O que os nanomateriais podem nos ensinar em termos de Física de sistemas de muitos corpos?

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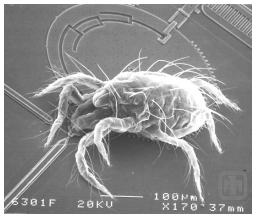
“The scale of things” (US DOE-BES)

Things Natural

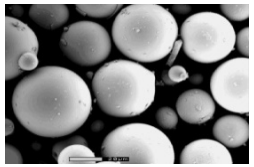


Dust mite

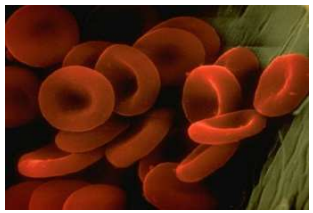
200 mm

Ant
~ 5 mm

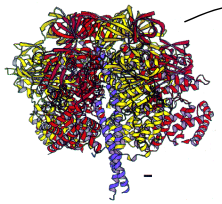
Human hair
~ 60-120 mm wide



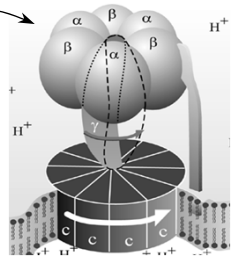
Fly ash
~ 10-20 mm



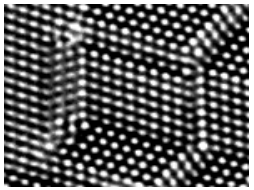
Red blood cells
(~7-8 mm)



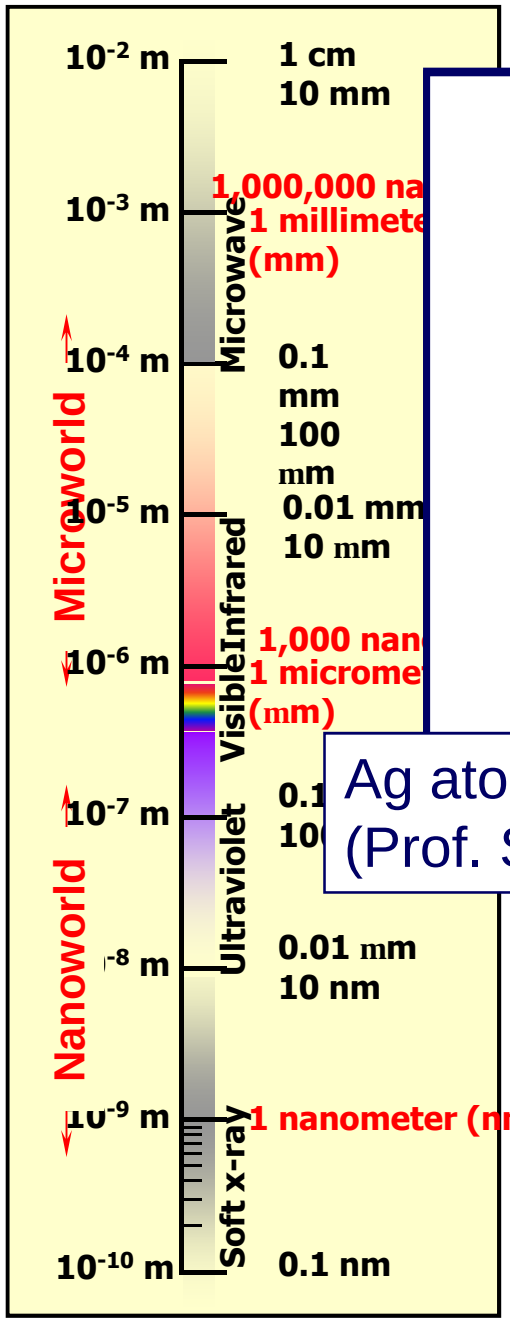
~10 nm diameter



ATP synthase

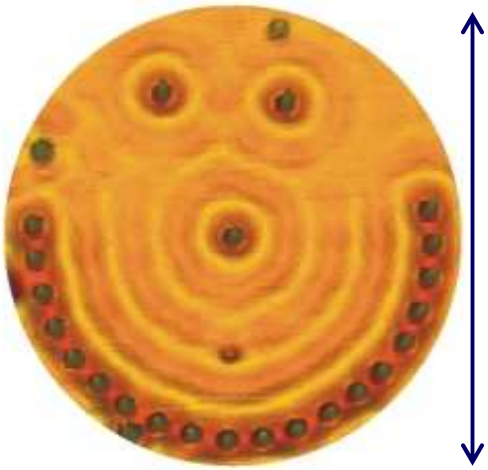


Atoms of silicon
spacing ~tenths of nm



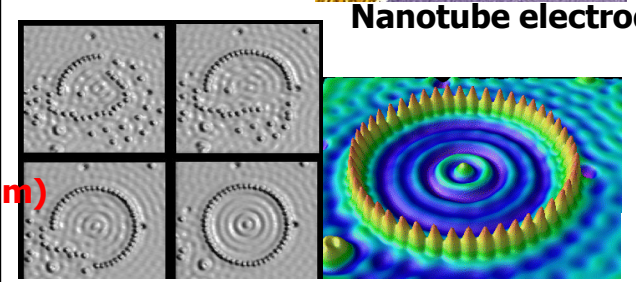
Things Manmade

“NanoSmiley”

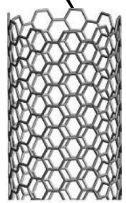


Ag atoms in a Ag(111) surface (STM).
(Prof. Saw Hla’s group, Ohio University)

Nanotube electrode



Quantum corral of 48 iron atoms on Cu surface positioned one at a time with an STM tip



Carbon nanotube
~1.3 nm diameter

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EBEE 2016

Let's start with a very simple question:

What's the solution of:

$$i\hbar\frac{\partial}{\partial t}\left|\Psi_{\mathrm{all}}\right\rangle = H_{\mathrm{all}}\left|\Psi_{\mathrm{all}}\right\rangle \quad ?$$

In other words….

What's the answer to life, the universe and everything?

And the answer is… (Hint: you can Google it!) **42**

According to "The Hitchhiker's Guide to the Galaxy, by Douglas Adams

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“Theory of Everything”

R. B. Laughlin and David Pines, PNAS **97** 28-31 (2000)

$$i\hbar\frac{\partial}{\partial t}|\Psi_{\rm all}\rangle = H_{\rm all}|\Psi_{\rm all}\rangle$$

In our everyday life, “everything” is made of electrons and nuclei.

Kinetic energy
electrons e nuclei

$$H_{\rm all} = \sum_j^{N_e}\frac{p_j^2}{2m_e} + \sum_\alpha^{N_n}\frac{P_\alpha^2}{2M_n}$$

Attractive/repulsive interactions between electrons e nuclei

$$-\sum_j^{N_e}\sum_\alpha^{N_n}\frac{Z_\alpha e^2}{|\mathbf{r}_j-\mathbf{R}_\alpha|} \qquad +\sum_{j,k}^{N_e}\frac{e^2}{|\mathbf{r}_j-\mathbf{r}_k|} \qquad +\sum_{\alpha,\beta}^{N_n}\frac{Z_\alpha Z_\beta e^2}{|\mathbf{R}_\alpha-\mathbf{R}_\beta|}$$

electron-nuclei | electron-electron | nuclei-nuclei

Not included: - Light and photons in general (which can be important)
- *Gravity* - *Nuclear forces* , etc.

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“Theory of Everything” does not predict everything!

$$i\hbar\frac{\partial}{\partial t}\left|\Psi_{\mathrm{all}}\right\rangle = H_{\mathrm{all}}\left|\Psi_{\mathrm{all}}\right\rangle$$

R. B. Laughlin and David Pines, PNAS **97** 28-31 (2000)

- Can only solve this equation exactly for small systems (N_e,N_n~10).
- Large systems: Much harder problem!
- Some approximations sometimes work well: Hartree-Fock, CI, DFT (+GGA, B3LYP), GW, etc.

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“Theory of Everything” does not predict everything!

$$i\hbar\frac{\partial}{\partial t}|\Psi_{\rm all}\rangle = H_{\rm all}|\Psi_{\rm all}\rangle$$

R. B. Laughlin and David Pines, PNAS **97** 28-31 (2000)

- Exact solution only for $N_{e,h}$~10!
- Even if one *could* solve it, this equation (as is) does not predict several fundamental behaviors!

Conductance quantum in the quantum Hall effect (=e^2/h).
- Quantum magnetic flux (=hc/2e) in superconduting rings (or in the Josephson effect).
- Magnetic field generated by rotating superconductors (=e/mc).

Experimental measurement of some of the fundamental physical constants: *h, m* and *c* !

Why???

These are *emergent* phenomena!

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In short:

Robert Laughlin - Stanford
Nobel Prize winner – 1998

> “We have succeeded in reducing all of ordinary physical behavior to a simple, correct Theory of Everything only to discover that it has revealed exactly nothing about many things of great importance.”

David Pines
U.C. Davis

Robert B. Laughlin and David Pines, “Theory of Everything”
PNAS **97** 28-31 (2000)

“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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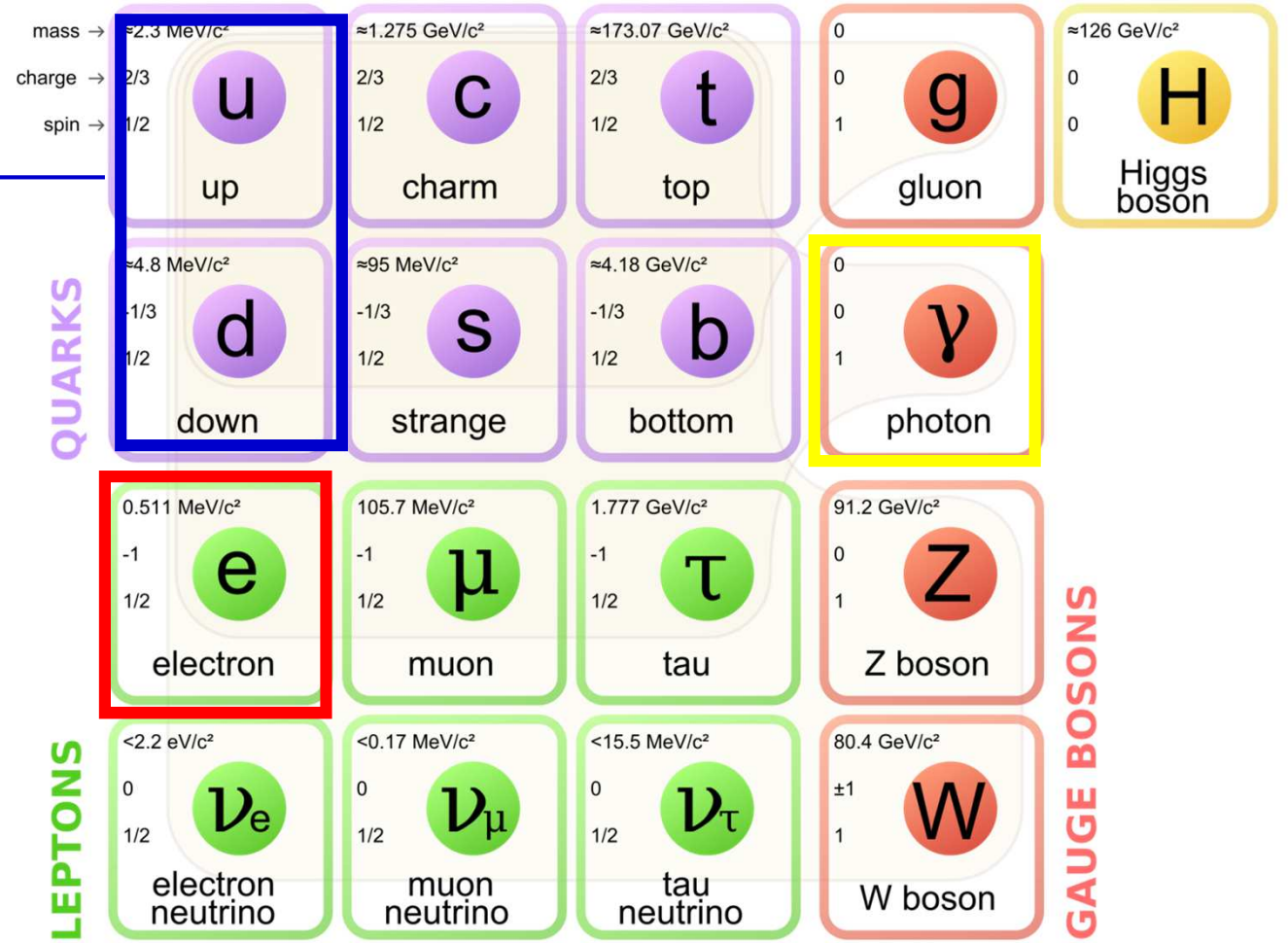
What is fundamental?

Nuclei



Standard Model Particles

Too much information!

All we need to make up all materials we have contact with is: electrons + nuclei

(and perhaps some photons?)

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How to do it then? *Model-based approach.*

In almost every case where I have been really successful it has been by dint of discarding almost all of the apparently relevant features of reality in order to create a “model” which has the two almost incompatible features:

1) enough *simplicity* to be solvable, or at least understandable;
2) enough *complexity* left to be interesting, in the sense that the remaining complexity actually contains some essential features which mimic the actual behavior of the real world, preferably in one of its as yet unexplained aspects.

Phillip W. Anderson, “More and Different: Notes from a Thoughtful Curmudgeon”

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Minicourse contents:

Lecture 1:

- Intro: “More is Different”.
- The Kondo effect: a true “More is Different” phenomenon.
- Wilson’s numerical renormalization group method.

Lecture 2:

- Applications I: Magnetic molecules on surfaces.
- Applications II: Vacancies in Graphene.

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Lecture 1:

Kondo effect and Wilson's Numerical Renormalization Group method.

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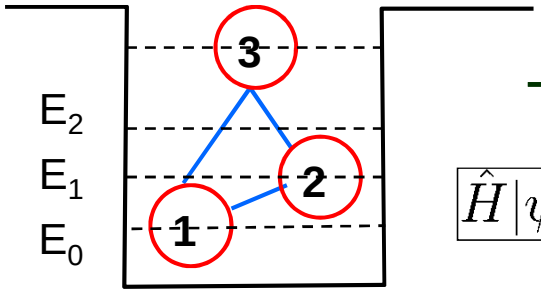
Example I: Many-body Quantum Well



"Particle in a box" :

$$\hat{H}^{(1)}|\phi_i^{(1)}\rangle = E_i^{(1)}|\phi_i^{(1)}\rangle$$

Two *interacting* particles

$$\hat{H} = \hat{H}^{(1)} + \hat{H}^{(2)} + \hat{V}_{1,2}$$

$$\hat{H}|\psi_k\rangle = E_k|\psi_k\rangle$$

$$|\psi_k\rangle = \sum_{ij} |\phi_i^{(1)}\rangle \otimes |\phi_j^{(2)}\rangle \otimes |\psi_j^{(2)}\rangle$$

$$E_k = E_k^{(1)} + E_k^{(2)} + ??$$

(via diagonalization…)

$$\bar{\psi}_k^{S,A}(\mathbf{r}_1, \mathbf{r}_2) = \pm \bar{\psi}_k^{S,A}(\mathbf{r}_2, \mathbf{r}_1)$$

Two *indistinguishable* particles (bosons/fermions)

Many-body system

$$\hat{H} = \sum_a \hat{H}^{(a)} + \sum_{a \neq b} \hat{V}_{a,b}$$

$$|\psi_0\rangle = \sum_{ij\cdots z} C^0_{ij\cdots z} |\psi_i^{(1)}\rangle \otimes |\psi_j^{(2)}\rangle \cdots \otimes |\psi_z^{(N)}\rangle$$

$$E_0 = ?$$

Ground state (sometimes, it's all you can do!)

$$\psi_0^{S,A}(\mathbf{r}_1, ..., \mathbf{r}_k, ..., \mathbf{r}_\ell, ...\mathbf{r}_N) = \pm \psi_0^{S,A}(\mathbf{r}_1, ..., \mathbf{r}_\ell, ..., \mathbf{r}_k, ...\mathbf{r}_N)$$

N *indistinguishable* particles (bosons/fermions)

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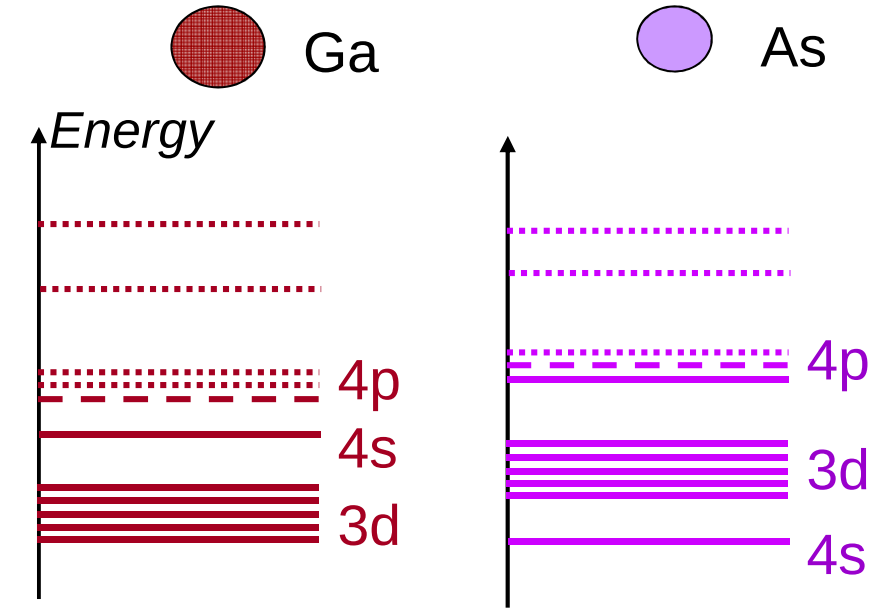
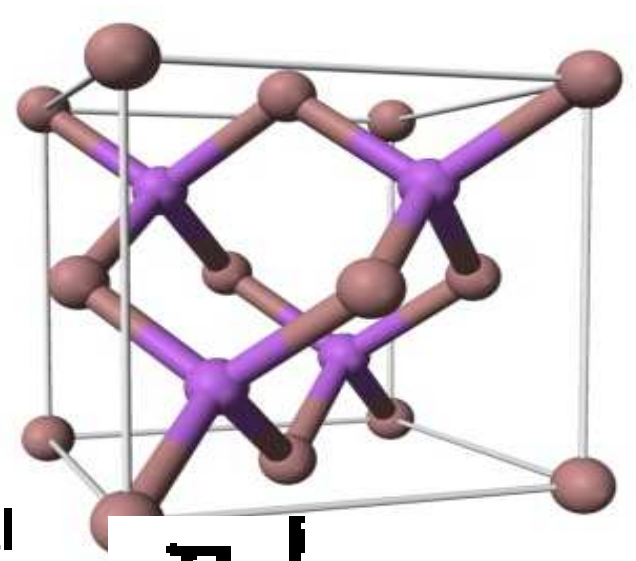
From atoms to solids



Atomic Energy levels

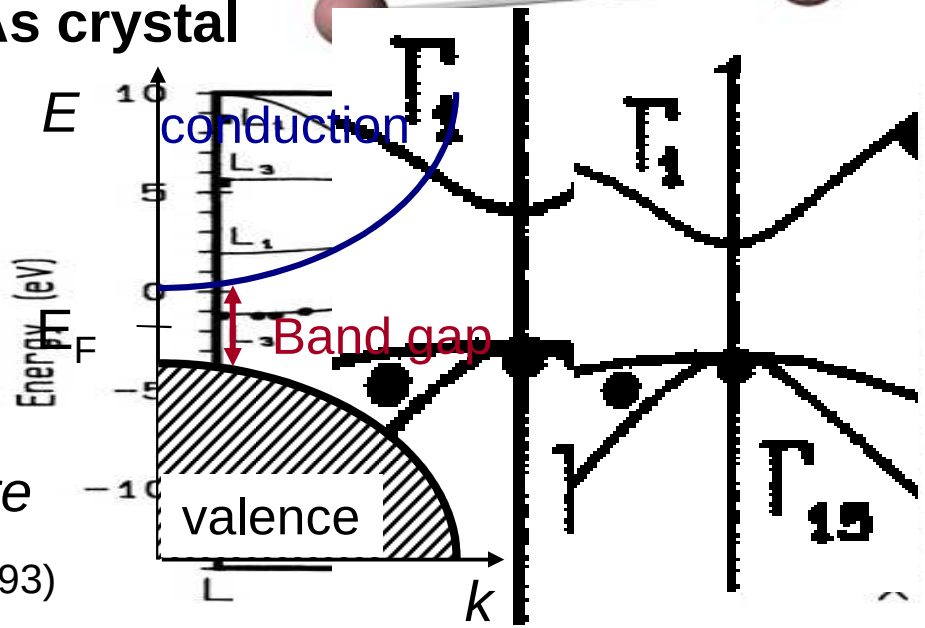
Many Atoms!



GaAs crystal

Many Atoms!

Band structure



M. Rohlfing et al. PRB **48** 17791 (1993)

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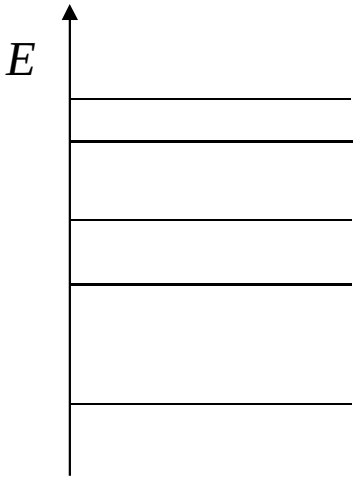
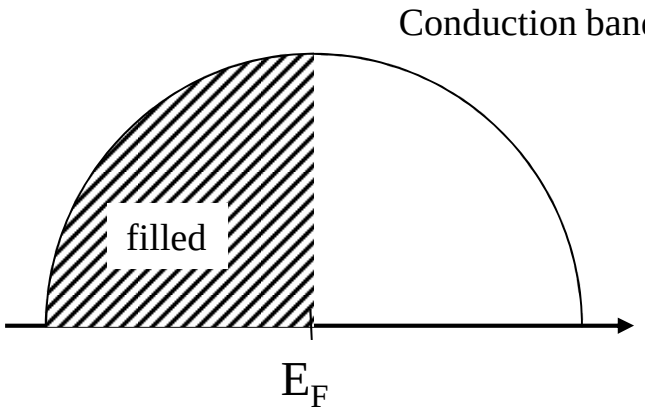
From atoms to metals + atoms…



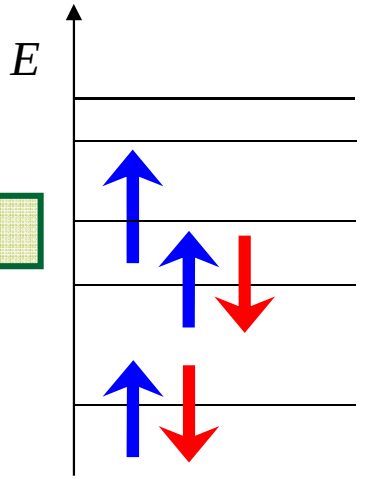
ATOM

Many Atoms!



Metal (non magnetic)

(few)



Magnetic “impurities” (e.g., transition atoms, with unfilled d-levels, f-levels (REarths…))

=

?

Is the resulting compound still a metal ?

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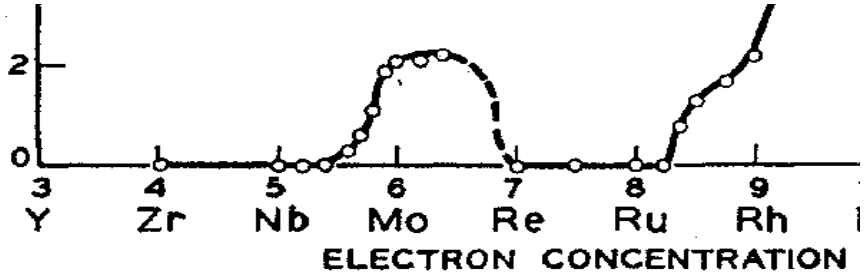
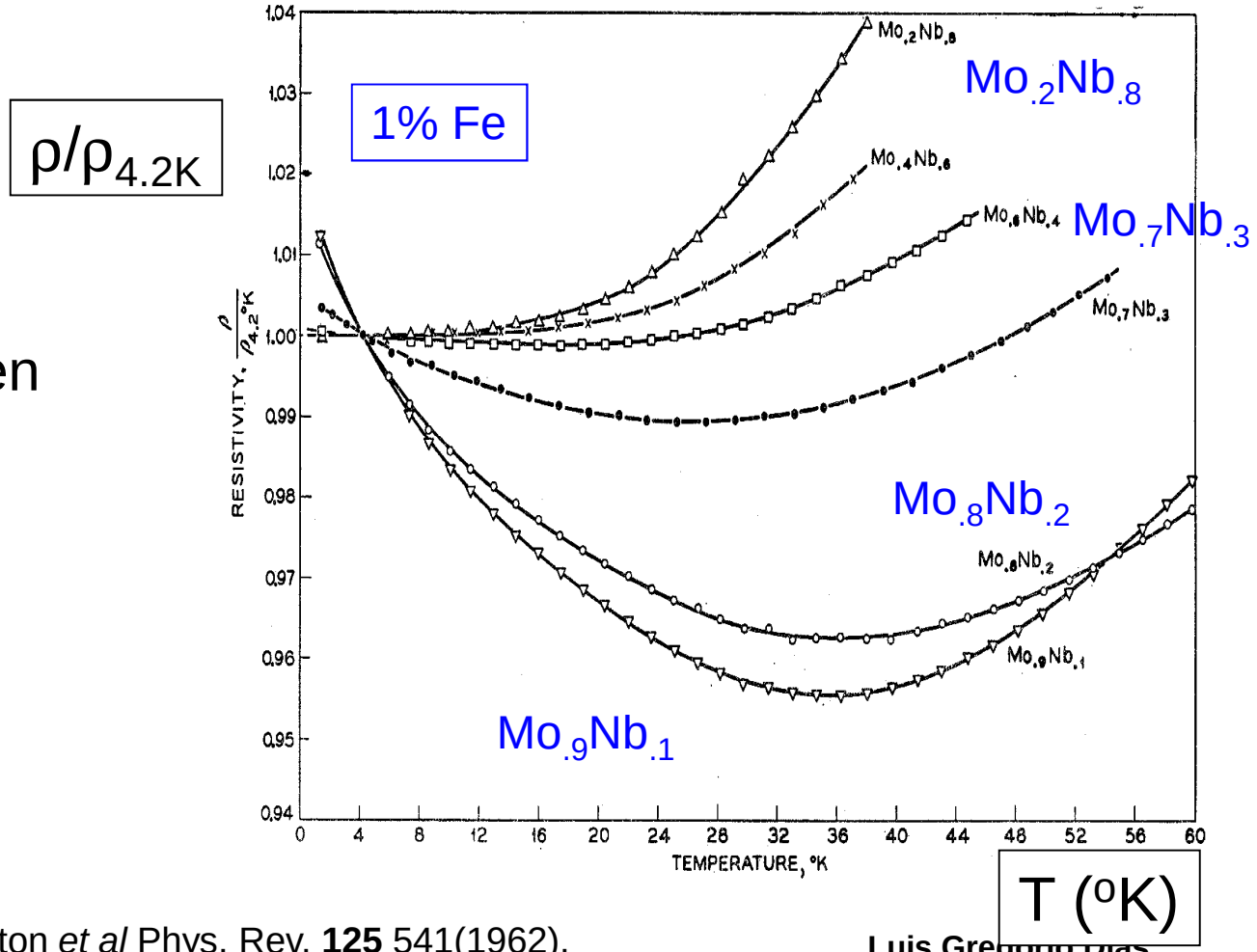
Kondo effect

- Magnetic impurity in a metal.
  - 30's - Resisivity measurements:

    minimum in ρ(T);

    T_{min} depends on $c_{imp.}$
  - 60's - Correlation between the existence of a Curie-Weiss component in the susceptibility (*magnetic moment*) and resistance minimum .





Top: A.M. Clogston *et al* Phys. Rev. **125** 541(1962).
Bottom: M.P. Sarachik *et al* Phys. Rev. **135** A1041 (1964).

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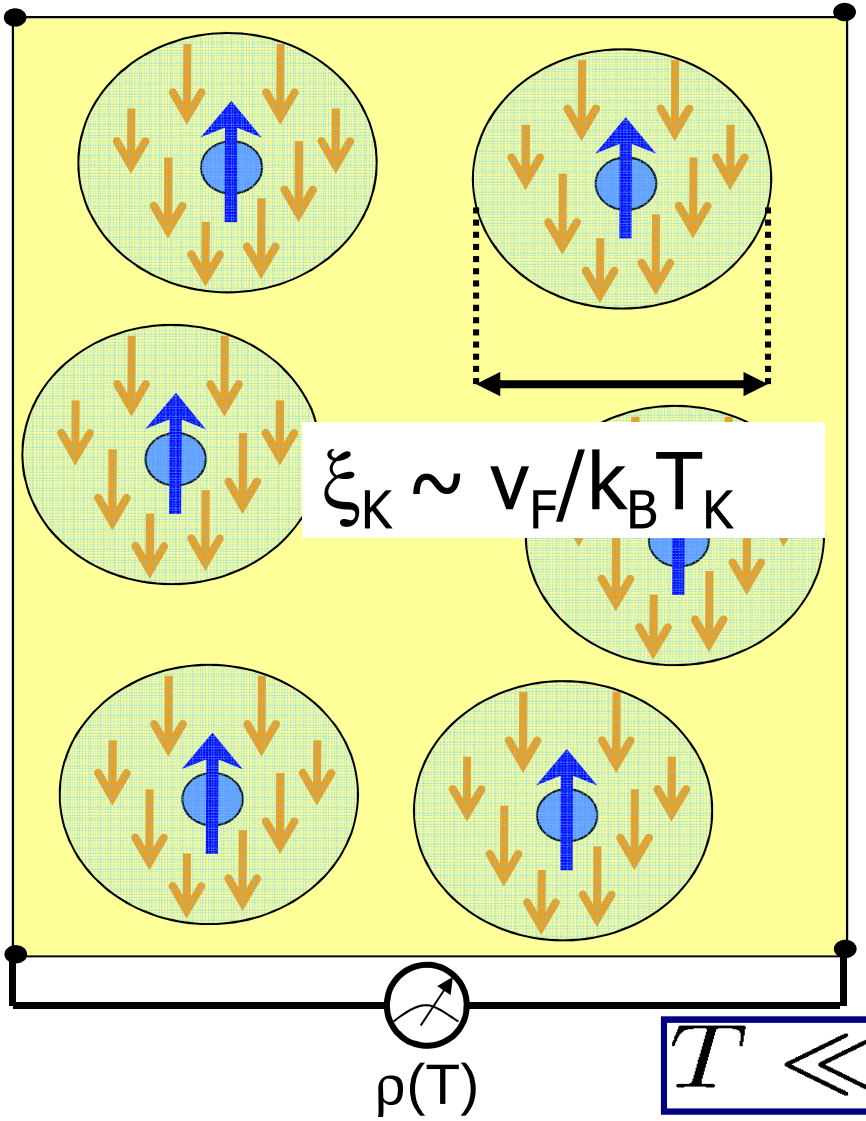
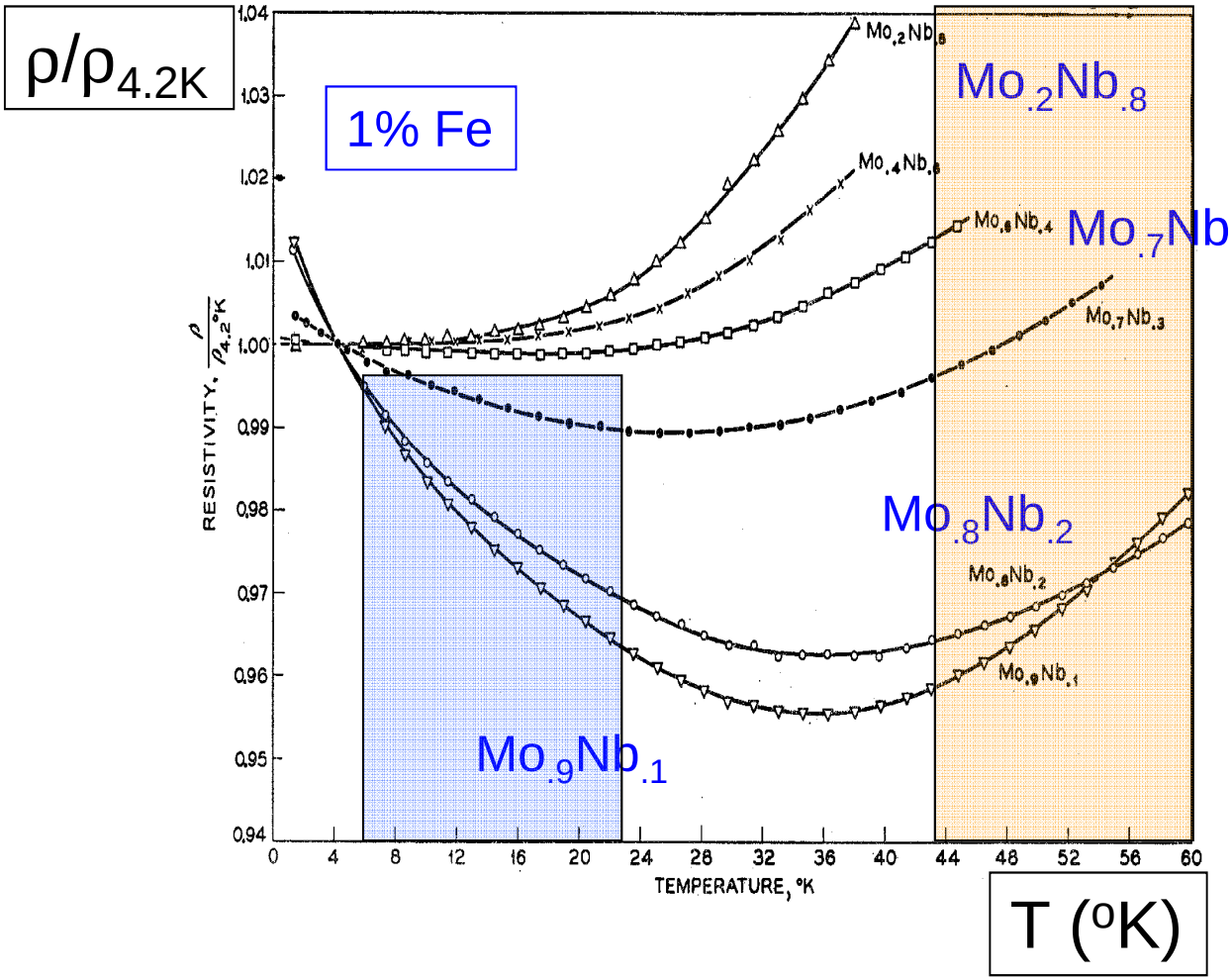
Kondo effect



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



$T \ll T_K$

Resistivity increases with decreasing T (Kondo effect)

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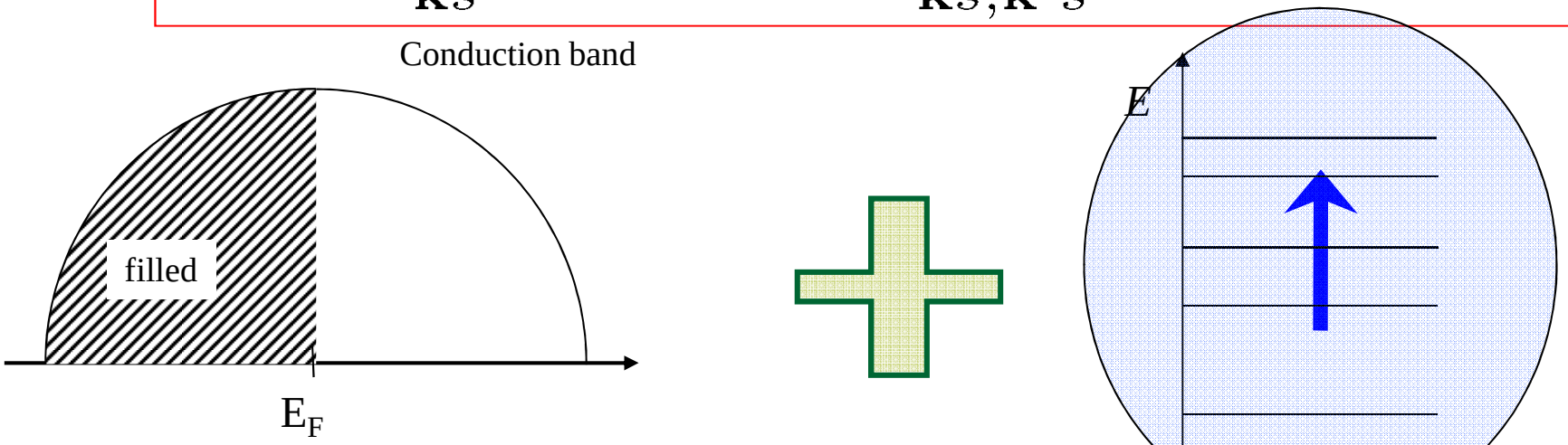
Kondo problem: s-d Hamiltonian

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

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



Metal (non magnetic, s-band)

Magnetic impurity (unfilled d-level)

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

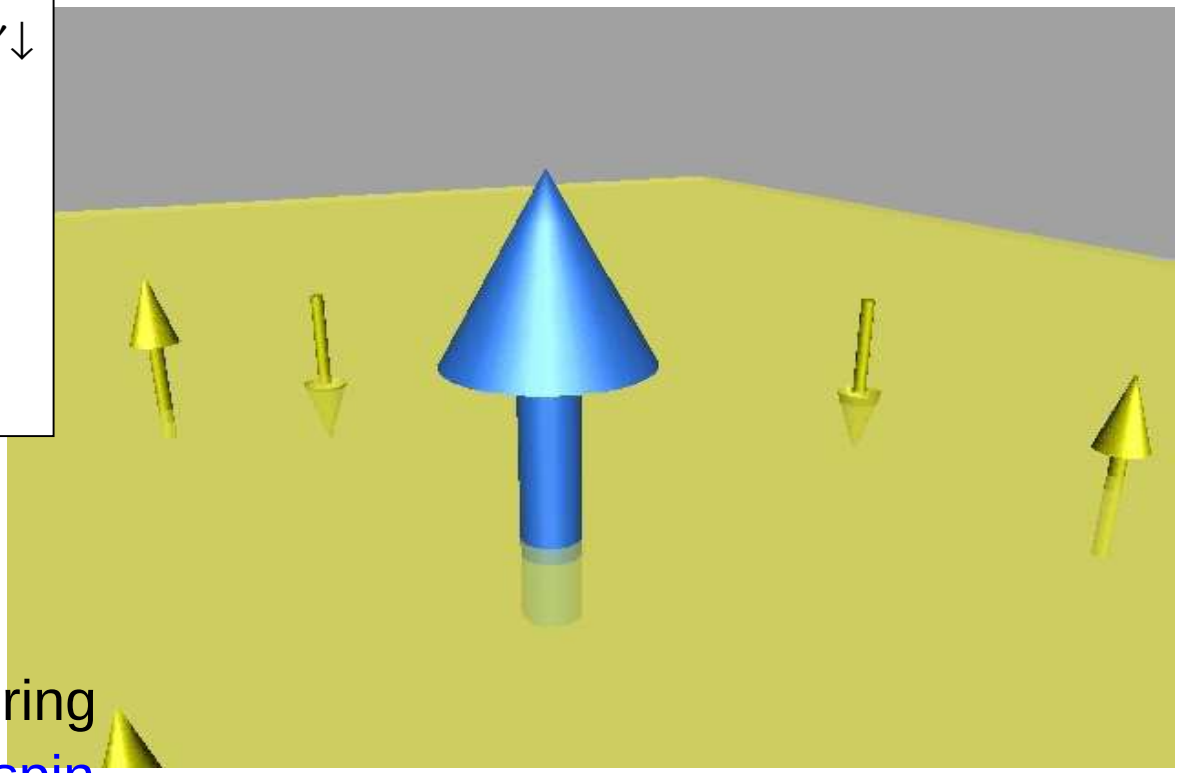
$$H_{s\text{-}d} = J \sum_{k,k'} S^{+} c^{\dagger}_{k\downarrow} c_{k'\uparrow} + S^{-} c^{\dagger}_{k\uparrow} c_{k'\downarrow}$$

Spin: J>0 AFM

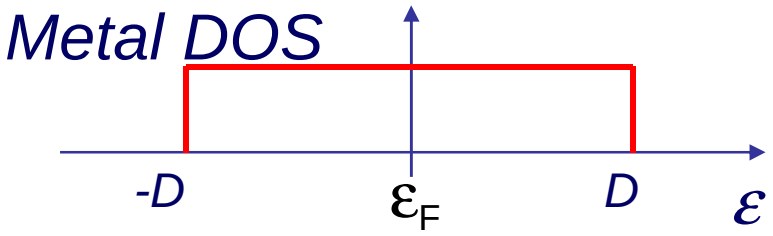
$$+ S_z \left(c^{\dagger}_{k\uparrow} c_{k'\uparrow} - c^{\dagger}_{k\downarrow} c_{k'\downarrow} \right)$$

$$+ \sum_{k} e_k \, c^{\dagger}_{k\sigma} c_{k\sigma}$$

Metal: Free waves



- **Many-body** effect: virtual bound state near the Fermi energy.
- AFM coupling (J>0)→ "spin-flip" scattering
- Kondo problem: s-wave coupling with spin impurity (**s-d model**):



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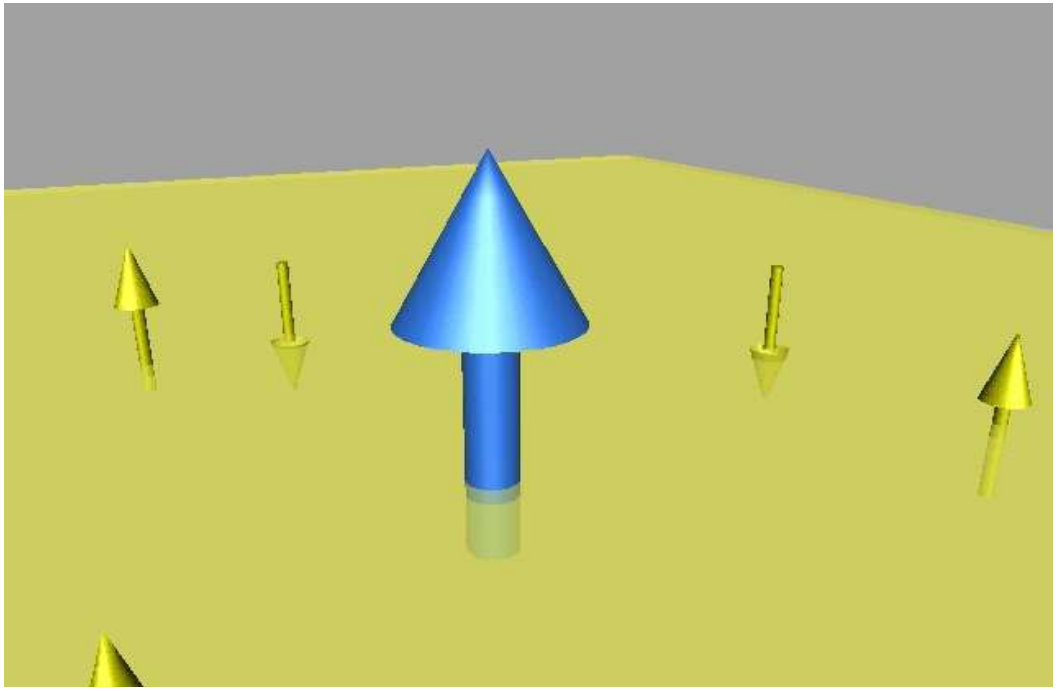
Kondo's explanation for T_{min} (1964)

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

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

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



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

- Only *one* free paramenter: the Kondo temperature T_K
  - Temperature at which the perturbative expansion ***diverges.***

$$k_B T_K \sim D e^{-1/2 J \rho_0}$$

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A little bit of Kondo history:

- Early ‘30s : Resistance minimum in some metals
- Early ‘50s : theoretical work on impurities in metals “Virtual Bound States” (Friedel)
- 1961: Anderson model for magnetic impurities in metals
- 1964: s-d model and Kondo solution (PT)
- 1970: Anderson “Poor’s man scaling”
- 1974-75: Wilson’s Numerical Renormalization Group (non PT)
- 1980 : Andrei and Wiegmann’s exact solution

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 minimum in s
- Early ‘50s : theoretical work on impur irtual Bound States” (Friedel)
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- 1964: s-d model and Kondo solution (PT)
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Kondo's explanation for T_{min} (1964)

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

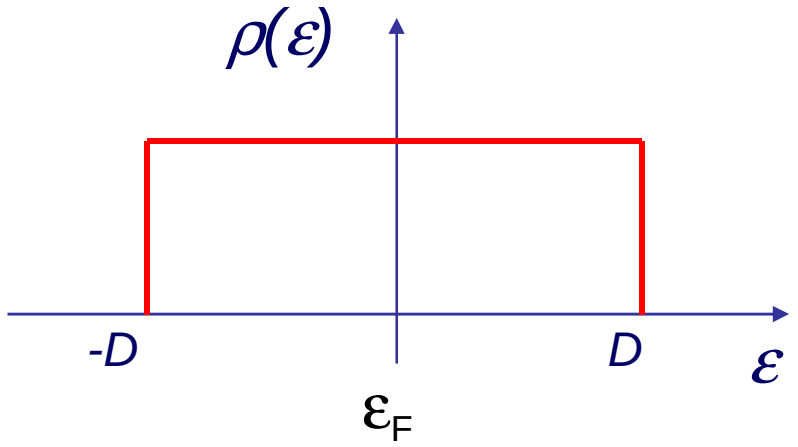
- Diverges *logarithmically* for T→0 or D→∞.

What is going on?

(T<T_K → perturbation expasion no longer holds)

- Experiments show *finite* R as T→0 or D→∞.
- The log comes from something like:

$$\int_{k_B T/D}^{1} \frac{d\varepsilon}{\varepsilon} = -\log\left(\frac{k_B T}{D}\right)$$



- *All* energy scales contribute!

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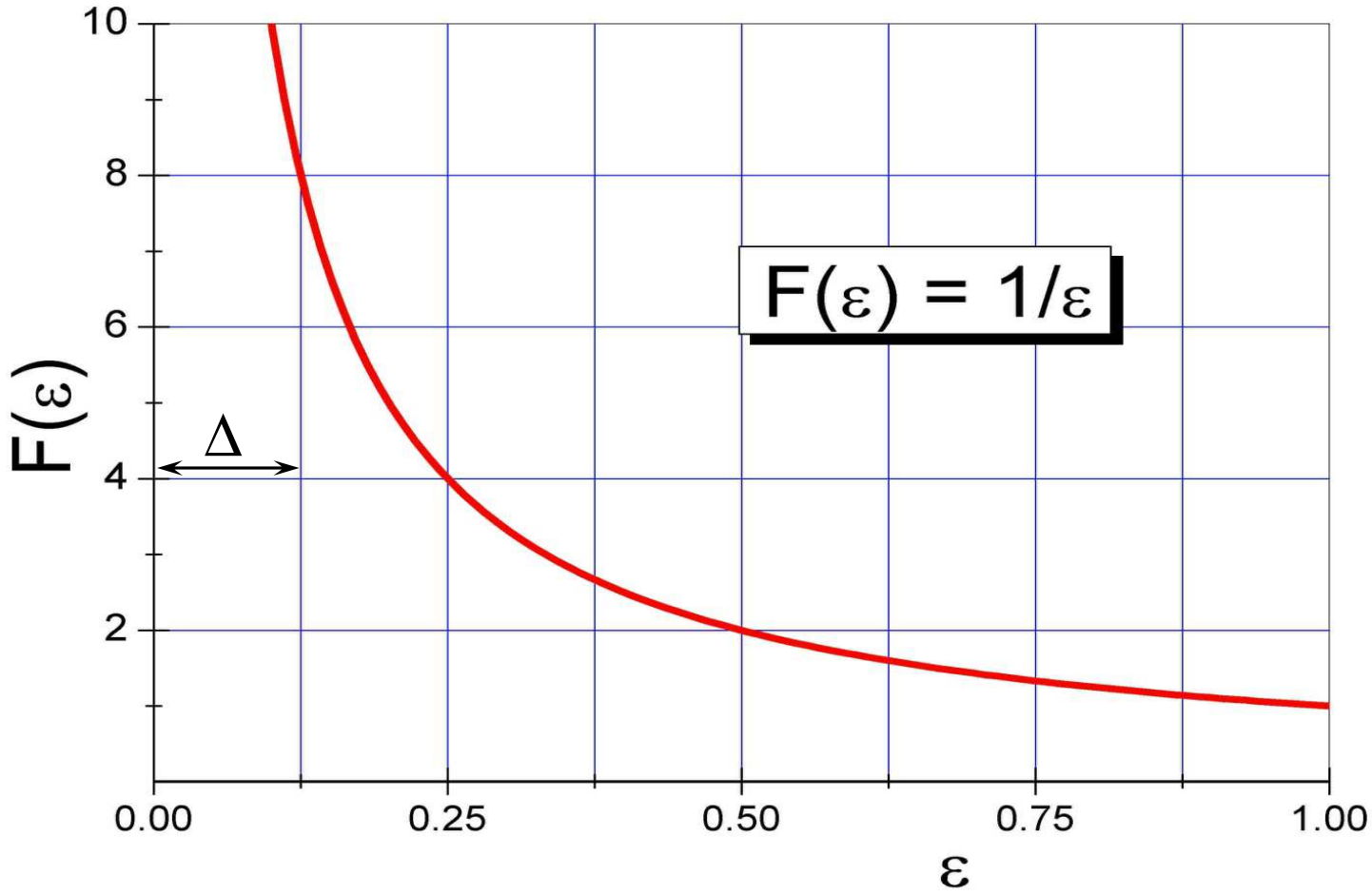
“Perturbative” Discretization of CB



$\varepsilon = (E-E_F)/D$

$\Delta = (\Delta E)/D$

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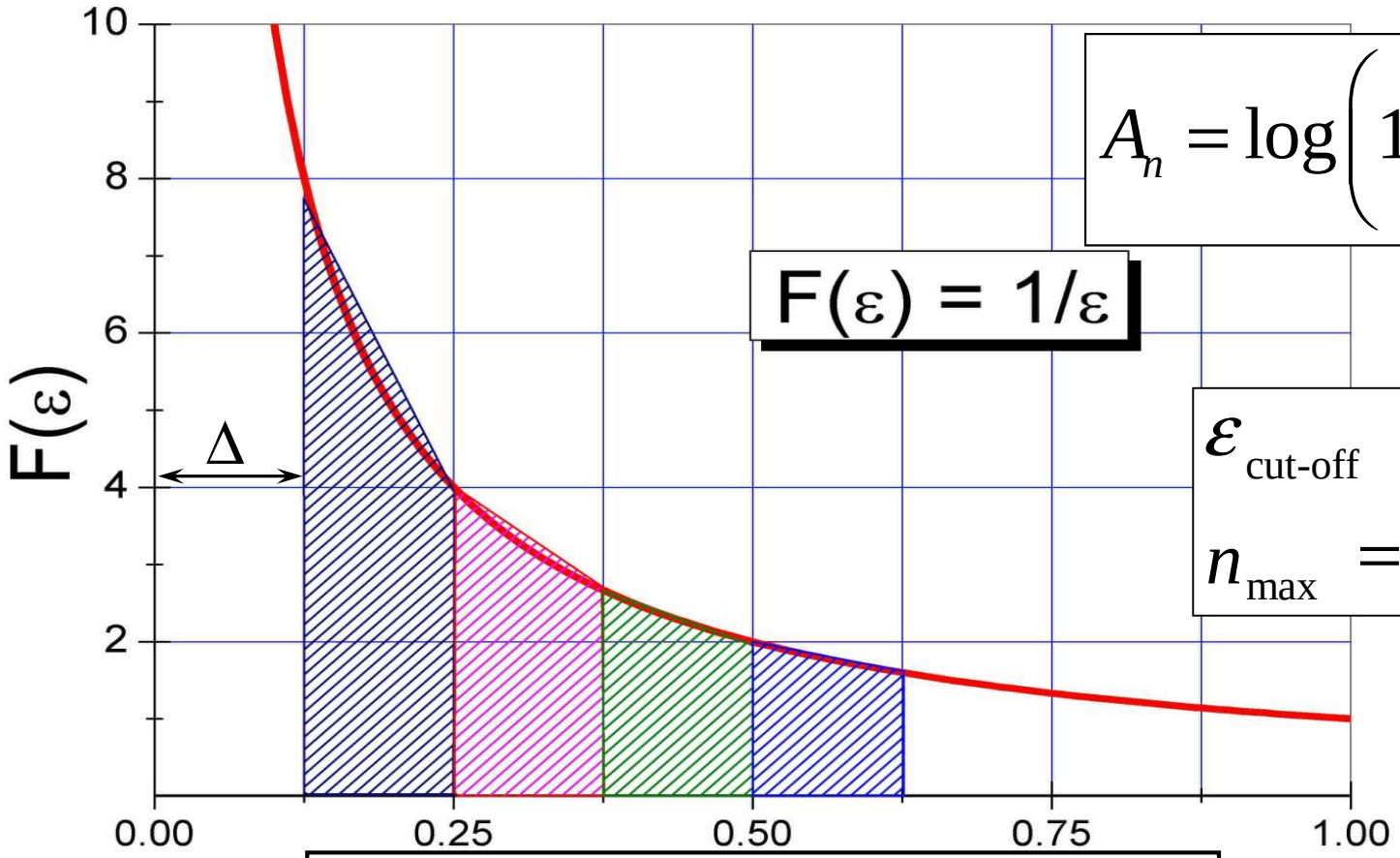
“Perturbative” Discretization of CB

$\Delta = (\Delta E)/D$



$$A_n = \log\left(1 - \frac{\Delta}{1 - n\Delta}\right)$$

$$\varepsilon_{\text{cut-off}} = \Delta$$

$$n_{\max} = \Delta^{-1} - 1$$

Want to keep all contributions

for D⟶∞?

$$A_7 > A_6 > A_5 > A_4 > A_3 > A_2 > A_1$$

Not a good approach!

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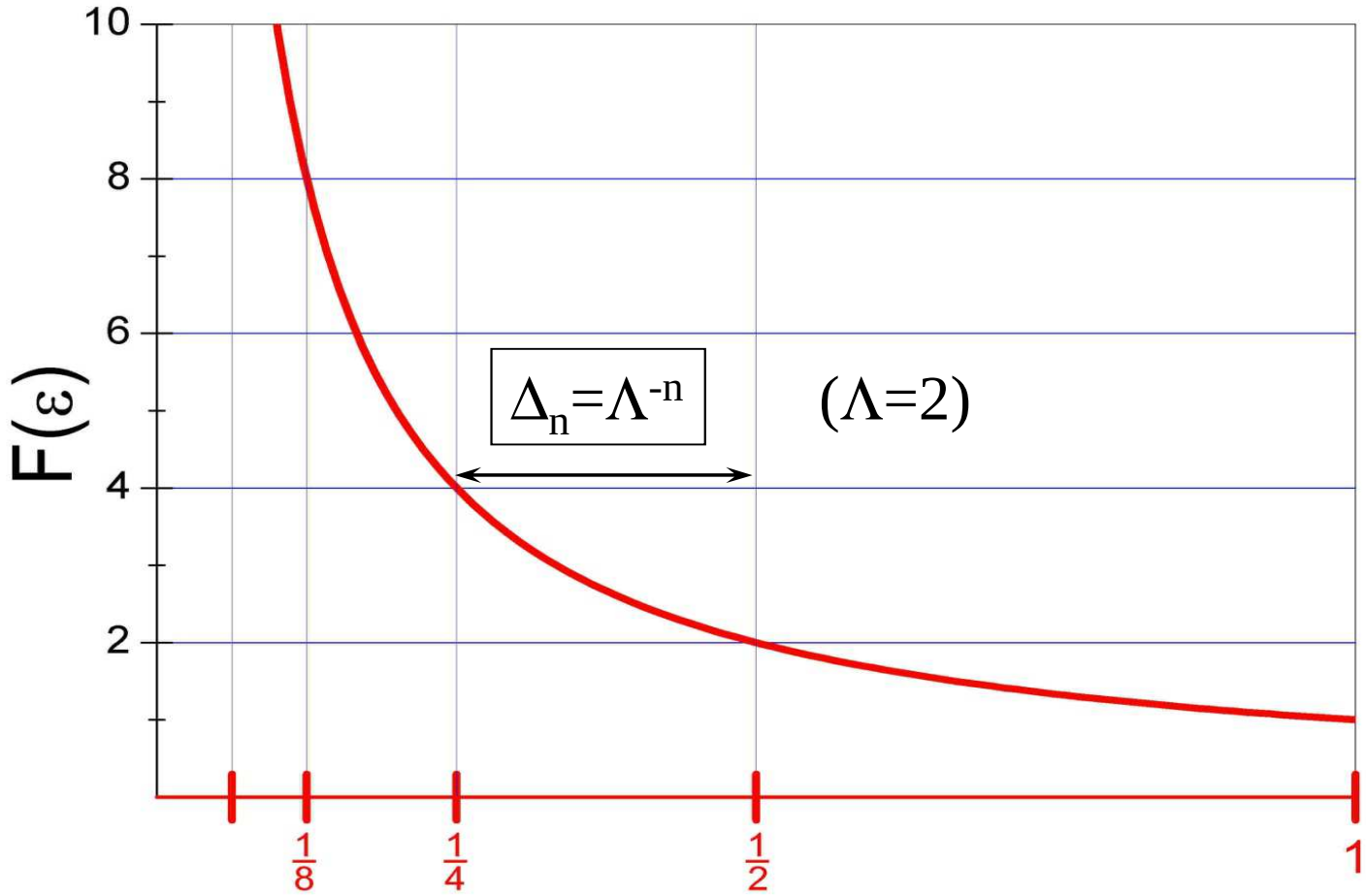
Wilson's CB Logarithmic Discretization



$\varepsilon = (E-E_F)/D$

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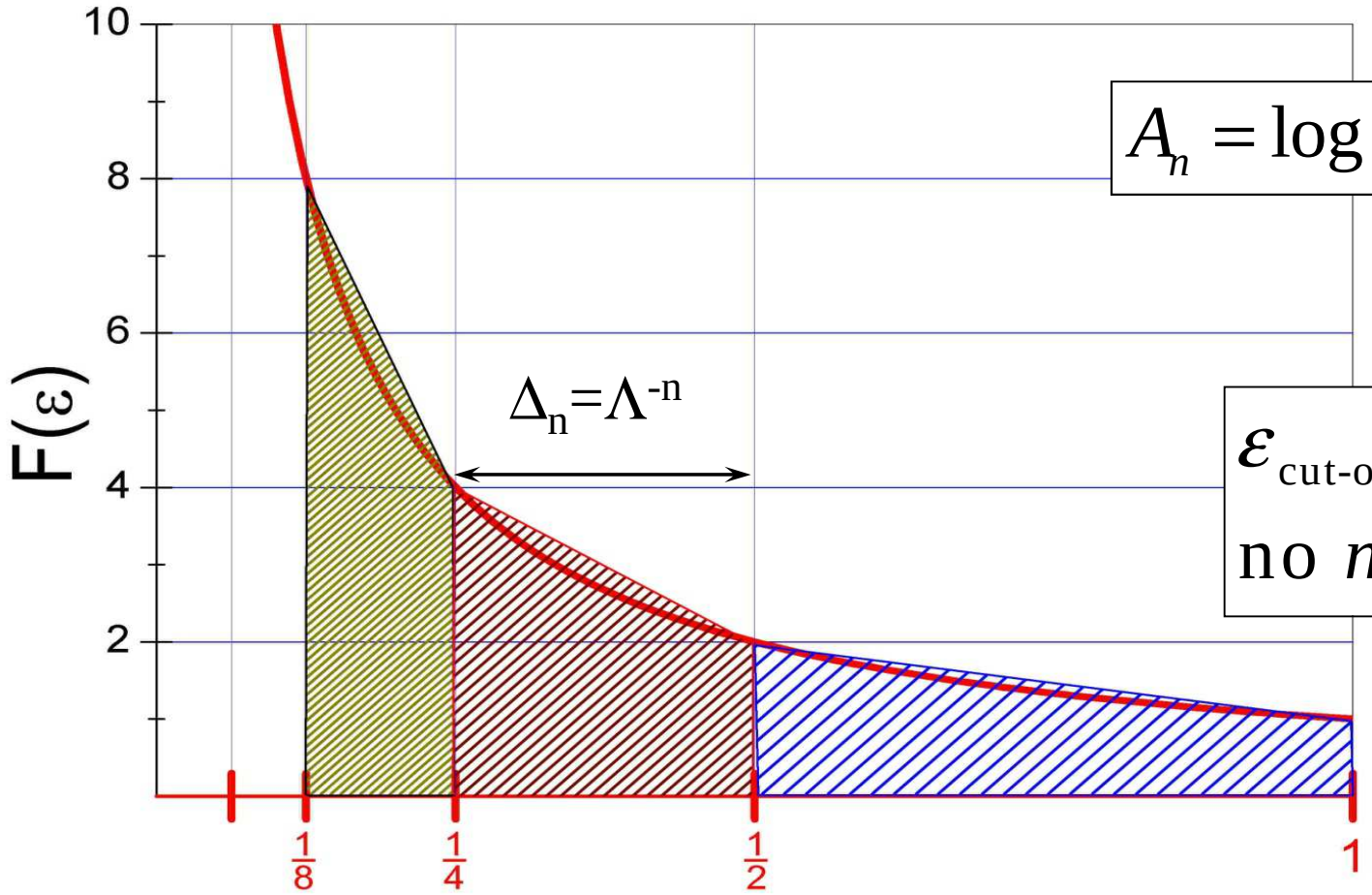
Wilson's CB Logarithmic Discretization



$$A_n = \log \Lambda = \text{const.}$$

$$\varepsilon_{\text{cut-off}} = \Lambda^{-n}$$

no $n_{\max}$

Now you're ok!

$\mathbf{A_3} = \mathbf{A_2} = \mathbf{A_1}$ $(\Lambda=2)$

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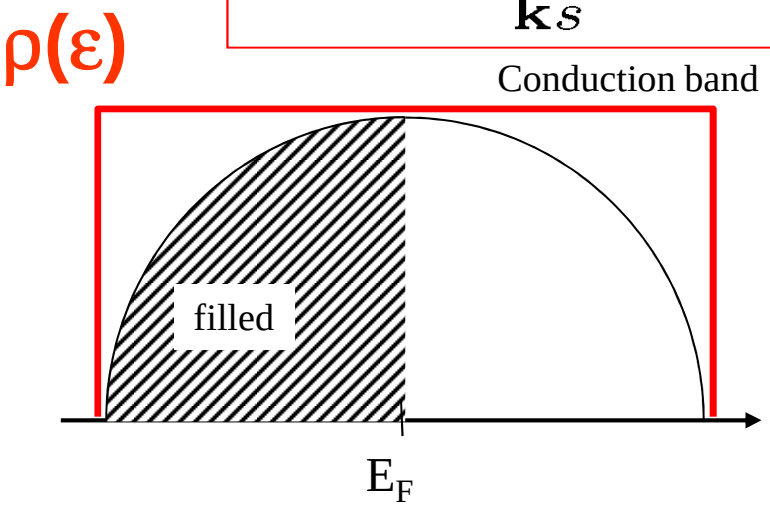
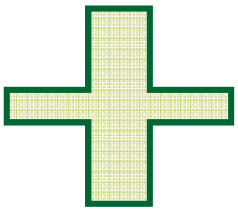
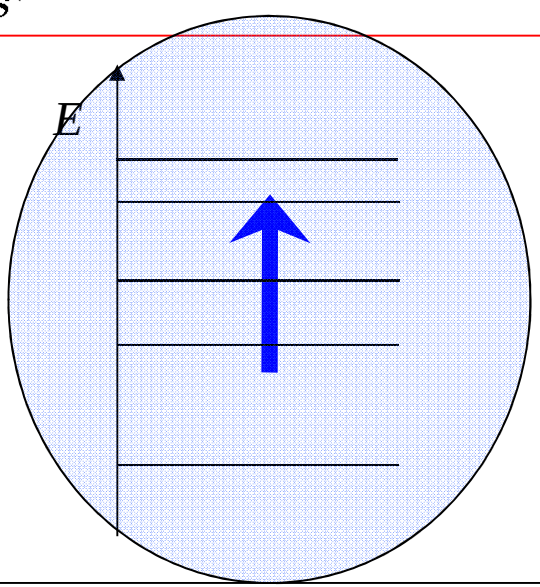
Kondo problem: s-d Hamiltonian

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

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







Metal (non magnetic, s-band)

Magnetic impurity (unfilled d-level)

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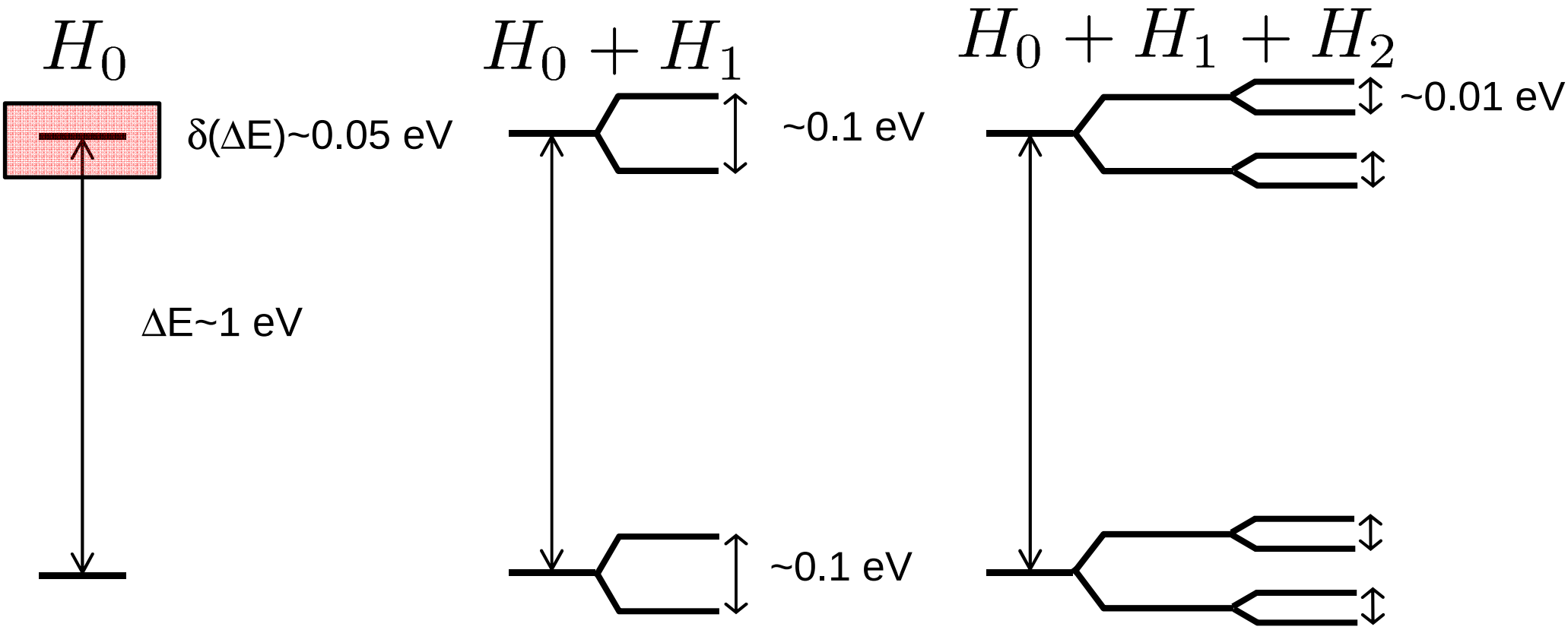
The problem: different energy scales!

(e.g.: all 2-level Hamiltonians)



Uncertainty of the calculation:
δ(ΔE)/ΔE~5%

How to calculate these splittings accurately?

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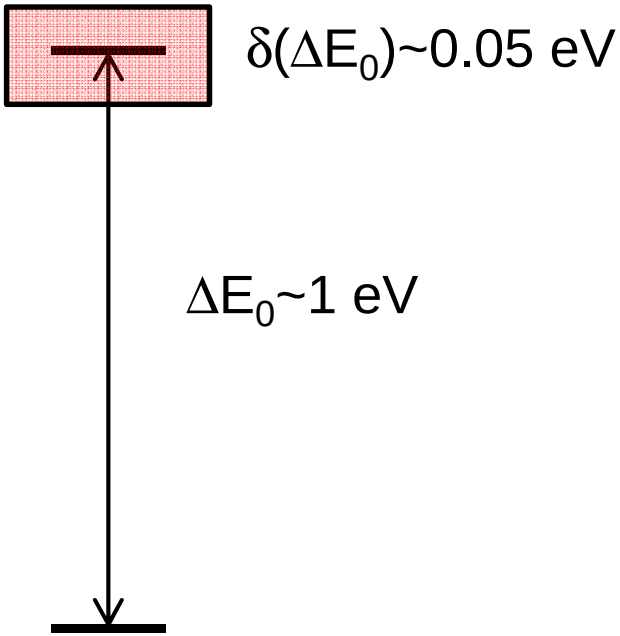
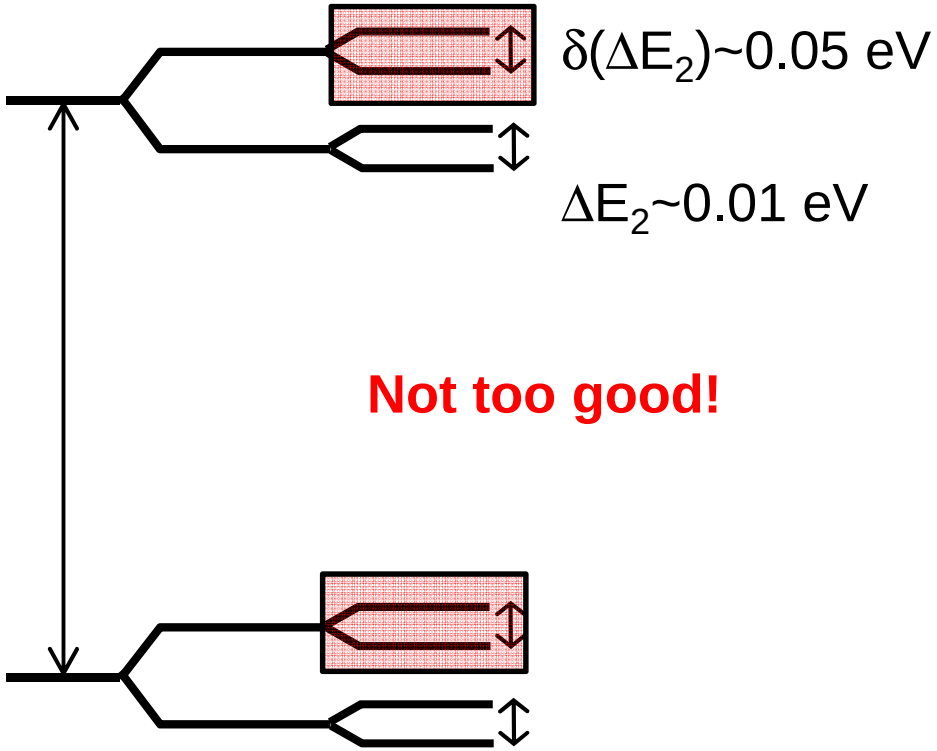
Option 1: “Brute force”

H_0 → **Directly diagonalize:** $H_0 + H_1 + H_2$



Uncertainty of the calculation:
δ(ΔE)/ΔE~5%



Not too good!

Uncertainty of the calculation:
δ(ΔE$_2$)/ΔE$_2$~500%!!!

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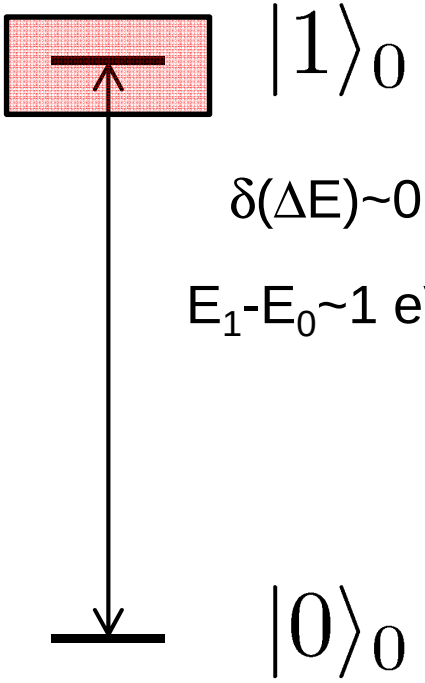
Option 2: Do it by steps.

$$H_0|n\rangle_0 = E_n^0|n\rangle_0$$



δ(ΔE)~0.05 eV

E_1-E_0~1 eV

Uncertainty of the calculation:
δ(ΔE)/ΔE~5%

New basis:

$$\{|0\rangle_0, |1\rangle_0\} \otimes \{|a\rangle_1, |b\rangle_1\}$$

H_0 is diagonal !

H_1 is not diagonal but can calculate matrix elements within 5%.

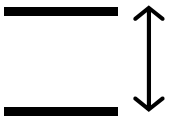
$$\tilde{H}_1 = H_0 + H_1$$

the uncertainty in diagonalizing it is still 5%!

$$\tilde{H}_1|n\rangle_1 = \tilde{E}_n^1|n\rangle_1$$

~0.1 eV

δ(ΔE_1)~0.005 eV



~0.1 eV

Uncertainty of the calculation:
δ(ΔE_1)/ΔE_1~5%

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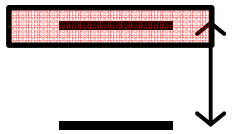
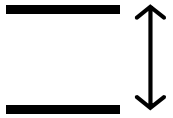
Option 2: Do it by steps, again.

$$\tilde{H}_1|n\rangle_1 = \tilde{E}_n^1|n\rangle_1$$



~0.1 eV

δ(ΔE$_1$)~0.005 eV



~0.1 eV

New basis:

$$\{|n\rangle_1\} \otimes \{|c\rangle_2, |d\rangle_2\}$$

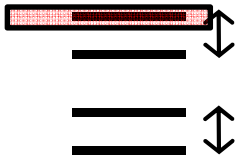
$\tilde{H}_1$ is diagonal!

H_2 is not diagonal but can calculate matrix elements within 5%.

$$\tilde{H}_2 = \tilde{H}_1 + H_2$$

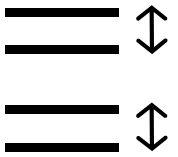
the uncertainty in diagonalizing it is still 5%!

$$\tilde{H}_2|n\rangle_2 = \tilde{E}_n^2|n\rangle_2$$



~0.01 eV

δ(ΔE$_2$)~0.0005 eV



Uncertainty of the calculation:
δ(ΔE$_2$)/ΔE$_2$~5%

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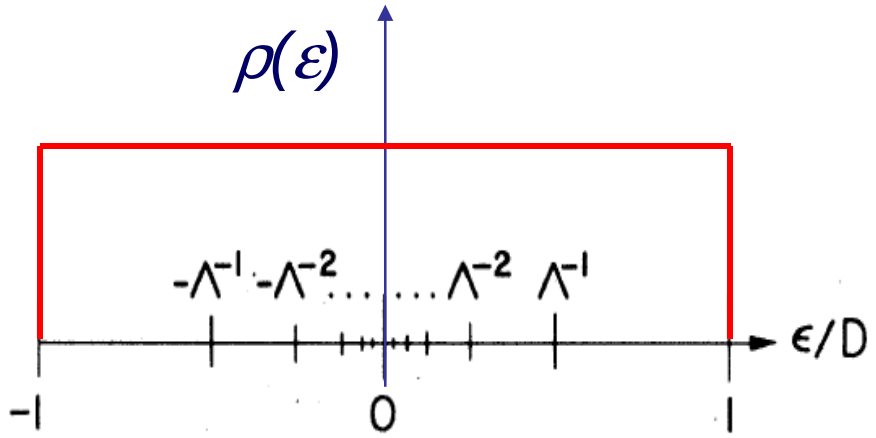
Kondo s-d Hamiltonian

$$H_{\text{s-d}} = J \sum_{k,k'} S^{+}\, c^{\dagger}_{k\downarrow} c_{k'\uparrow} + S^{-}\, c^{\dagger}_{k\uparrow} c_{k'\downarrow} + S_z \left(c^{\dagger}_{k\uparrow} c_{k'\uparrow} - c^{\dagger}_{k\downarrow} c_{k'\downarrow} \right) + \sum_{k} e_k\, c^{\dagger}_{k\sigma} c_{k\sigma}$$



- From continuum *k* to a *discretized* band.
- Transform $H_{\text{s-d}}$ into a linear chain form (exact, as long as the chain is infinite):

$$H_K = \sum_{n=0}^{\infty} \epsilon_n (f_n^{+} f_{n+1} + f_{n+1}^{+} f_n) - 2J\, f_0^{+} \boldsymbol{\sigma} f_0 \cdot \boldsymbol{\tau},$$

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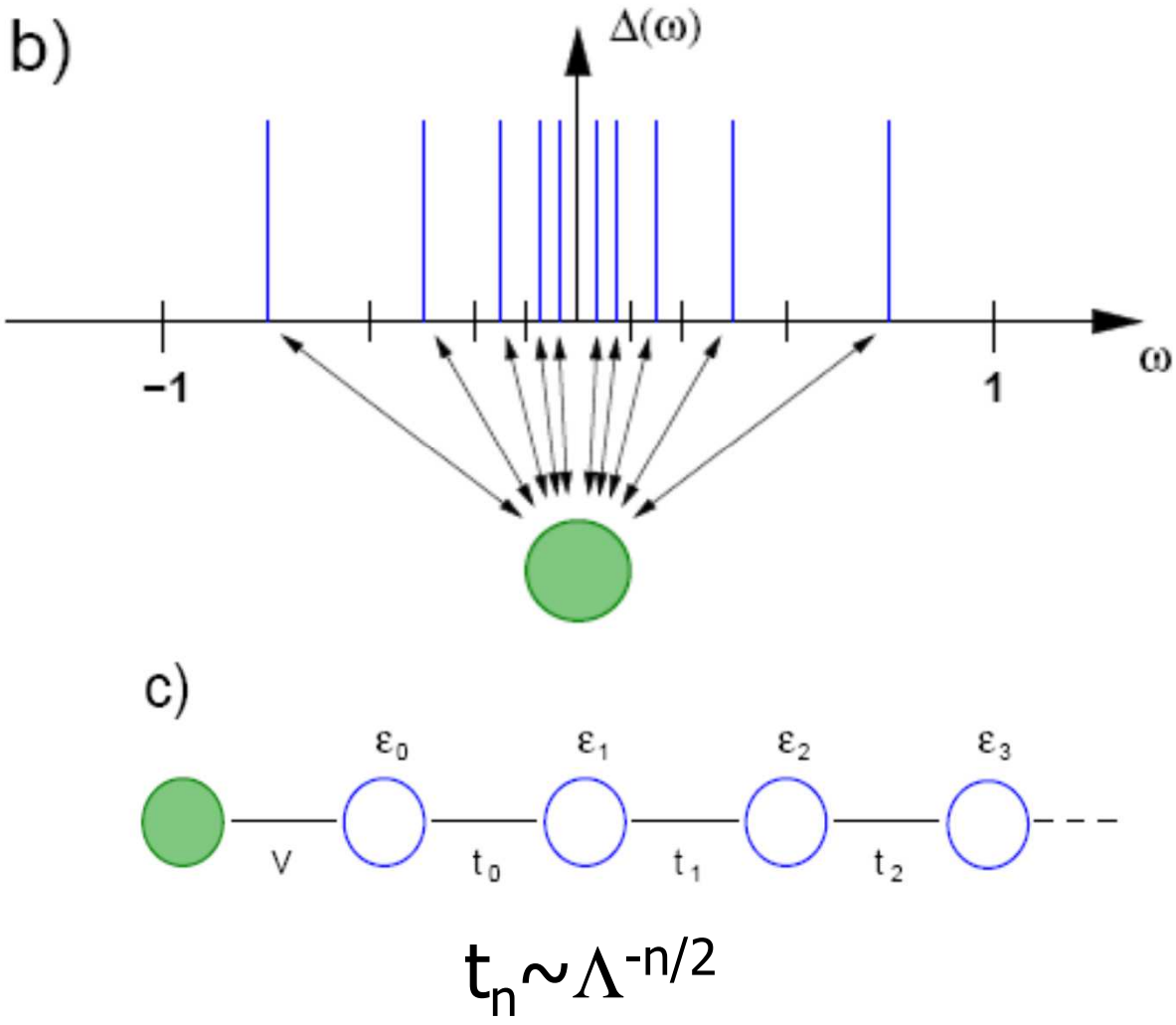
Logarithmic Discretization.

Steps:

1. Slice the conduction band in intervals in a log scale (parameter Λ)
2. Continuum spectrum approximated by a single state
3. Mapping into a tight binding chain: sites correspond to different energy scales.



$t_n \sim \Lambda^{-n/2}$

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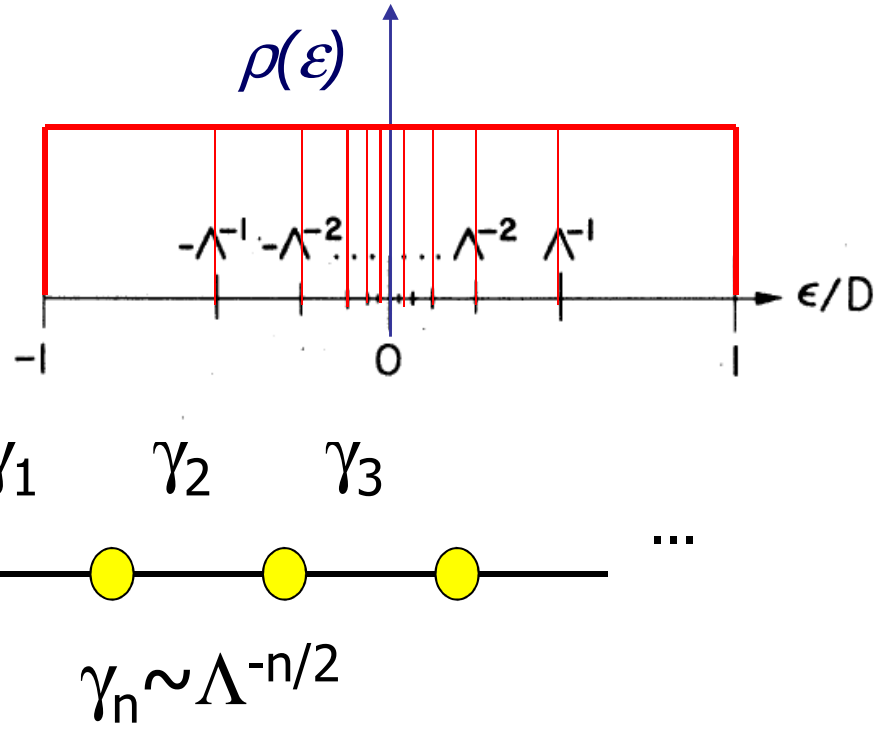
“New” Hamiltonian (Wilson’s RG method)

- Logarithmic CB discretization is the key to avoid divergences!
- Map: conduction band $\rightarrow$ Linear Chain
  - Lanczos algorithm.
  - Site $n \rightarrow$ new energy scale:
  - $D\Lambda^{-(n+1)} < |\varepsilon_k - \varepsilon_F| < D\Lambda^{-n}$
  - Iterative numerical solution



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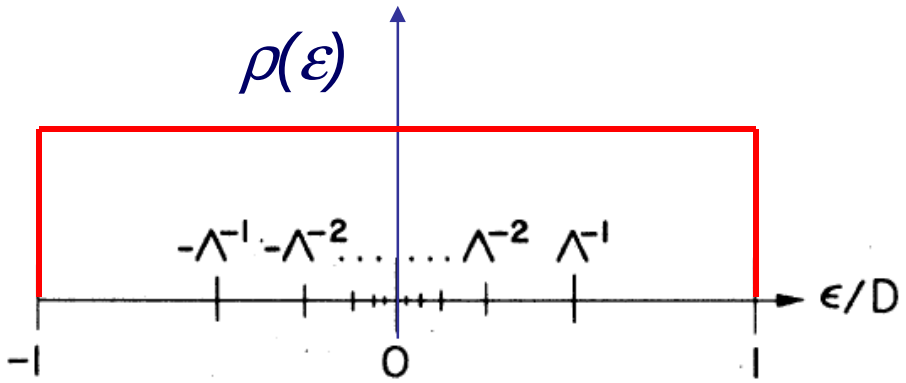
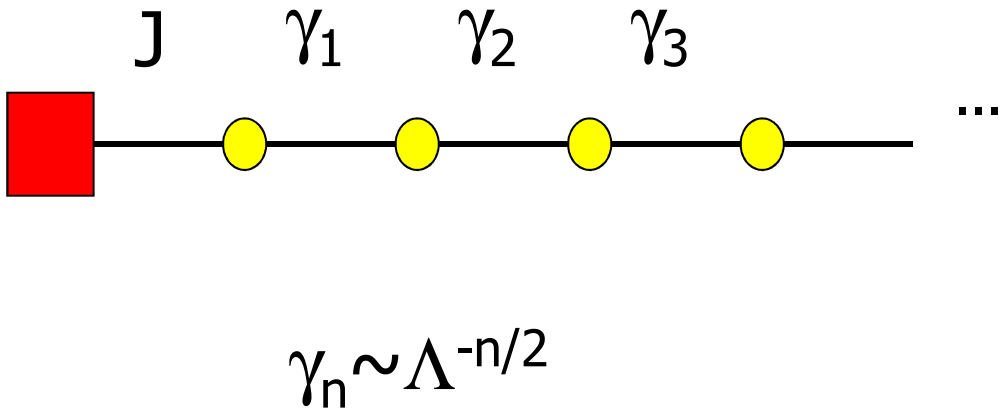
“New” Hamiltonian (Wilson)

- Recurrence relation (Renormalization procedure).

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





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“New” Hamiltonian (Wilson)

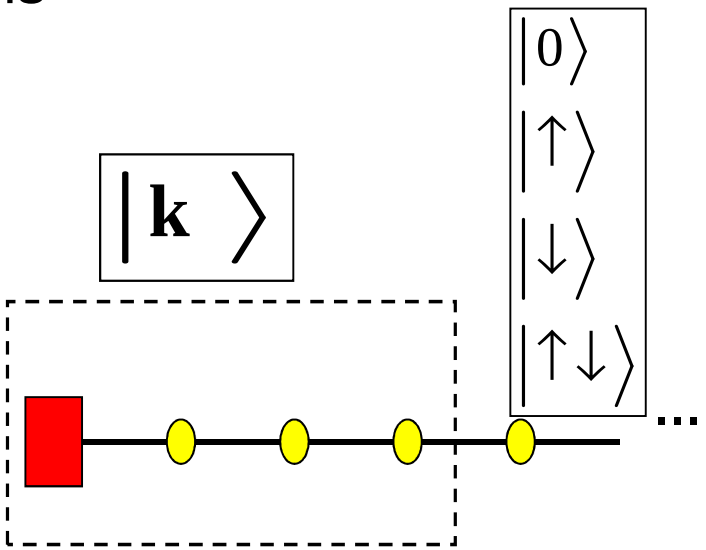
- Suppose you diagonalize H_N getting E_k and |k> and you want to diagonalize H_{N+1} using this basis.
- First, you expand your basis:

$$|\Omega;\, k\rangle = |k\rangle,$$

$$|\tfrac{1}{2};\, k\rangle = f_{N+1,\frac{1}{2}}{}^{+}|k\rangle,$$

$$|-\tfrac{1}{2};\, k\rangle = f_{N+1,-\frac{1}{2}}{}^{+}|k\rangle,$$

$$|\tfrac{1}{2},\, -\tfrac{1}{2};\, k\rangle = f_{N+1,\frac{1}{2}}{}^{+} f_{N+1,-\frac{1}{2}}{}^{+}|k\rangle.$$



- Then you calculate <*k*,a|f^{+}_{N}|*k*’,a’>, <*k*,a|f_{N}|*k*’,a’>and you have the matrix elements for H_{N+1} (sounds easy, right?)

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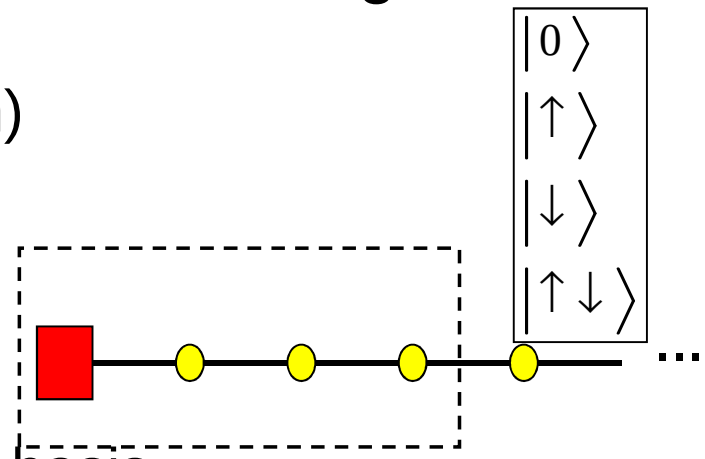
Intrinsic Difficulty

- You ran into problems when N~5. The basis is too large! (grows as $2^{(2N+1)}$)
  - N=0; (just the impurity); 2 states (up and down)
  - N=1; 8 states
  - N=2; 32 states
  - N=5; 2048 states
  - (…) N=20; 2.199×10^{12} states:
    - 1 byte per state $\rightarrow$ 20 HDs just to store the basis.
  - And we might go up to N=180; 1.88×10^{109} states.
    - Can we store this basis?

      (Hint: The number of atoms in the universe is ~ 10^{80})
- Cut-off the basis $\rightarrow$ lowest ~1500 or so in the next round (Even then, you end up having to diagonalize a 4000x4000 matrix…).



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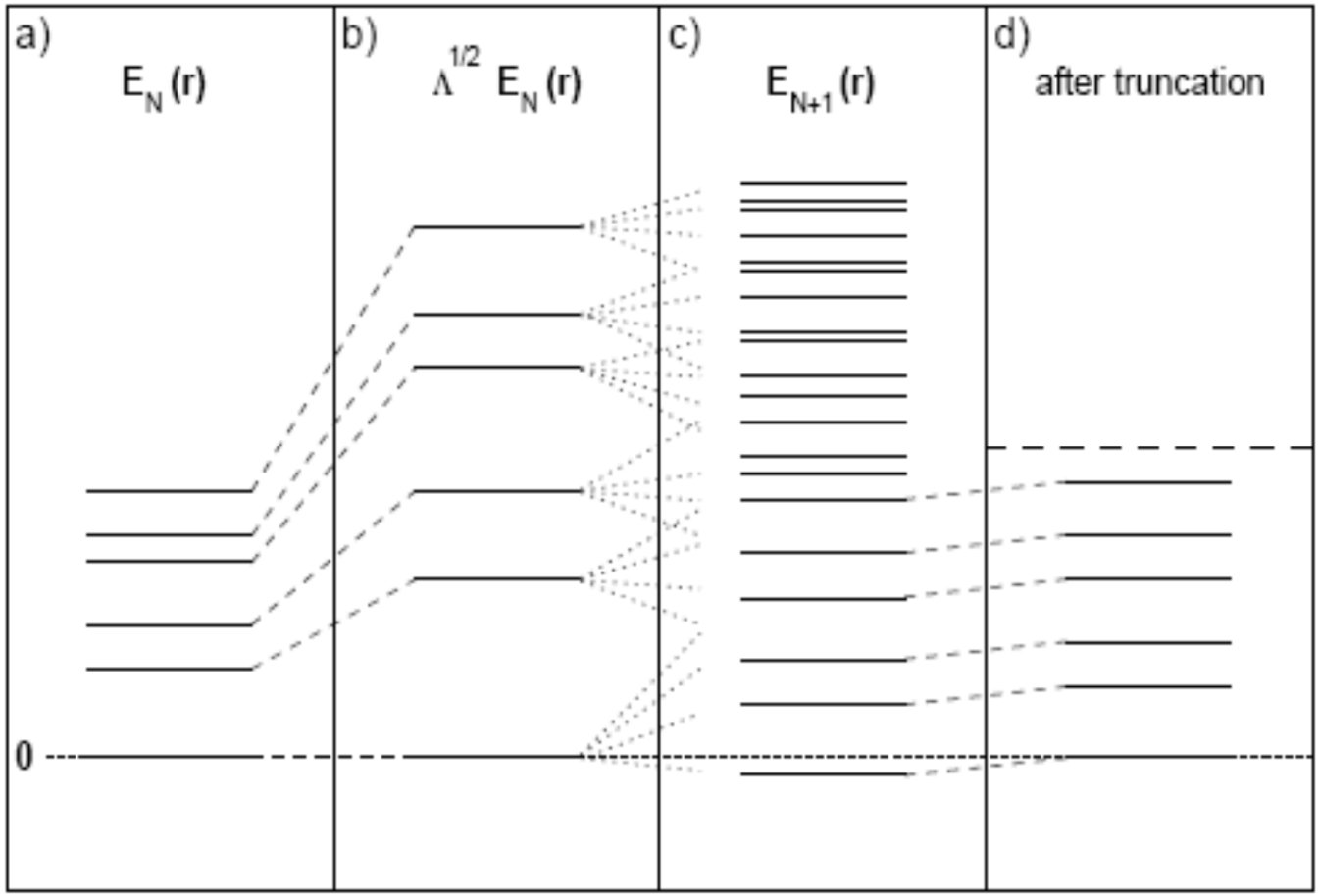
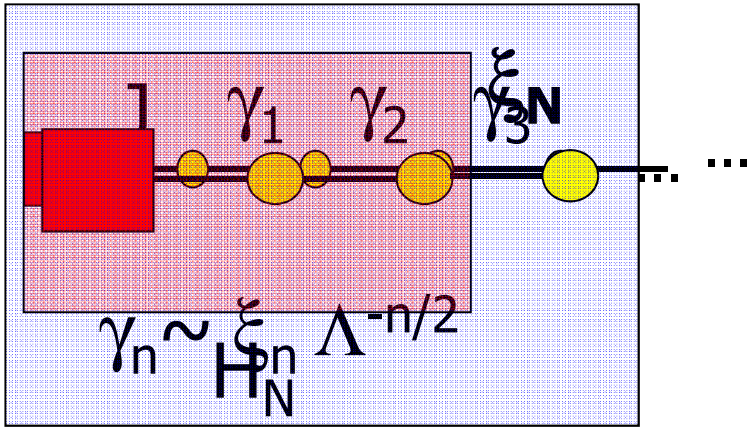
Renormalization Procedure

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



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



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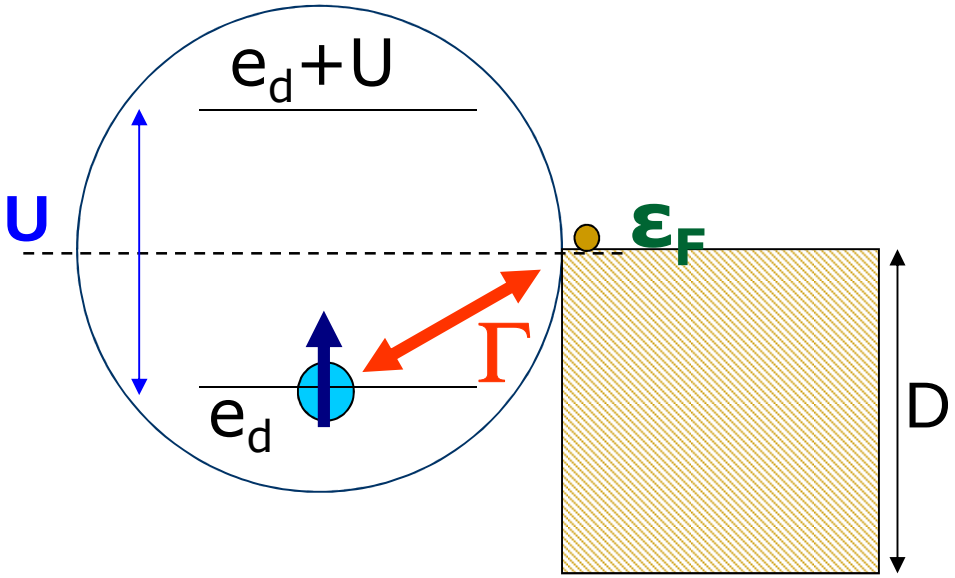
Anderson Model



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

with

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

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

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

Level broadening:

$$\Gamma = \pi \rho(\epsilon_F) t^2$$

Strong interacting limit:

$$U \gg \Gamma, |\varepsilon_d - \epsilon_F|$$

NRG: fixed points

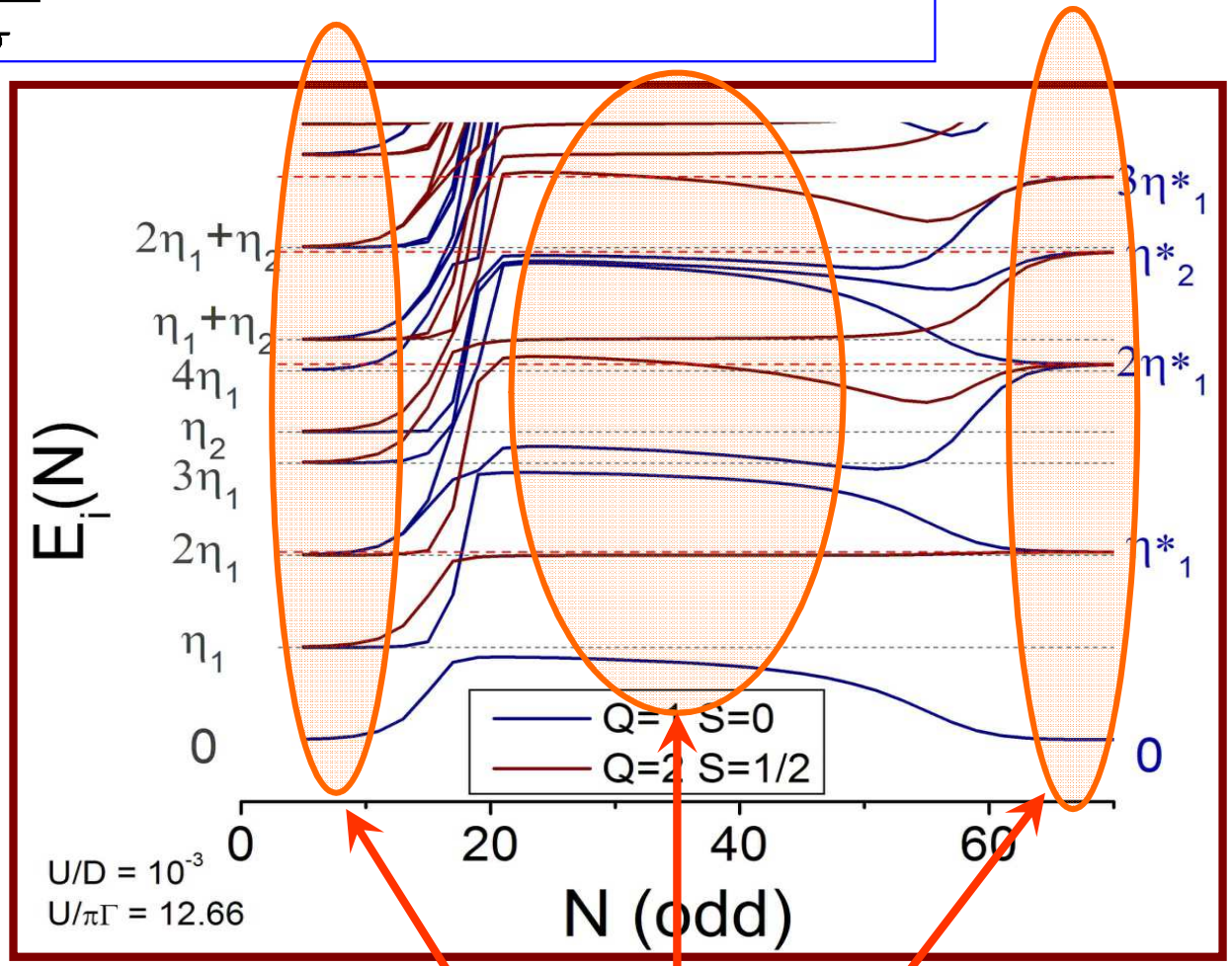
$$H_{N+1} = \sqrt{\Lambda} H_N + \xi_N \sum_\sigma f^\dagger_{N+1\sigma} f_{N\sigma} + f^\dagger_{N\sigma} f_{N+1\sigma}$$

- **Renormalization Group transformation**: (Re-scale energy by $\Lambda^{1/2}$).

$$H_{N+1} = R(H_N)$$

- **Fixed point H***: indicates *scale invariance.*

$$H^* = R^2(H^*)$$



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NRG: fixed points

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- **Renormalization Group transformation**: (Re-scale energy by $\Lambda^{1/2}$).

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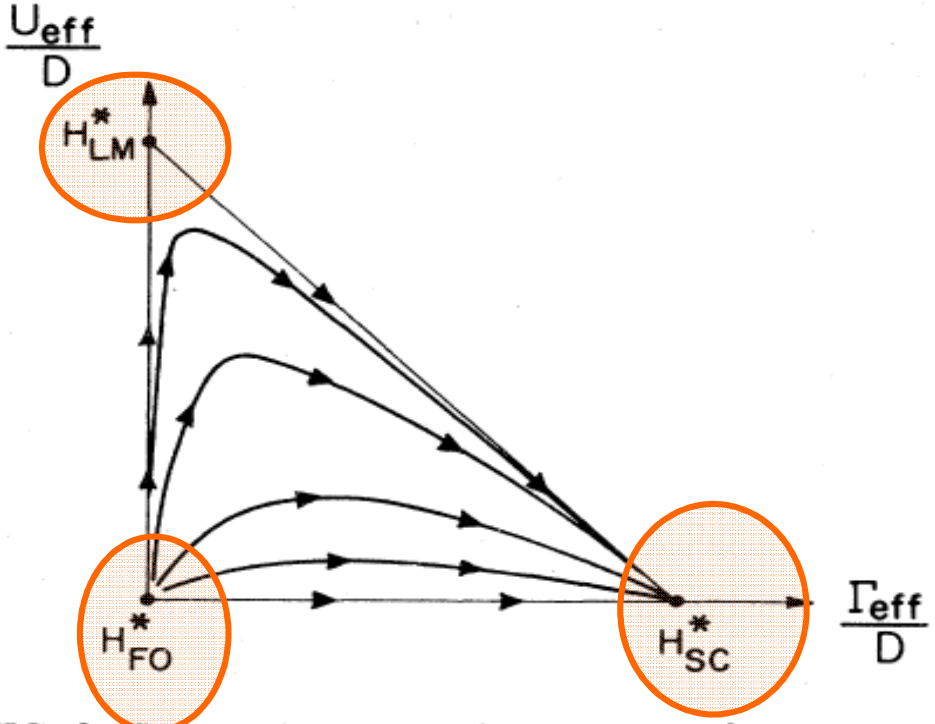
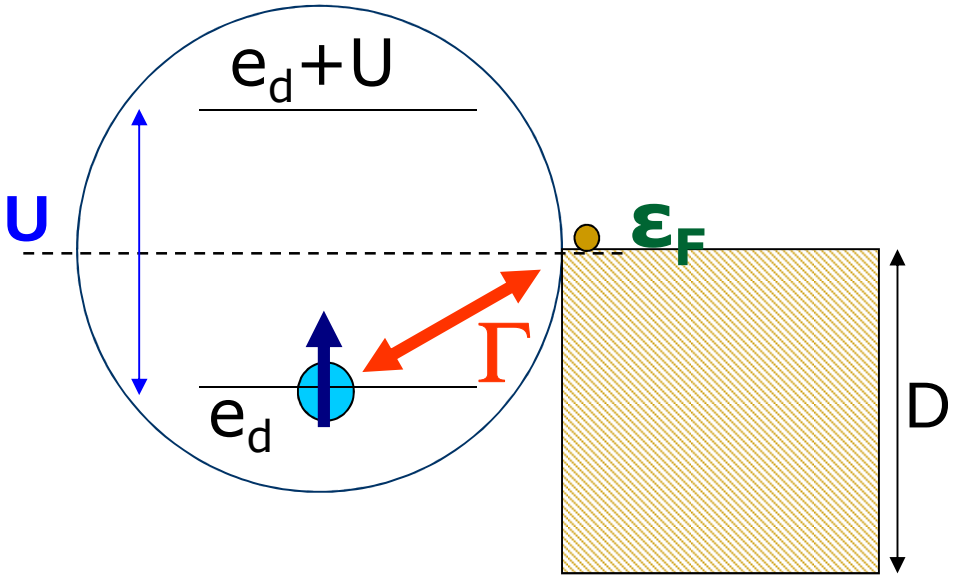


FIG. 8. Schematic renormalization-group flow diagram. Each H_N is thought of as associated with a U_{eff} and Γ_{eff}. Trajectories depict the flow of H_N with increasing N. Note that only the strong-coupling fixed point is stable.

Fixed points of the Anderson Model



Level broadening:

$$\Gamma = \pi \rho(\epsilon_F) t^2$$

Strong interacting limit:

$$U \gg \Gamma, |\varepsilon_d - \epsilon_F|$$

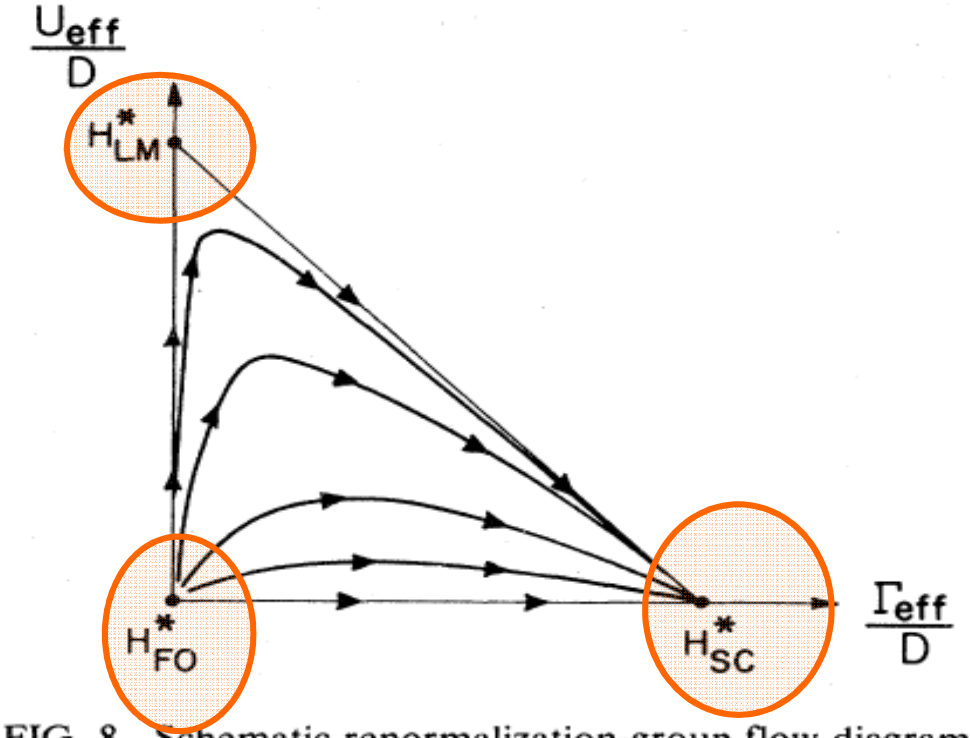


FIG. 8. Schematic renormalization-group flow diagram. Each H_N is thought of as associated with a U_{eff} and Γ_{eff}. Trajectories depict the flow of H_N with increasing N. Note that only the strong-coupling fixed point is stable.

Fixed points

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Spectral function

At each NRG step:

$$H_N |r\rangle_N = E_r^N |r\rangle_N ,$$

$$M^N_{r,r'} = {}_N\langle r| f_\sigma |r'\rangle_N ,$$

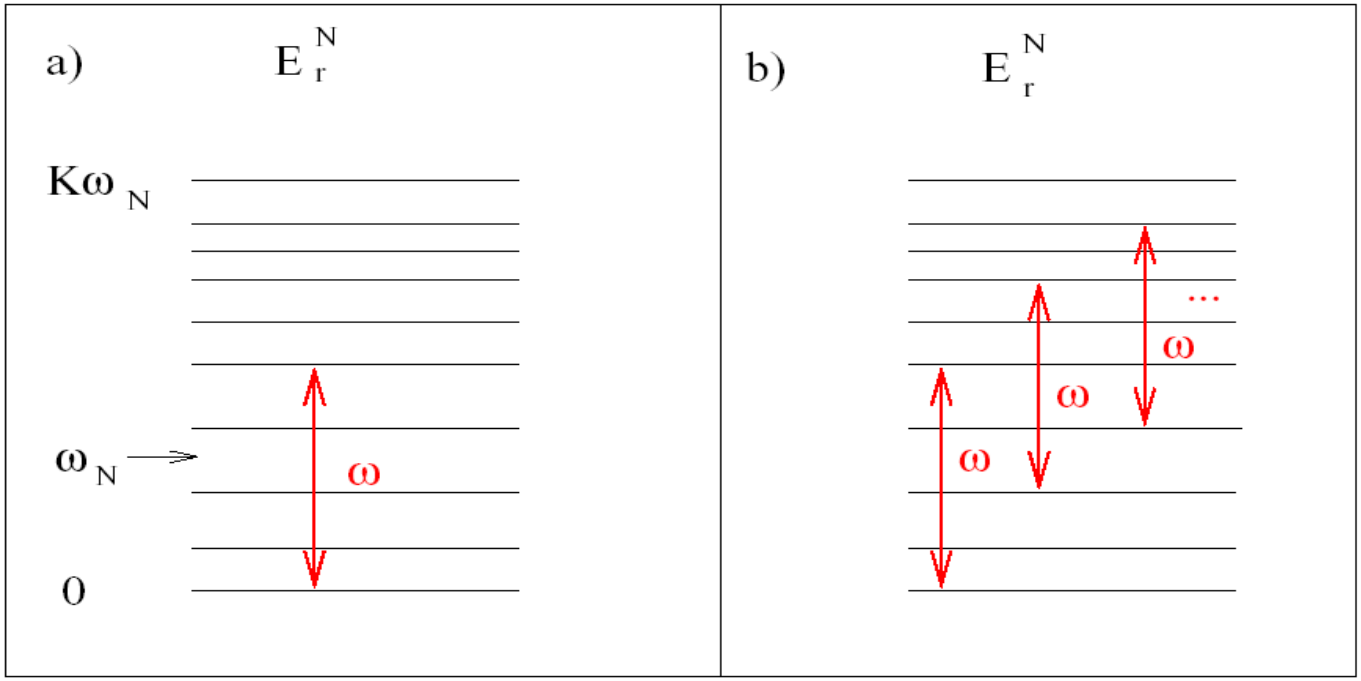

FIG. 9 Excitations of H_N contributing to the spectral function at frequency ω for, (a), $T = 0$, and, (b), $T > 0$.

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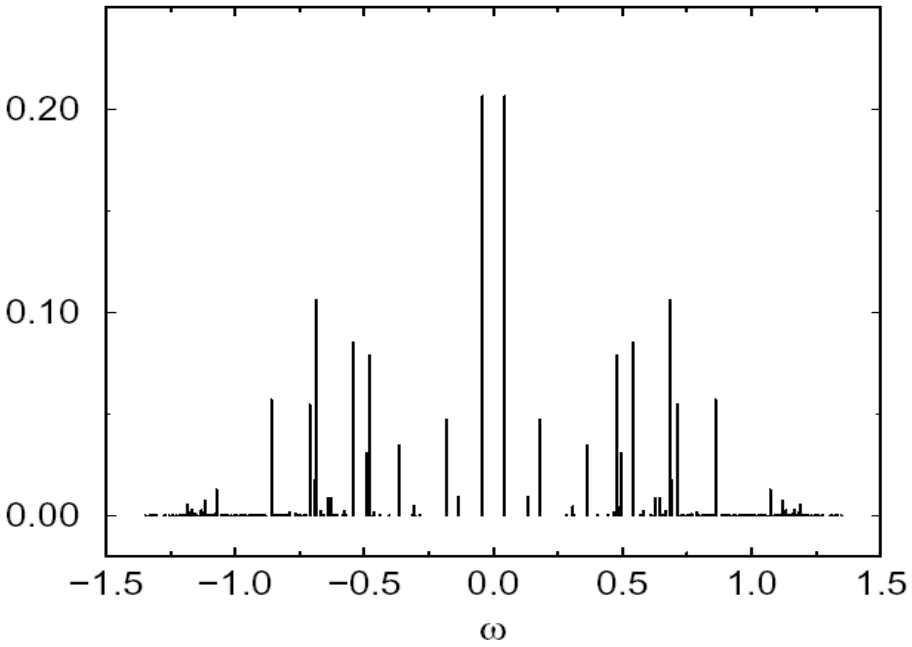
Spectral function calculation (Costi)

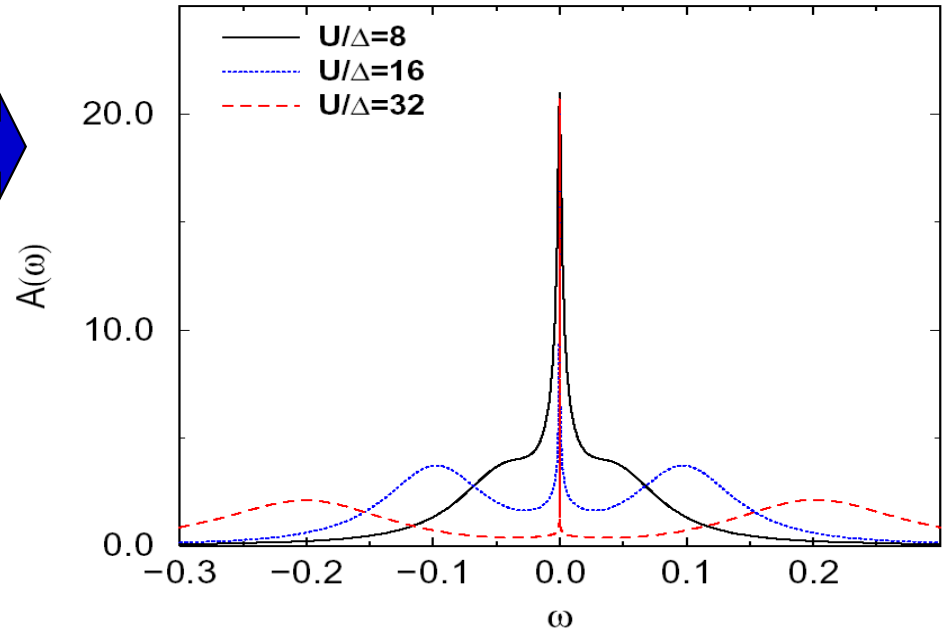
$$A_\sigma^N(\omega, T=0) = \frac{1}{Z_N(0)} \sum_r |M_{r,0}^N|^2 \delta(\omega + E_r^N)$$

$$+ \frac{1}{Z_N(0)} \sum_{r'} |M_{0,r'}^N|^2 \delta(\omega - E_{r'}^N).$$

To get a continuos curve, need to broaden deltas.
Best choice: log gaussian

$$\delta(\omega - \omega_n) \rightarrow \frac{e^{-b^2/4}}{b\omega_n\sqrt{\pi}} \exp\left[-\frac{(\ln\omega - \ln\omega_n)^2}{b^2}\right]$$





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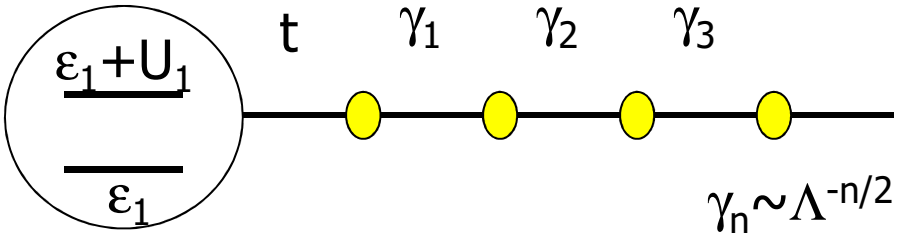
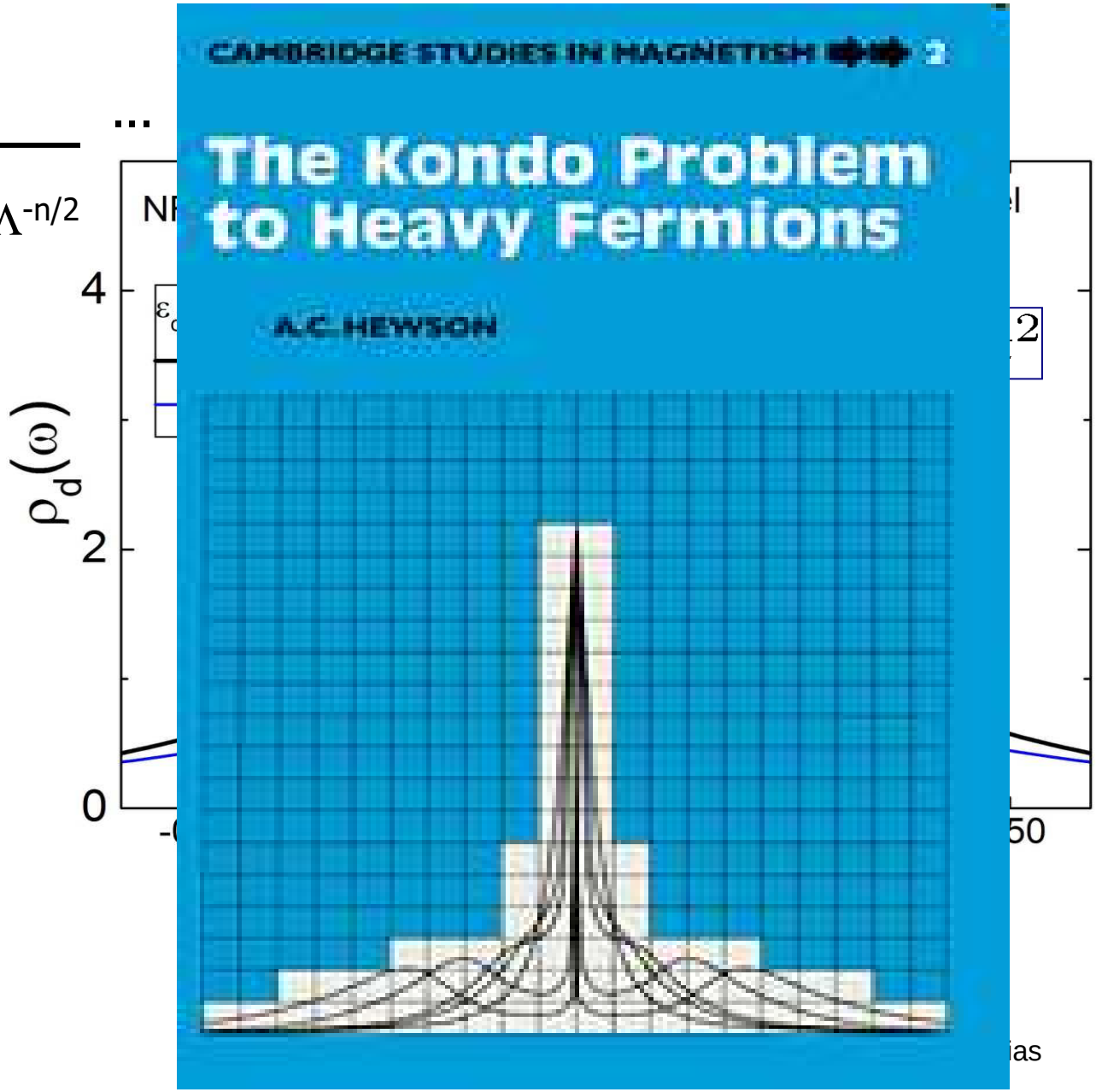
NRG on Anderson model: LDOS



- Single-particle peaks at ε_d and ε_d+U.
- *Many-body* peak at the Fermi energy: ***Kondo resonance*** (width ~T_K).
- NRG: good resolution at low ω (log discretization).



Summary: NRG overview

- NRG method: designed to handle quantum impurity problems
- All energy scales treated on the same footing.
- Non-perturbative: can access transitions between fixed points in the parameter space
- Calculation of physical properties

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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”)
- ...

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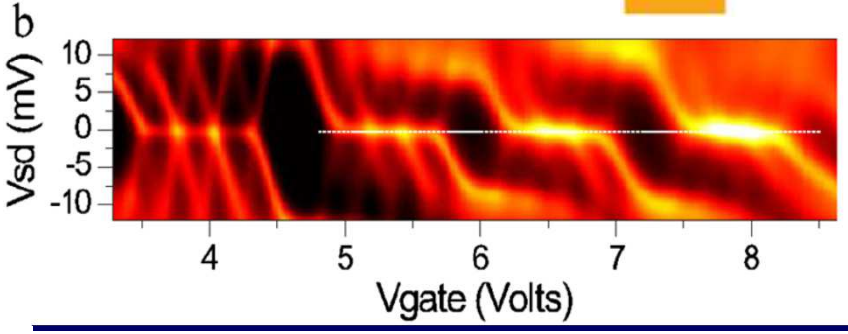
Kondo everywhere!

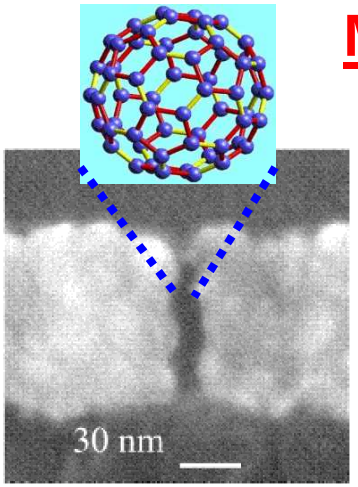
Carbon Nanotubes



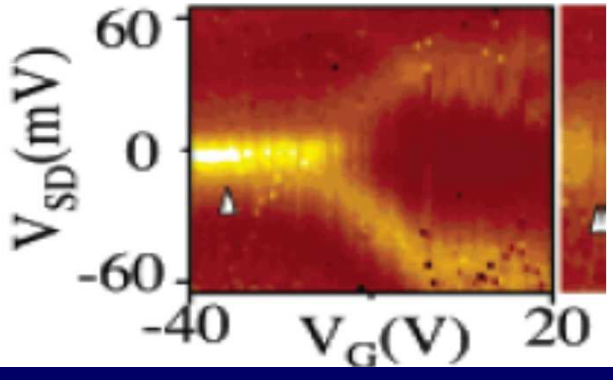
Makarovski, Liu, Filkenstein *PRL* **99** 066801 (2007).

T_K ~ 40 K

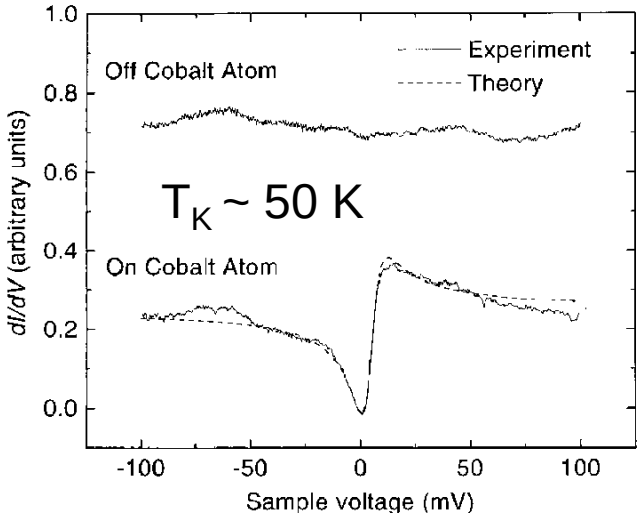
Molecular Junctions



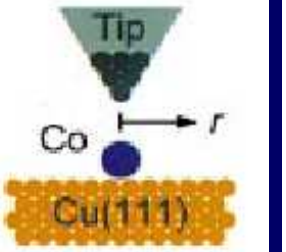
Yu, Natelson, *NanoLett.* **4** 79 (2004).

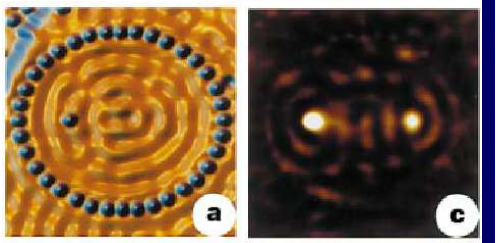


Magnetic atoms on surfaces



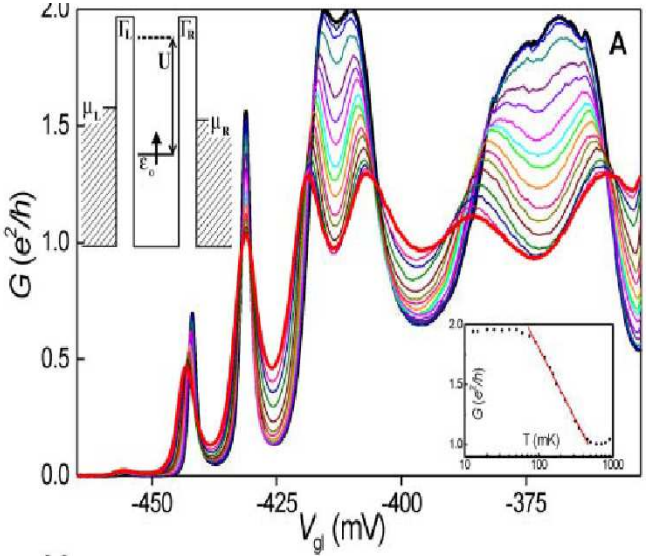
Madhavan et al., *Science* **280** 567 (1998).

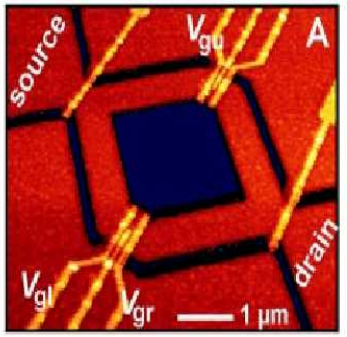




Manoharan et al., *Nature* **403** 512 (2000).

Semiconductor Quantum dots





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

T_K ~ 5 mK

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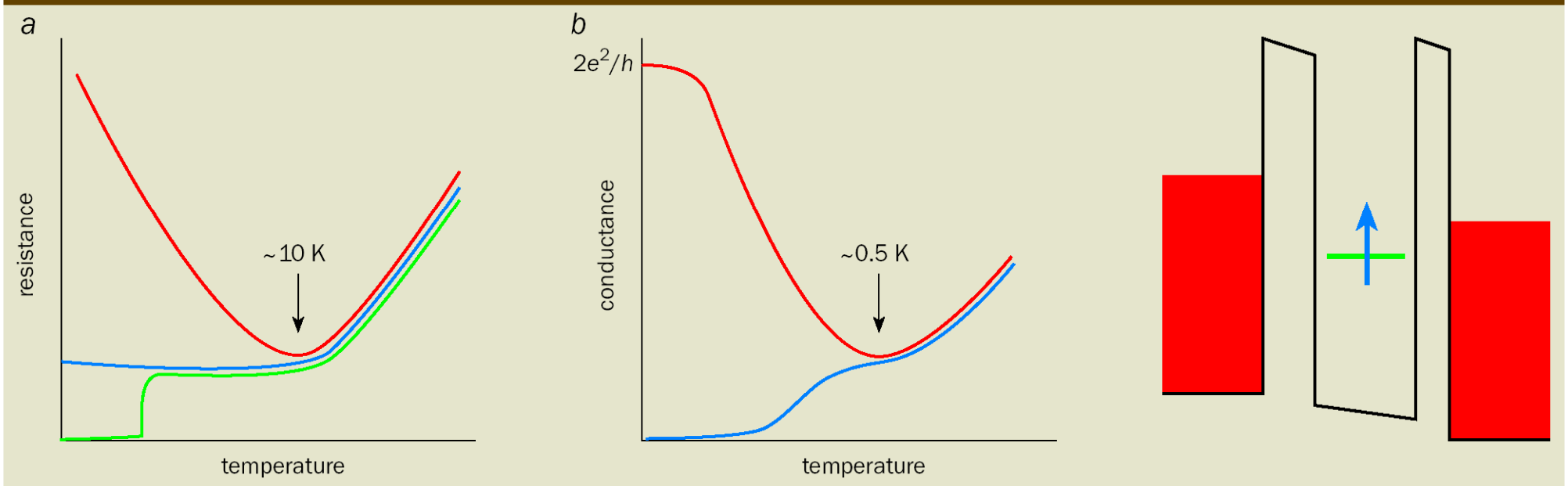
Kondo Effect in Quantum Dots

Revival of the Kondo effect

Leo Kouwenhoven and Leonid Glazman

1 The Kondo effect in metals and in quantum dots



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

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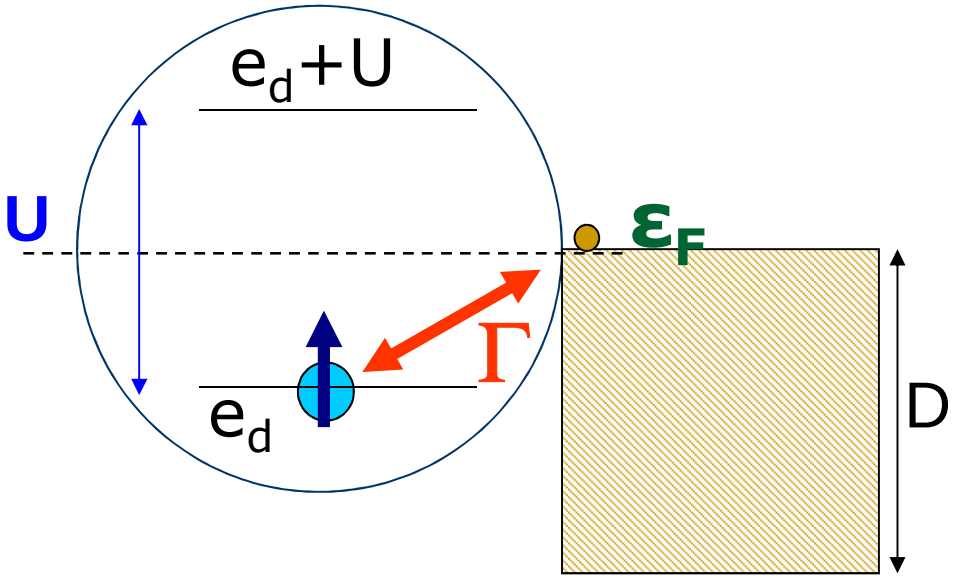
Anderson Model



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

with

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

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

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

"Quantum dot language"

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

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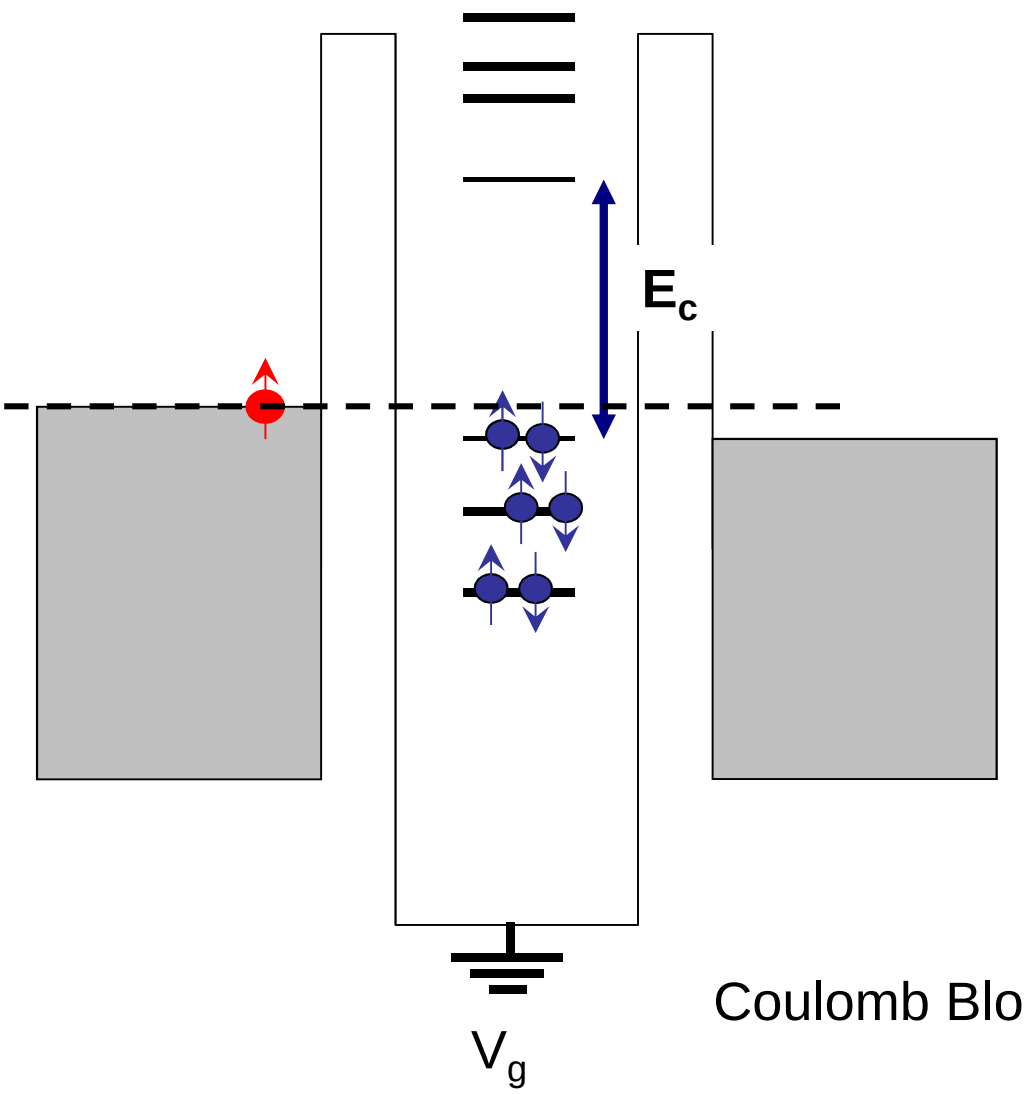
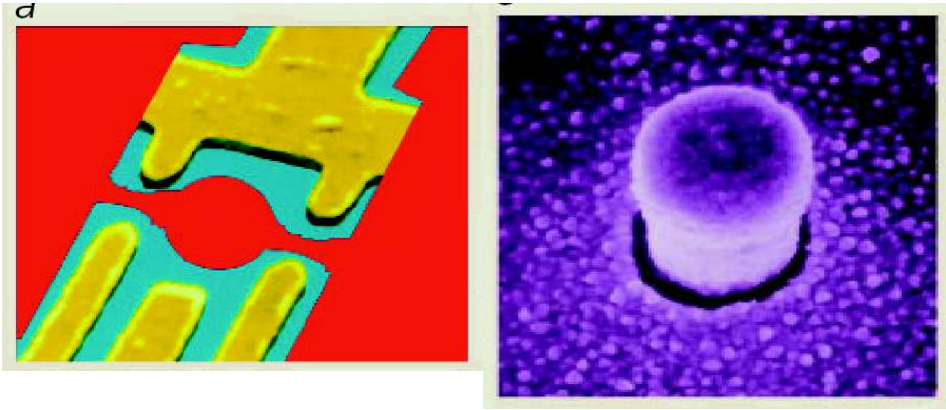
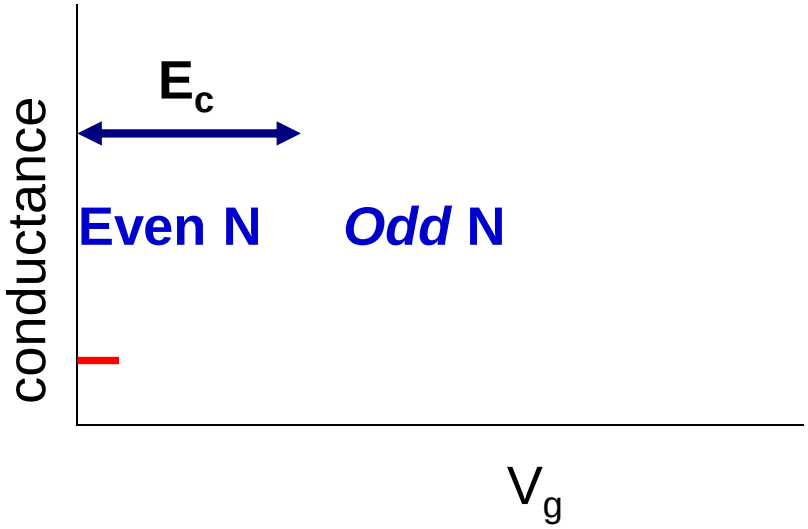
Coulomb Blockade in Quantum Dots







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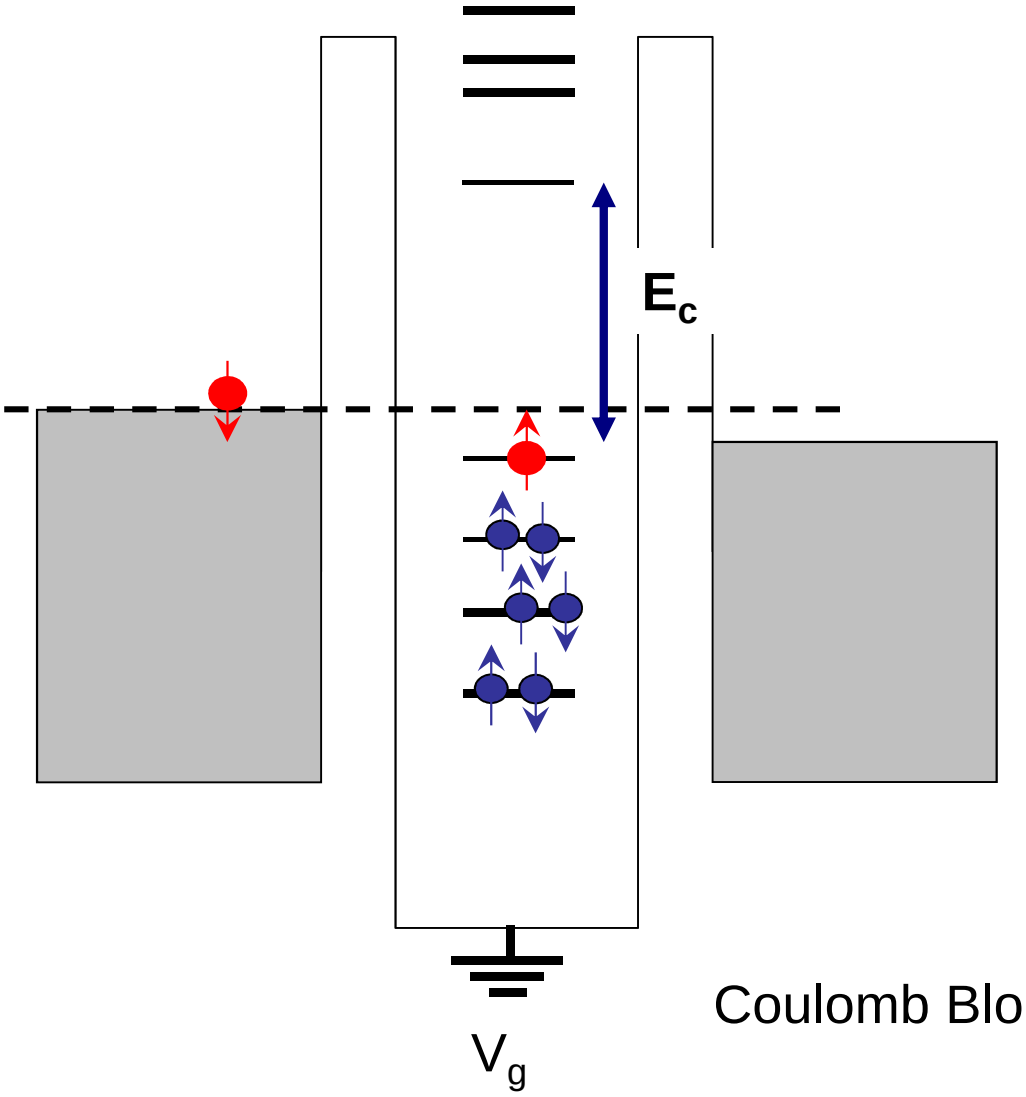
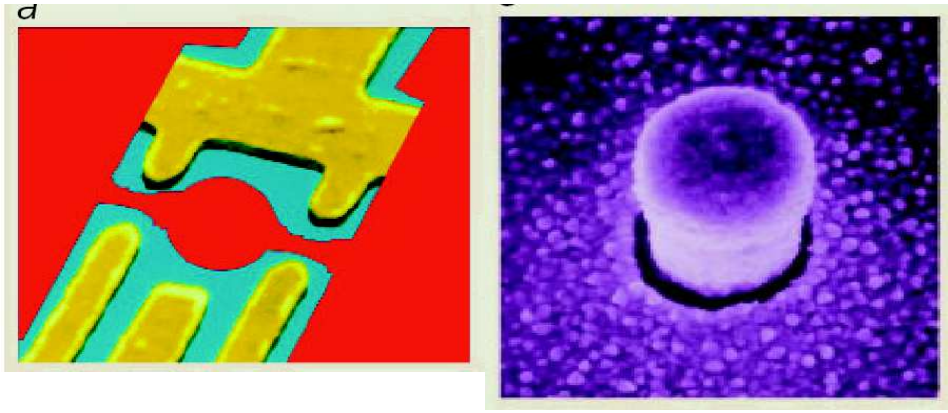
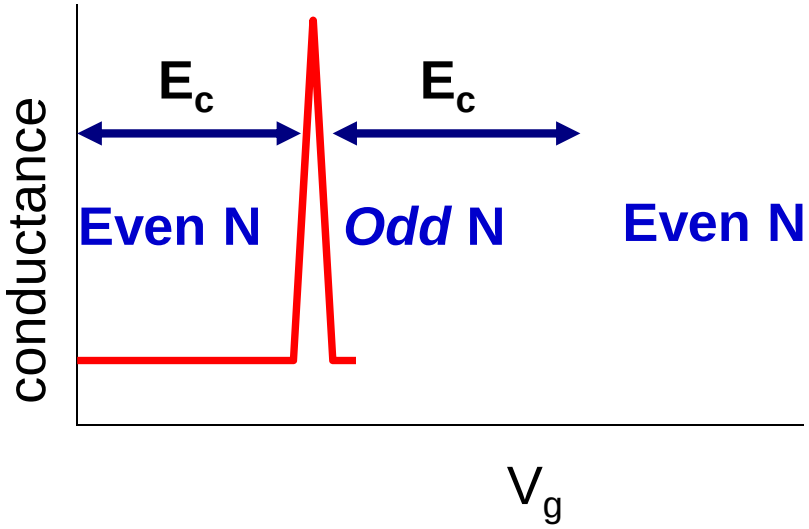
Coulomb Blockade in Quantum Dots







Coulomb Blockade in Quantum Dots

Y. Alhassid *Rev. Mod. Phys.* **72** 895 (2000).

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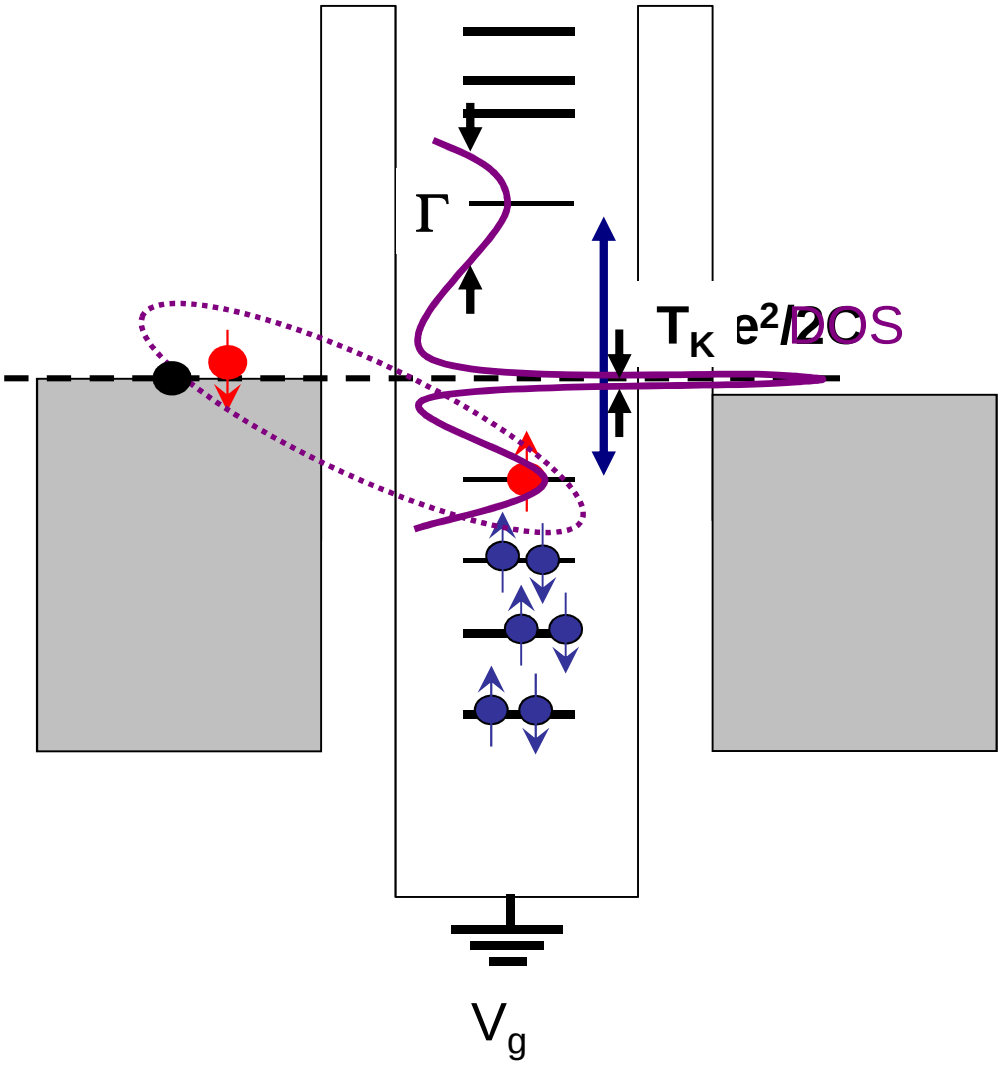
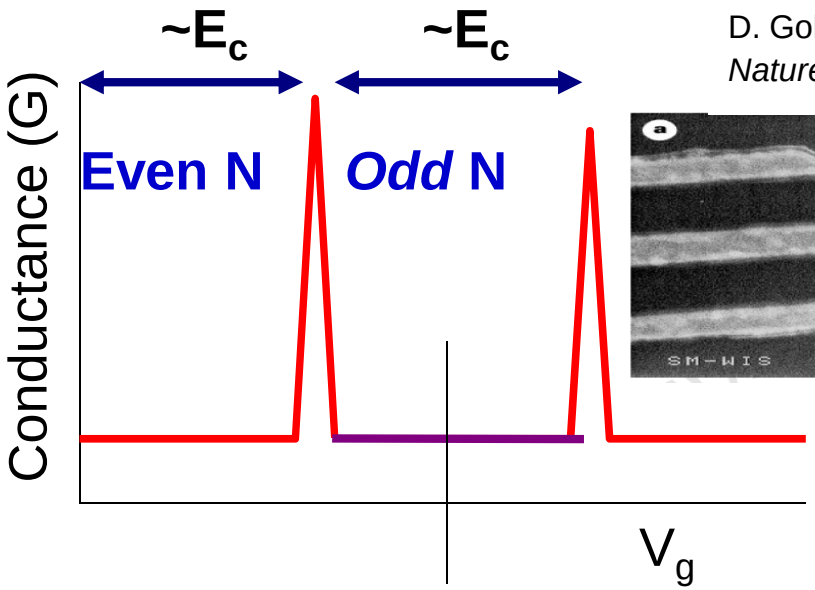
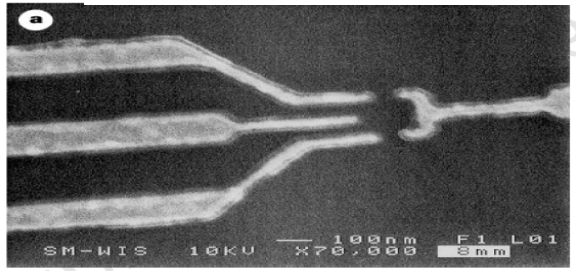
Kondo Effect in Quantum Dots





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

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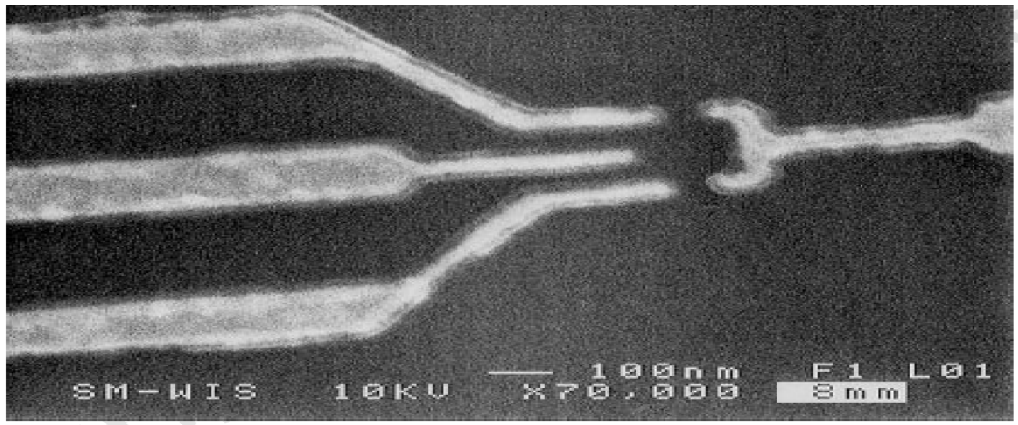
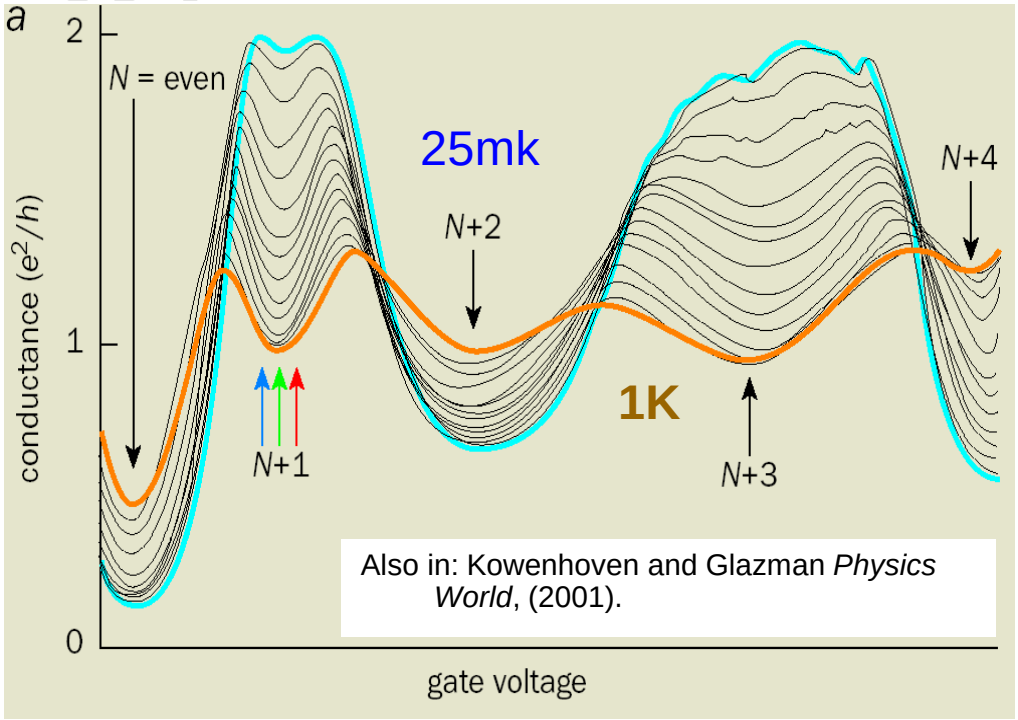
Kondo effect in Quantum Dots

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





Also in: Kowenhoven and Glazman *Physics World*, (2001).

Semiconductor Quantum Dots:

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

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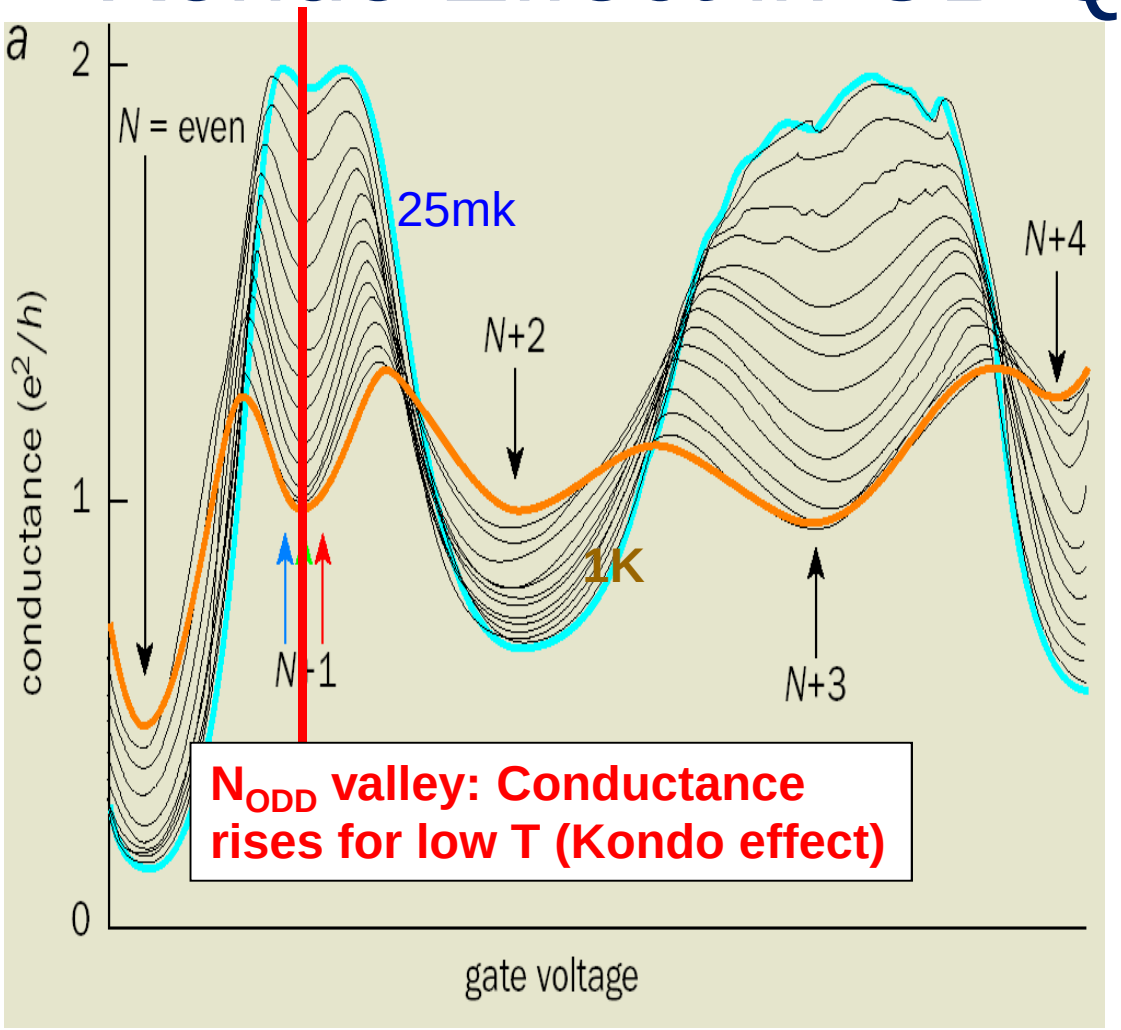
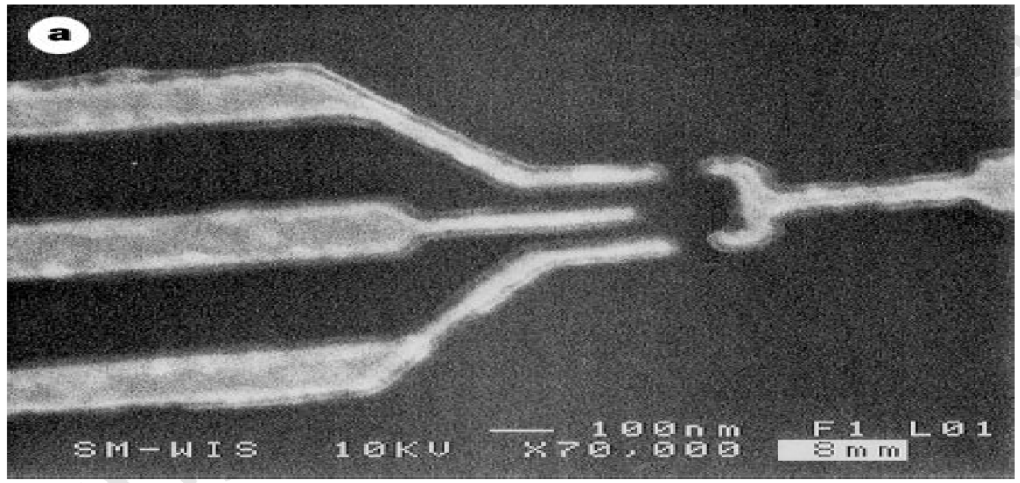
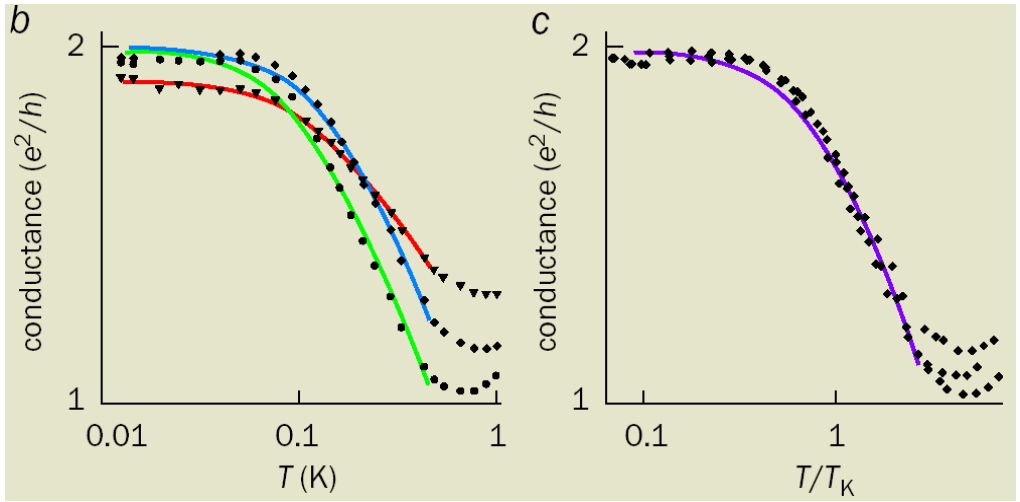
Kondo Effect in CB-QDs







Kondo Temperature T_k : only scaling parameter (~0.5K, depends on V_g)

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

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

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