Quantum Theory of Many-Body systems in Condensed Matter (4302112) 2020

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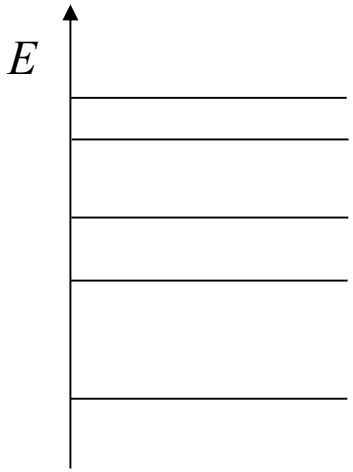
Today's class: *Kondo effect in quantum dots.*

- Kondo effect and the "Kondo problem".
- Wilson's numerical renormalization group.
- Application: Kondo effect in nanostructures.
- Kondo signatures in quantum dot transport.

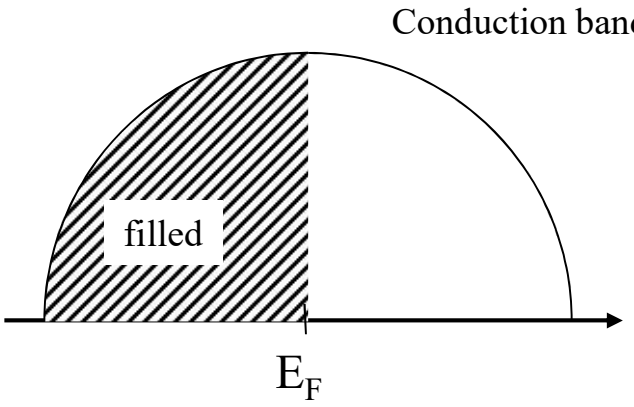
Kondo effect and Wilson's Numerical Renormalization Group method.

From atoms to metals + atoms…



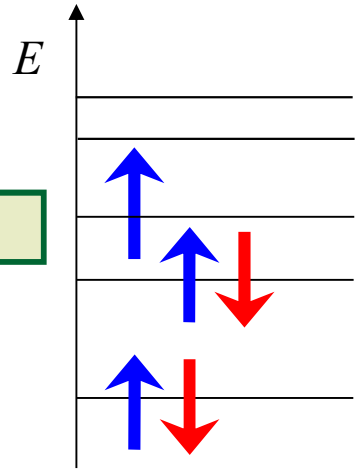
ATOM

Many Atoms!



Metal (non magnetic)

(few)



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

=

?

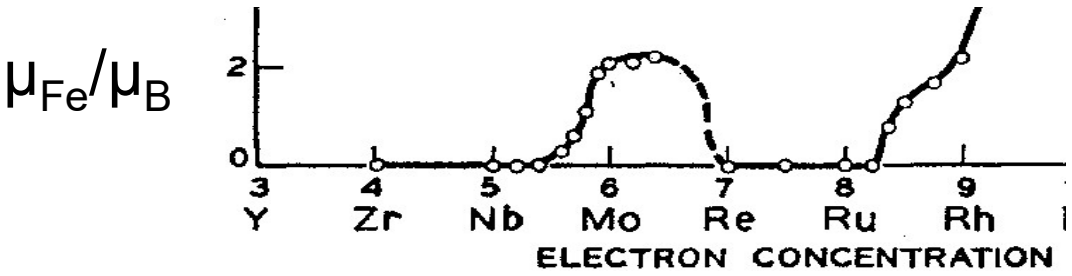
Is the resulting compound still a metal ?

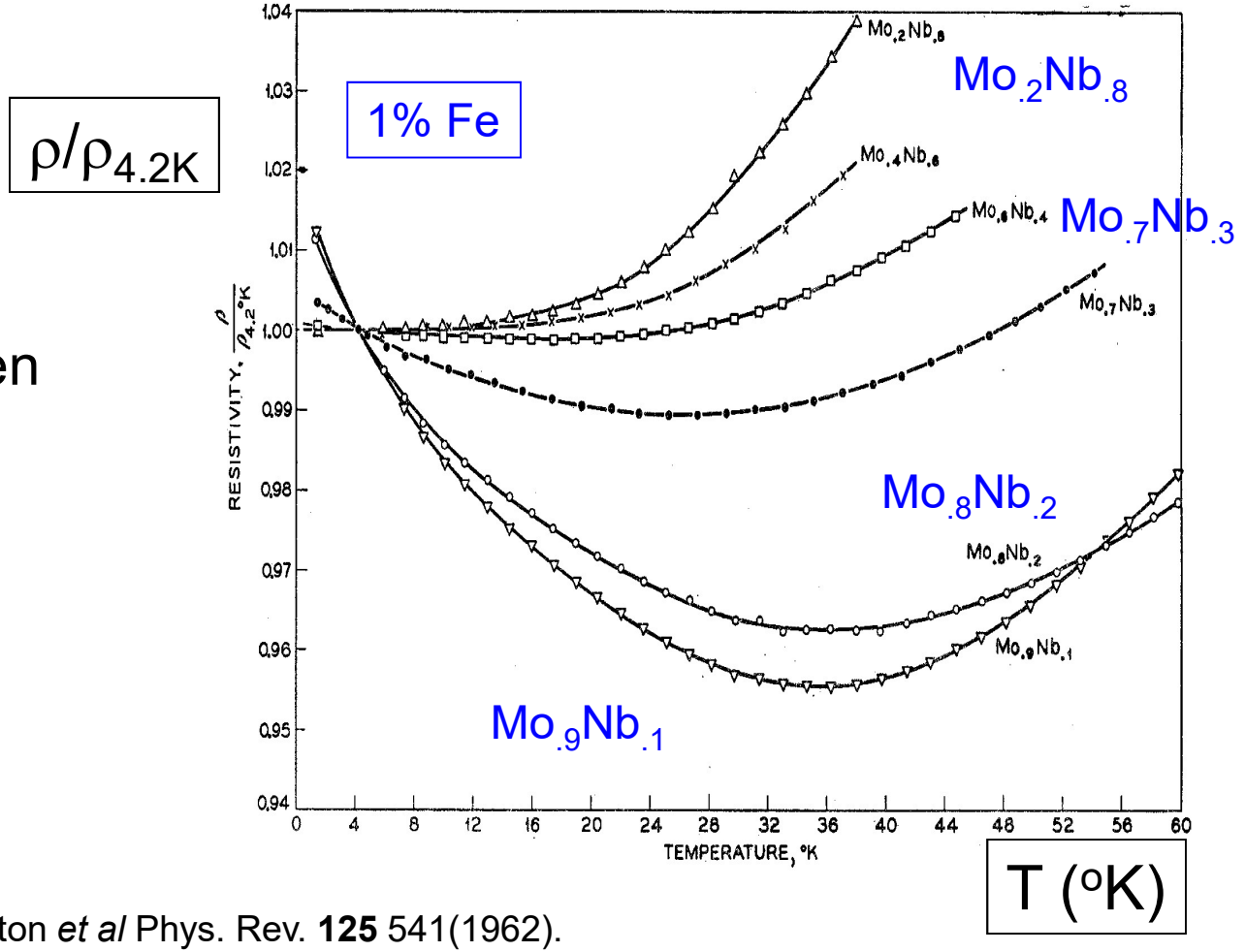
Kondo effect

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

    minimum in ρ(T);

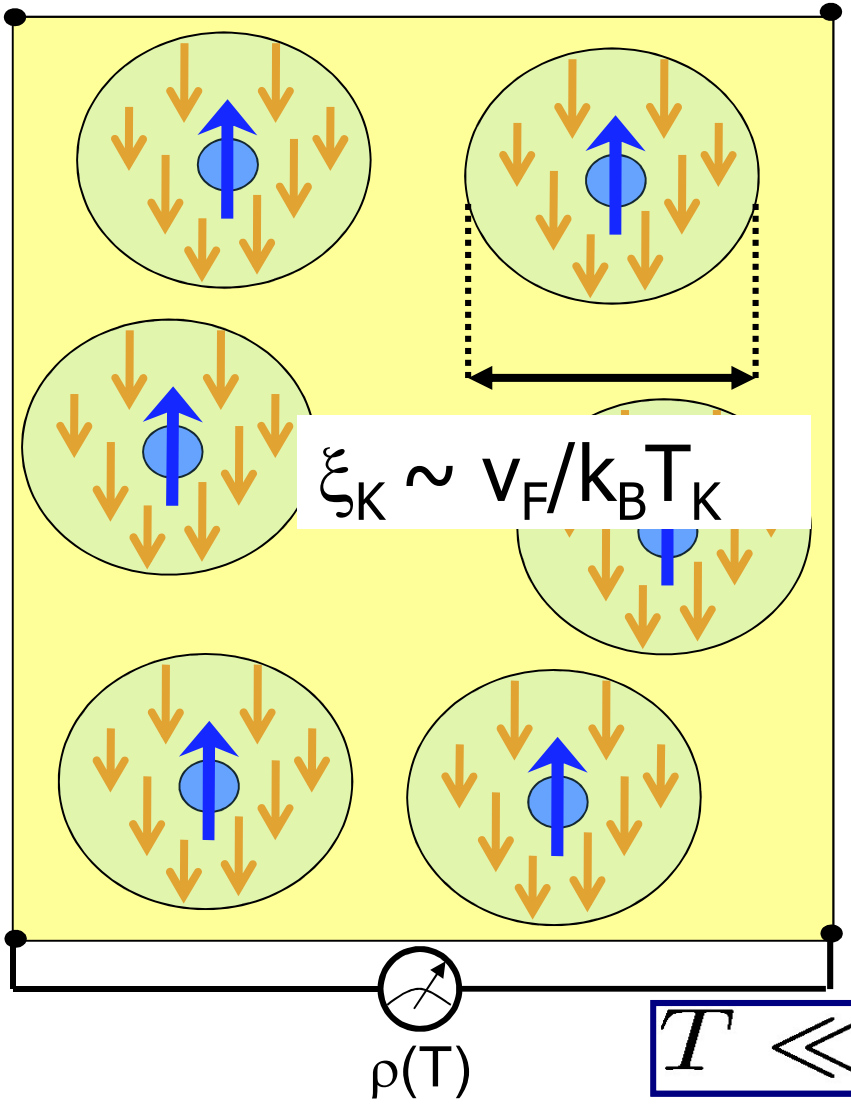
    T_{min} depends on $c_{imp.}$
  - 60's - Correlation between the existence of a Curie-Weiss component in the susceptibility (*magnetic moment*) and resistance minimum .





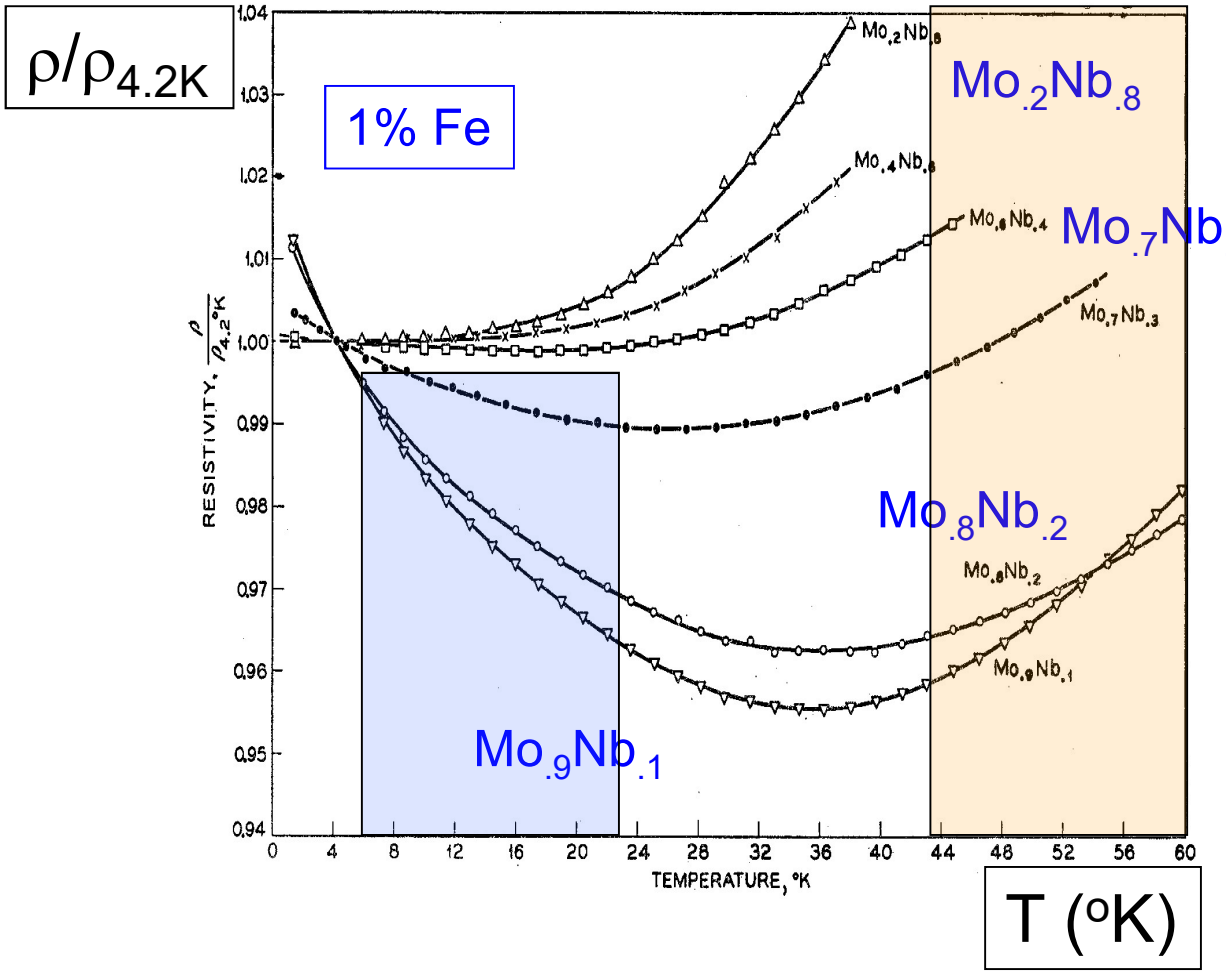
Top: A.M. Clogston *et al* Phys. Rev. **125** 541(1962).
Bottom: M.P. Sarachik *et al* Phys. Rev. **135** A1041 (1964).

Kondo effect



$T \ll T_K$

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

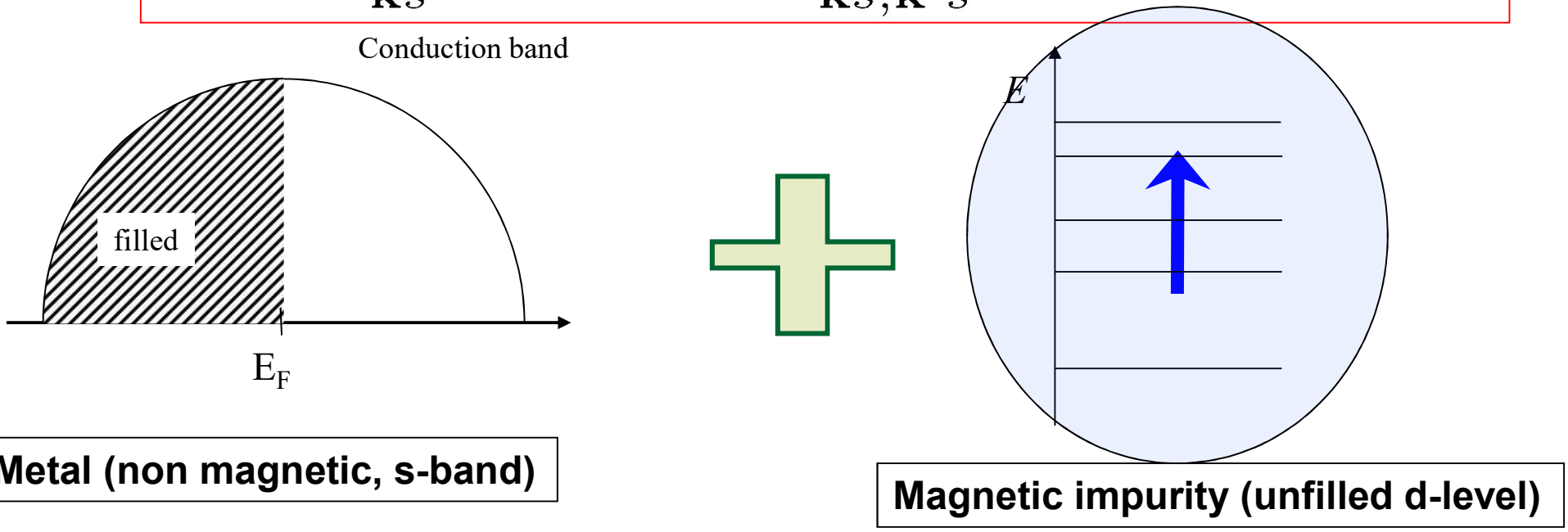


Resistivity *increases* with decreasing T (Kondo effect)

Kondo problem: s-d Hamiltonian

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

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



Metal (non magnetic, s-band)

Magnetic impurity (unfilled d-level)

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

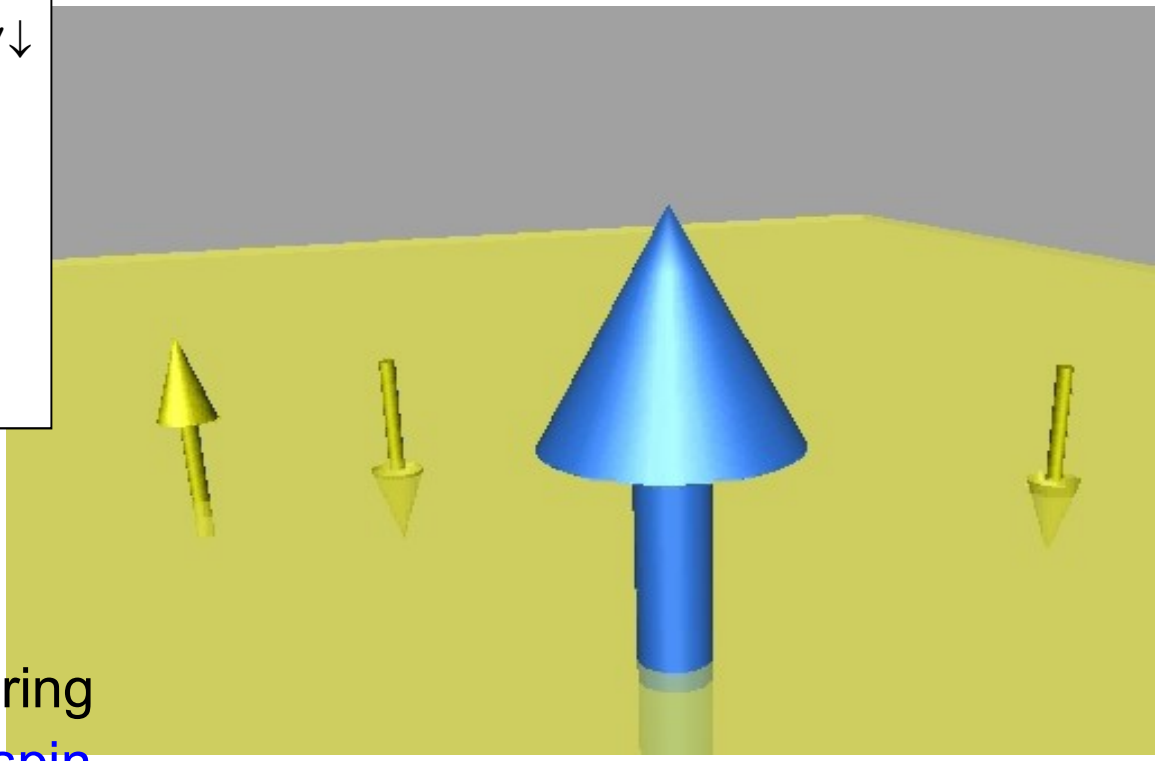
$$H_{\text{s-d}} = J \sum_{k,k'} S^{+} c^{\dagger}_{k\downarrow} c_{k'\uparrow} + S^{-} c^{\dagger}_{k\uparrow} c_{k'\downarrow}$$

Spin: J>0 AFM

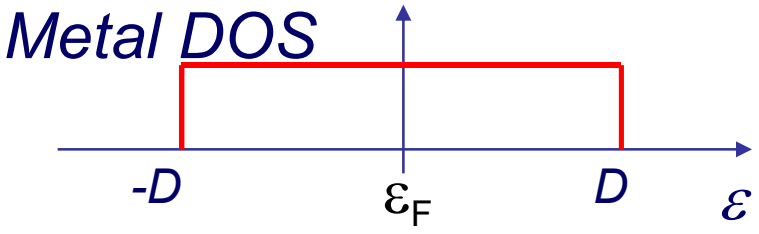
$$+ S_z \left(c^{\dagger}_{k\uparrow} c_{k'\uparrow} - c^{\dagger}_{k\downarrow} c_{k'\downarrow} \right)$$

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

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**):

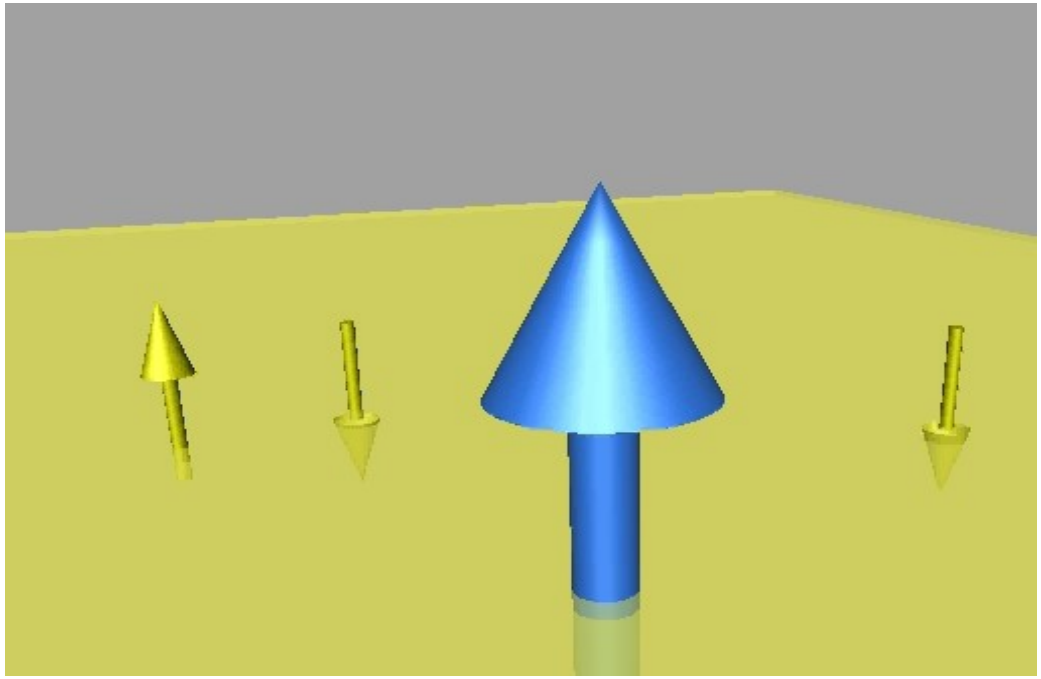


Kondo's explanation for T_{min} (1964)

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

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

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



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

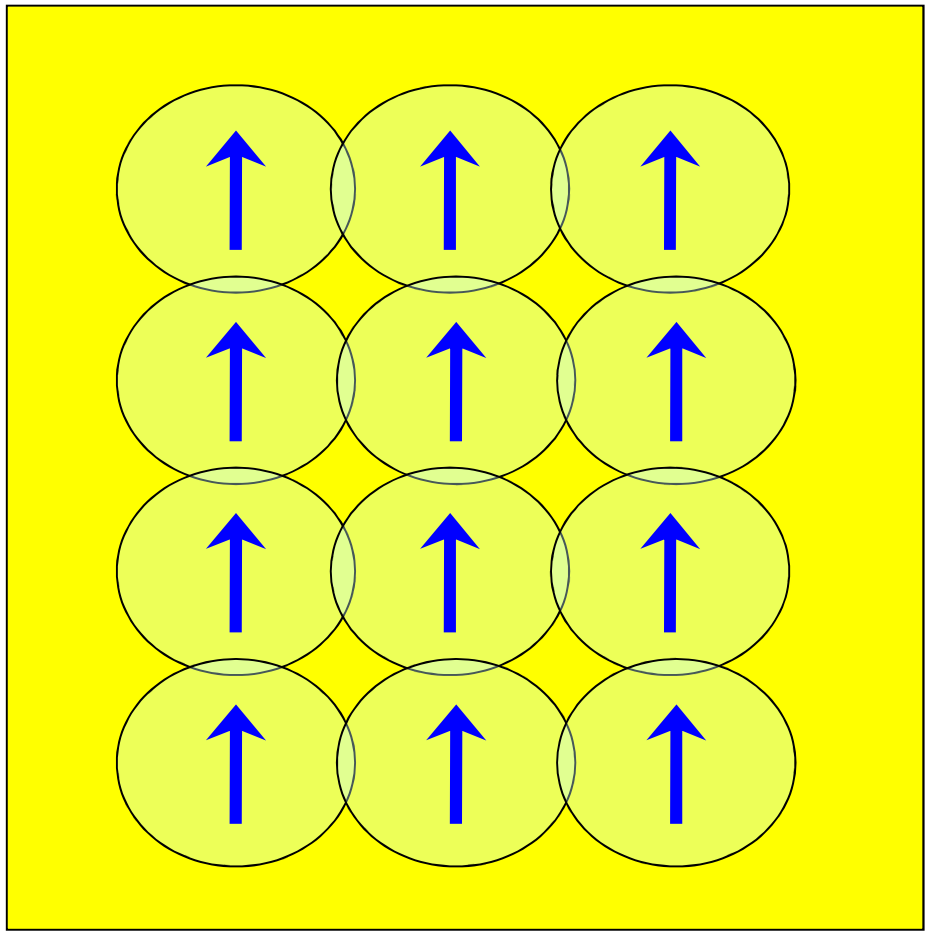
- Only *one* free paramenter: the Kondo temperature T_K
  - Temperature at which the perturbative expansion ***diverges.***

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

J. Kondo, Resistance Minimum in Dilute Magnetic Alloys, *Prog. Theo. Phys.* 37–49 **32** (1964).

Kondo Lattice models

"Concentrated" case: Kondo Lattice (e.g., some heavy-Fermion materials)



- Kondo impurity model suitable for diluted impurities in metals.
- Some rare-earth compounds (localized 4f or 5f shells) can be described as "Kondo lattices".
- This includes so called "heavy fermion" materials (e.g. Cerium and Uranium-based compounds $CeCu_2Si_2$, UBe_{13}).

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)
- 1961: Anderson model for
- 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

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

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

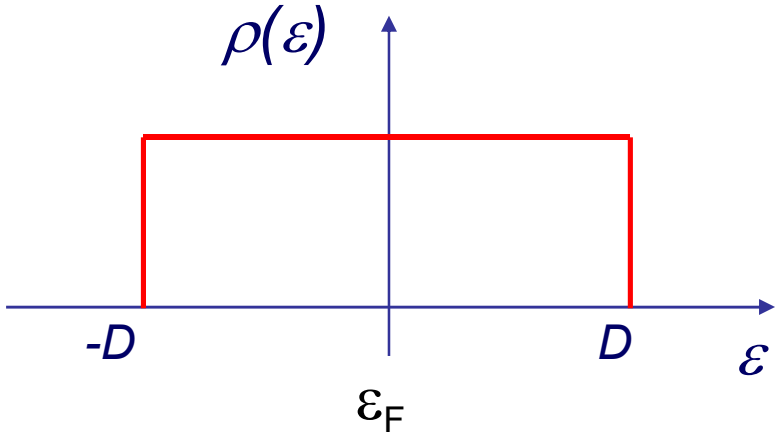
- Diverges *logarithmically* for $T \to 0$ or $D \to \infty$.

What is going on?

($T < T_K \to$ perturbation expasion no longer holds)

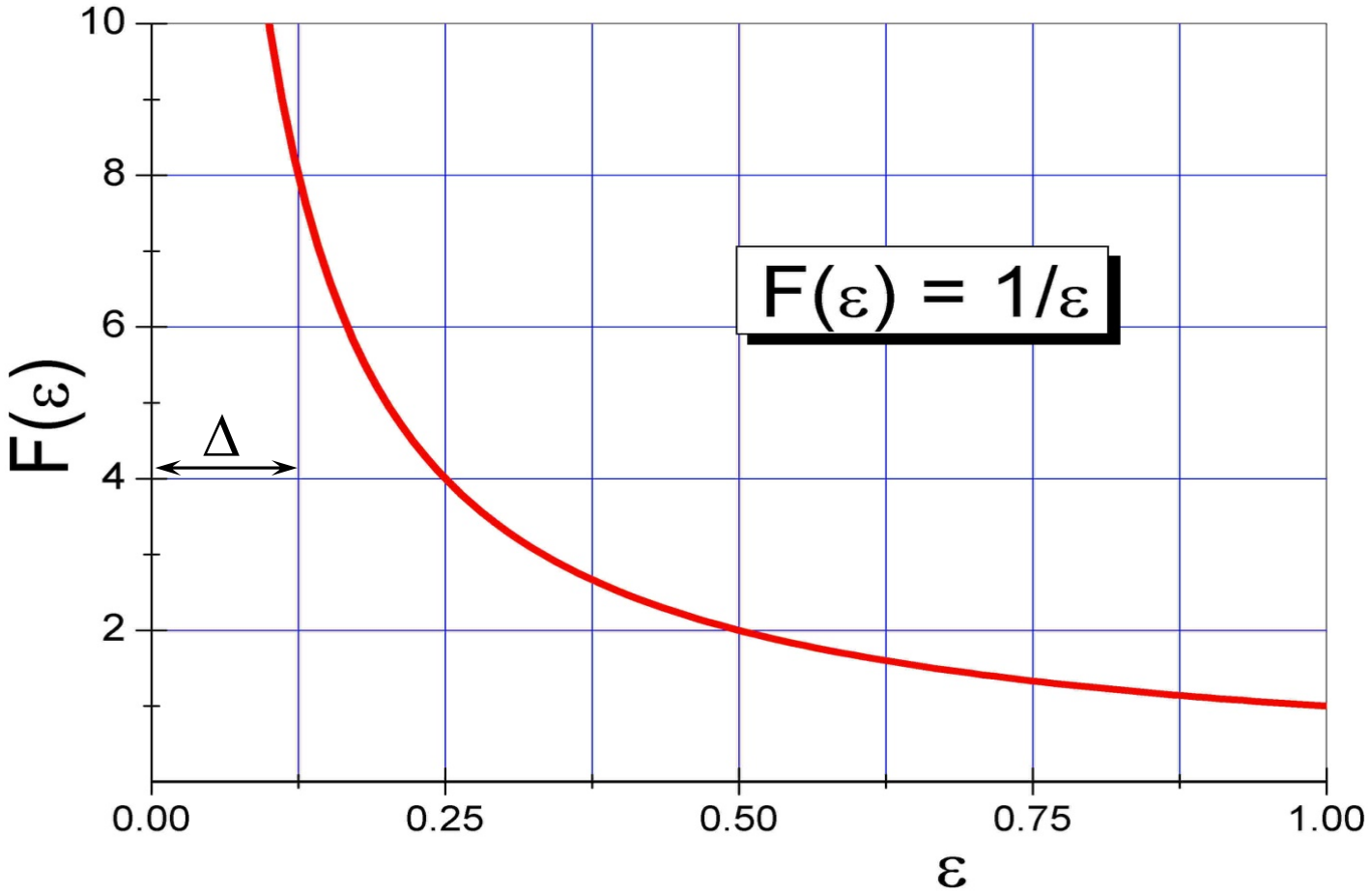
- Experiments show *finite* R as $T \to 0$ or $D \to \infty$.
- The log comes from something like:

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



- *All* energy scales contribute!

“Perturbative” Discretization of CB

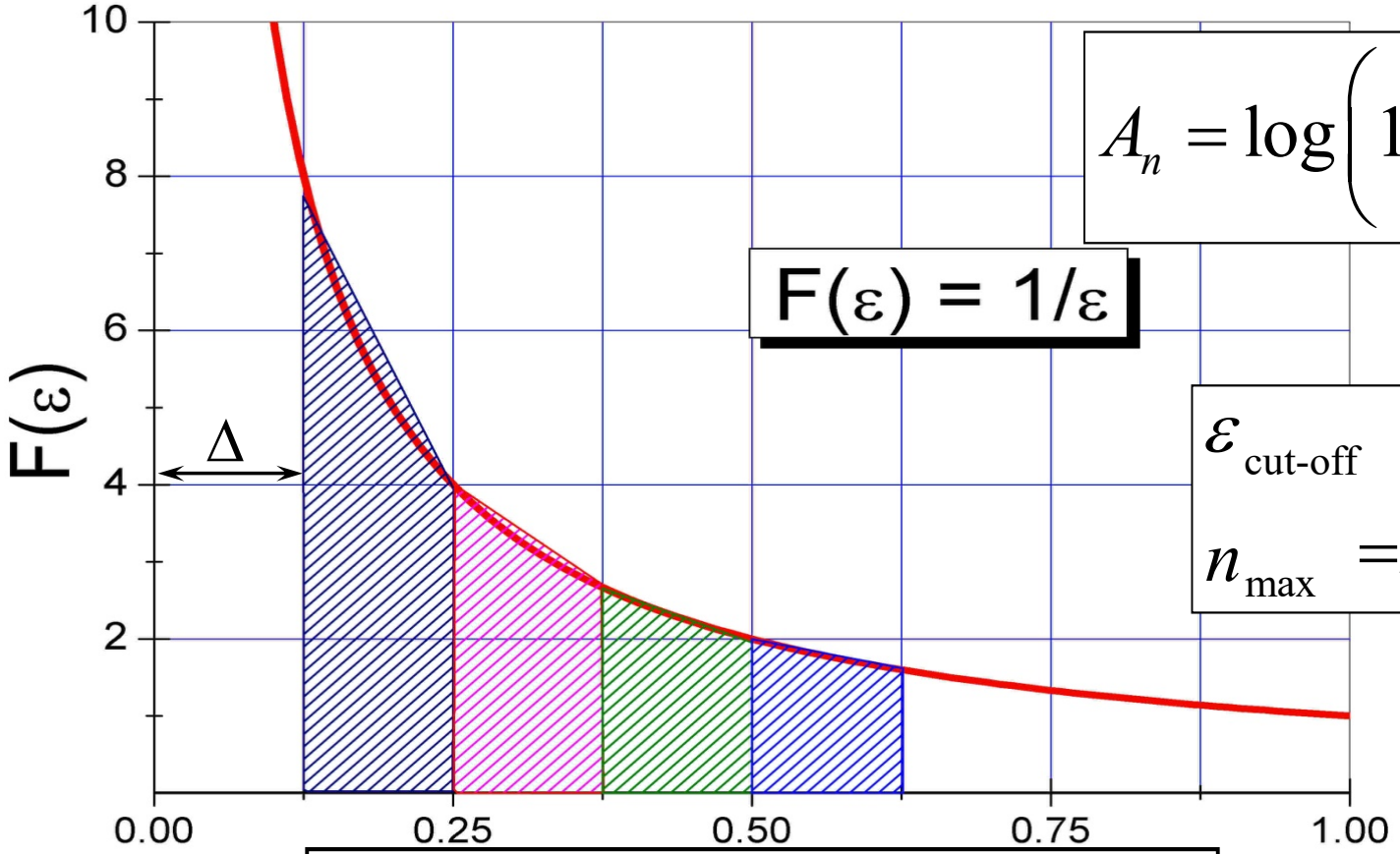


$\varepsilon = (E-E_F)/D$

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

“Perturbative” Discretization of CB

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



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

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

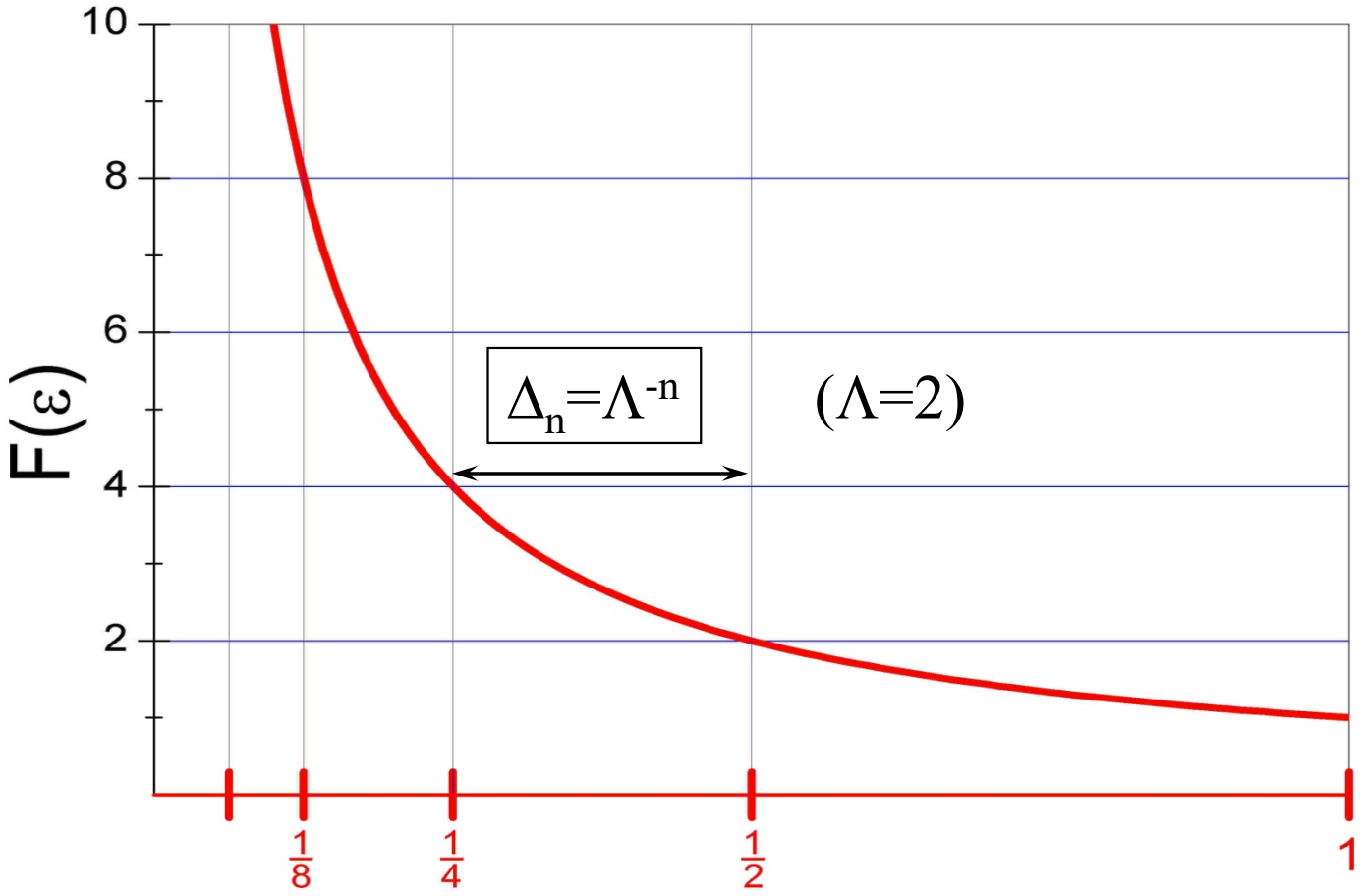
$$n_{\max} = \Delta^{-1} - 1$$

Want to keep all contributions for $D \to \infty$?

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

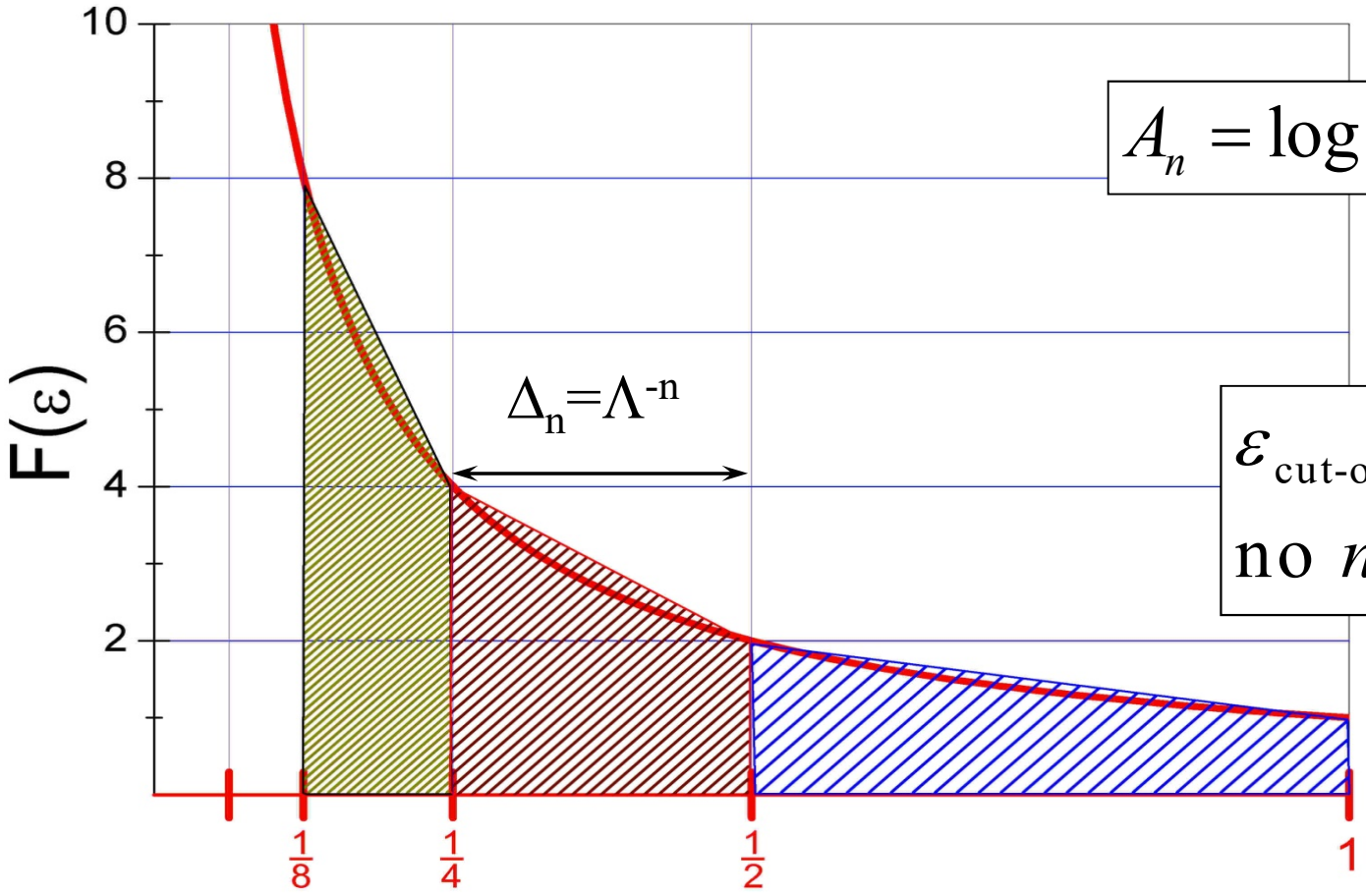
Not a good approach!

Wilson's CB Logarithmic Discretization



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

Wilson's CB Logarithmic Discretization



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

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

$$\text{no } n_{\max}$$

Now you're ok!

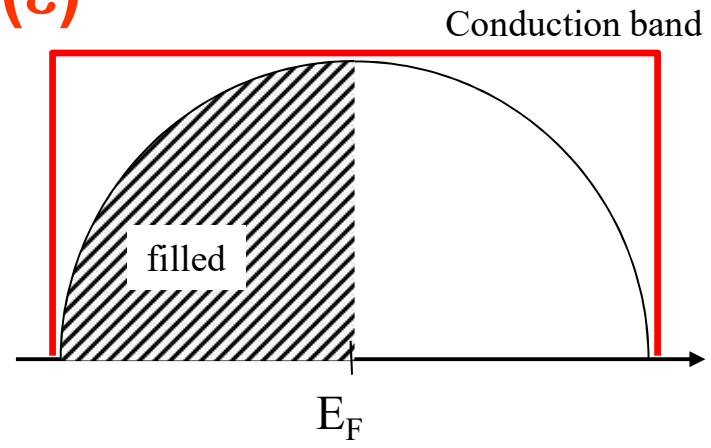
$A_3 = A_2 = A_1$ ($\Lambda=2$)

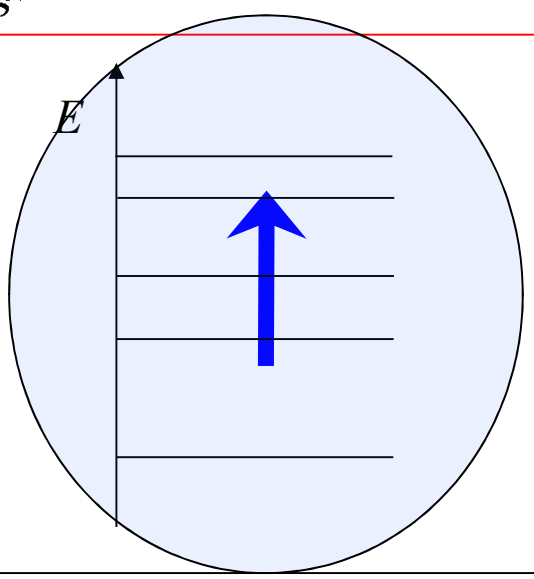
Kondo problem: s-d Hamiltonian

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

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

ρ(ε)



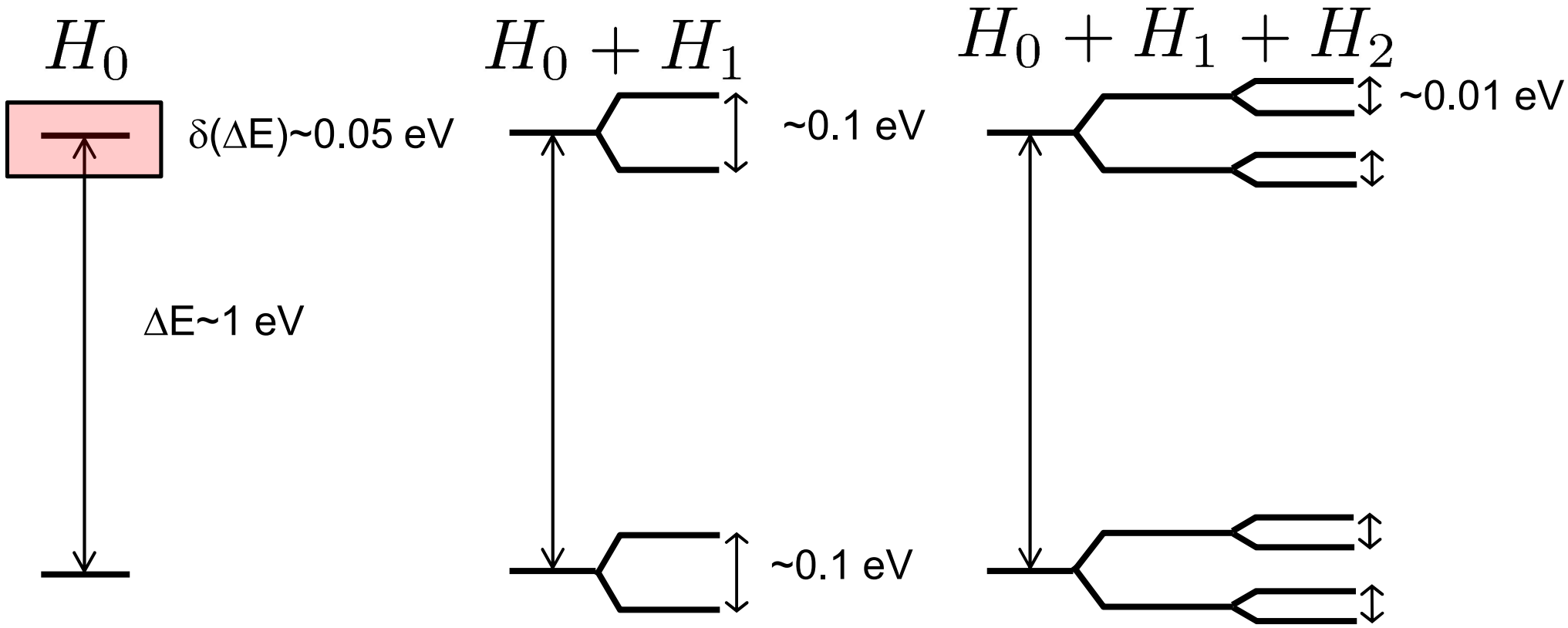


Metal (non magnetic, s-band)

Magnetic impurity (unfilled d-level)

The problem: different energy scales!

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

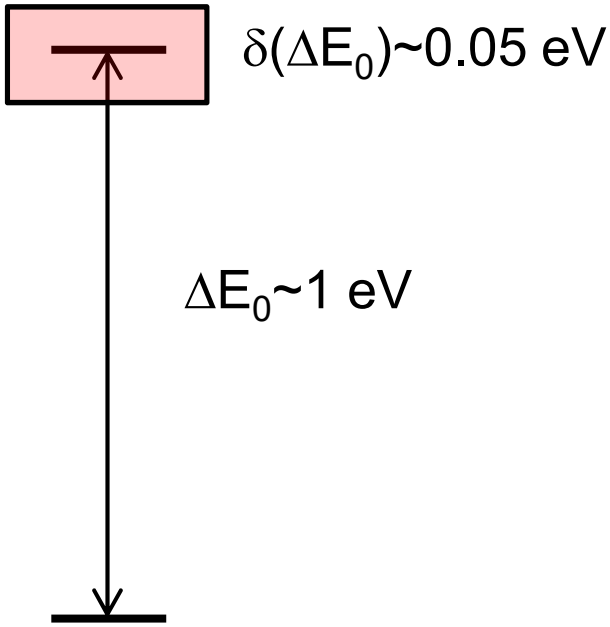


Uncertainty of the calculation:
$\delta(\Delta E)/\Delta E \sim 5\%$

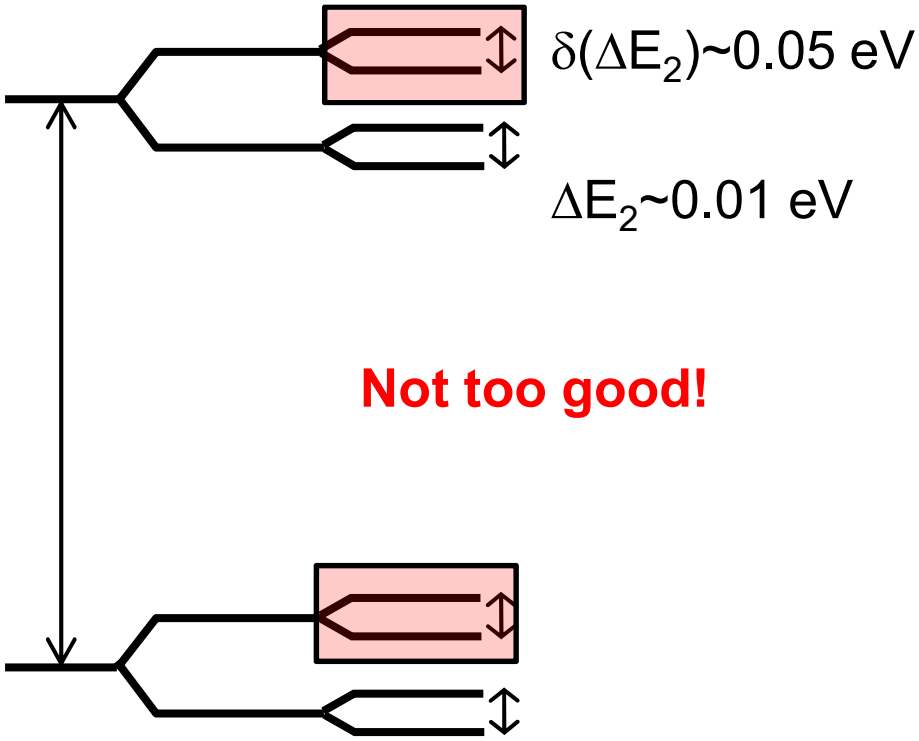
How to calculate these splittings accurately?

Option 1: “Brute force”

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



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

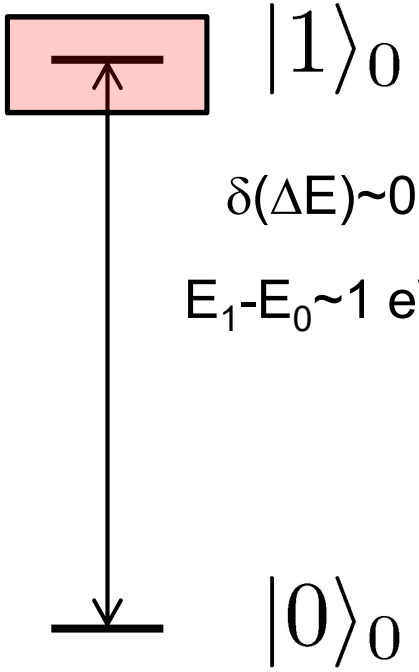


Not too good!

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

Option 2: Do it by steps.

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



$\delta(\Delta E)$~0.05 eV

E_1-E_0~1 eV

Uncertainty of the calculation:
$\delta(\Delta E)/\Delta E$~5%

New basis:

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

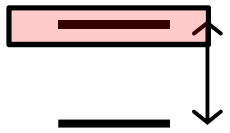
H_0 is diagonal !

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

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

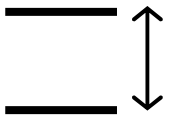
the uncertainty in diagonalizing it is still 5%!

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



~0.1 eV

$\delta(\Delta E_1)$~0.005 eV

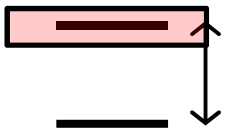


~0.1 eV

Uncertainty of the calculation:
$\delta(\Delta E_1)/\Delta E_1$~5%

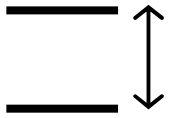
Option 2: Do it by steps, again.

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



~0.1 eV

$\delta(\Delta E_1)$~0.005 eV



~0.1 eV

New basis:

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

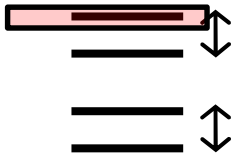
$\tilde{H}_1$ is diagonal!

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

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

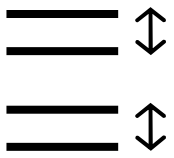
the uncertainty in diagonalizing it is still 5%!

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



~0.01 eV

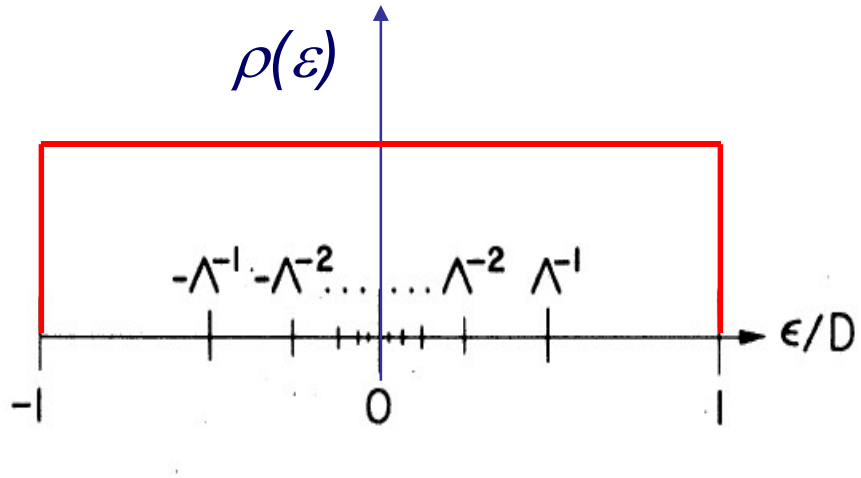
$\delta(\Delta E_2)$~0.0005 eV



Uncertainty of the calculation:
$\delta(\Delta E_2)/\Delta E_2$~5%

Kondo s-d Hamiltonian

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



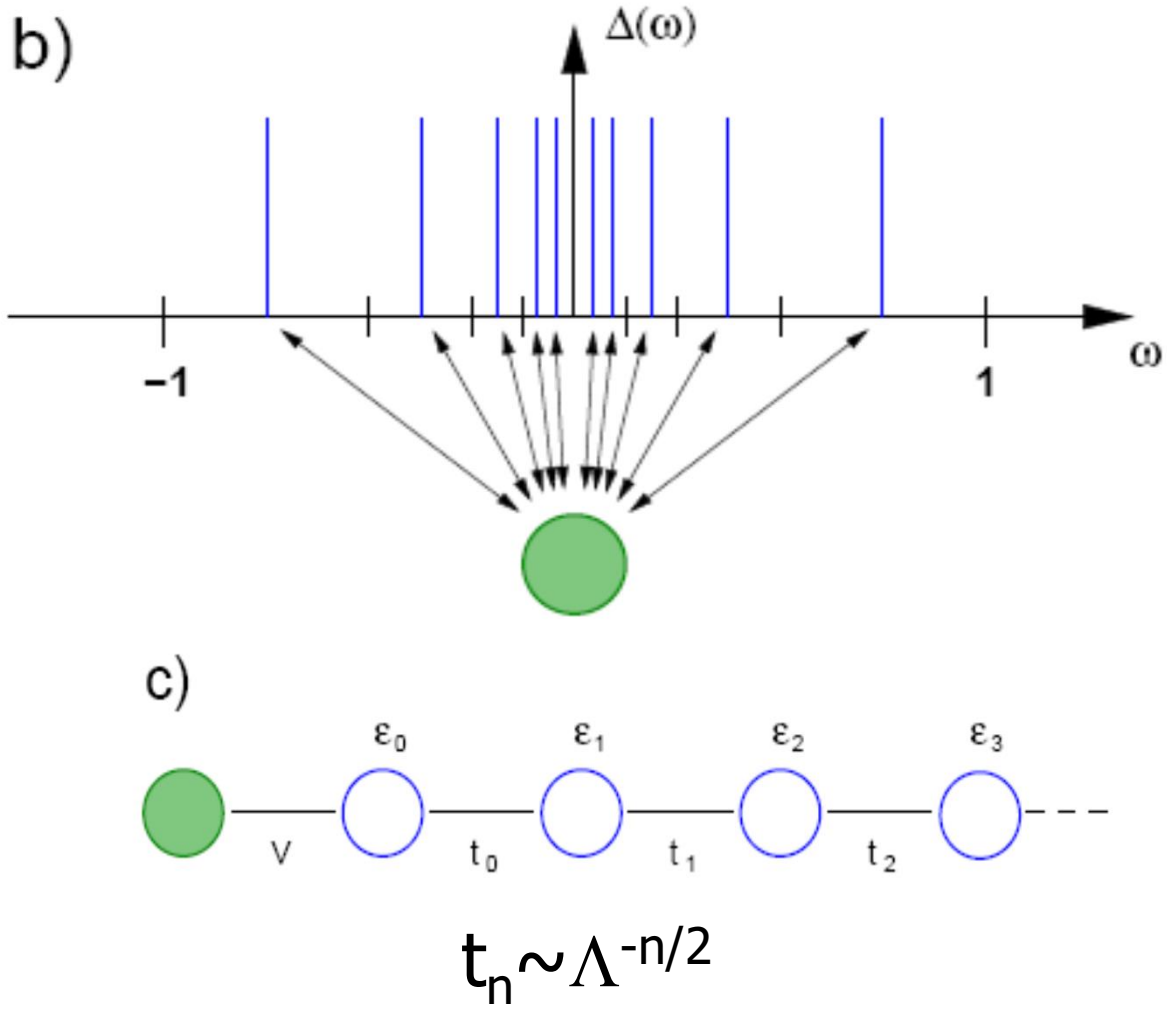
- From continuum *k* to a *discretized* band.
- Transform $H_{\text{s-d}}$ into a linear chain form (exact, as long as the chain is infinite):

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

Logarithmic Discretization.

Steps:

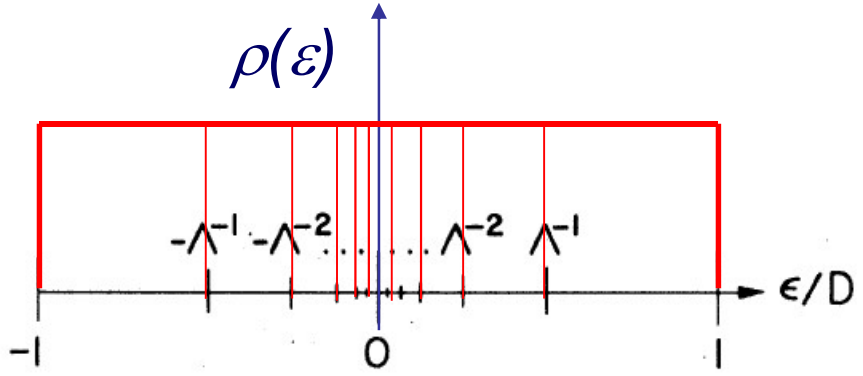
1. Slice the conduction band in intervals in a log scale (parameter Λ)
2. Continuum spectrum approximated by a single state
3. Mapping into a tight binding chain: sites correspond to different energy scales.

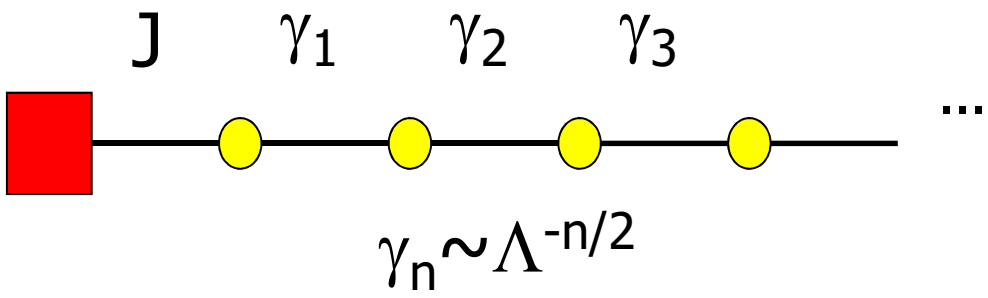


$t_n \sim \Lambda^{-n/2}$

“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

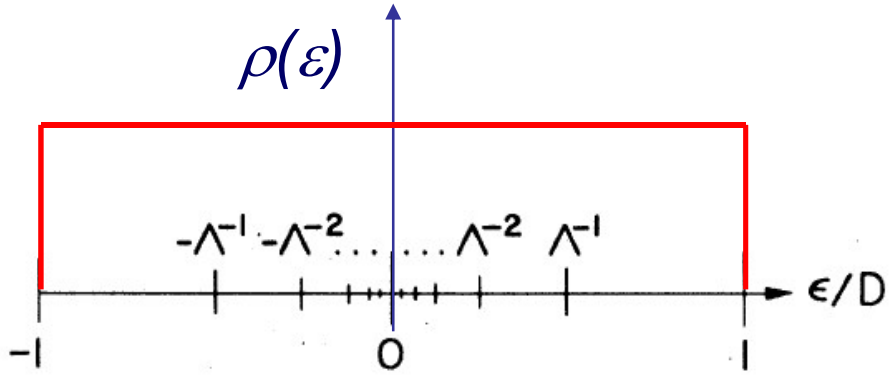


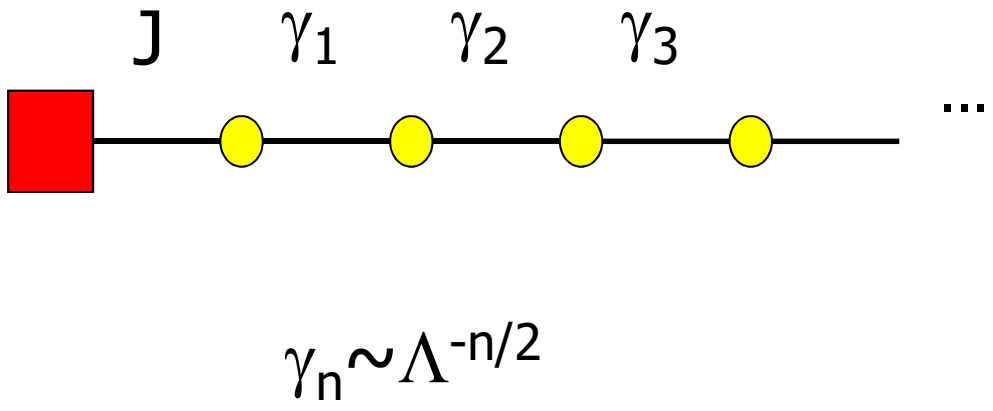


“New” Hamiltonian (Wilson)

- Recurrence relation (Renormalization procedure).

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



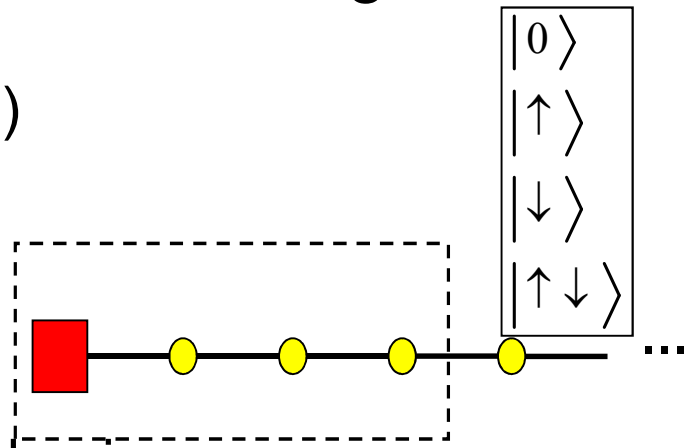


$\gamma_n \sim \Lambda^{-n/2}$

Intrinsic Difficulty

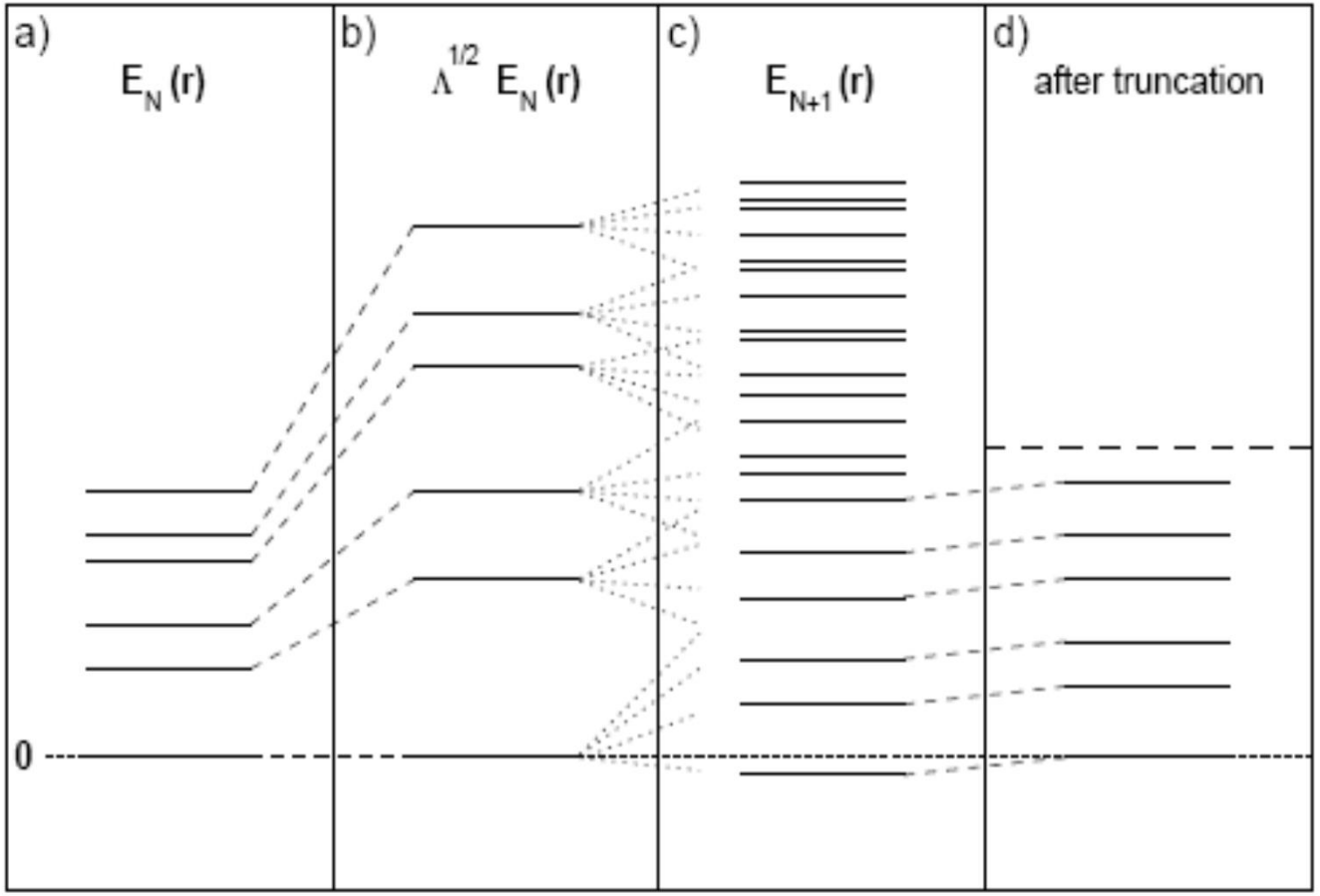
- You ran into problems when N~5. The basis is too large! (grows as $2^{(2N+1)}$)
  - N=0; (just the impurity); 2 states (up and down)
  - N=1; 8 states
  - N=2; 32 states
  - N=5; 2048 states
  - (…) N=20; 2.199×10^{12} states:
    - 1 byte per state → 20 HDs just to store the basis.
  - And we might 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 → lowest ~1500 or so in the next round (Even then, you end up having to diagonalize a 4000x4000 matrix…).

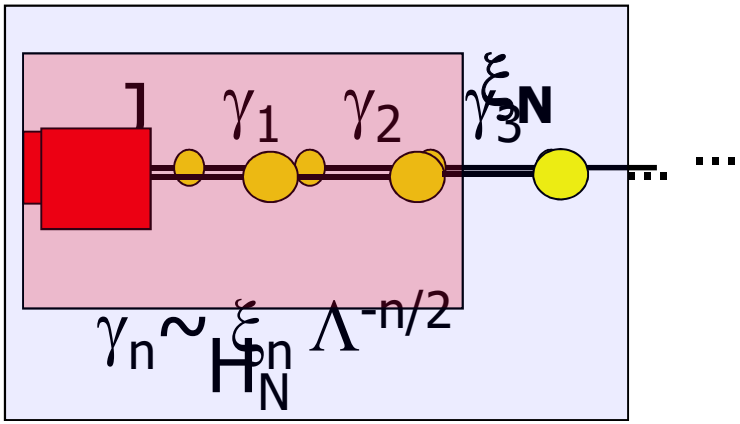


Renormalization Procedure

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

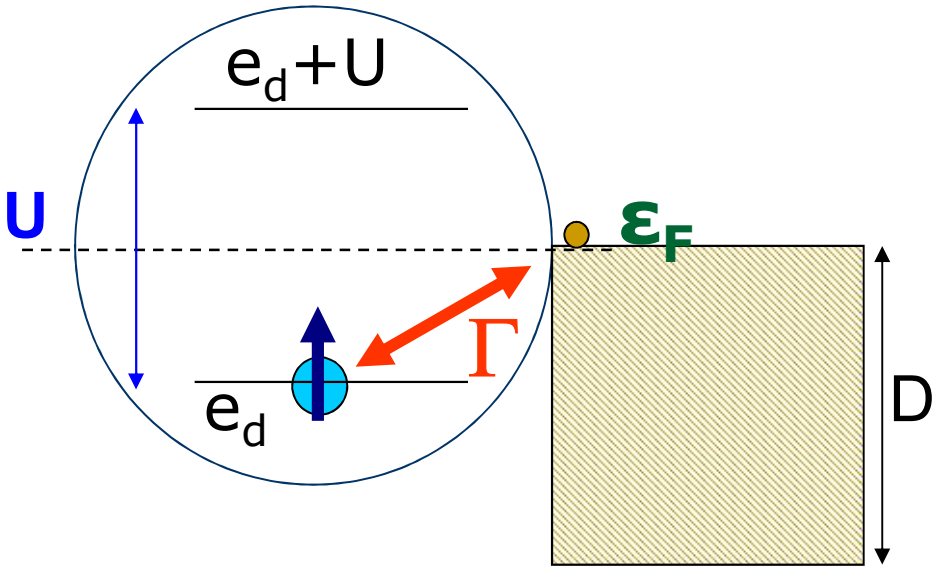


- Iterative numerical solution.
- Renormalize by $\Lambda^{1/2}$.
- Keep low-energy states.



H_{N+1}

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

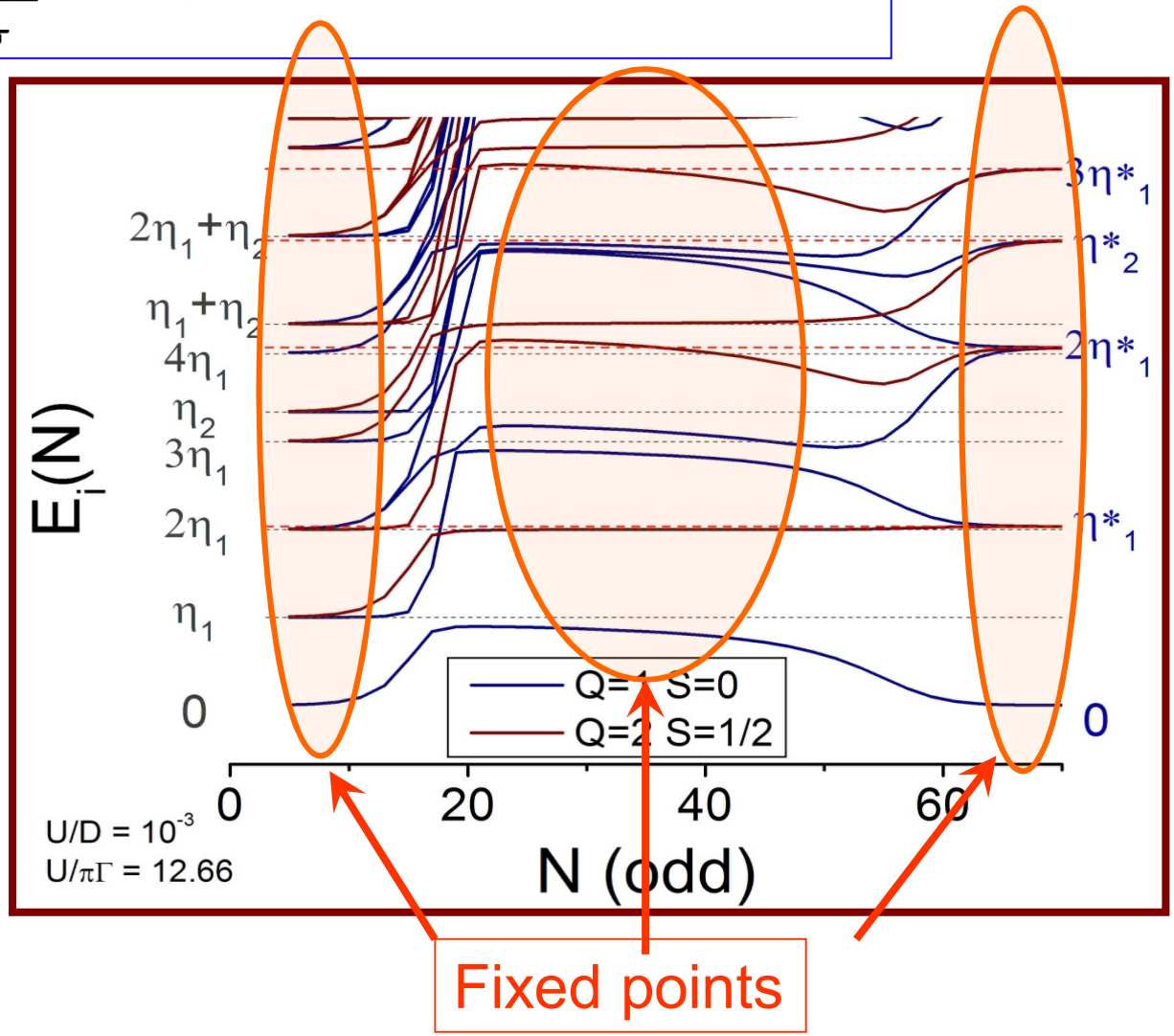
$$H_{N+1} = \sqrt{\Lambda} H_N + \xi_N \sum_\sigma f^\dagger_{N+1\sigma} f_{N\sigma} + f^\dagger_{N\sigma} f_{N+1\sigma}$$

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

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

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

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



NRG: fixed points

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

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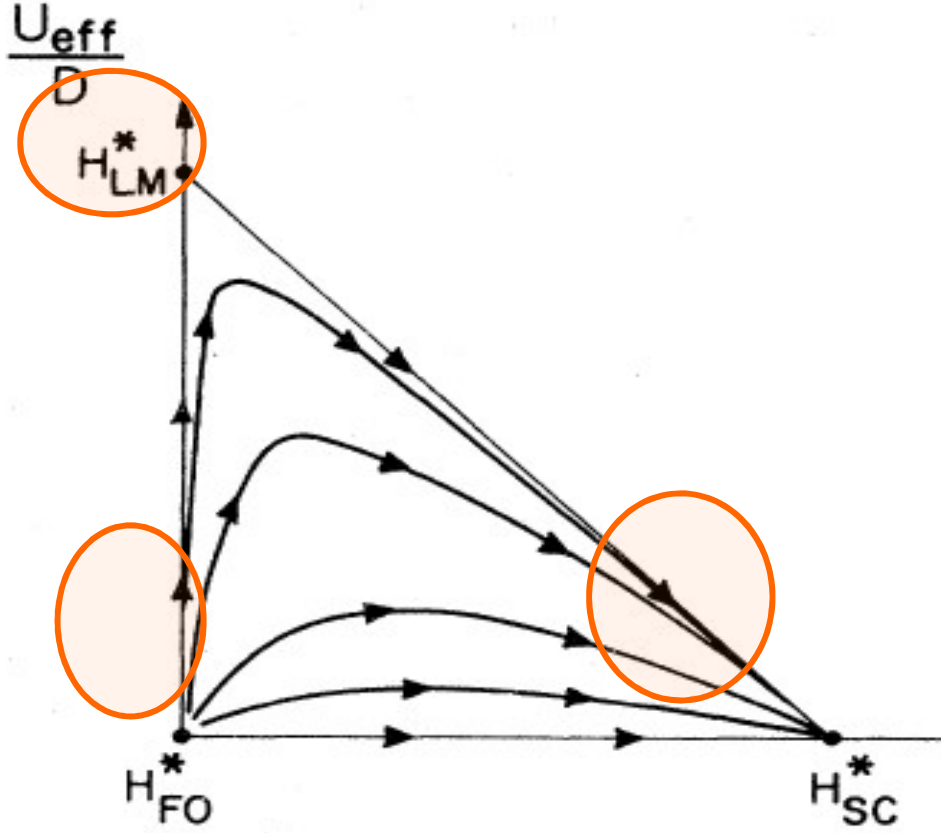
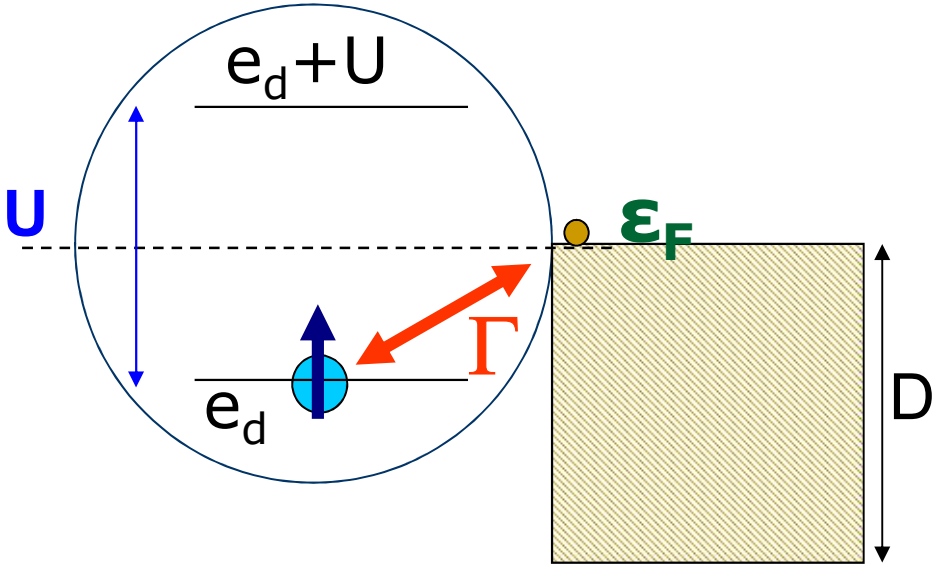


Fixed points

Fixed points of the Anderson Model

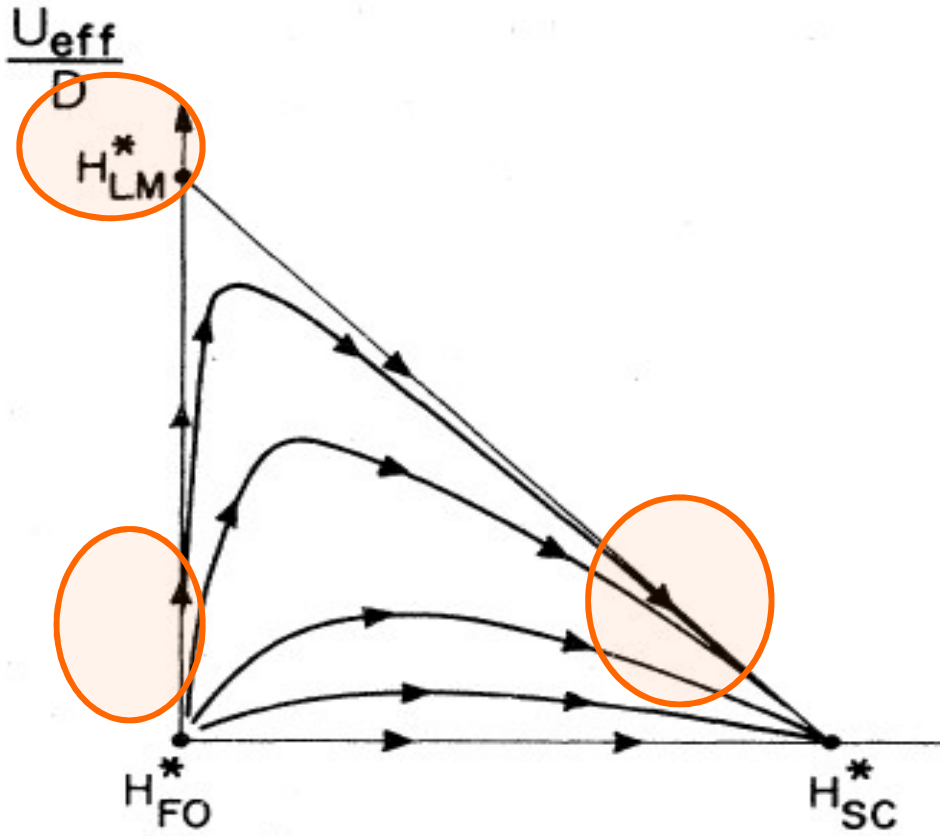


Level broadening:

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

Strong interacting limit:

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



Fixed points

Spectral function

At each NRG step:

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

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

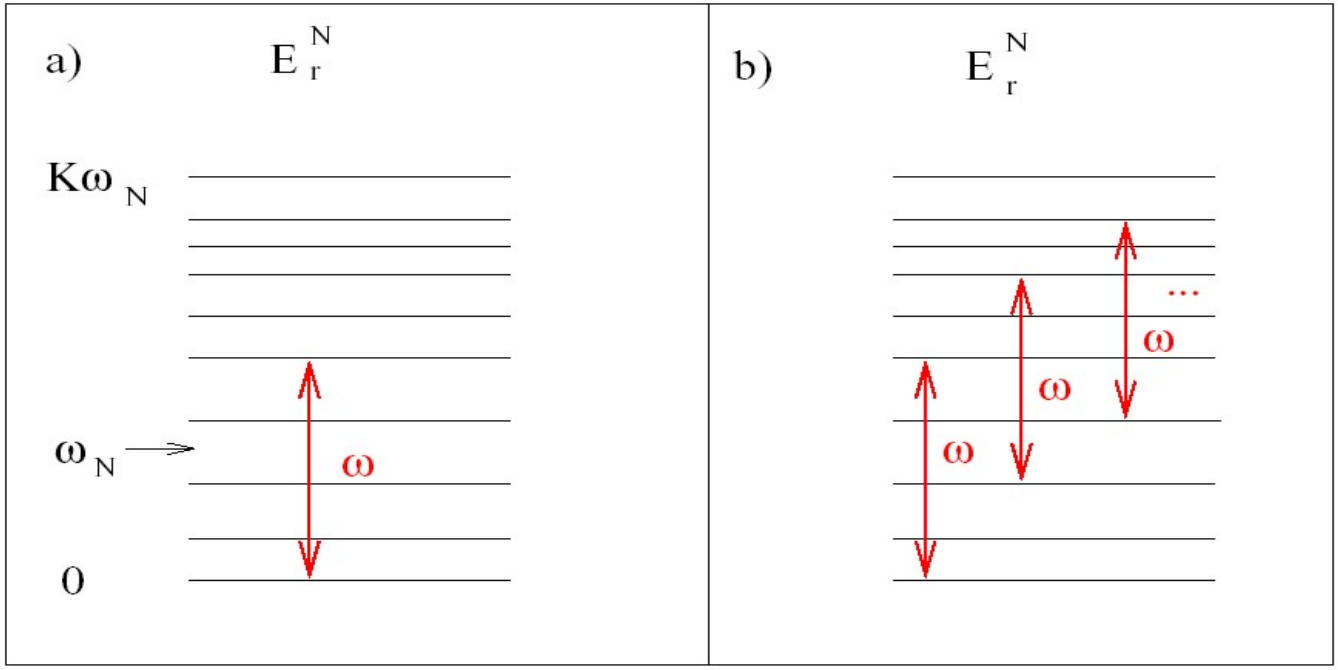


FIG. 9 Excitations of H_N contributing to the spectral function at frequency ω for, (a), $T = 0$, and, (b), $T > 0$.

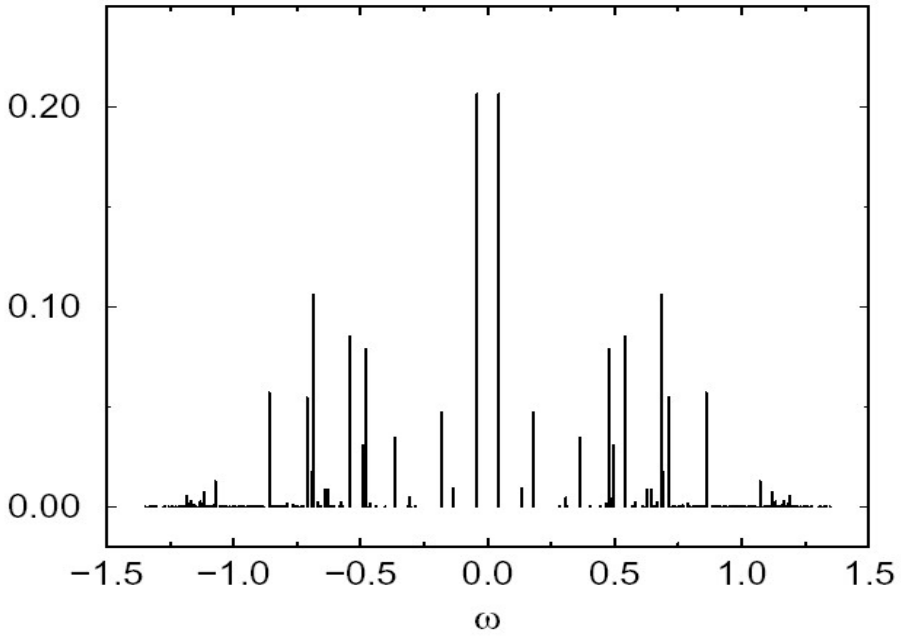
Spectral function calculation (Costi)

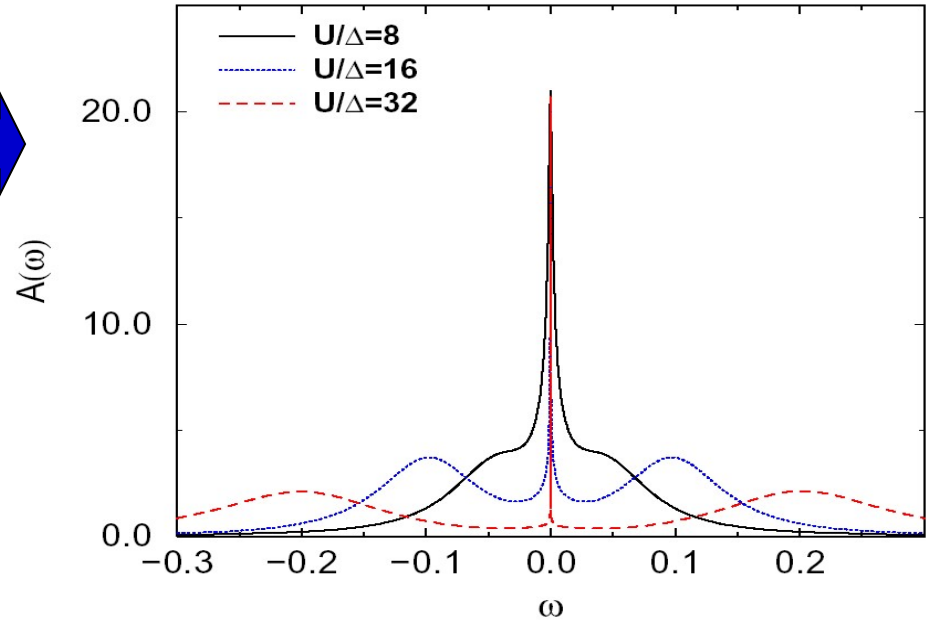
$$A_\sigma^N(\omega, T=0) = \frac{1}{Z_N(0)} \sum_r |M_{r,0}^N|^2 \delta(\omega + E_r^N)$$

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

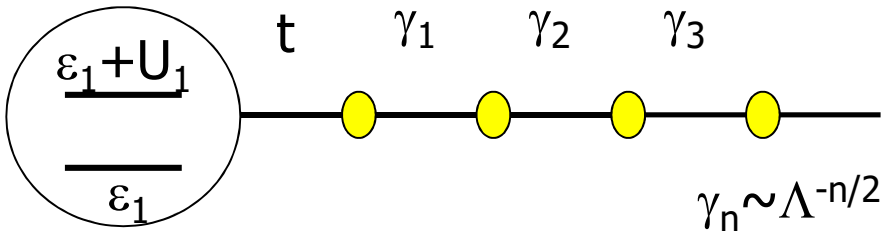
To get a continuos curve, need to broaden deltas.
Best choice: log gaussian

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

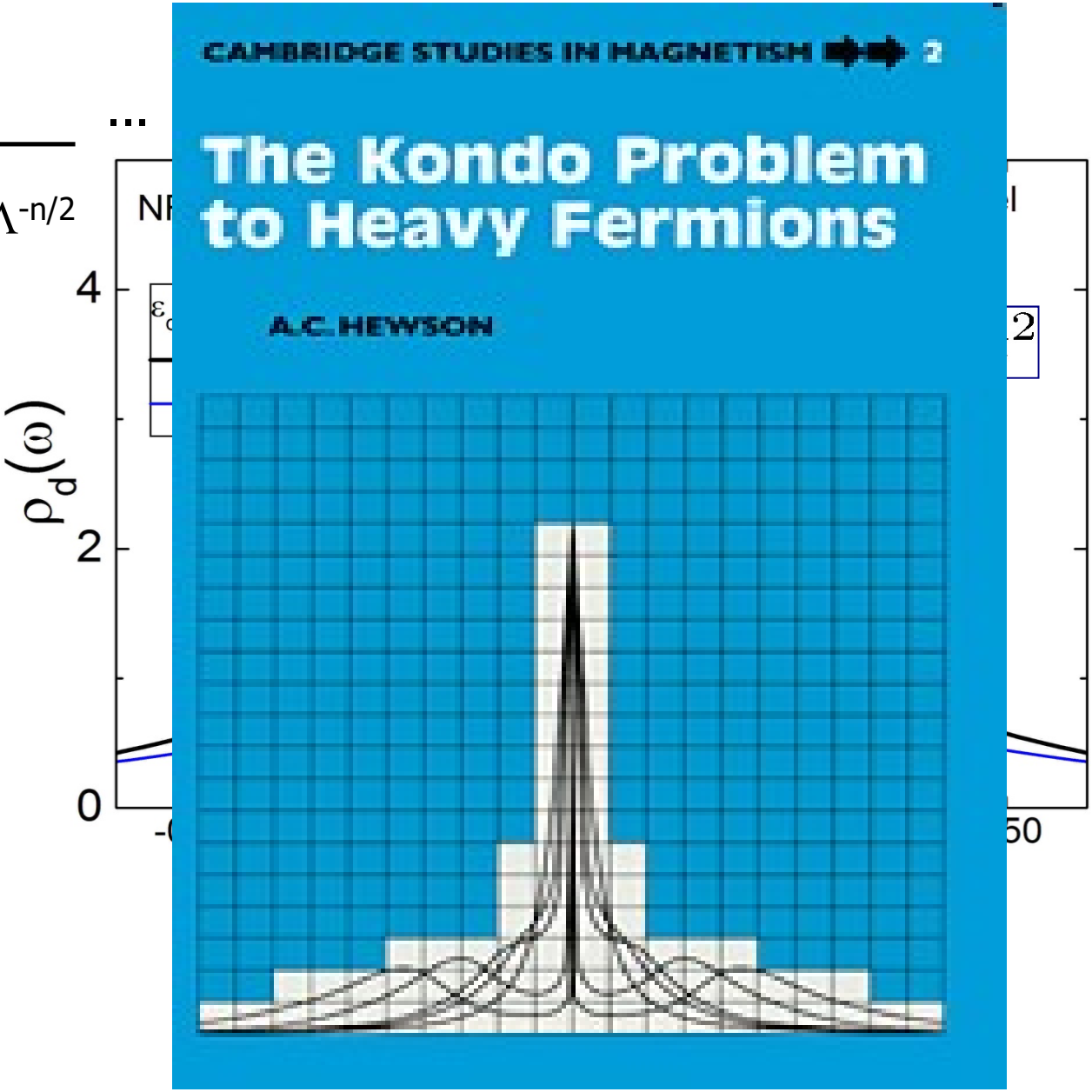




NRG on Anderson model: LDOS



- 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

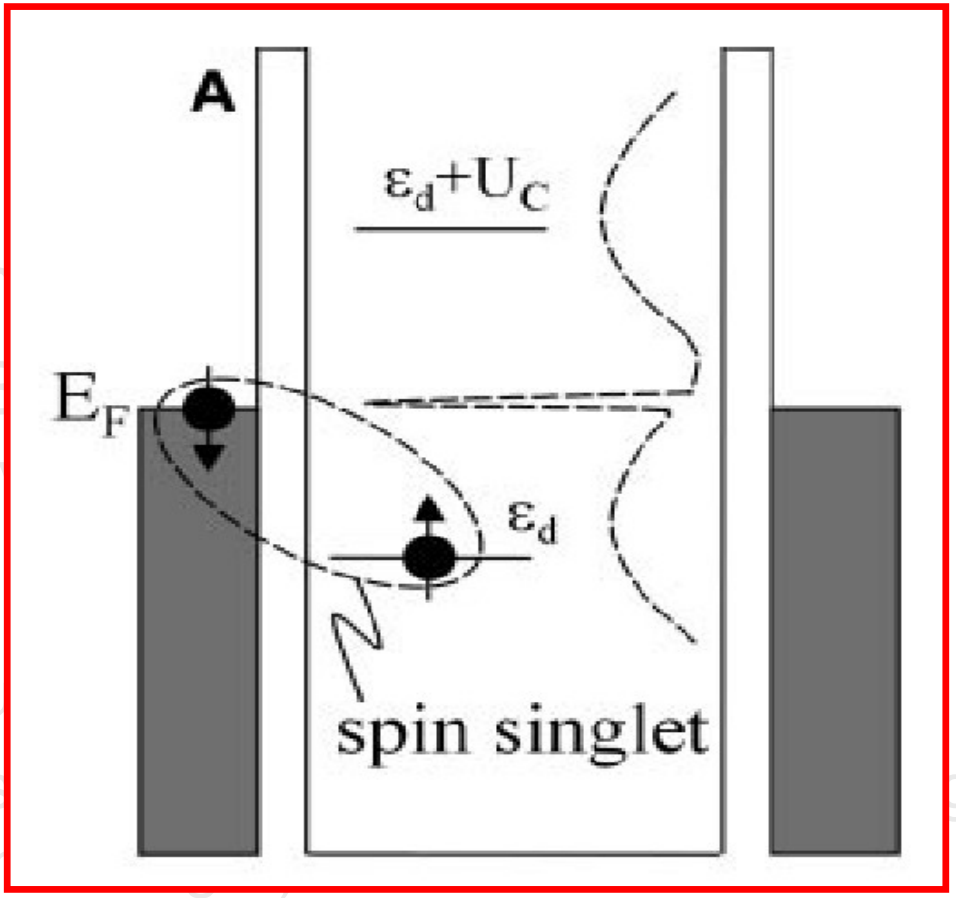
History of Kondo Phenomena

- Observed in the ‘30s
- Explained in the ‘60s
- Numerically Calculated in th
- Exactly solved in the ‘80s (E

So, what’s ne

Kondo correlations observed in m

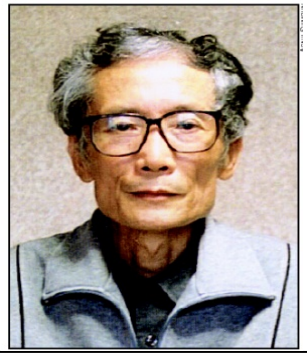
- Transport in quantum dots, quantu
- STM measurements of magnetic s g.,
  single atoms, molecules. “Quantur
- ...



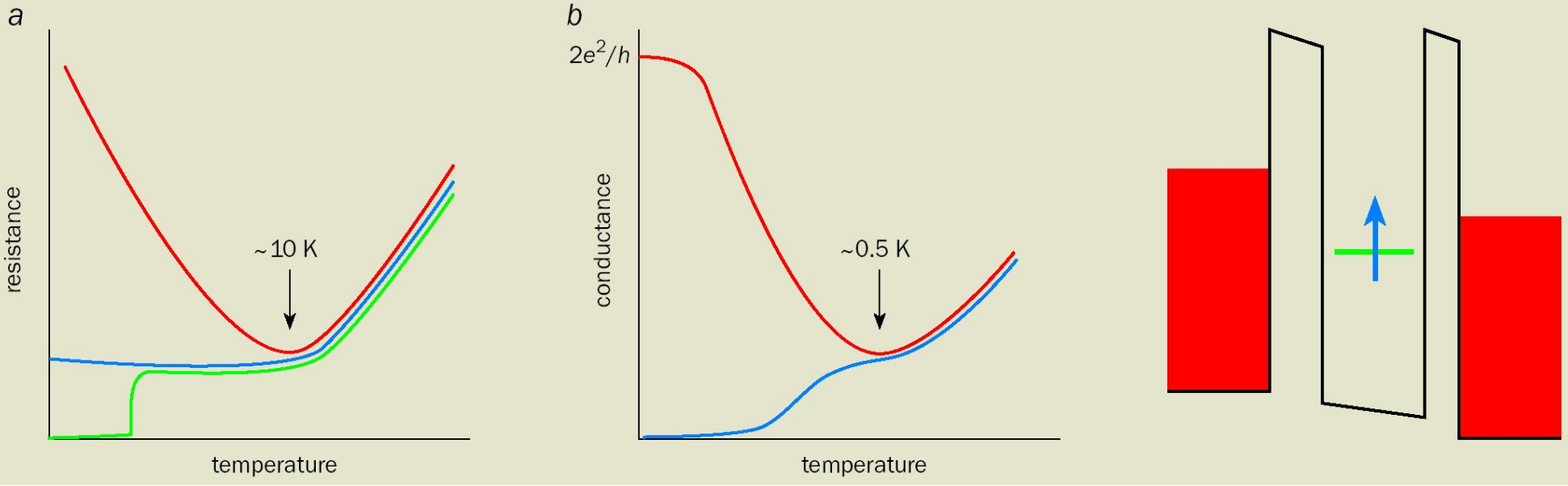
Kondo Effect in Quantum Dots

Revival of the Kondo effect

Leo Kouwenhoven and Leonid Glazman

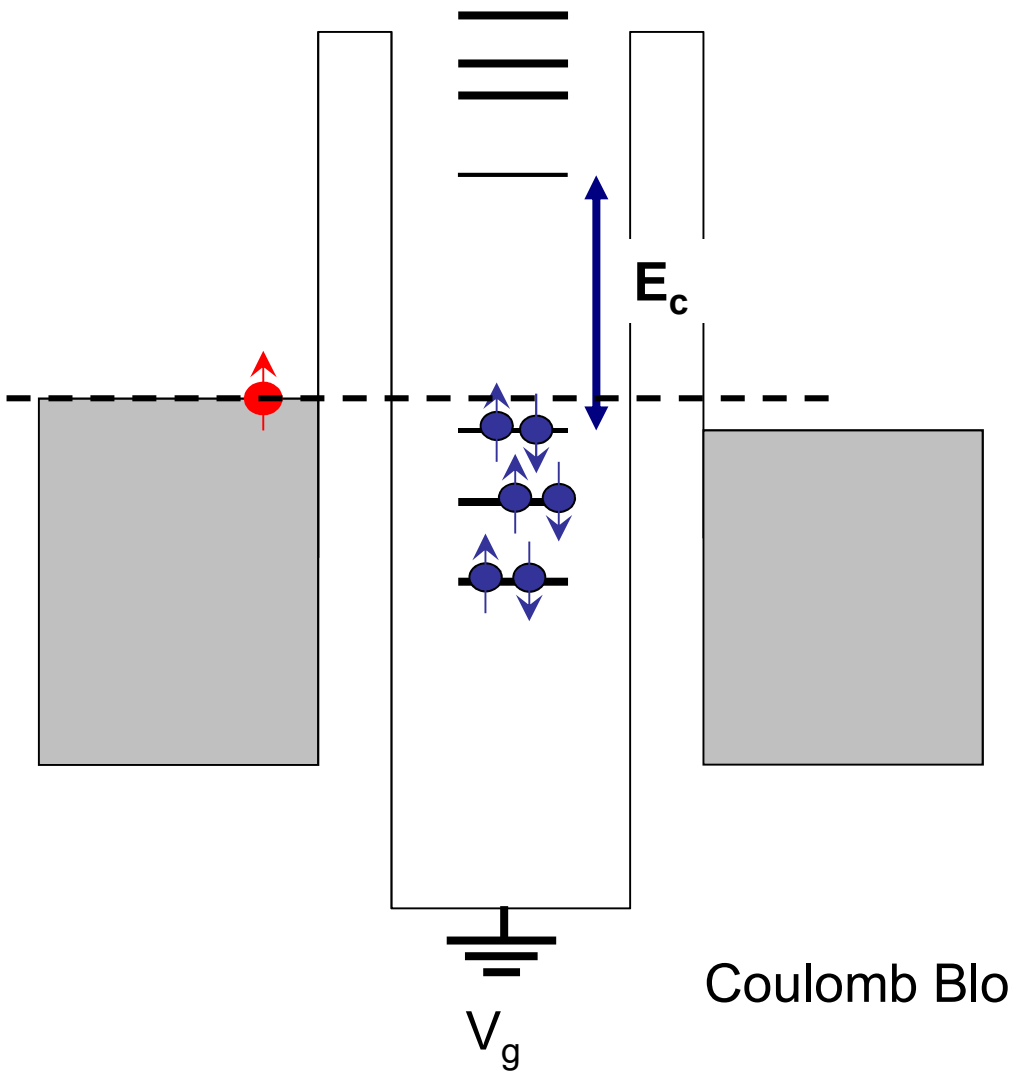


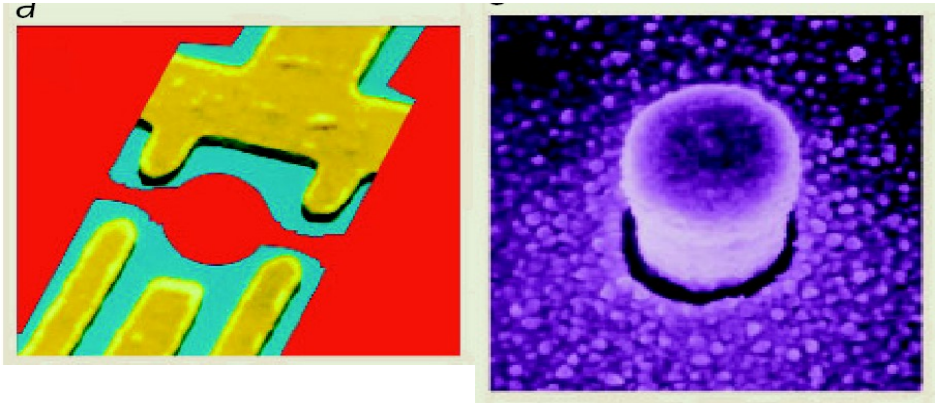
1 The Kondo effect in metals and in quantum dots

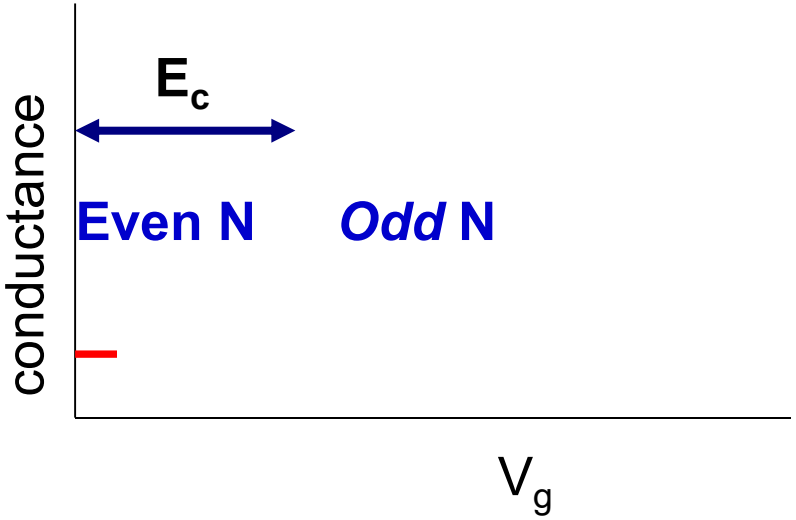


Kowenhoven and Glazman *Physics World* – Jan. 2001.

Coulomb Blockade in Quantum Dots

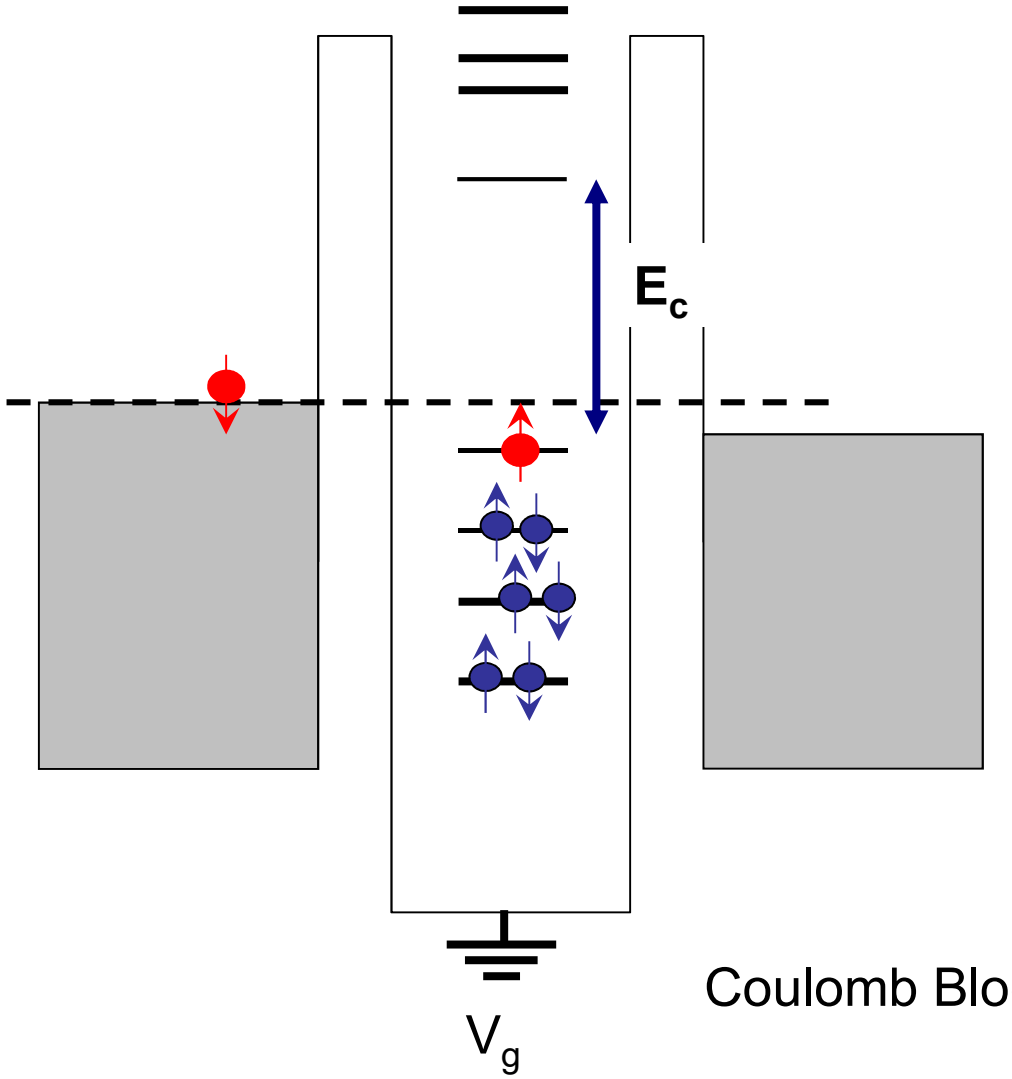


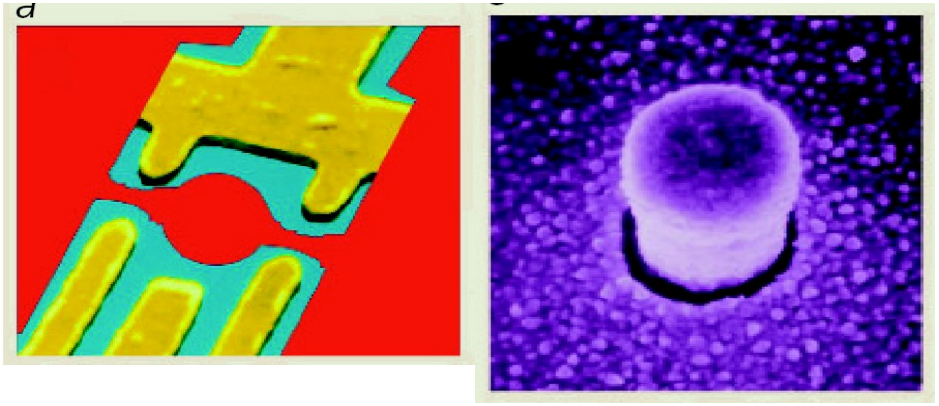


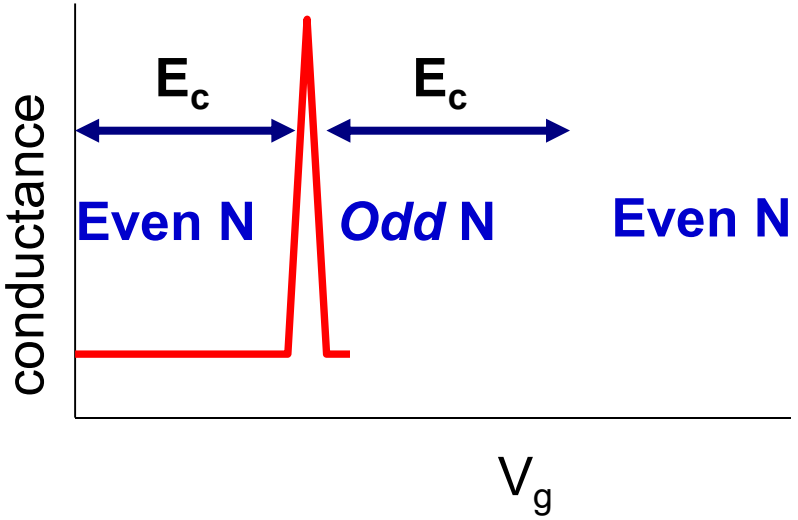


Coulomb Blockade in Quantum Dots

Coulomb Blockade in Quantum Dots



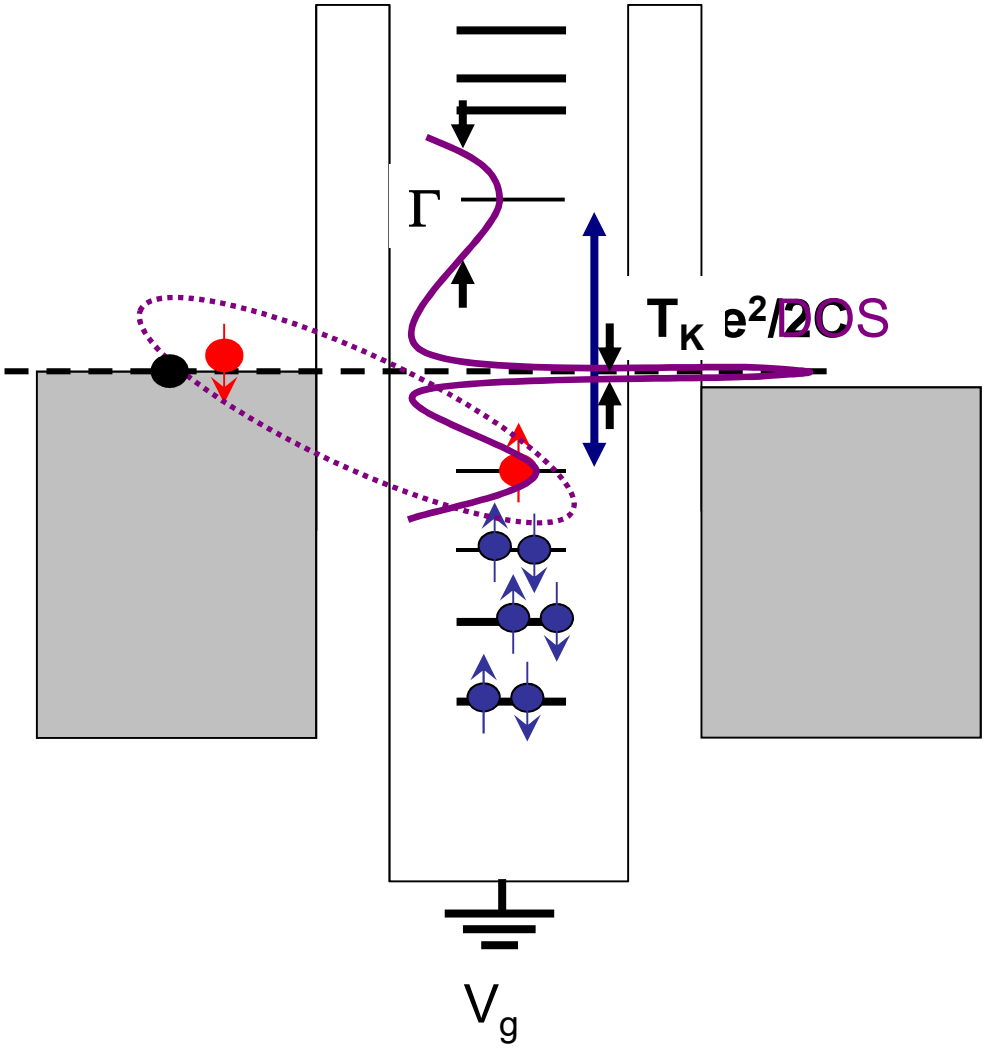


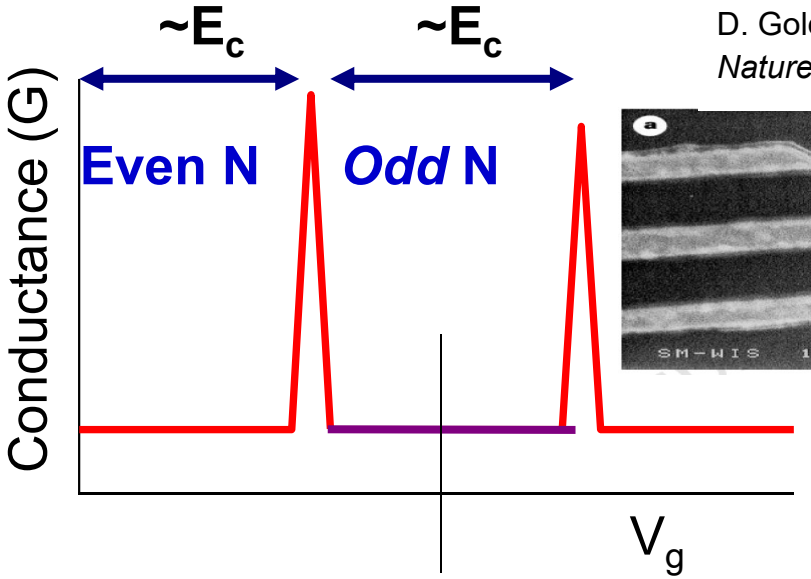


Coulomb Blockade in Quantum Dots

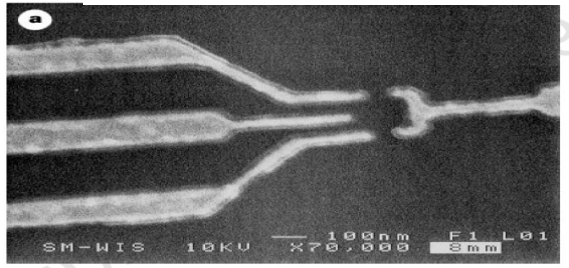
Y. Alhassid *Rev. Mod. Phys.* **72** 895 (2000).

Kondo Effect in Quantum Dots





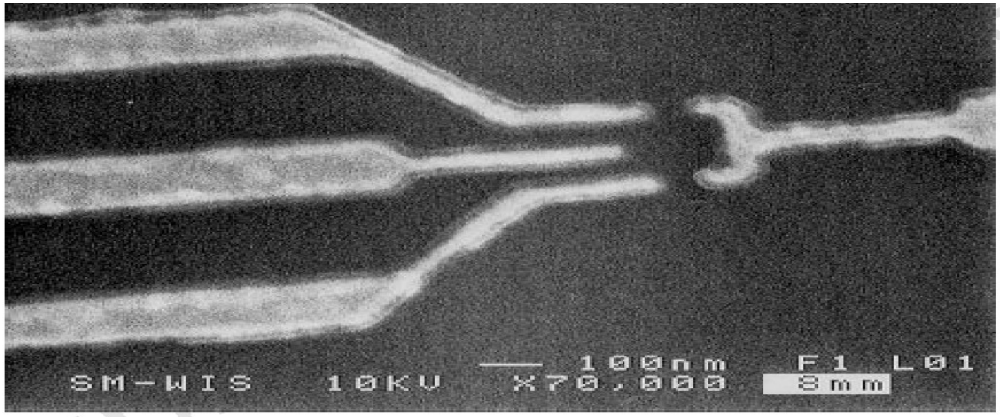
D. Goldhaber-Gordon et al
Nature **391** 156 (1998)

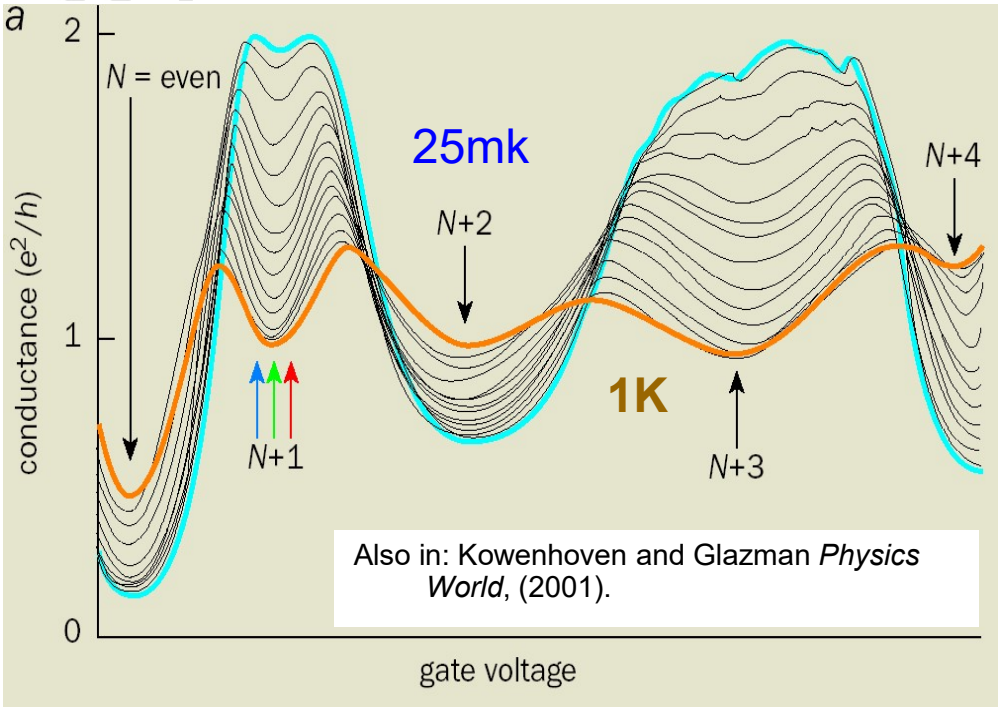


- $T>T_K$: Coulomb blockade (low G)
- $T<T_K$: Kondo singlet formation
- Kondo resonance at E_F (width T_K).
- New conduction channel at E_F:
  Zero-bias enhancement of G

Kondo effect in Quantum Dots

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

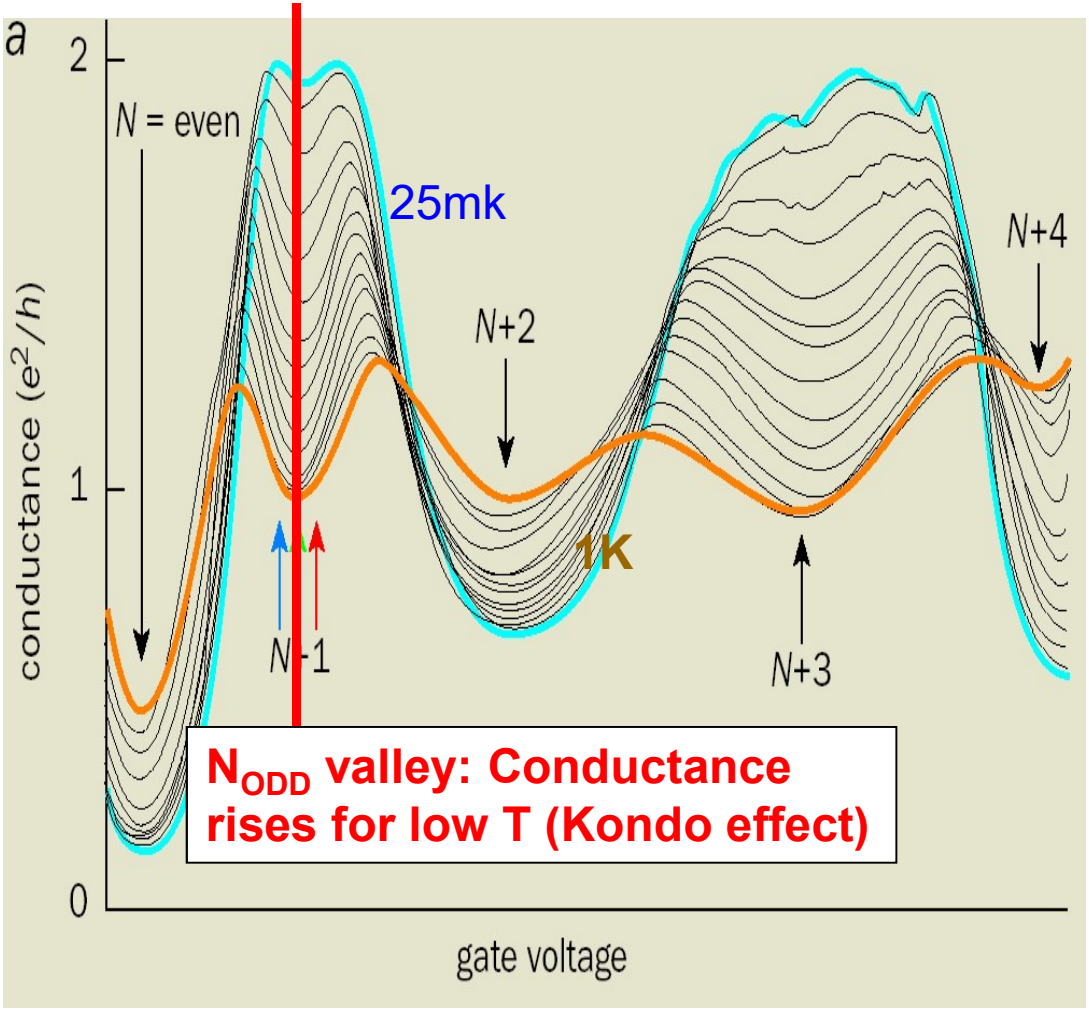


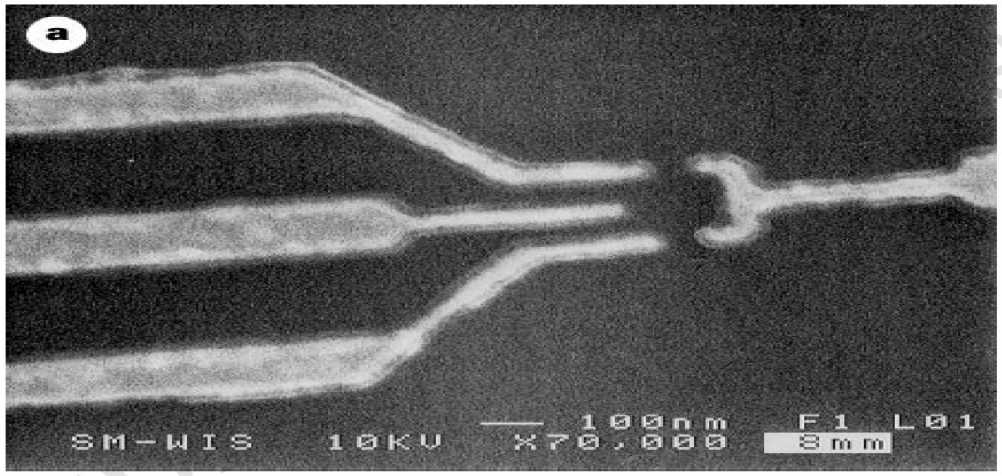


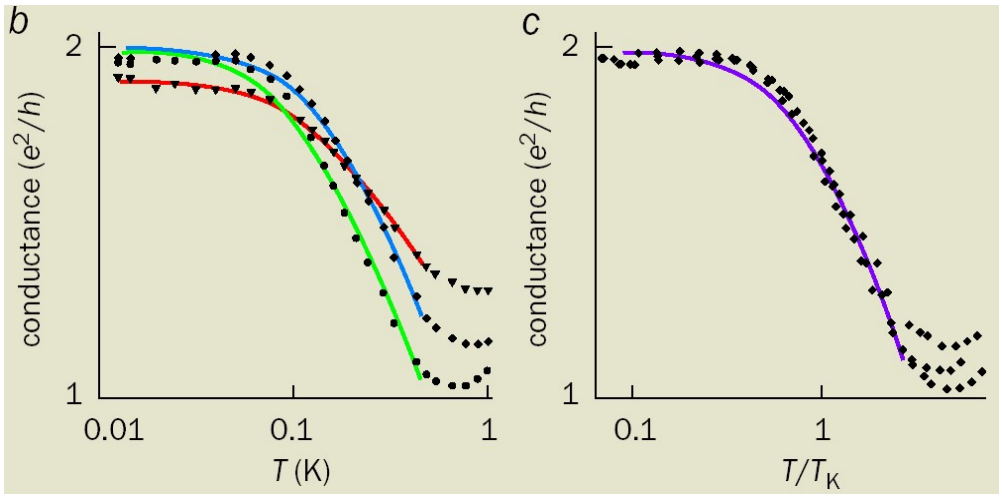
Semiconductor Quantum Dots:

- Allow for systematic and *controllable* investigations of the Kondo effect.
- QD in N_{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 (~0.5K, depends on V_g)

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

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

That’s it!