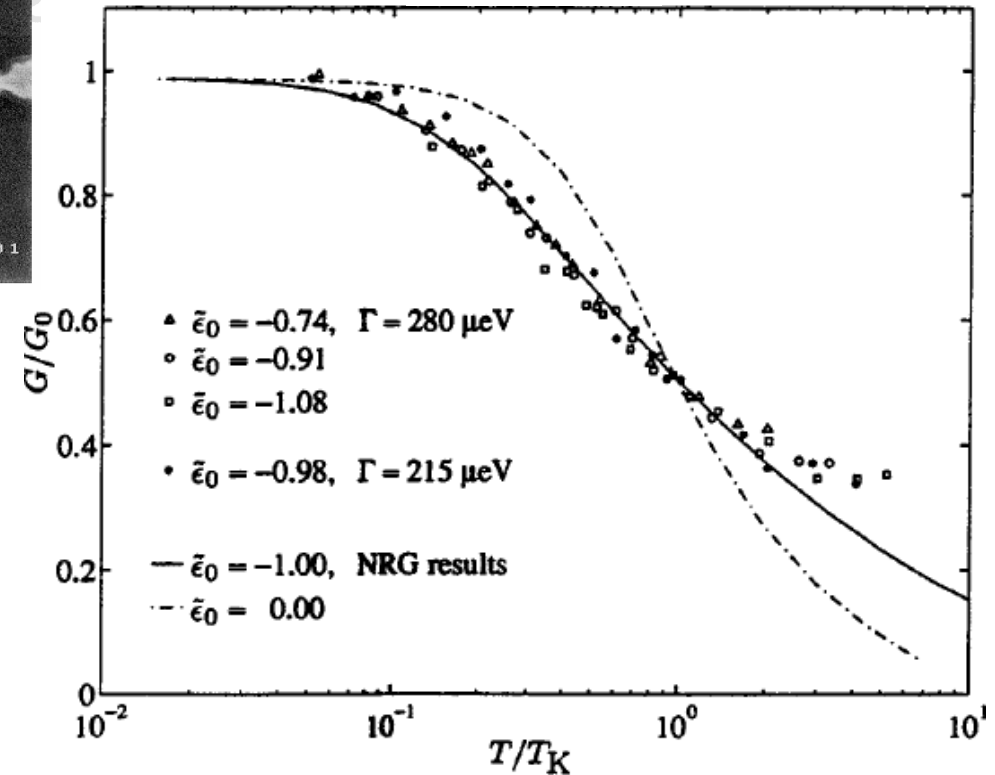
- Zero-bias conductance in semiconductor quantum dots:

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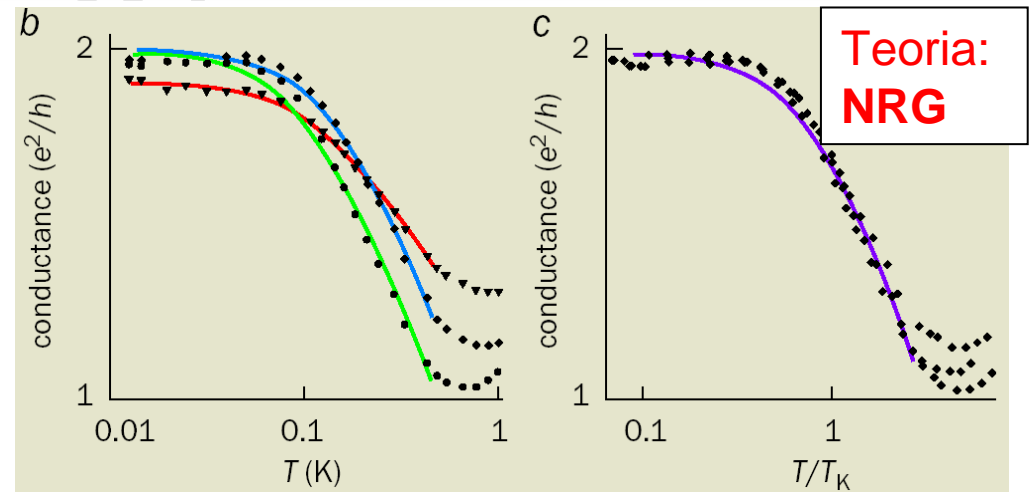
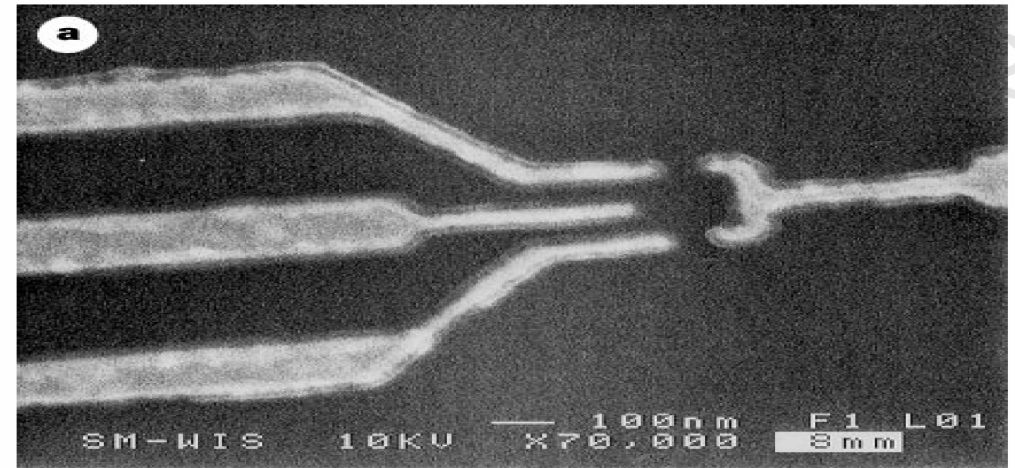
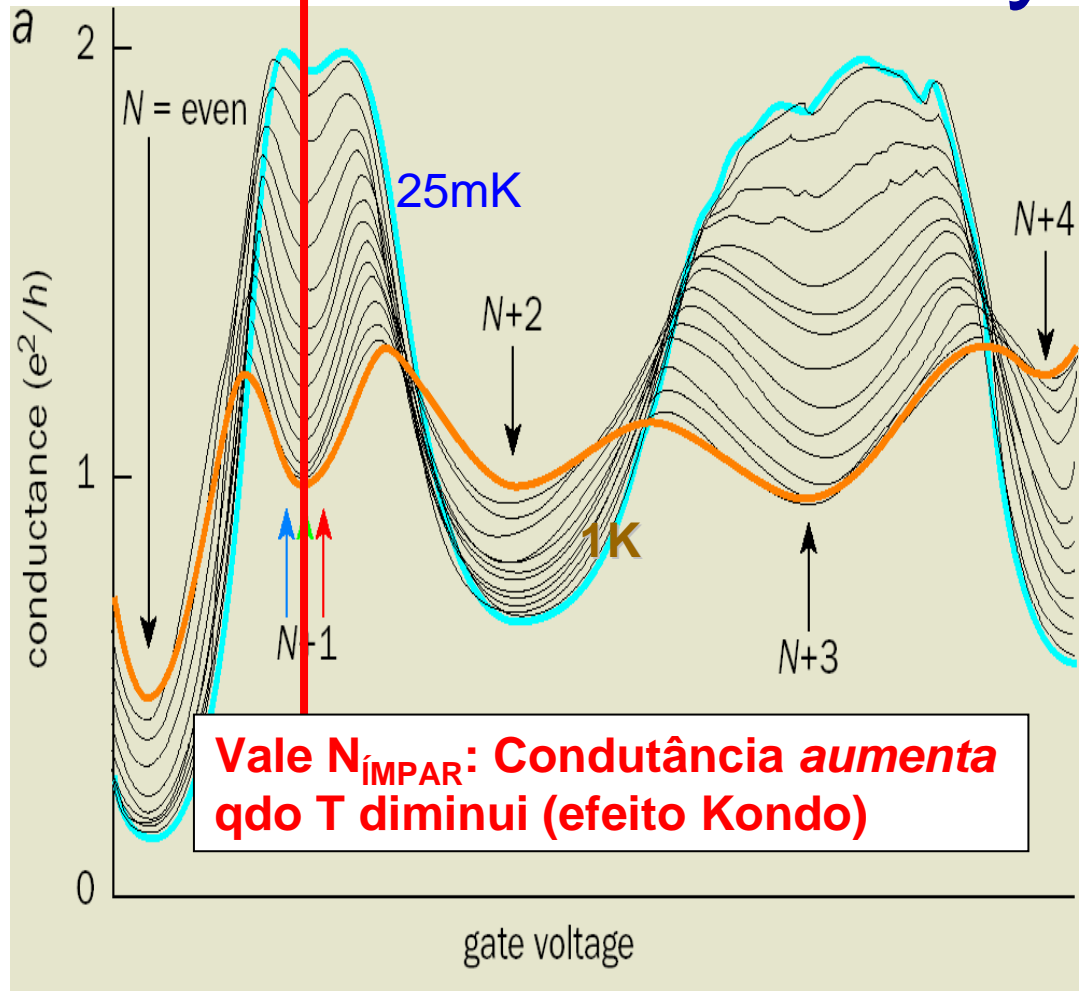
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July 1998



D. Goldhaber-Gordon et al. *PRL* **81** 5225 (1998)

1998: "The Kondo year"

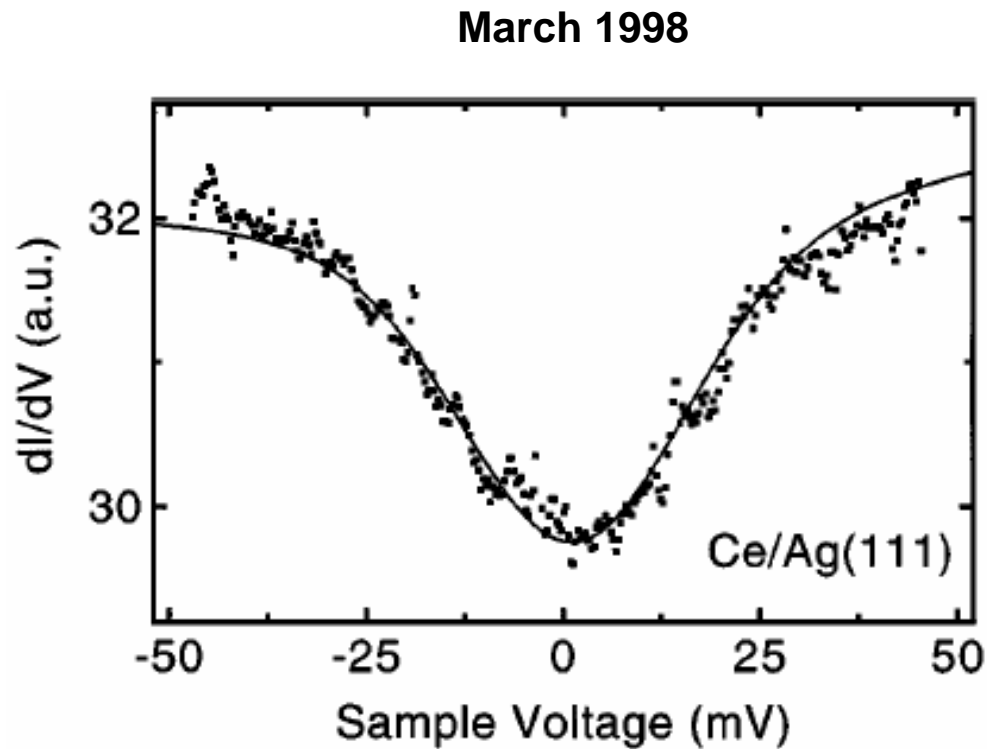


Temperatura de Kondo T_K ($\sim 0.5\text{K}$): um ÚNICO parâmetro escala todas as curvas G vs T

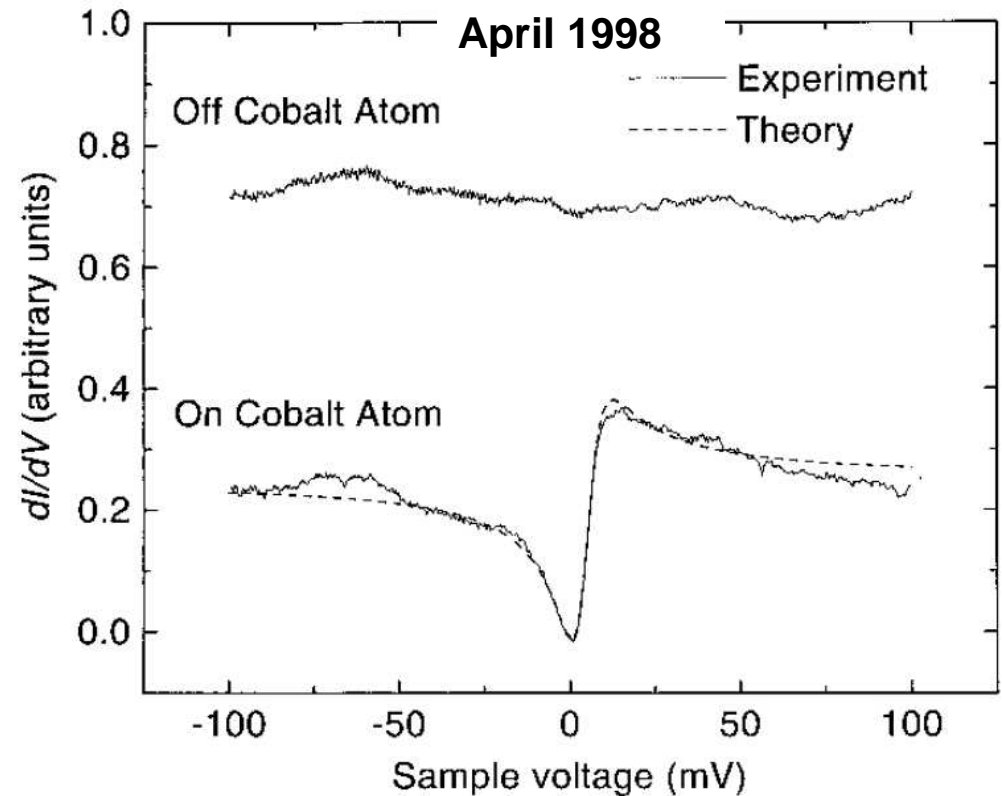
Kowenhoven and Glazman *Physics World* – Jan. 2001.

1998: “The Kondo year”

- Magnetic atoms on surfaces: zero-bias anomaly in STM dI/dV

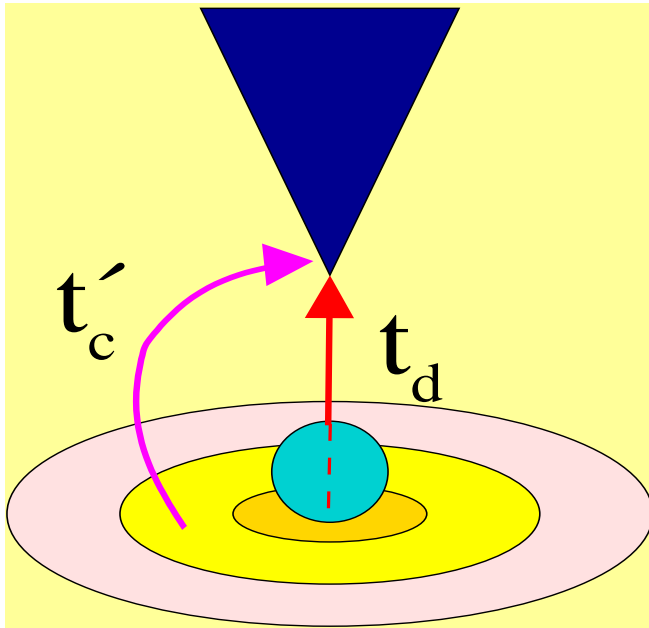


J. Li, et al. *PRL* **80** 2893 (1998)



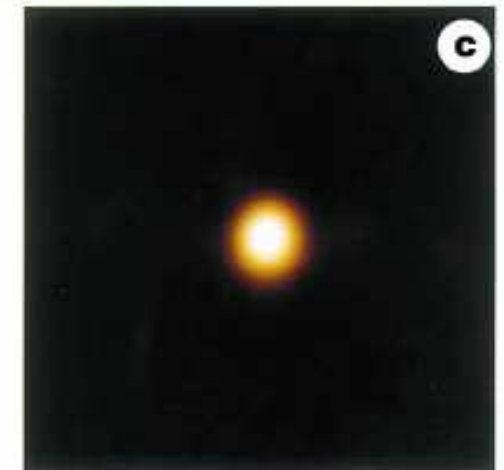
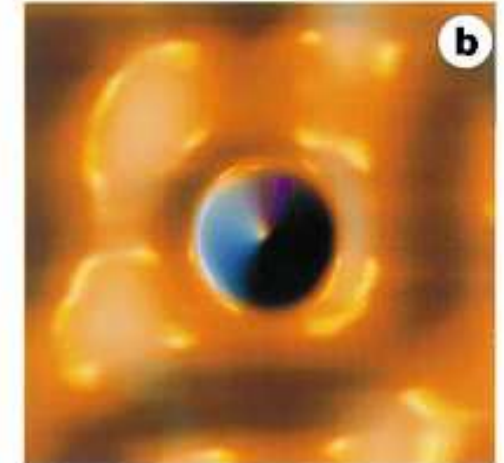
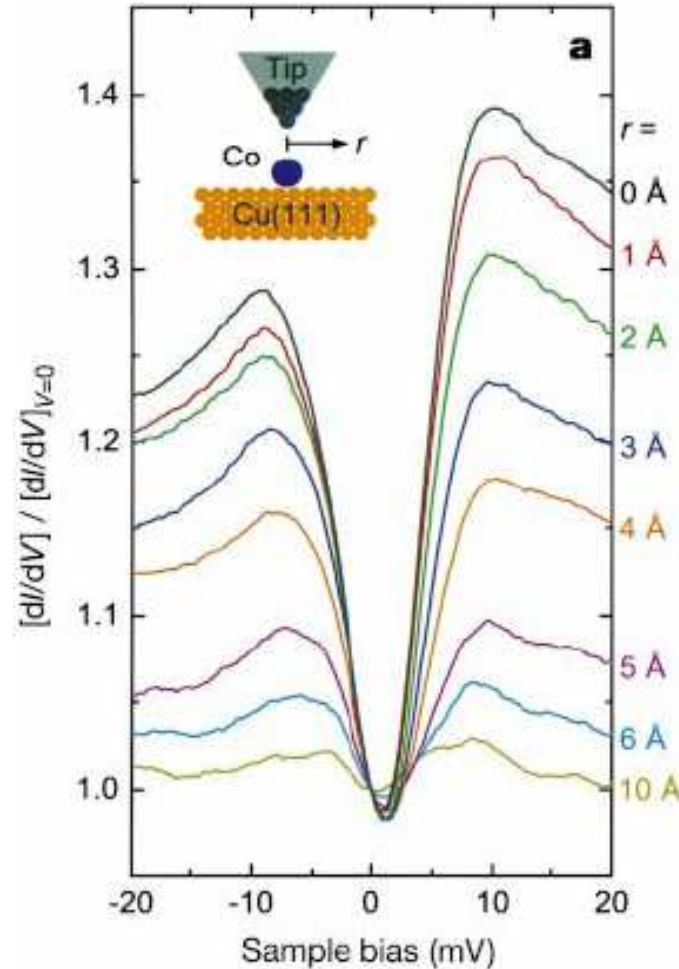
Madhavan et al., *Science* **280** 567 (1998).

Kondo effect in surfaces (STM images).



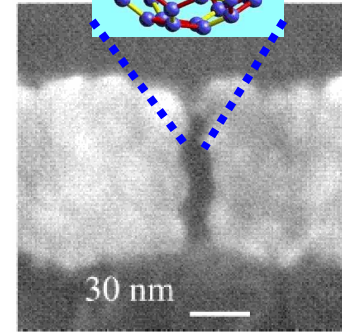
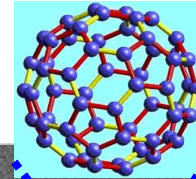
- Magnetic (Co, Fe) atoms on metallic *surfaces*!
- Right ingredients for Kondo.
- In this case, Kondo is marked by a *dip* at zero-bias conductance (dI/dV at $V_{\text{bias}}=0$).

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



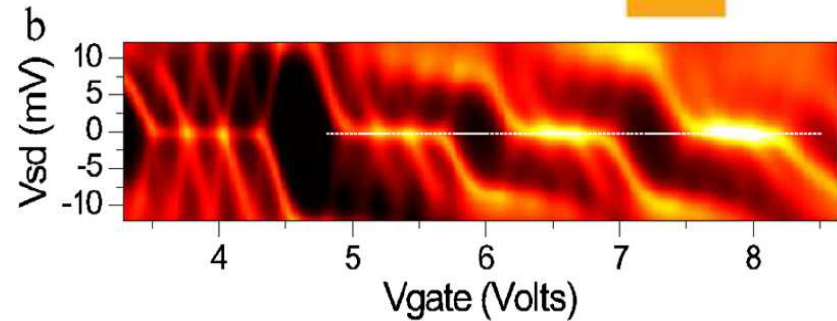
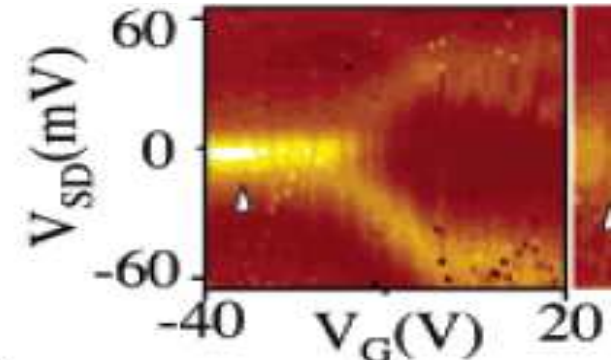
Kondo everywhere!

Carbon Nanotubes



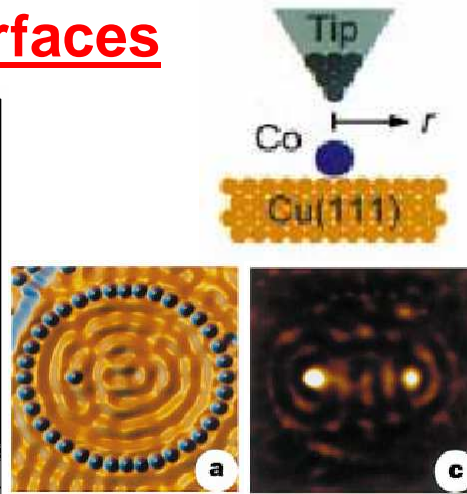
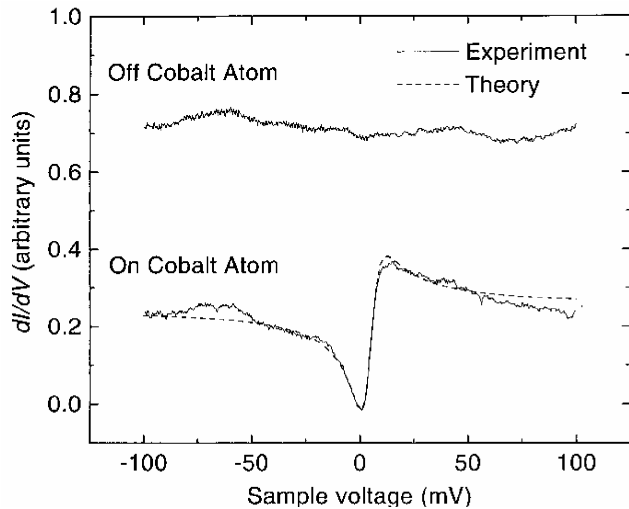
Molecular Junctions

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



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

Magnetic atoms on surfaces

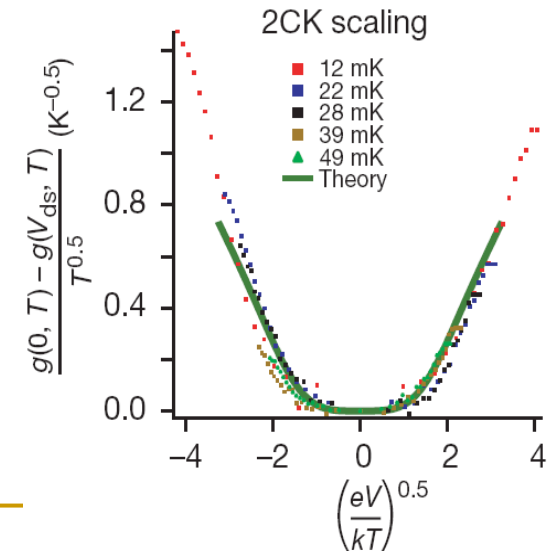
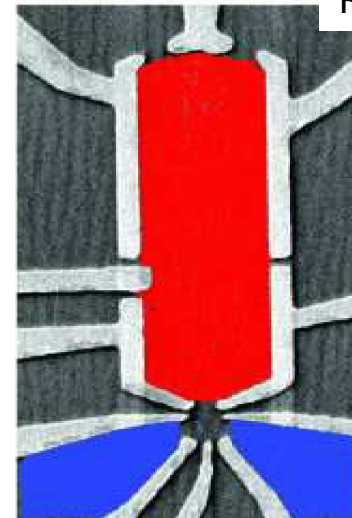


Manoharan et al.,
Nature **403** 512 (2000).

Madhavan et al., *Science* **280** 567 (1998).

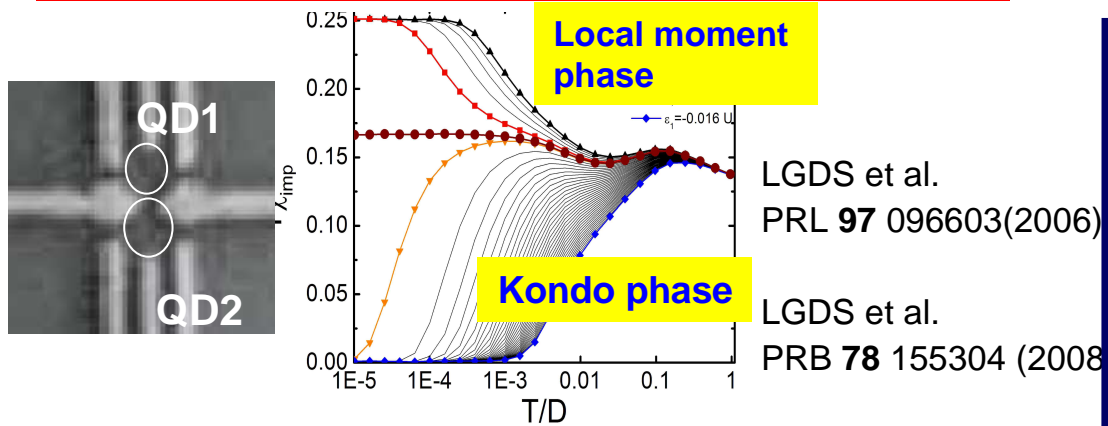
Semiconductor Quantum dots

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

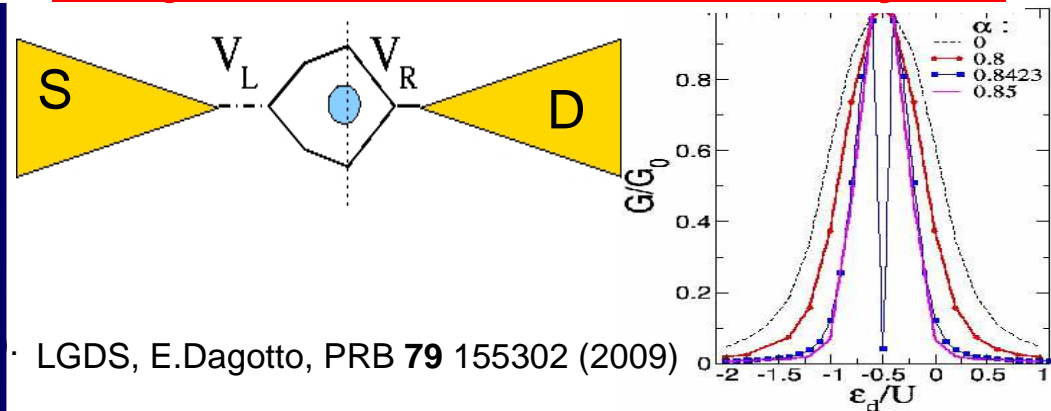


Kondo+NRG em nanoestruturas: exemplos

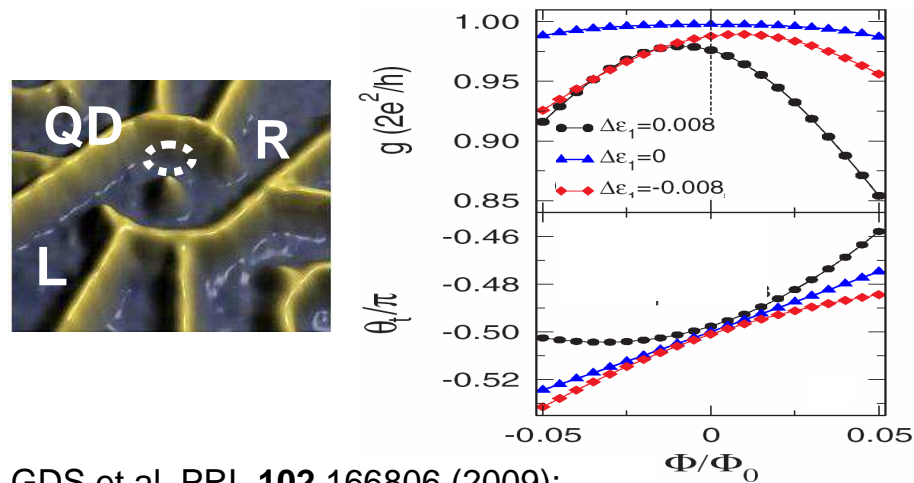
Pontos Quânticos semicondutores



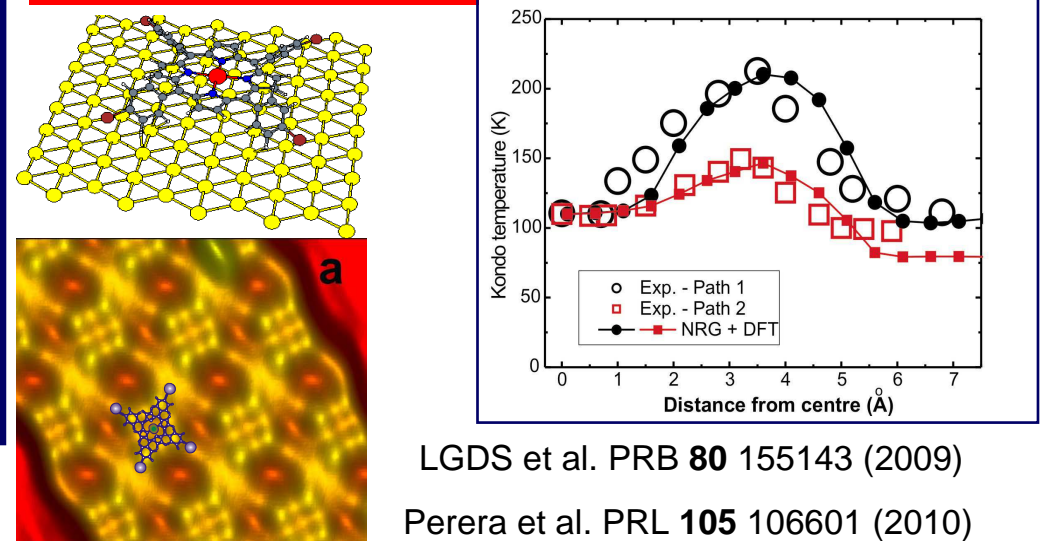
Junções moleculares c/ vibrações



Anéis Quânticos + efeito Aharonov Bohm



Moléculas magnéticas em superfícies



Mapa do Seminário

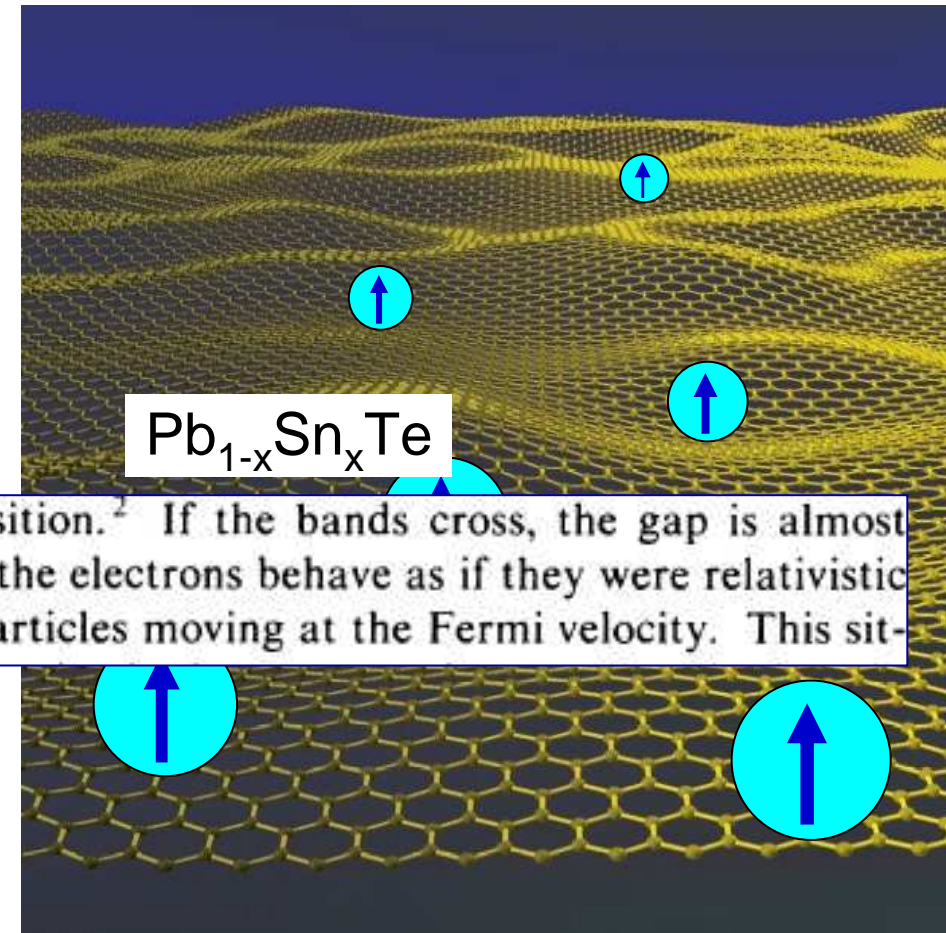
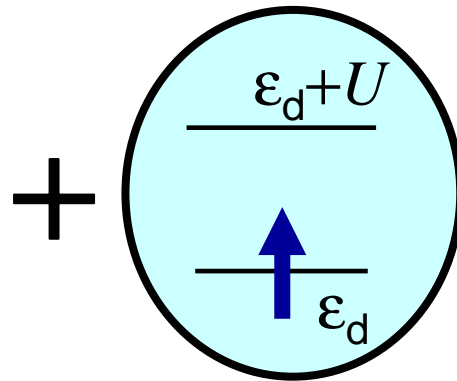
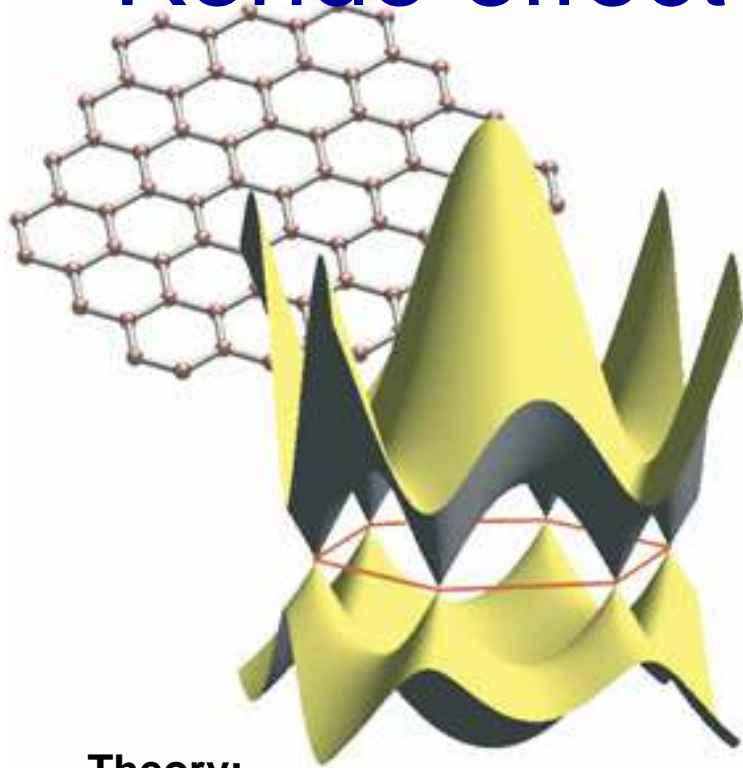
◆ 15 anos do Efeito Kondo em nanoestruturas.

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◆ E hoje? Alguns desenvolvimentos recentes.

- Efeito Kondo com Férmions de Dirac.
- Ação combinada com outros efeitos quânticos (graus de liberdade orbitais, efeito Zeeman, etc.): transições de fase quânticas e “filtros de spin”.

Kondo effect with Dirac Fermions



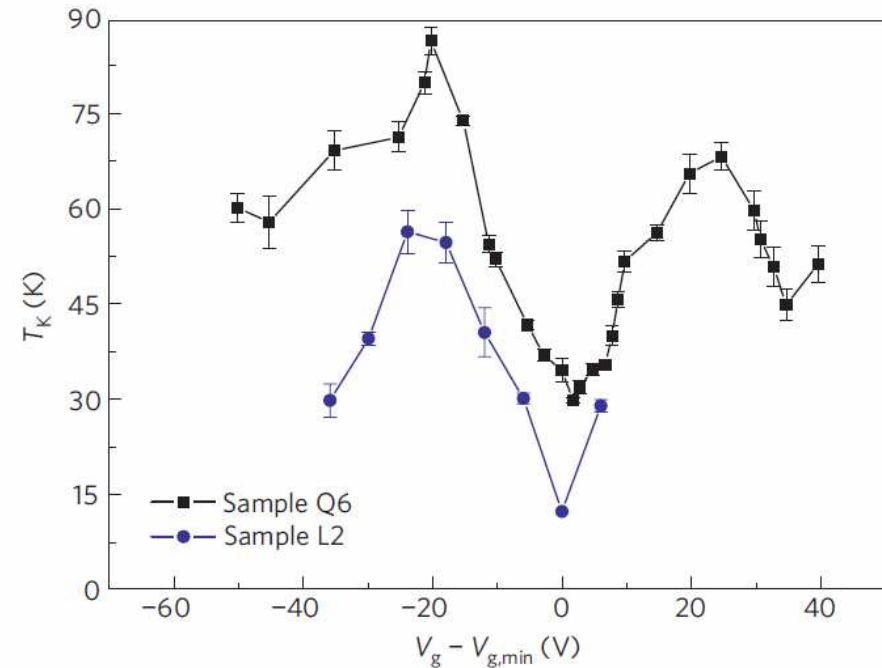
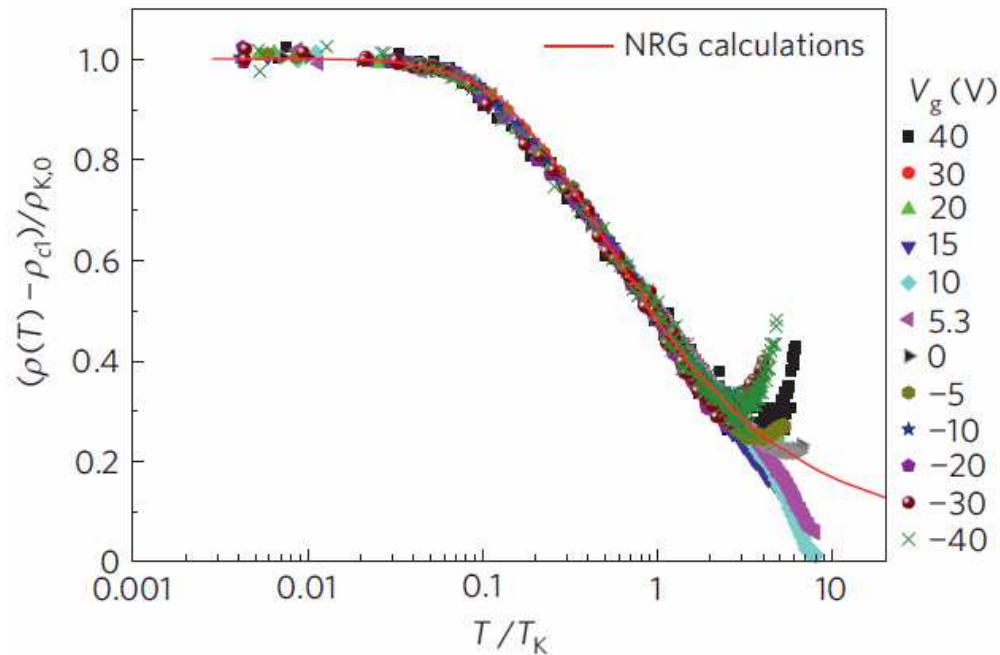
cal composition.² If the bands cross, the gap is almost linear and the electrons behave as if they were relativistic massless particles moving at the Fermi velocity. This sit-

Theory:

- D. Withoff and E. Fradkin, PRL **64** 1835 (1990).
- C. Gonzalez-Buxton, K. Ingersent, PRB **57**, 14254 (1998)
- P.S. Cornaglia et al. PRL **102** 046801 (2009).
- M. Vojtá, et al., Europhys. Lett. **90**, 27006 (2010).
- Review: L. Fritz and M. Vojtá, arXiv:1208.3113 (2012)

Experiment?

Kondo-like $\rho(T)$ features in irradiated graphene



Jian-Hao Chen et al., *Nature Phys.* **7** 535 (2011)

- Resistivity vs Temperature measurements in disordered graphene.
- Short-range disorder intentionally caused by irradiation.
- Left: Kondo-like scaling in T/T_K . Right: T_K vs gate voltage.

Kondo effect in graphene: questions.

- Where does the localized (magnetic) state come from?

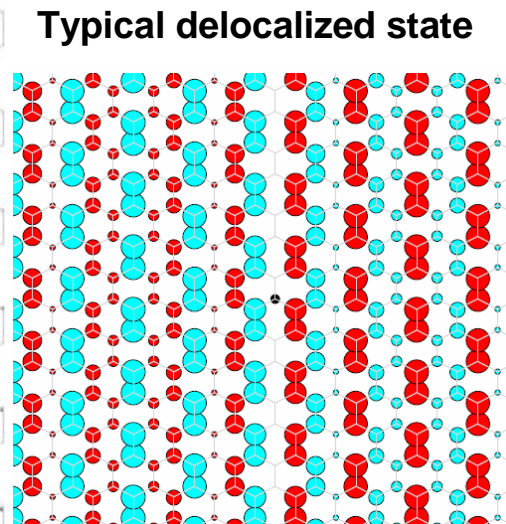
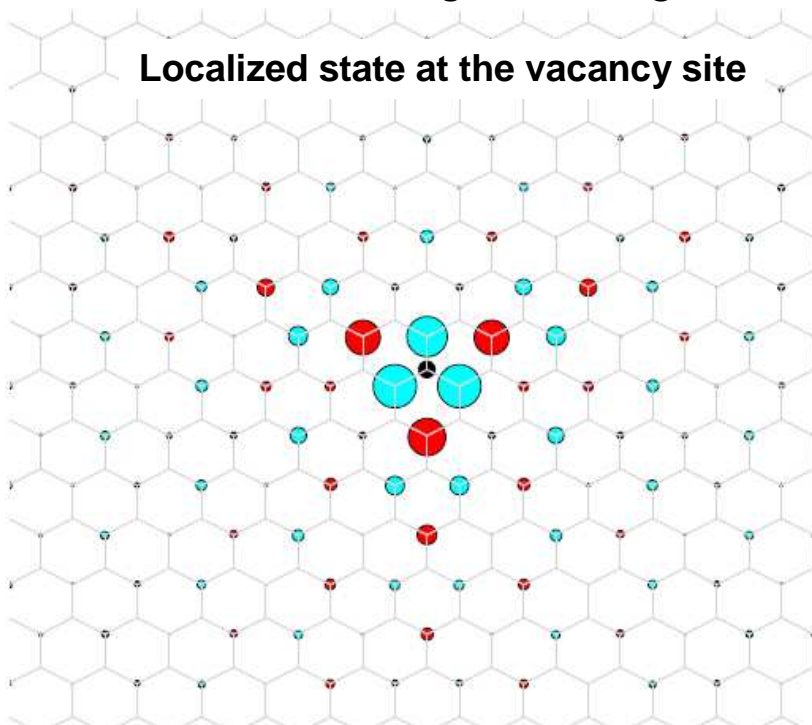
R: Vacancies (=mid gap states) V. M. Pereira et al., *PRB* **77** 115109 (2008)

- How does it couple to the continuous band?

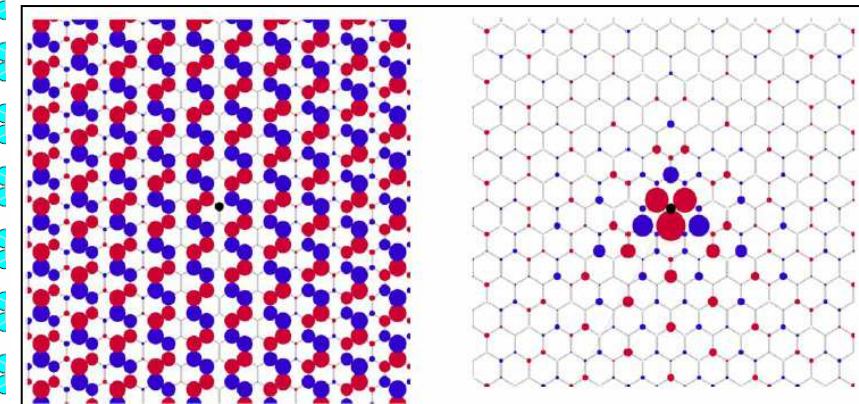
- Does this system retain features of an Anderson model coupled to Dirac fermions?

Mid-gap state in the presence of vacancies.

- Tight-binding calculations: single vacancy leads to midgap state



Agreement with previous results



V. M. Pereira et al., *PRB* **77** 115109 (2008)

- Vacancy tight-binding model:

$$H_v = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + t \sum_{\langle v,j \rangle} c_v^\dagger c_j + \text{H.c.}$$

$$H_v |\nu\rangle = \begin{cases} \varepsilon_\nu |\nu\rangle & \text{for } \varepsilon \neq 0, |\nu\rangle \text{ is extended,} \\ 0 |\nu\rangle & \text{for } \nu = v, |v\rangle \text{ is localized.} \end{cases}$$

Kondo effect in graphene: questions.

- Where does the localized (magnetic) state comes from?

R: Vacancies (=mid gap states) V. M. Pereira et al., *PRB* **77** 115109 (2008)

- How does it couple to the continuous band?

R1: Rippling, Jahn Teller like distortion M. A. Cazallila et al., arXiv 1207.3135 (2012)

R2: Long range disorder (this work)

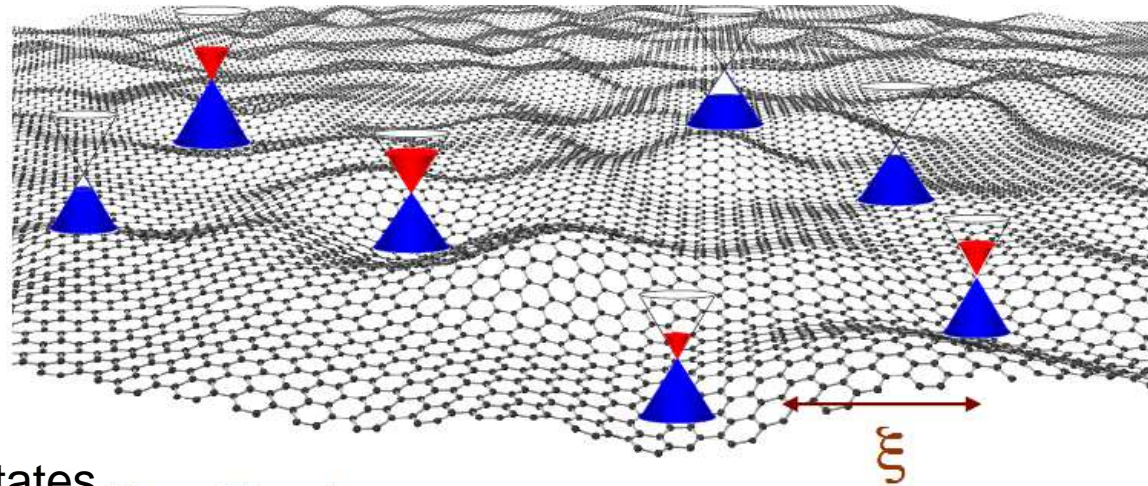
- Does this system retain features of an Anderson model coupled to Dirac fermions?

Tight-binding: long-range disorder+vacancy.

- How to couple the localized state to the graphene band? Disorder (weak)

$$U_{\text{dis}}(\mathbf{r}_i) = \sum_{j=1}^{N_{\text{imp}}} W_j e^{-\frac{(\mathbf{r}_i - \mathbf{R}_j)^2}{2\xi^2}}$$

$$H = H_{\text{v}} + U_{\text{dis}}$$



- Our “basis”: localized and extended states

$$H_{\text{v}} = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + t \sum_{\langle \text{v},j \rangle} c_{\text{v}}^\dagger c_j + \text{H.c.}$$

$$H_{\text{v}}|\nu\rangle = \begin{cases} \varepsilon_\mu |\mu\rangle & \text{and } \varepsilon_\mu \neq 0, \quad |\mu\rangle \text{ is extended,} \\ \varepsilon_0 |0\rangle & \text{and } \varepsilon_0 = 0 \quad |0\rangle \text{ is localized.} \end{cases}$$

- Projectors:

$$\mathbf{1} = \hat{P} + \hat{Q} \equiv \sum_{\mu} |\mu\rangle \langle \mu| + |0\rangle \langle 0|$$

$$H = \hat{P}H\hat{P} + \hat{Q}H\hat{P} + \hat{P}H\hat{Q} + \hat{Q}H\hat{Q}$$

Tight-binding: long-range disorder+vacancy.

- How to couple the localized state to the graphene band? Disorder (weak)

Extended

Coupling

Localized

$$H = \hat{P}H\hat{P} + \hat{Q}H\hat{P} + \hat{P}H\hat{Q} + \hat{Q}H\hat{Q}$$

$$\hat{P}H\hat{P} = \sum_{\mu} |\mu\rangle \varepsilon_{\mu} \langle \mu| + \sum_{\mu\mu'} |\mu\rangle \langle \mu| U_{\text{dis}} |\mu'\rangle \langle \mu'|$$

Effective band density of states.

$$\rho_{\text{dis}}(\omega) = \sum \delta(\omega - \varepsilon_{\beta})$$

$$\hat{Q}H\hat{P} + \text{h.c.} = \sum_{\mu} |0\rangle \langle 0| U_{\text{dis}} |\mu\rangle \langle \mu| + \text{h.c.}$$

Coupling to the localized state

$$t_{\beta 0} \equiv \langle \beta | U_{\text{dis}} | 0 \rangle$$

$$\hat{Q}H\hat{Q} = \sum_{\mu} |0\rangle \varepsilon_0 \langle 0| + |0\rangle \langle 0| U_{\text{dis}} |0\rangle \langle 0| = |0\rangle \varepsilon_0^{\text{dis}} \langle 0|$$

Renormalized state energy

$$\varepsilon_0^{\text{dis}} \equiv \langle 0 | U_{\text{dis}} | 0 \rangle$$

Hybridization function from TB

calculations

For each realization:

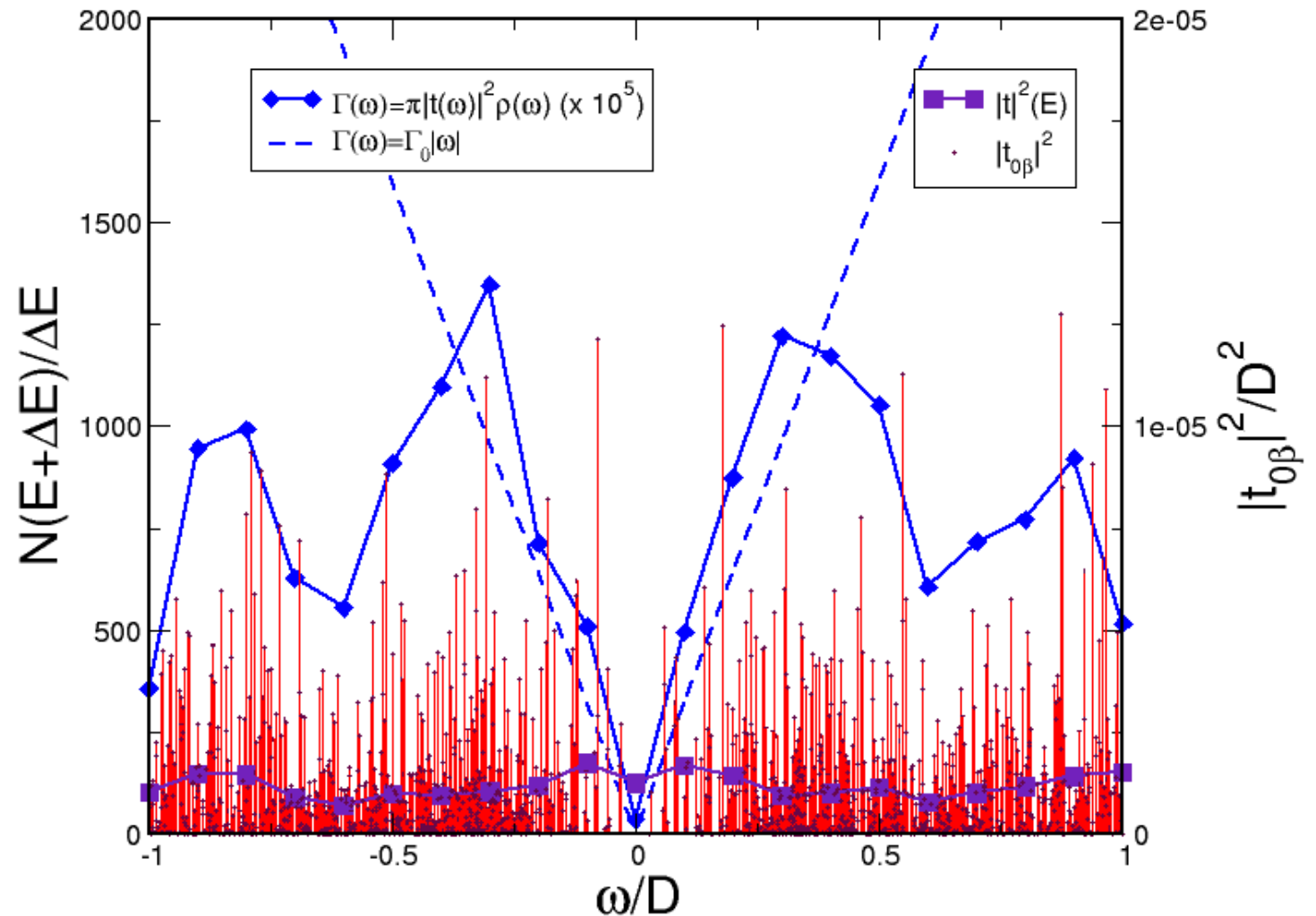
$$|t_{0\beta}|^2 \quad \varepsilon_\beta$$



$$\Gamma_{\text{dis}}(\omega) = \pi |t_\omega|^2 \rho_{\text{dis}}(\omega)$$

And also:

$$\varepsilon_0^{\text{dis}} \equiv \langle 0 | U_{\text{dis}} | 0 \rangle$$



Kondo effect in graphene: questions.

- Where does the localized (magnetic) state comes from?

R: Vacancies (=mid gap states) V. M. Pereira et al., *PRB* **77** 115109 (2008)

- How does it couple to the continuous band?

R1: Rippling, Jahn Teller like distortion M. A. Cazallila et al., arXiv 1207.3135 (2012)

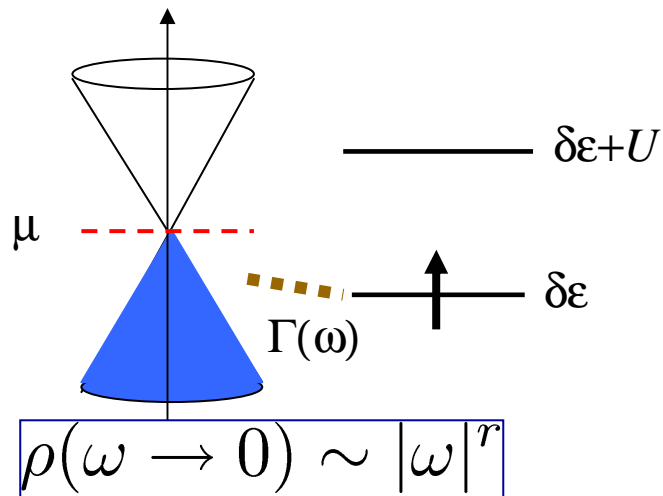
R2: Long range disorder (this work)

- Does this system retain features of an Anderson model coupled to Dirac fermions?

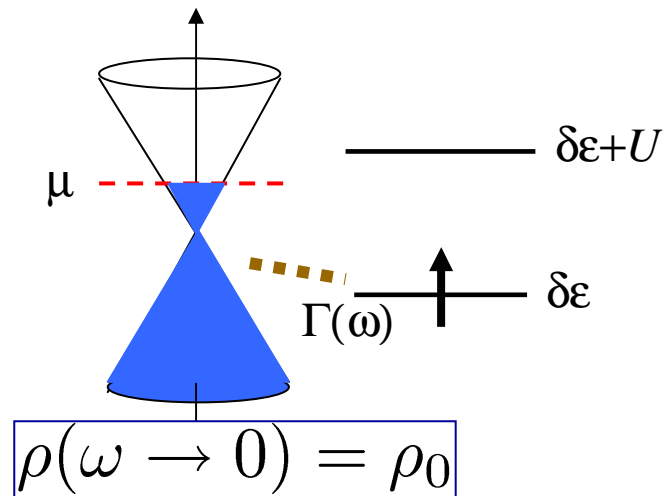
NRG calculations: TB derived Anderson model

Anderson model with Dirac fermions

“Pseudogap” model



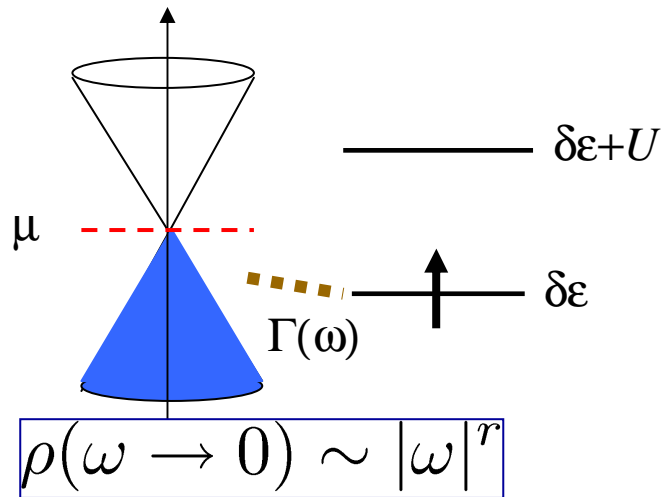
“metallic” model



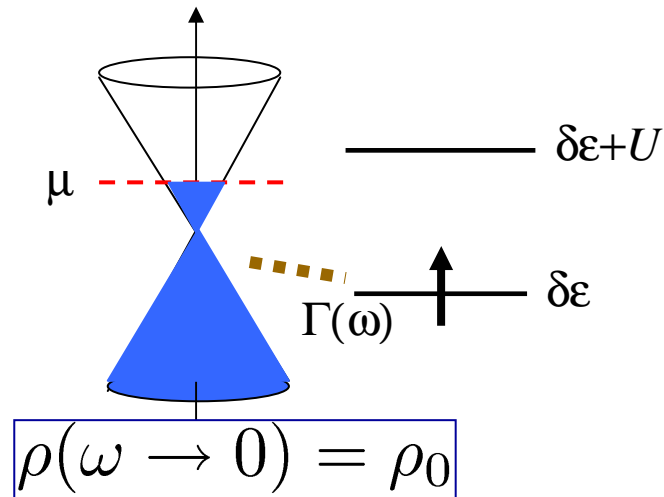
- Anderson impurity coupled to a “Dirac band” with linear dispersion.
- $\delta\varepsilon$: impurity state energy
- $\mu(V_g)$: Fermi energy (gate-dependent)
- $\mu(0)$: Fermi energy at charge neutrality
- Realization of the “pseudogap Anderson model” for $V_g=0$.

Anderson model with Dirac fermions.

“Pseudogap” model



“metallic” model



- Anderson impurity coupled to a “Dirac band” with linear dispersion.
- $\delta\epsilon$: impurity state energy
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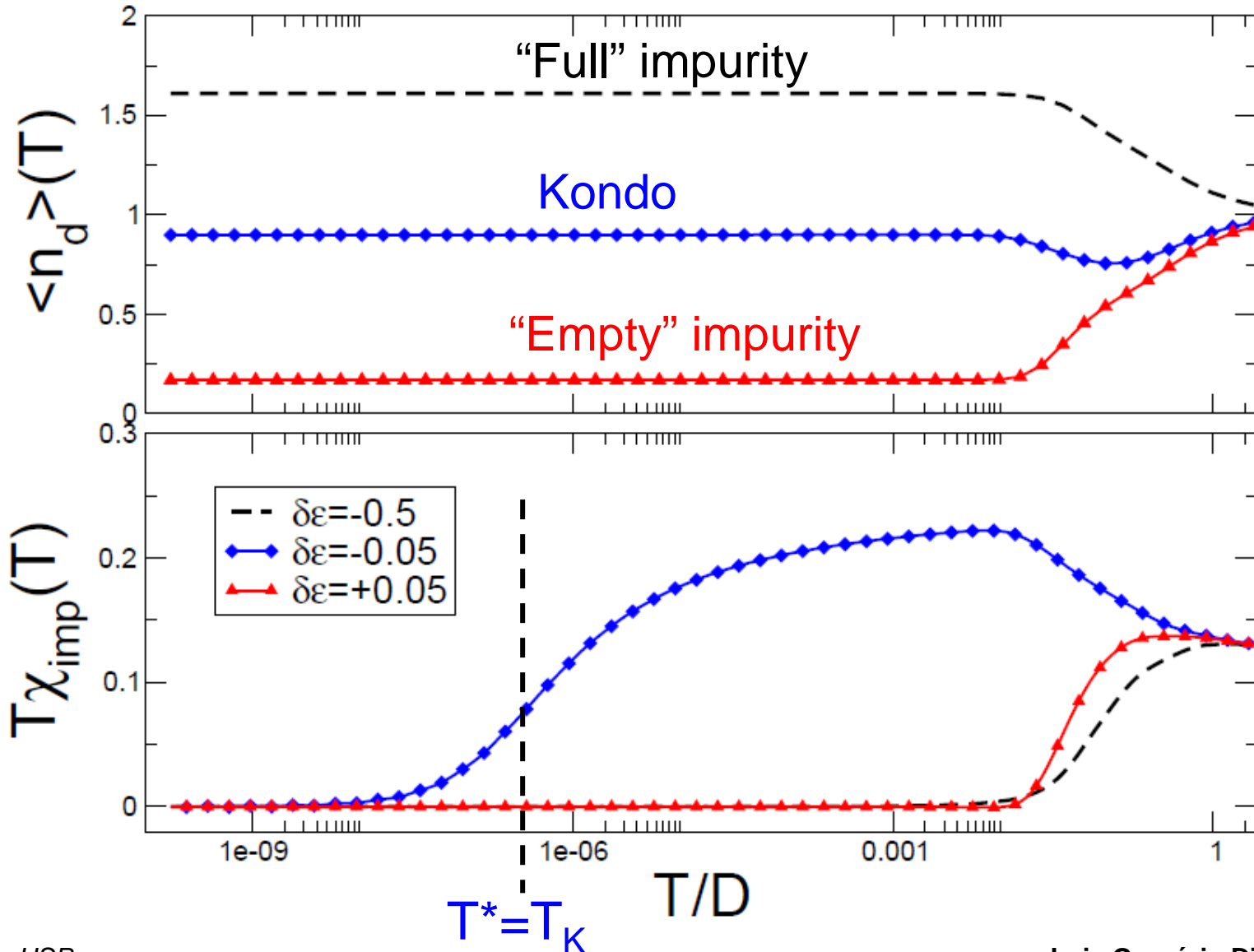
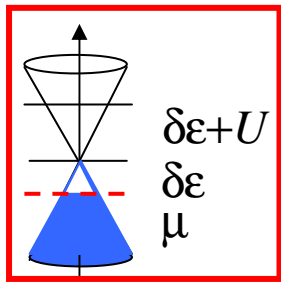
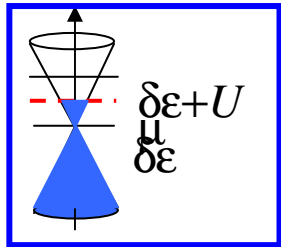
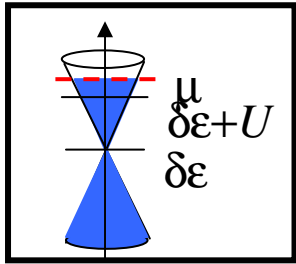
$H_A = H_{\text{state}} + H_{\text{band}} + H_{s-b}$ where:

$$H_{\text{state}} = \delta\epsilon n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} \quad (\delta\epsilon = \epsilon_0 - \mu(V_g))$$

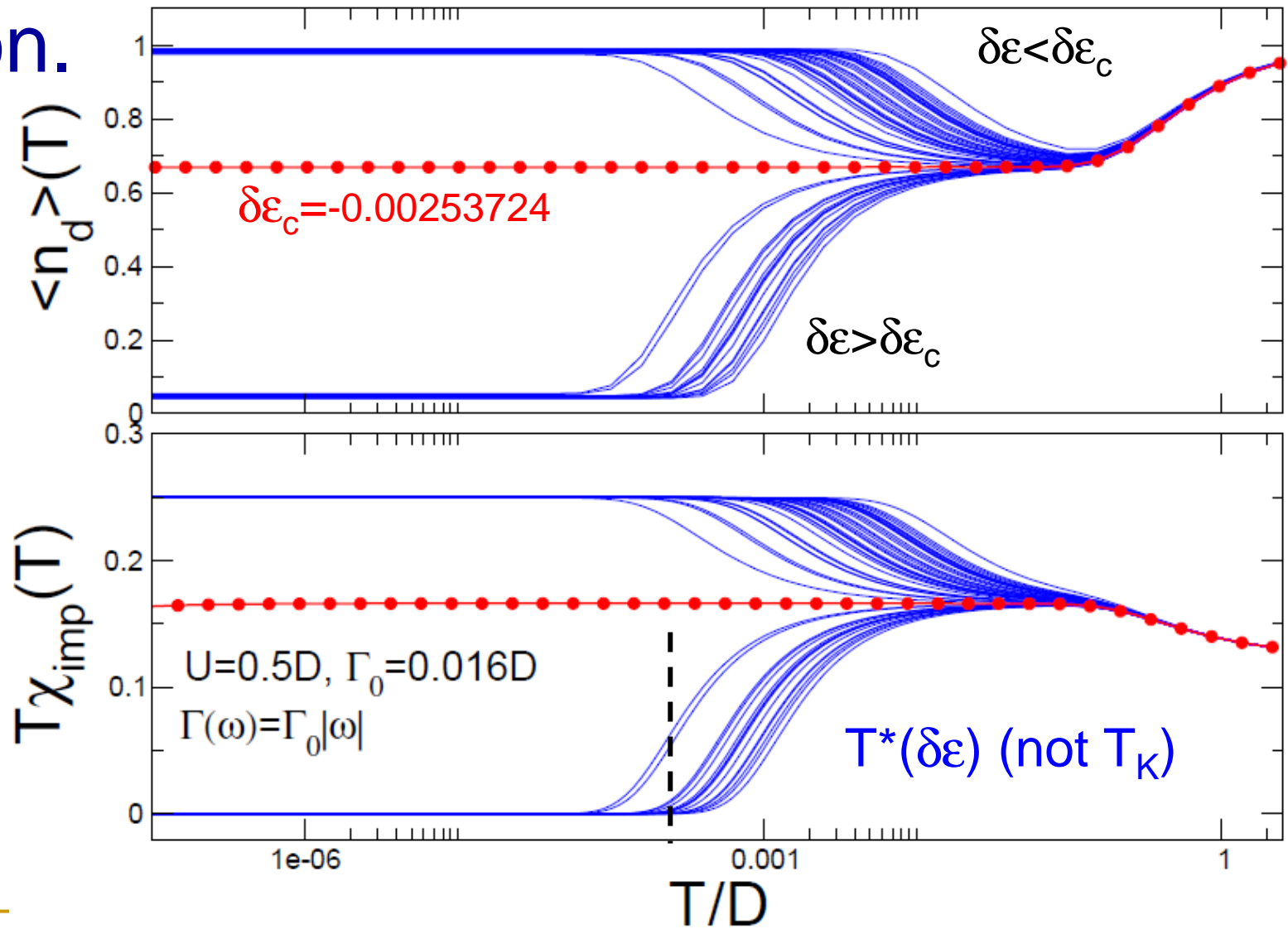
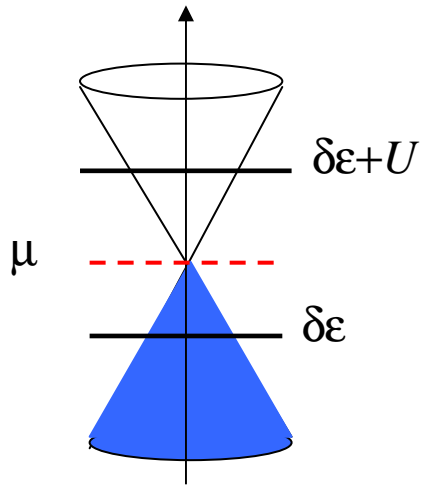
$$H_{\text{band}} = \frac{1}{D} \int_{-D}^D d\omega \omega c_{\omega\sigma}^\dagger c_{\omega\sigma} \quad (\rho(\omega) = \rho_0 |\omega - \Delta\mu|)$$

$$H_{s-b} = \frac{1}{\sqrt{D}} \int_{-D}^D d\omega \sqrt{\rho(\omega)} t_{s-b} \left(c_{d\sigma}^\dagger c_{\omega\sigma} + \text{h.c.} \right) .$$

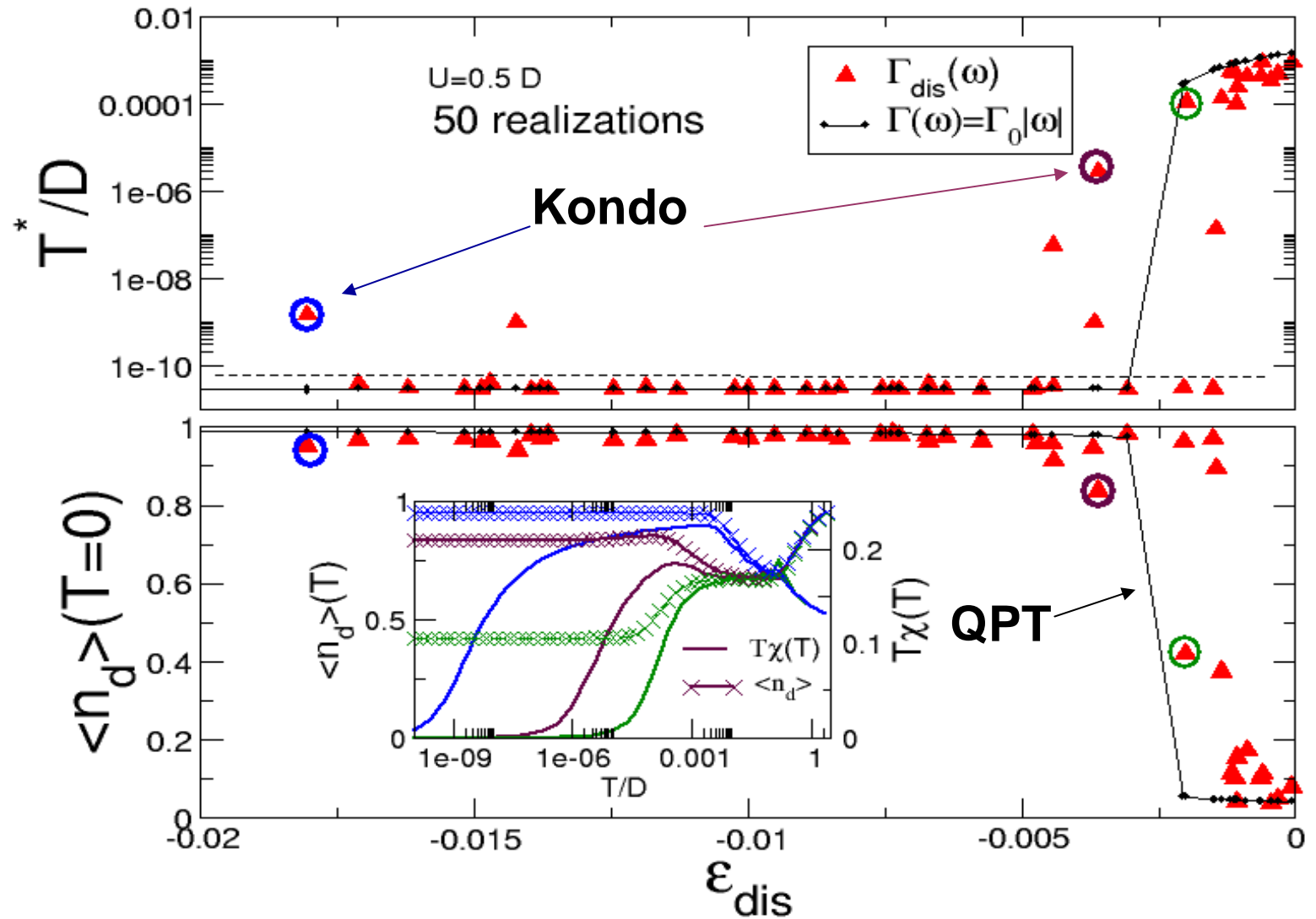
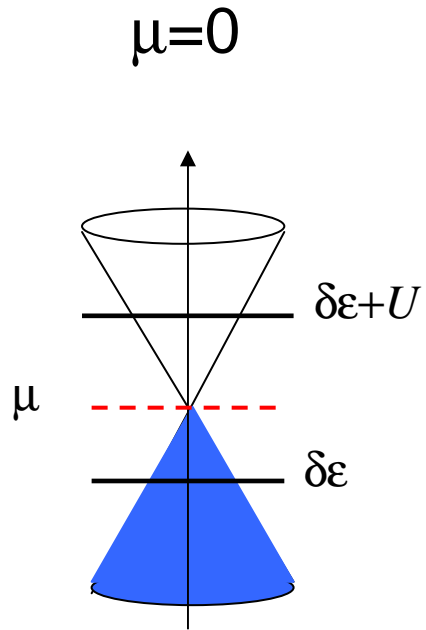
Metallic model: “vanilla” Kondo effect (NRG)



Pseudogap model: quantum phase transition.



Tight-binding + NRG.



Mapa do Seminário

◆ 15 anos do Efeito Kondo em nanoestruturas.

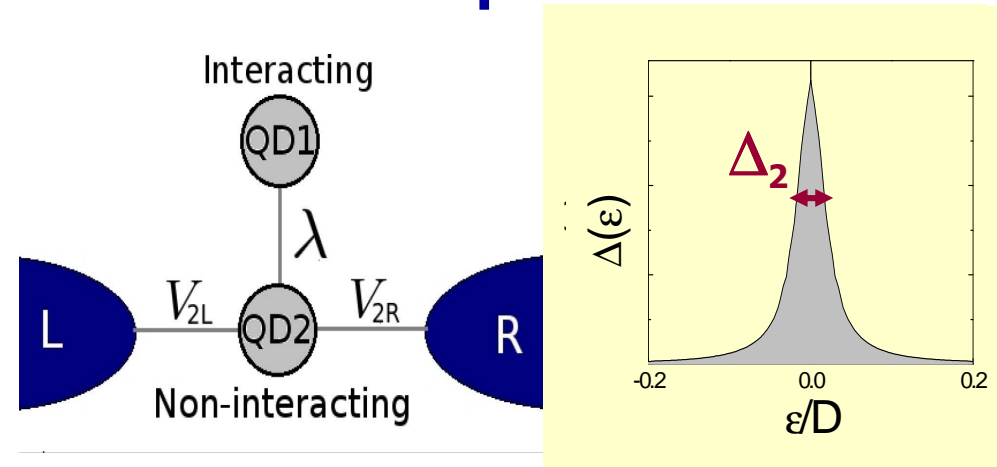
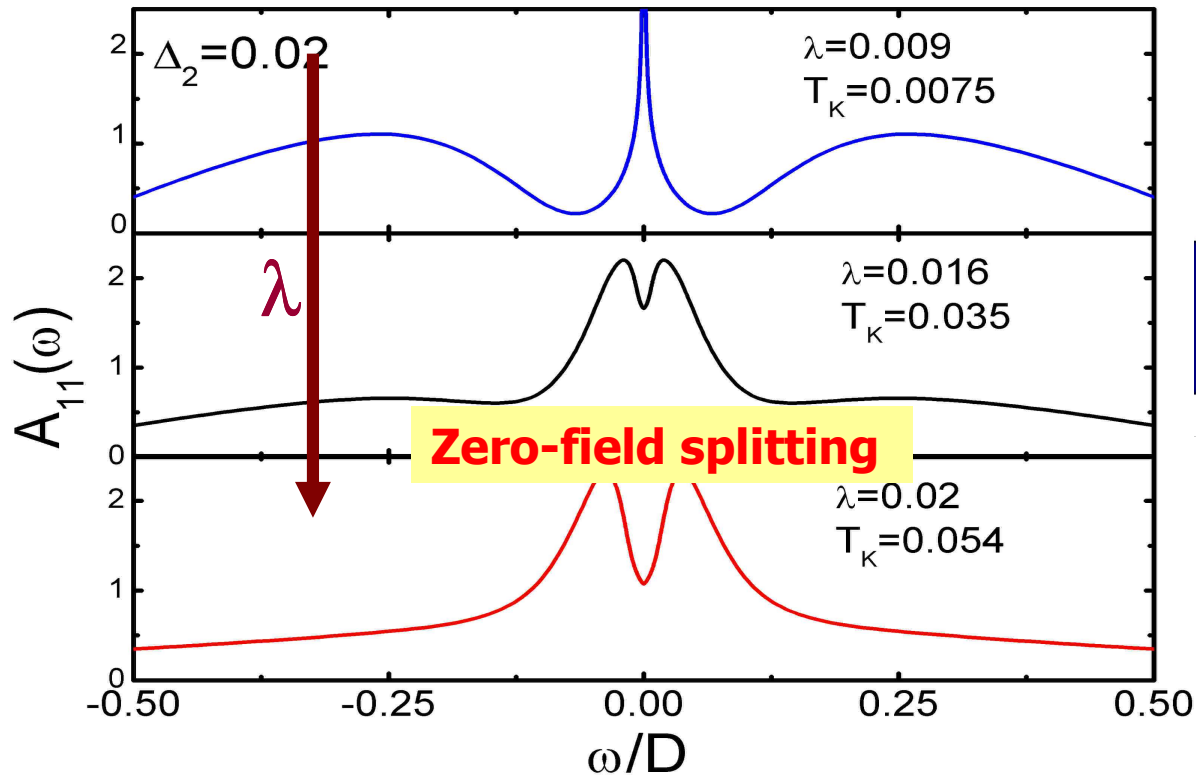
- Review: Efeito Kondo em metais com impurezas.
- 1998: “Revival of the Kondo effect”: pontos quânticos e átomos em superfícies.

◆ E hoje? Alguns desenvolvimentos recentes.

- Efeito Kondo com Férmions de Dirac.
- Ação combinada com outros efeitos quânticos (graus de liberdade orbitais, efeito Zeeman, etc.): transições de fase quânticas e “filtros de spin”.

LDS, E. Vernek, K. Ingersent, N. Sandler, S. Ulloa,
PRB **87** 205313 (2013)

Zero-field splitting of the Kondo peak



Side-coupled QDs Splitting of the Kondo peak at $T_K > \Delta_2$.

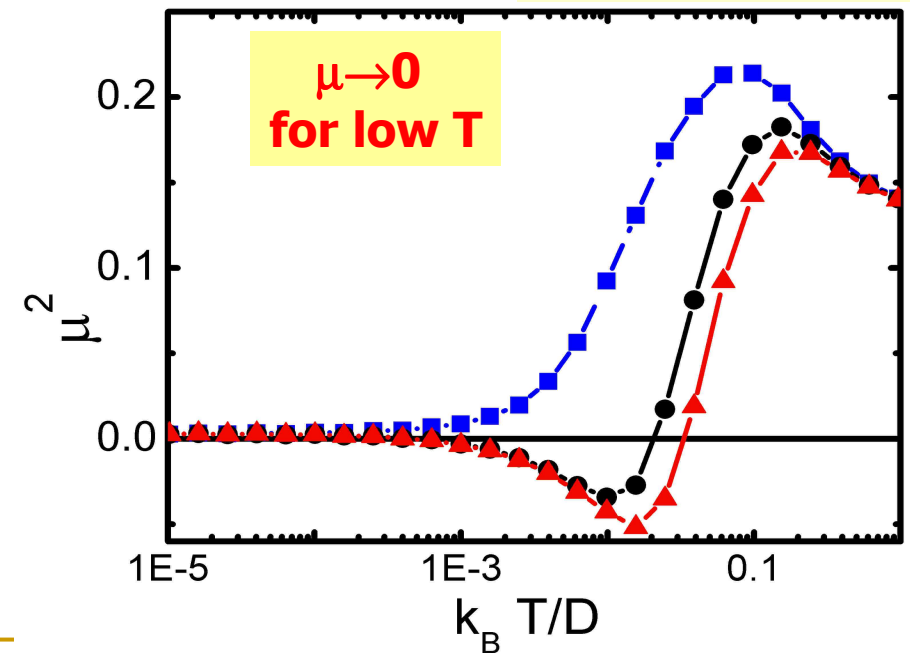
LDS et al PRL **97**, 096603 (2006).

Vaugier et al. PRL **99**, 209701 (2007).

LDS et al. PRL **99**, 209702 (2007).

Vaugier et al. PRB **76**, 165112 (2007).

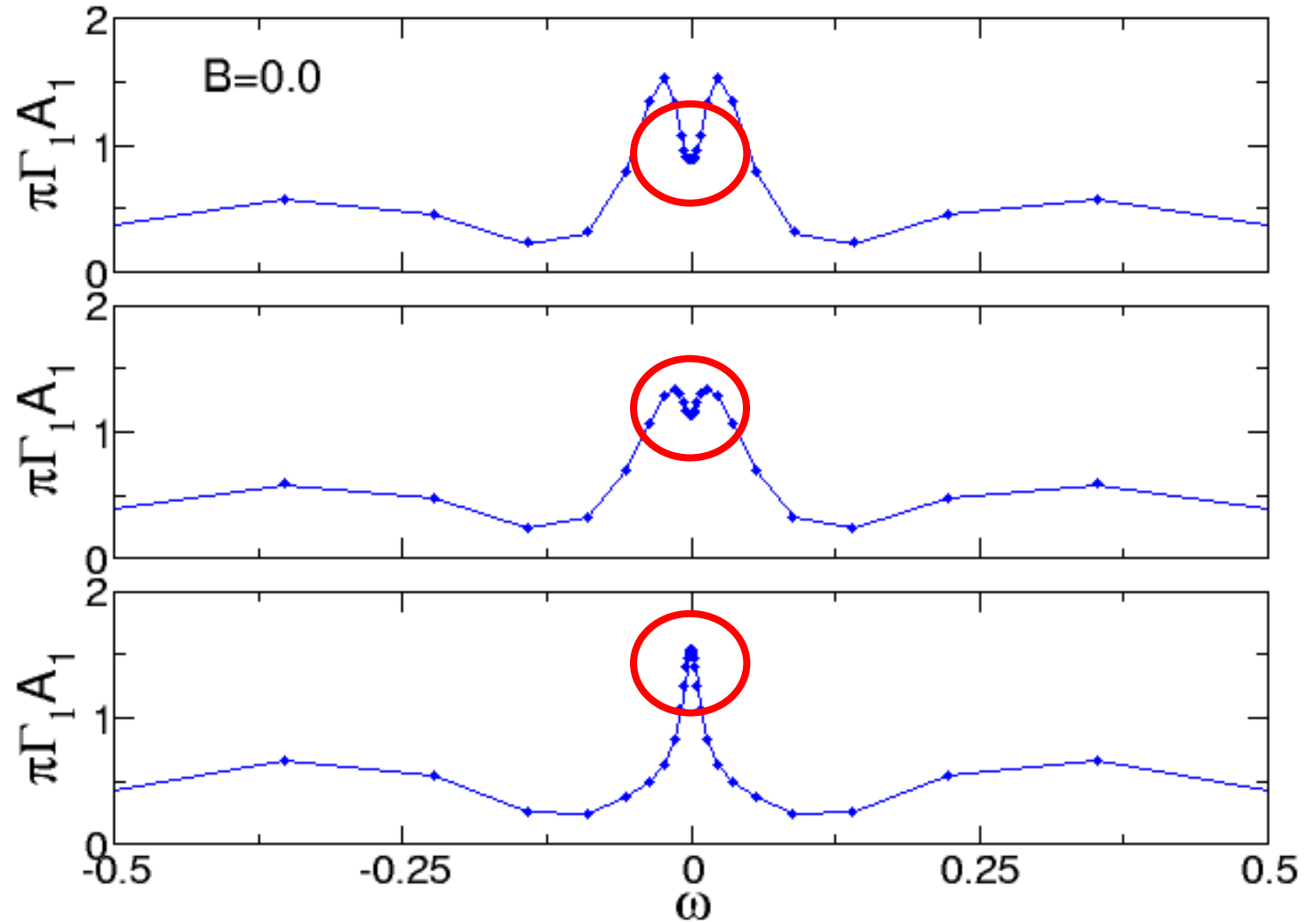
LDS et al PRB **78**, 153304 (2008).



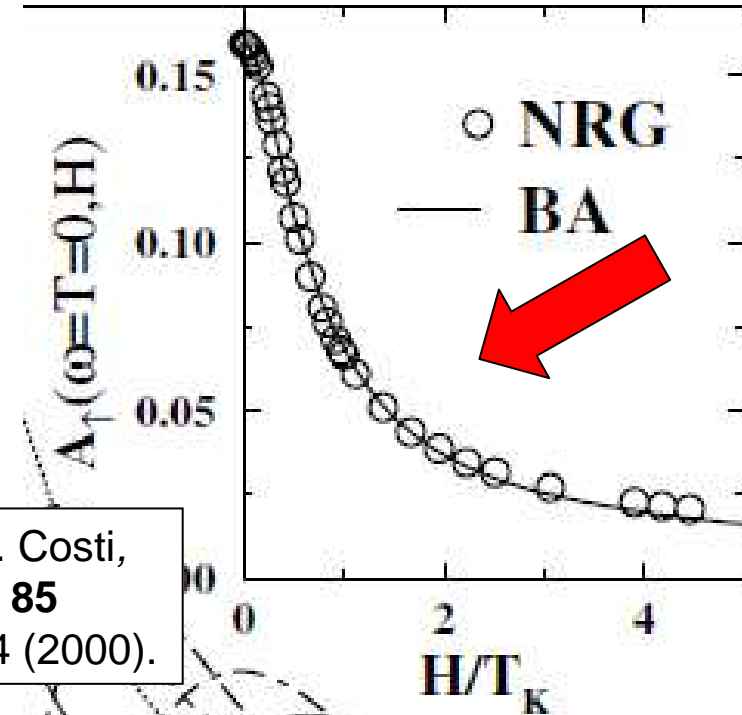
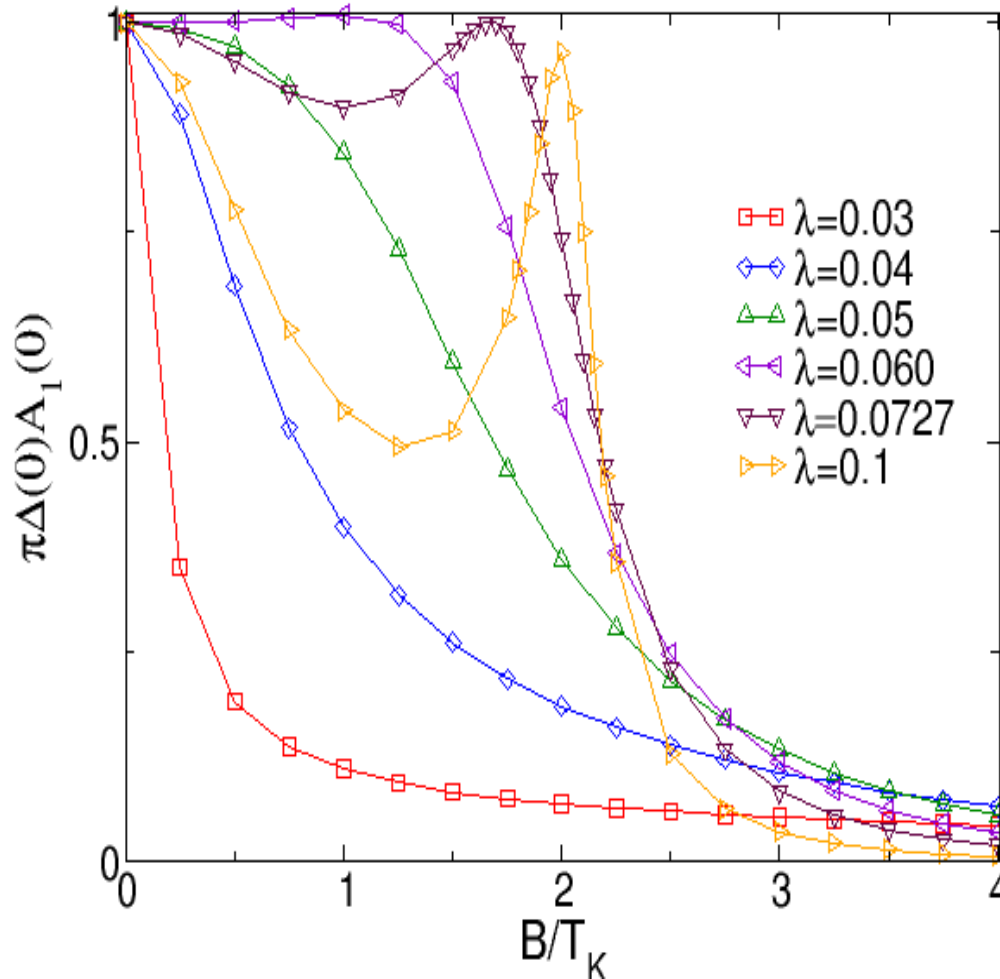
Kondo Peak Splitting: Zeeman + orbital

$$A_{1\sigma}(\omega) = -\frac{\text{Im } \mathcal{G}_{1\sigma}(\omega)}{\pi}$$

$$A_1(\omega) = \frac{A_{1\uparrow}(\omega) + A_{1\downarrow}(\omega)}{2}$$



A(0) vs field: non-universal decay?



T. A. Costi,
PRL **85**
1504 (2000).

p-h-s: **monotonic decay with h!**

$$\pi\Gamma A_d(0, h) = \cos^2(\pi M_d)$$

D.E. Logan, N.L. Dickens,
JPCM **13** 9713 (2001)

$$M_d(h) = \frac{1}{2} (\langle n_{d\uparrow} \rangle - \langle n_{d\downarrow} \rangle)$$

Friedel Sum Rule revisited

Langreth, PR **150** 516 (1966).

Vaugier et al. PRB **76**, 165112 (2007).

$\mathcal{G}_{1\sigma}(\omega, T) \rightarrow$ Fully interacting GF in dot 1

$\Sigma_{1\sigma}^0(\omega) \rightarrow$ Non-interacting self-energy

$$A_{1\sigma}(\omega) = -\frac{1}{\pi} \text{Im} \mathcal{G}_{1\sigma}(\omega)$$

$$\Delta_{\sigma}(\omega) = -\text{Im} \Sigma_{1\sigma}^0(\omega)$$

$$\pi \Delta_{\sigma}(0) A_{1\sigma}(0, 0) = \sin^2 (\pi \langle n_{1\sigma} \rangle + \varphi_{\sigma})$$

where

$$\varphi_{\sigma} = \text{Im} \int_{-\infty}^0 \frac{\partial \Sigma_{1\sigma}^0(\omega)}{\partial \omega} \mathcal{G}_{1\sigma}(\omega) d\omega$$

“Usual” case:

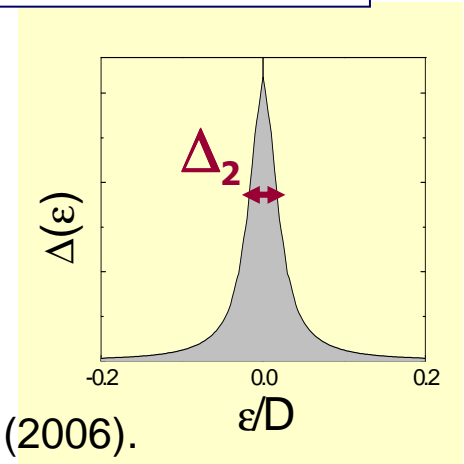
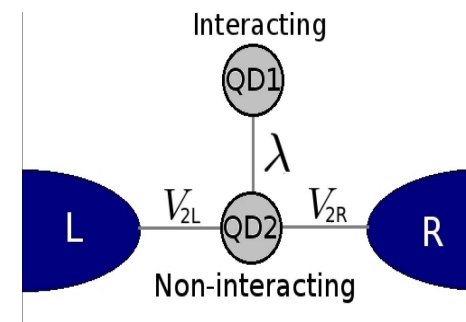
$$\Delta_{\sigma}(\omega) = \Delta_0$$

$$\varphi_{\sigma} = 0$$

DQD mapping:

$$\Delta_{\sigma}(\omega) = \frac{\lambda^2 \Delta_2}{(\omega - \varepsilon_{2\sigma})^2 + \Delta_2^2}$$

$$\varphi_{\sigma} \neq 0$$



LDS et al PRL **97** 096603 (2006).

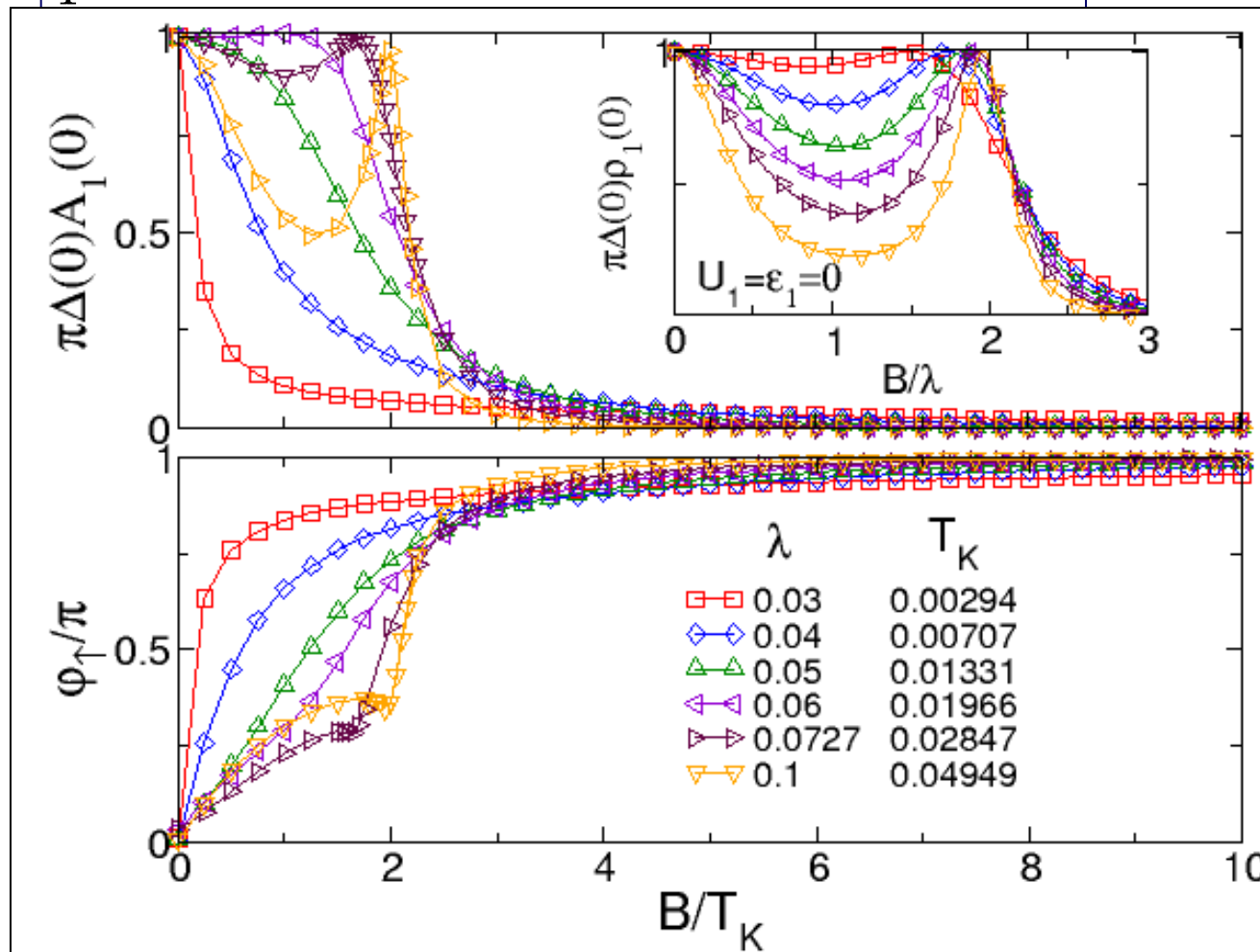
Magnetic Field dependence at the Fermi energy:

$$\frac{\pi}{4} \sum_{\sigma} \Delta_{\sigma}(0) A_{1\sigma}(0, h) = \cos^2 (\pi M_1 + \varphi_{1\uparrow})$$

$$M_1(h) = \frac{1}{2} (\langle n_{1\uparrow} \rangle - \langle n_{1\downarrow} \rangle)$$

FSR revisited: B -dependence

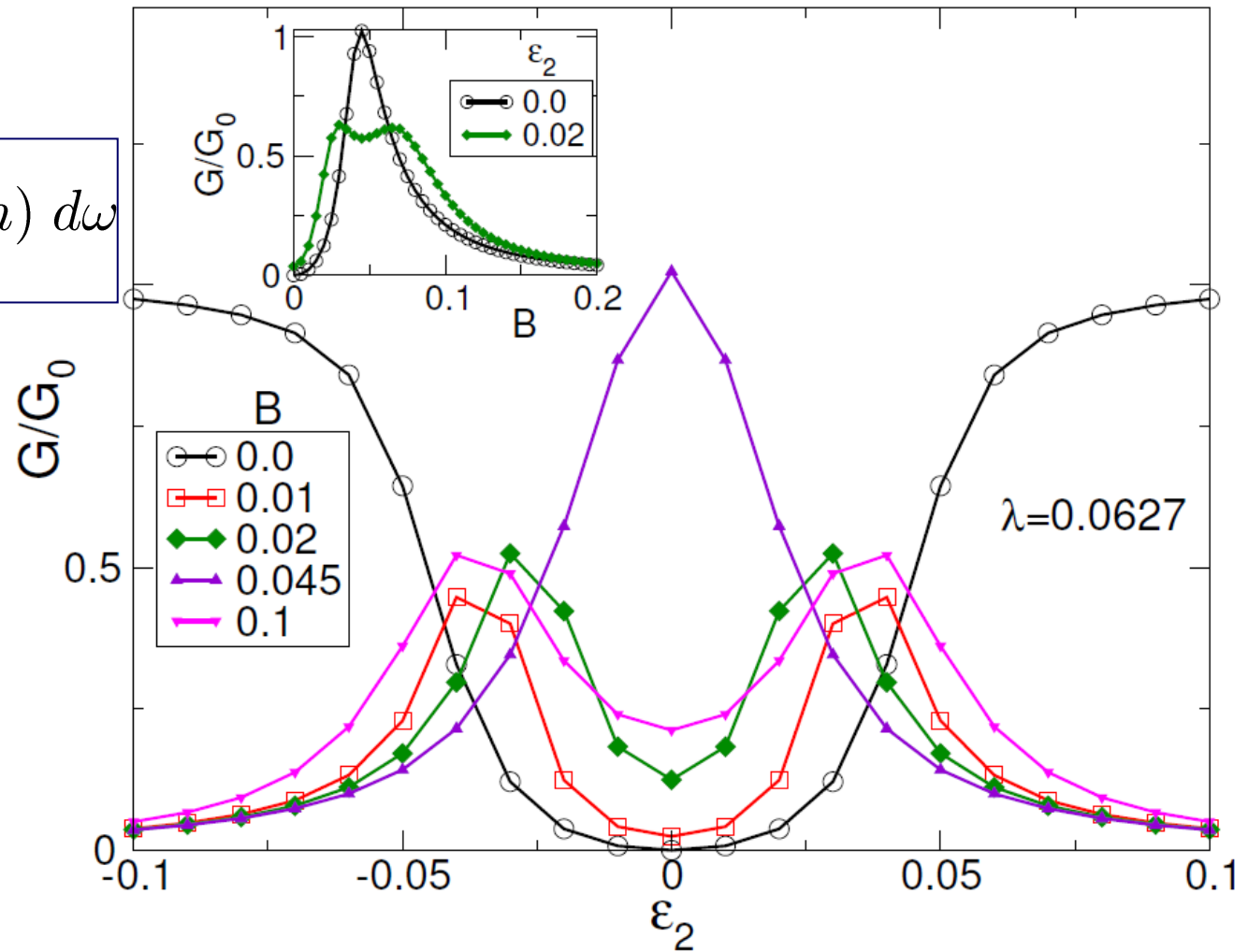
$$\frac{\pi}{4} \sum \Delta_{\sigma}(0) A_{1\sigma}(0, h) = \cos^2(\pi M_1 + \varphi_{1\uparrow})$$



Conductance

$$G_{\sigma} = \frac{\pi e^2}{4h} \sum_{\sigma} \int \Delta_{\sigma}(0) A_{1\sigma}(0, h) d\omega$$

$$G = \frac{G_{\uparrow} + G_{\downarrow}}{2}$$

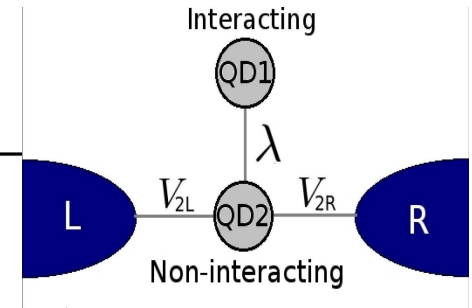
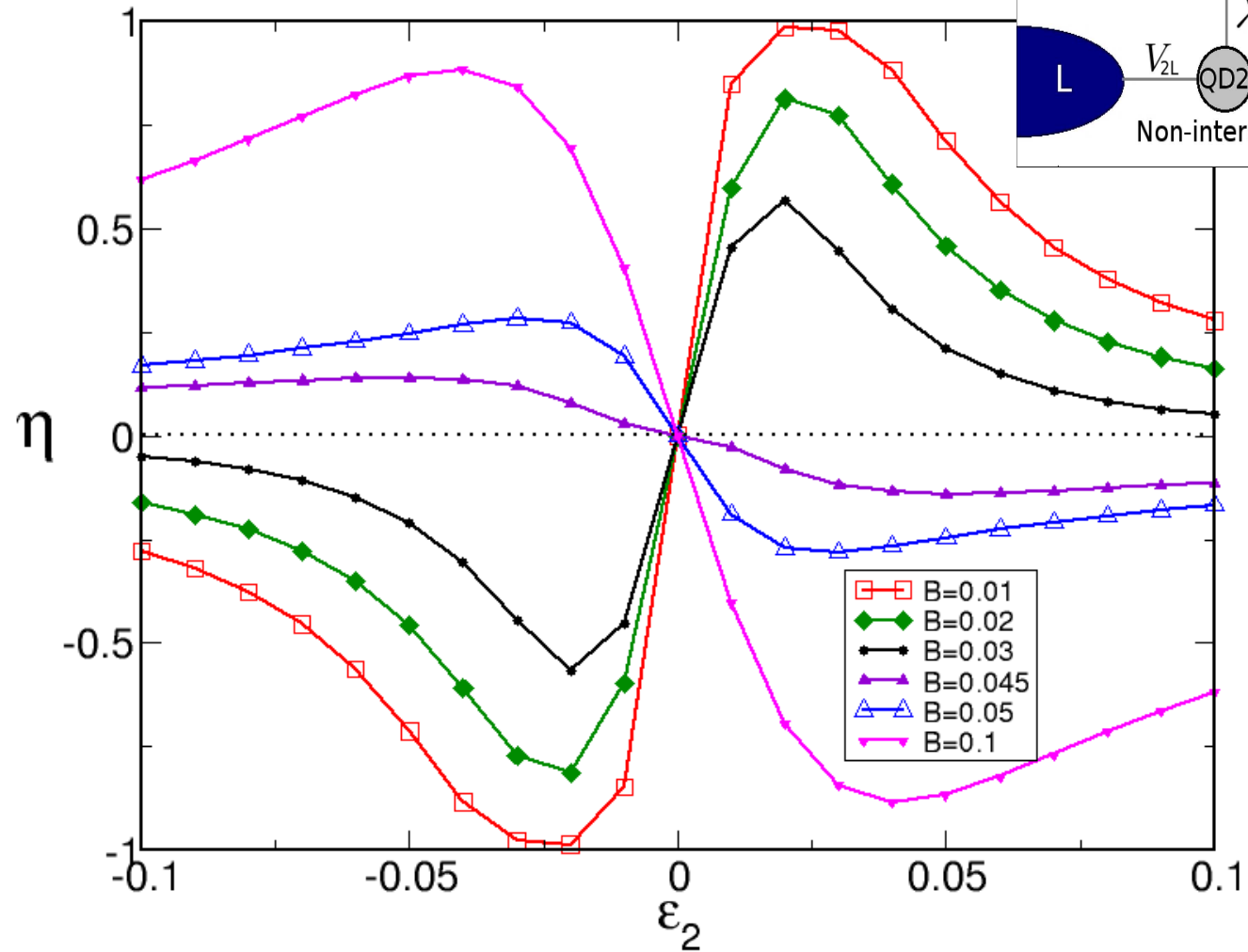


Spin-polarization: conductance

$$\eta = \frac{G_{\uparrow} - G_{\downarrow}}{G_{\uparrow} + G_{\downarrow}}$$

Wire + side-coupled QD
(non-Kondo)

Aligia and Salguero,
PRB **70**, 075307 (2004).
M. E. Torio, et al.
EPJ B **37**, 399 (2004).



LDS, E. Vernek, K. Ingersent, N. Sandler, S. Ulloa,
PRB **87** 205313 (2013)

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George Martins (Oakland U)

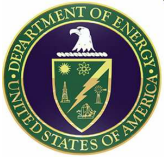
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Adrian Feiguin (Northeastern)

Support (USA):

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NSF: DMR-0706020 (TN);



Brazil: CNPq, FAPESP, PRP-USP



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