PG5295 – Muitos Corpos

1 – Electronic Transport in Quantum dots

2 – Kondo effect: Intro/theory.

3 – Kondo effect in nanostructures

Prof. Luis Gregório Dias – DFMT

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1 – Electronic Transport in Quantum dots

➡ 2 – Kondo effect: Intro/theory.

3 – Kondo effect in nanostructures

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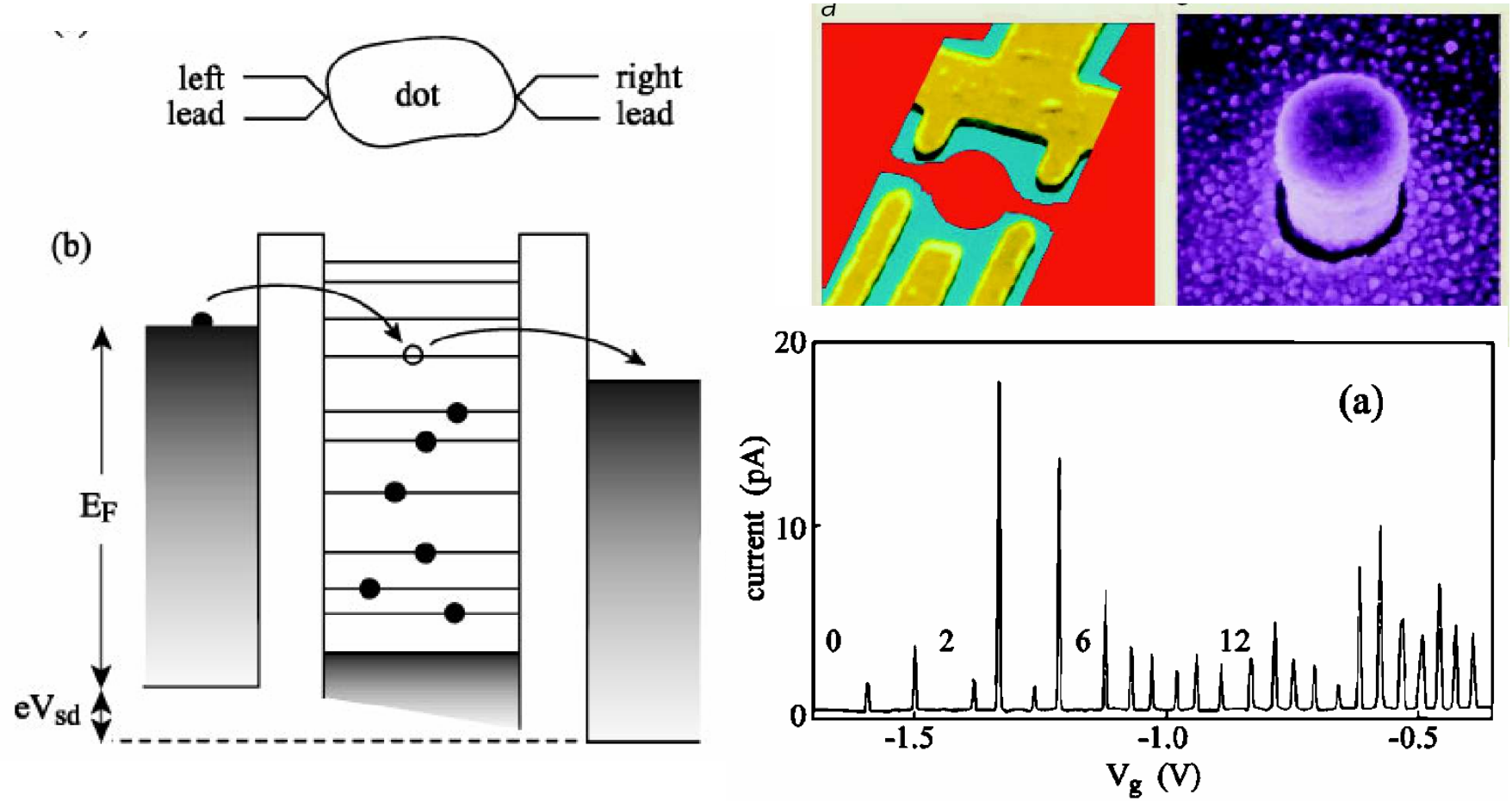
Basic references for today's lecture:

A.C. Hewson, *The Kondo Problem to Heavy Fermions*, Cambridge Press, 1993.
R. Bulla, T. Costi, Prushcke, *Rev. Mod. Phys* (in press) arXiv 0701105.
K.G. Wilson, *Rev. Mod. Phys.* **47** 773 (1975).

Lecture 2: Outline

- Kondo effect: Intro.
- Kondo's original idea: Perturbation theory.
- Numerical Renormalization Group (NRG).
- s-d and Anderson models.
- NRG results for the local density of states.

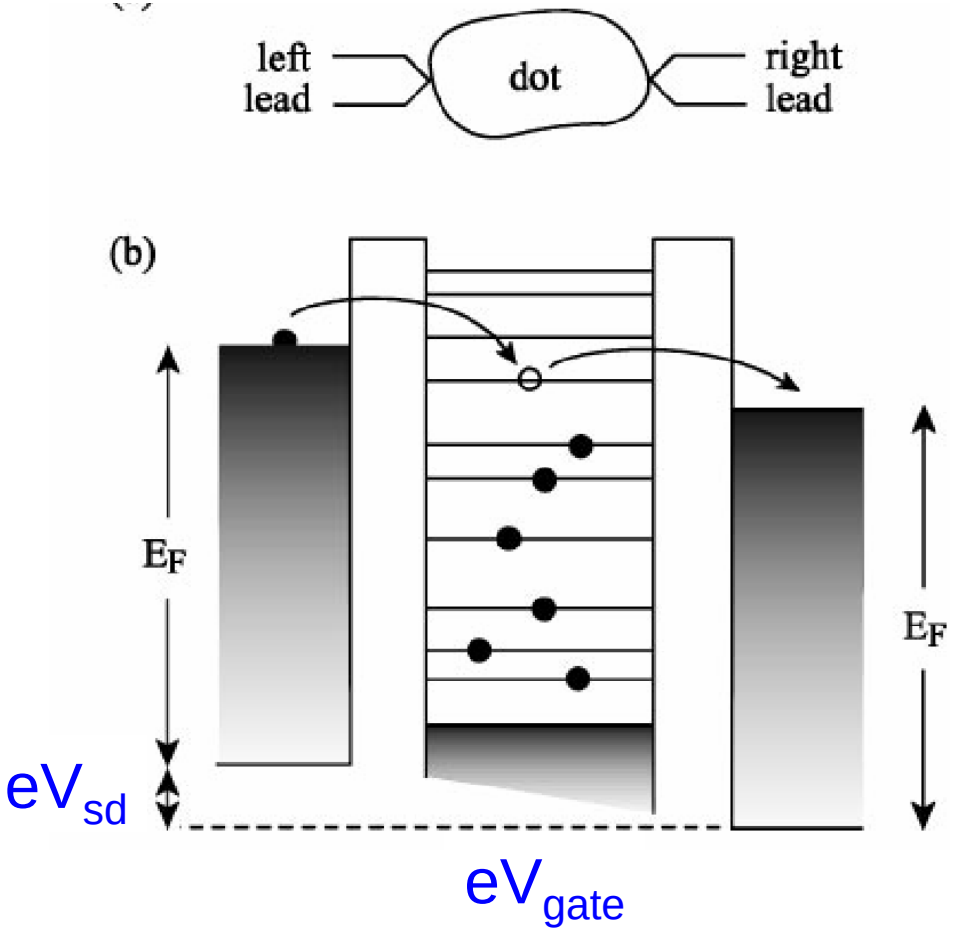
Coulomb Blockade in Quantum Dots



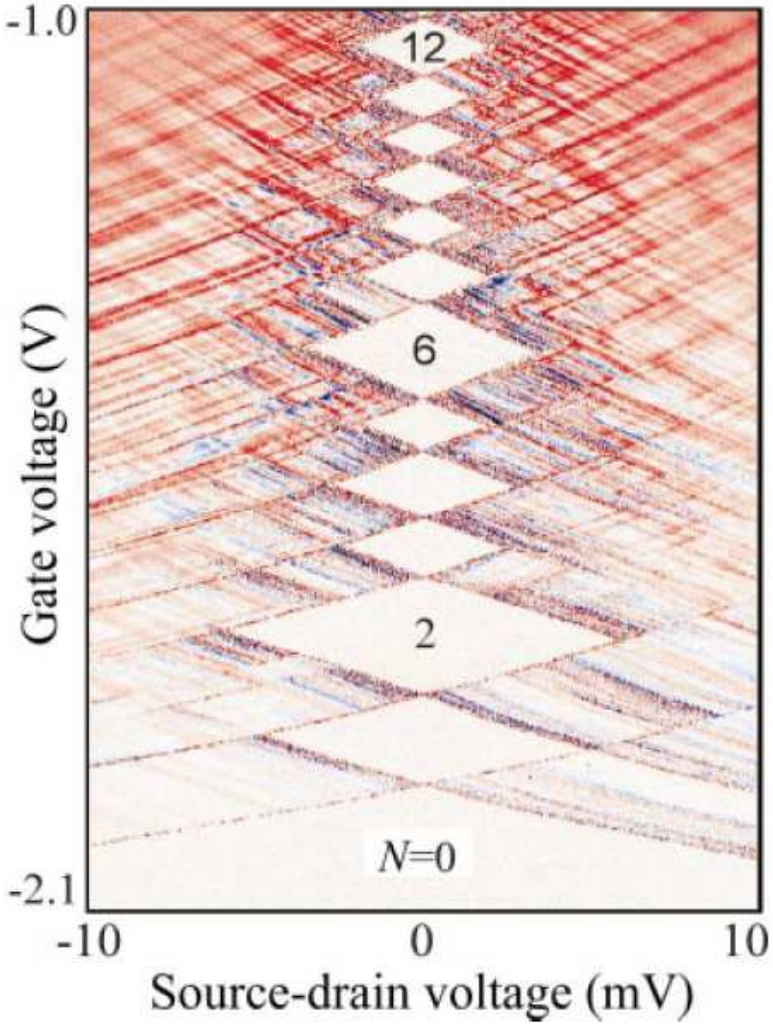
Coulomb Blockade in Quantum Dots: “dot spectroscopy”

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

“Coulomb Diamonds” (Stability Diagram)

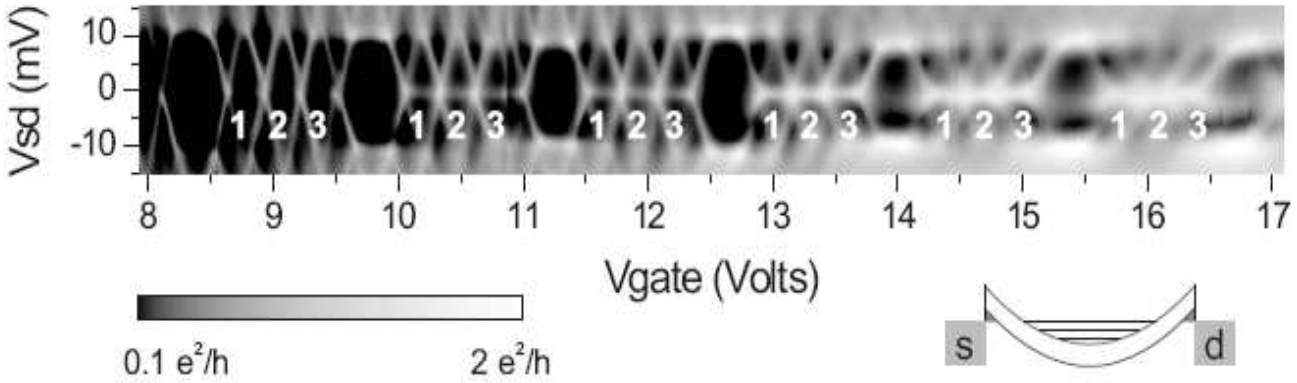


Coulomb Blockade in Quantum Dots



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

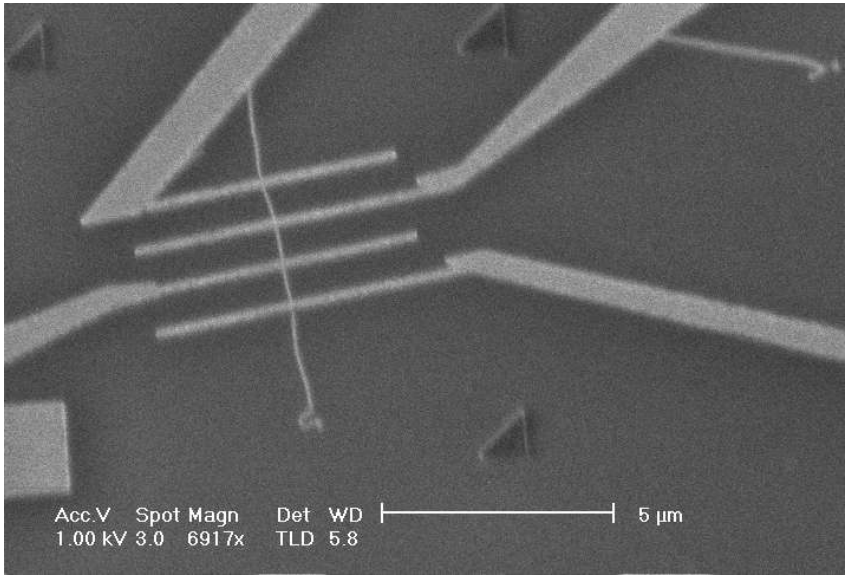
“Carbon nanotube Quantum dots”.



$$\Gamma_S \gg \Gamma_D$$

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

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



Gleb Filkenstein’s webpage: http://www.phy.duke.edu/~gleb/

Lecture 2 (coming up…)

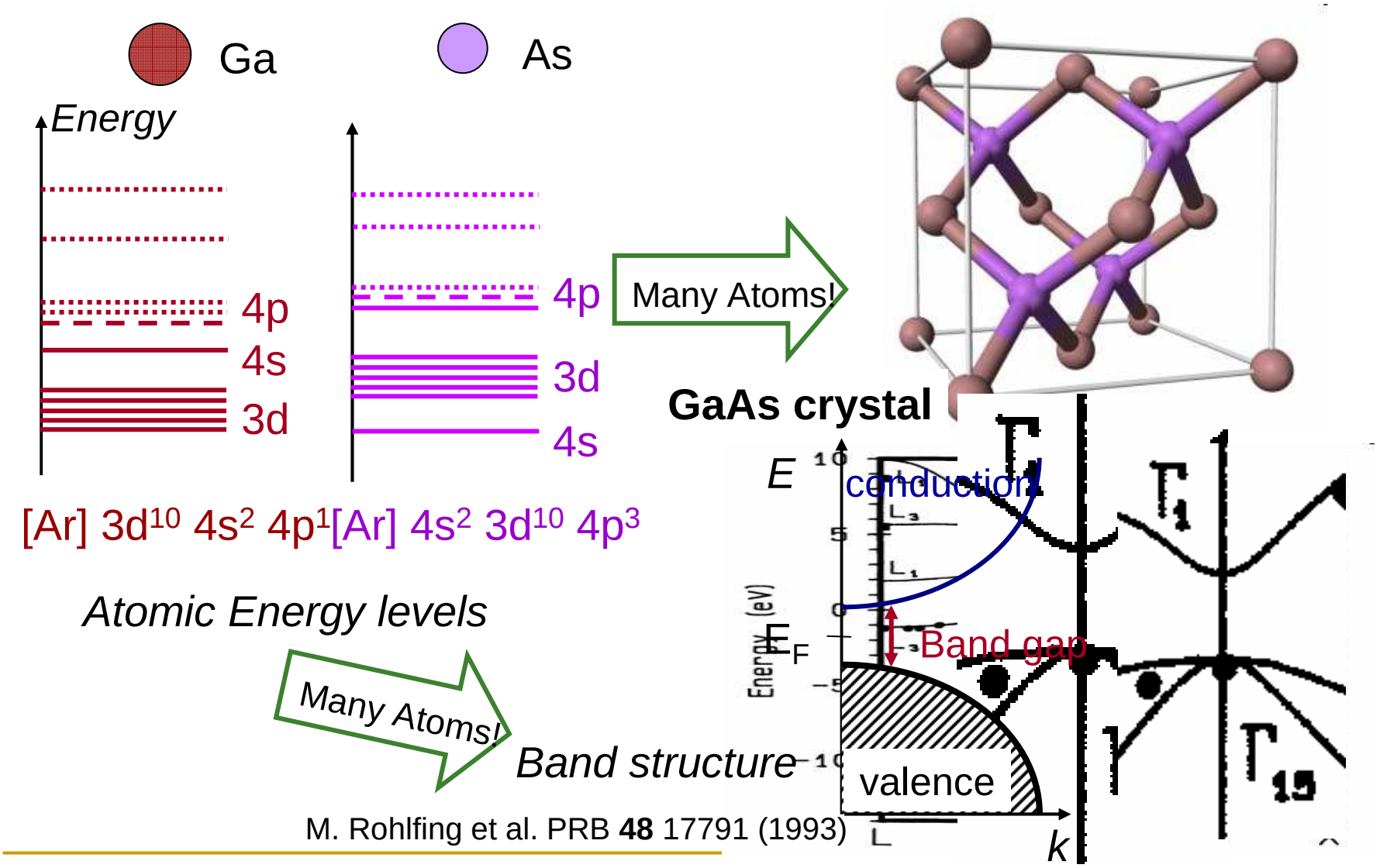
“More is Different”

“ 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.“

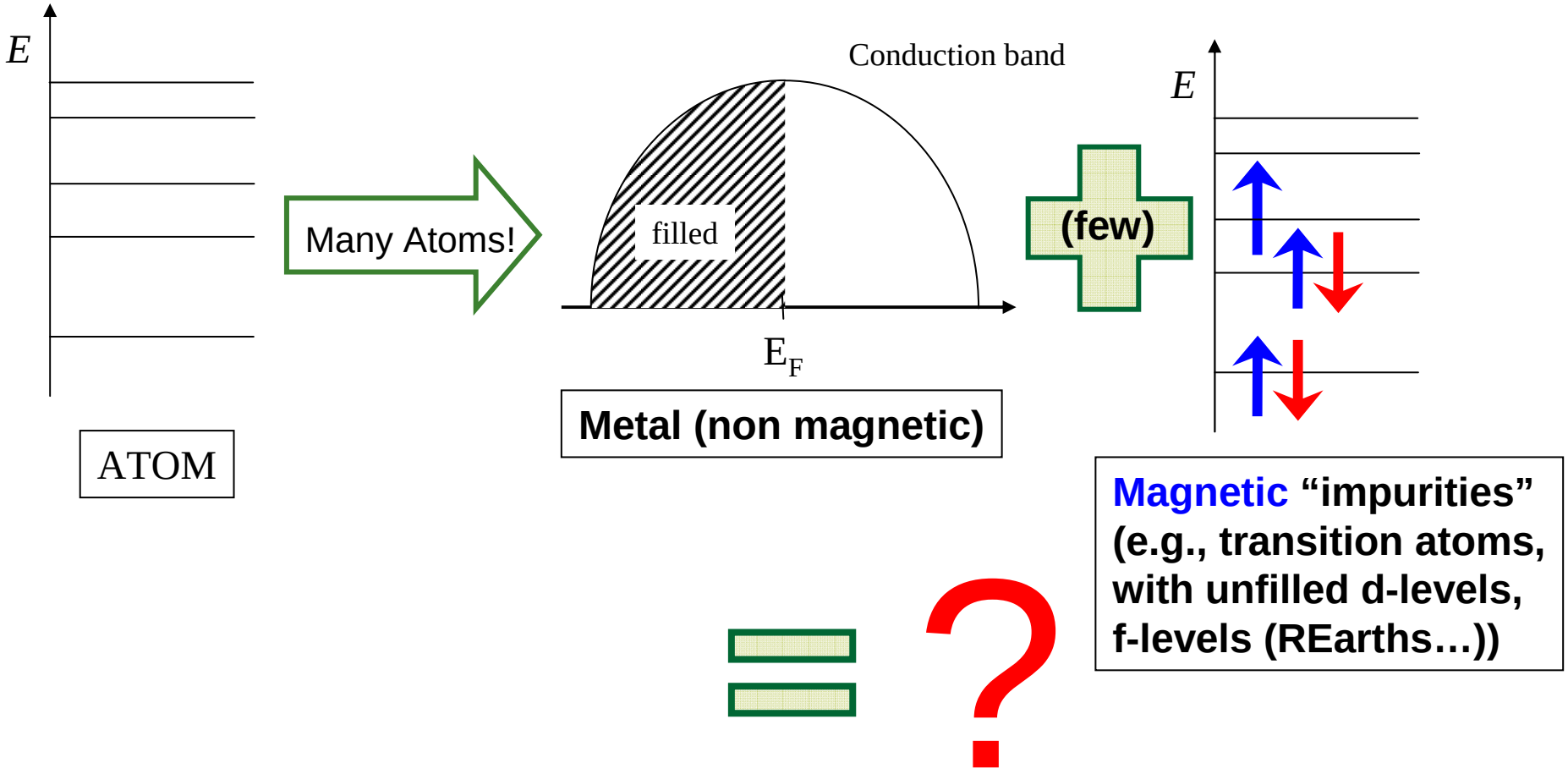
Phillip W. Anderson, “More is Different”, *Science* **177** 393 (1972)

Can you make “atoms” out of atoms?



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

From atoms to metals, plus atoms…

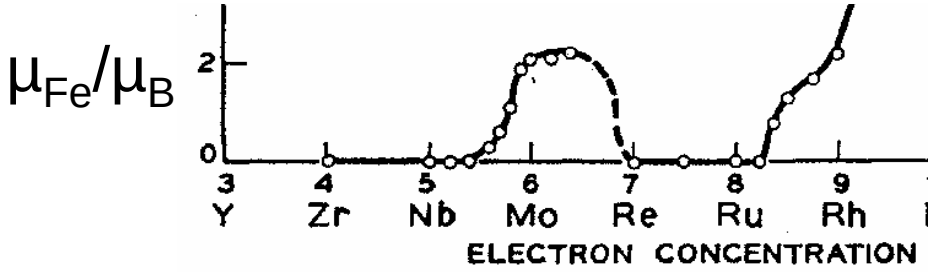


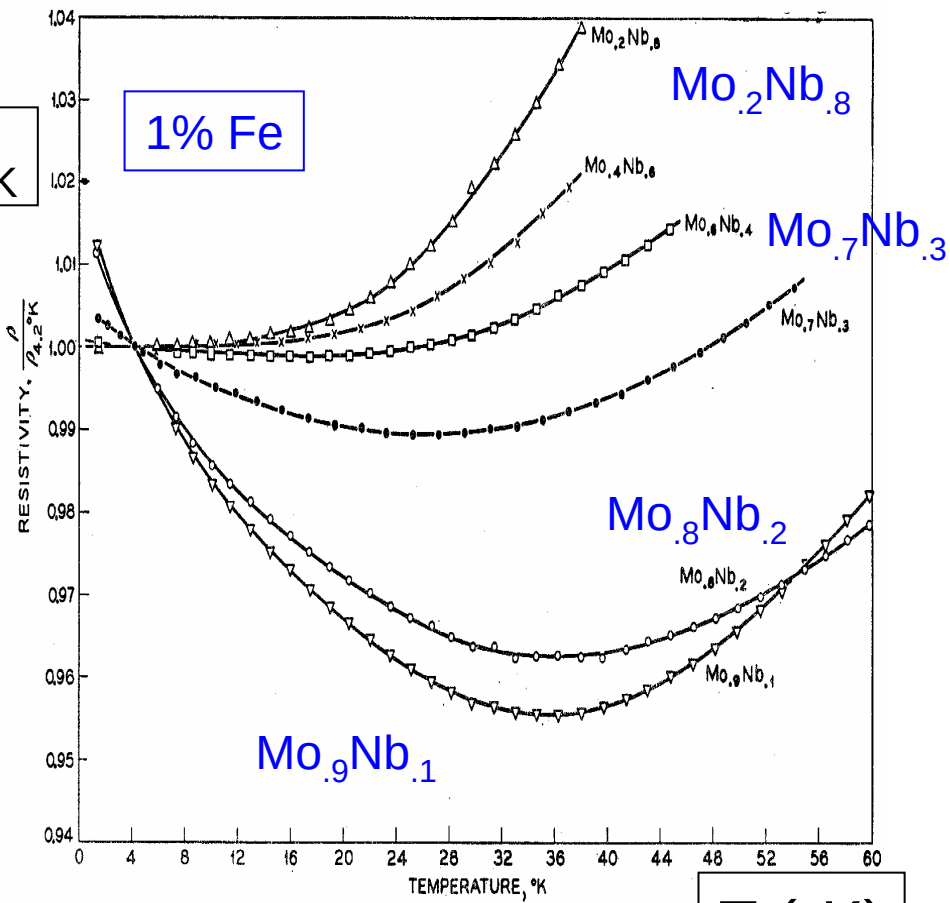
Is the resulting compound still a metal ?

Kondo effect

- Magnetic impurity in a metal.
  - 30's - Resisivity measurements: **minimum in ρ(T)**;

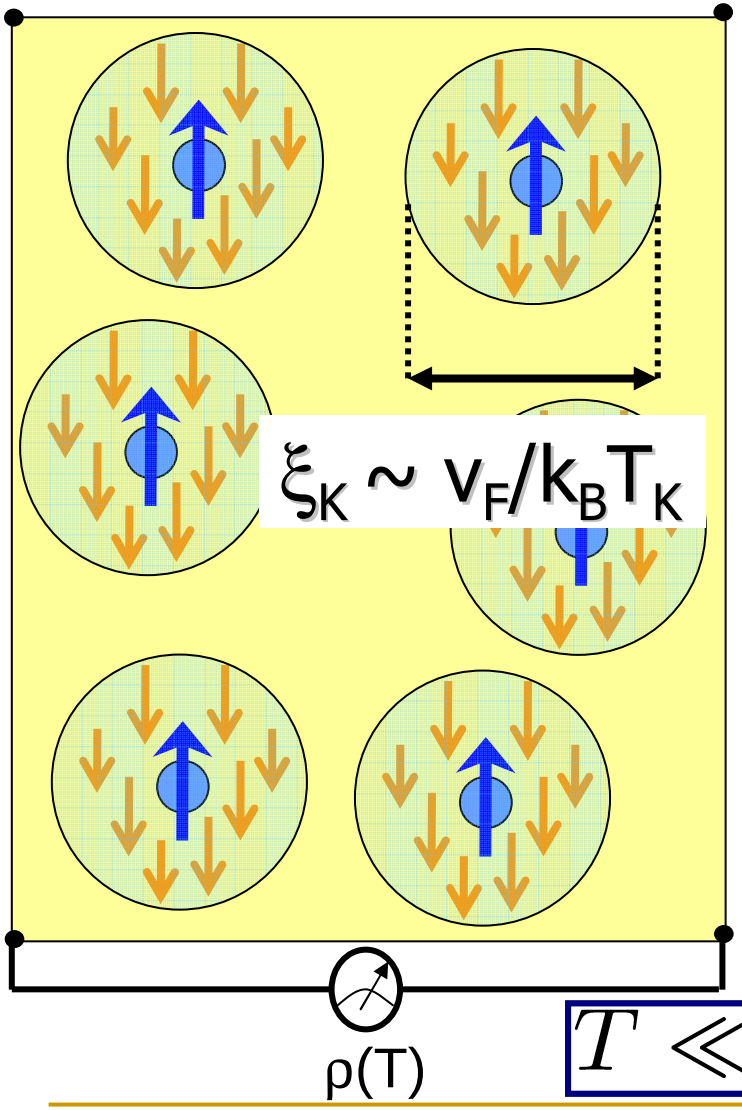
    T_{min} depends on $c_{imp.}$
  - 60's - Correlation between the existence of a Curie-Weiss component in the susceptibility (*magnetic moment*) and resistance minimum .





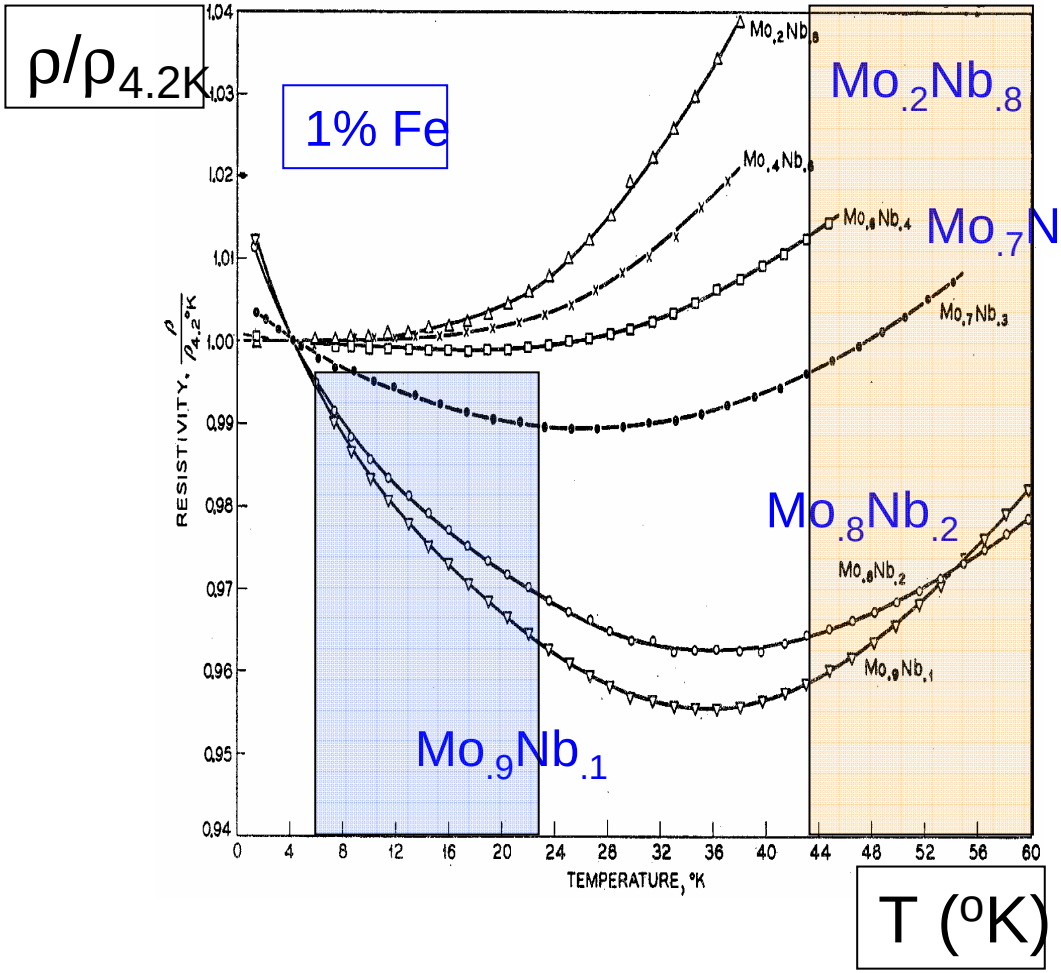
Top: A.M. Clogston *et al* Phys. Rev. **125** 541(1962).
Bottom: M.P. Sarachik *et al* Phys. Rev. **135** A1041 (1964).

Kondo effect



$T \ll T_K$

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



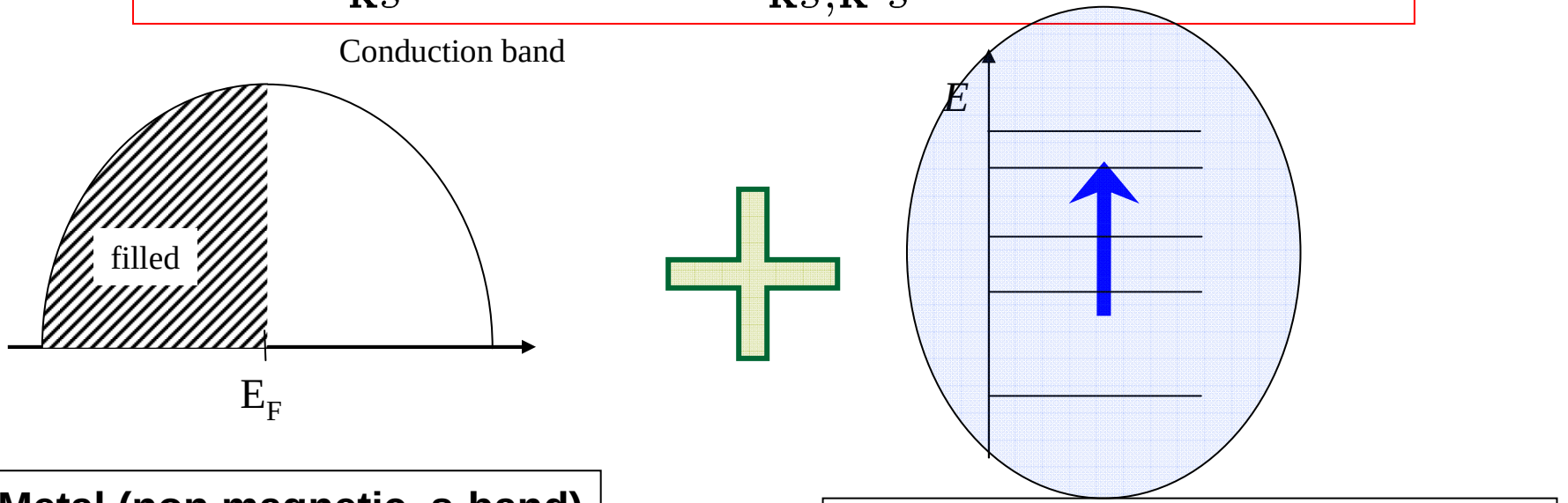
Resistivity increases with decreasing T (Kondo effect)

Resistivity saturates at low 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)

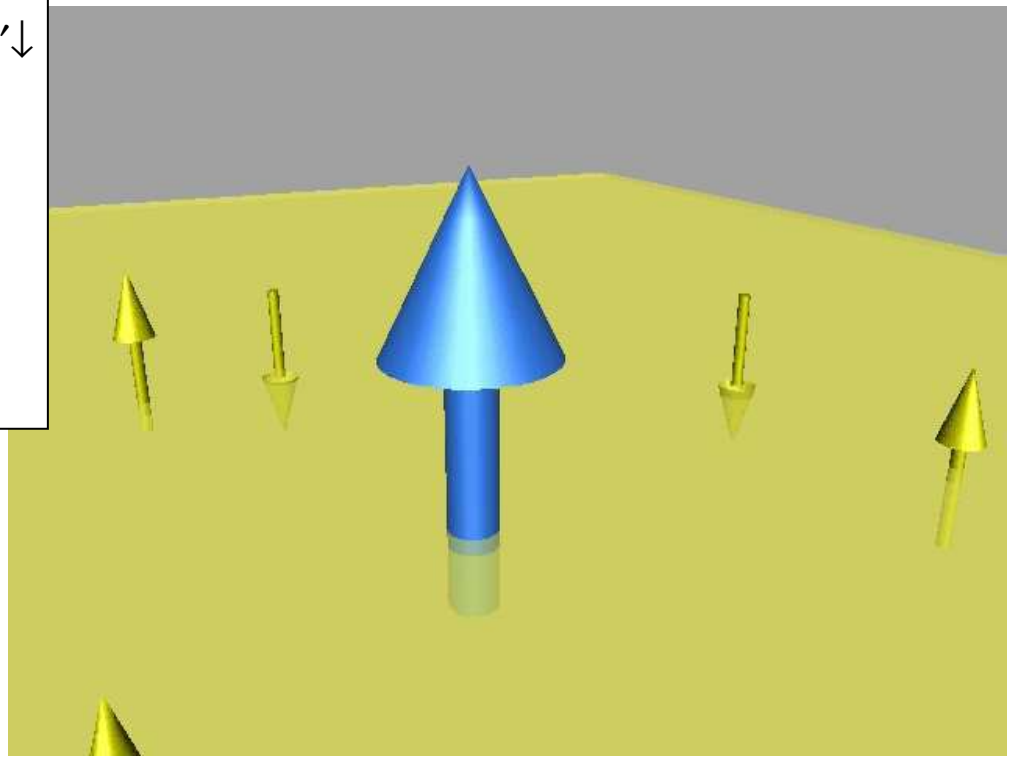
$$H_{\text{s-d}} = J\sum_{k,k'} S^{+}\, c^{\dagger}_{k\downarrow} c_{k'\uparrow} + S^{-}\, c^{\dagger}_{k\uparrow} c_{k'\downarrow}$$

Spin: J>0 AFM

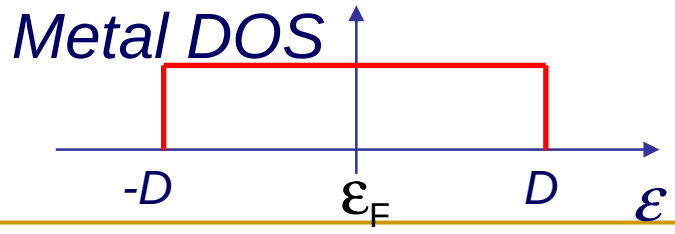
$$+ S_z \left(c^{\dagger}_{k\uparrow} c_{k'\uparrow} - c^{\dagger}_{k\downarrow} c_{k'\downarrow} \right)$$

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

Metal: Free waves



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

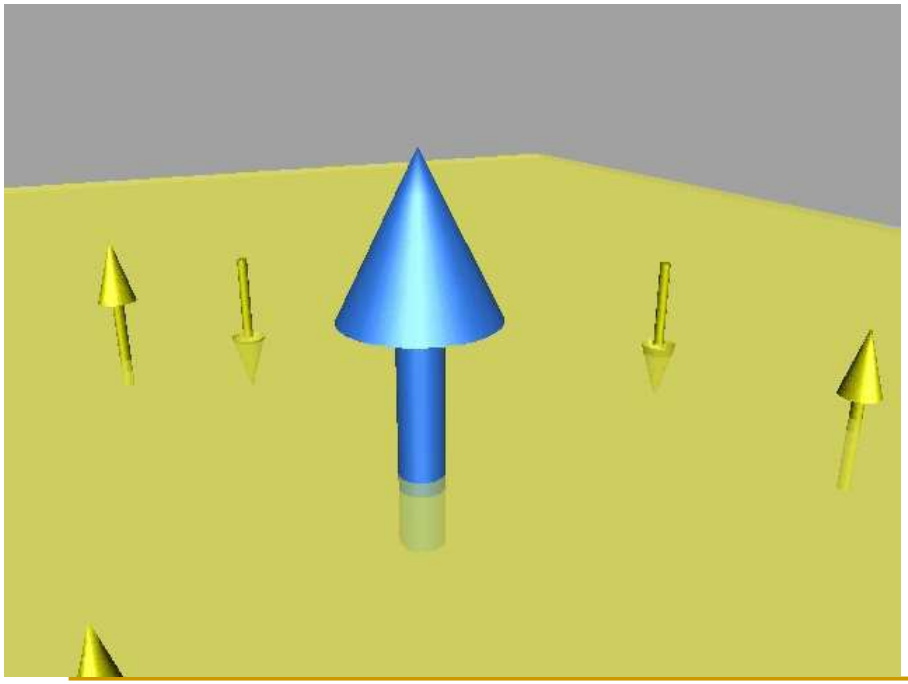


Kondo's explanation for T_{min} (1964)

- 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.***

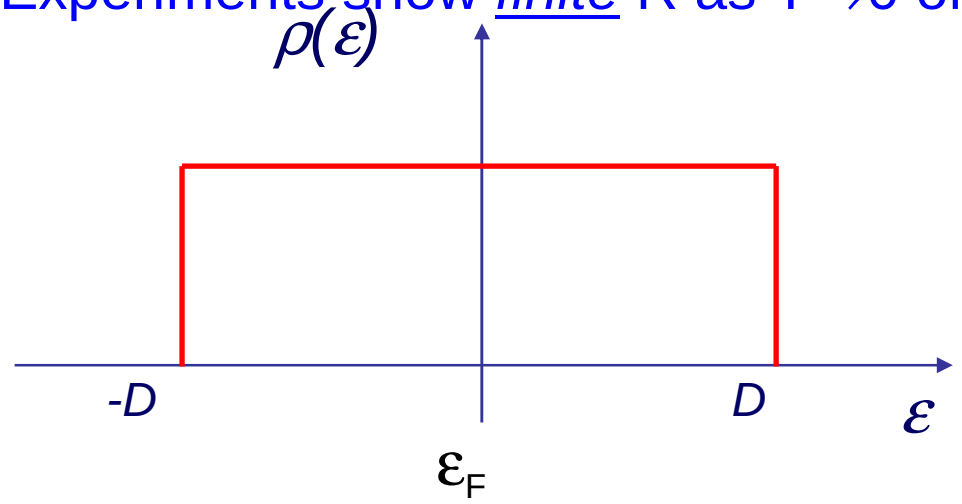
$$k_B T_K \sim D e^{-1/2 J \rho_0}$$

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

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

What is going on?

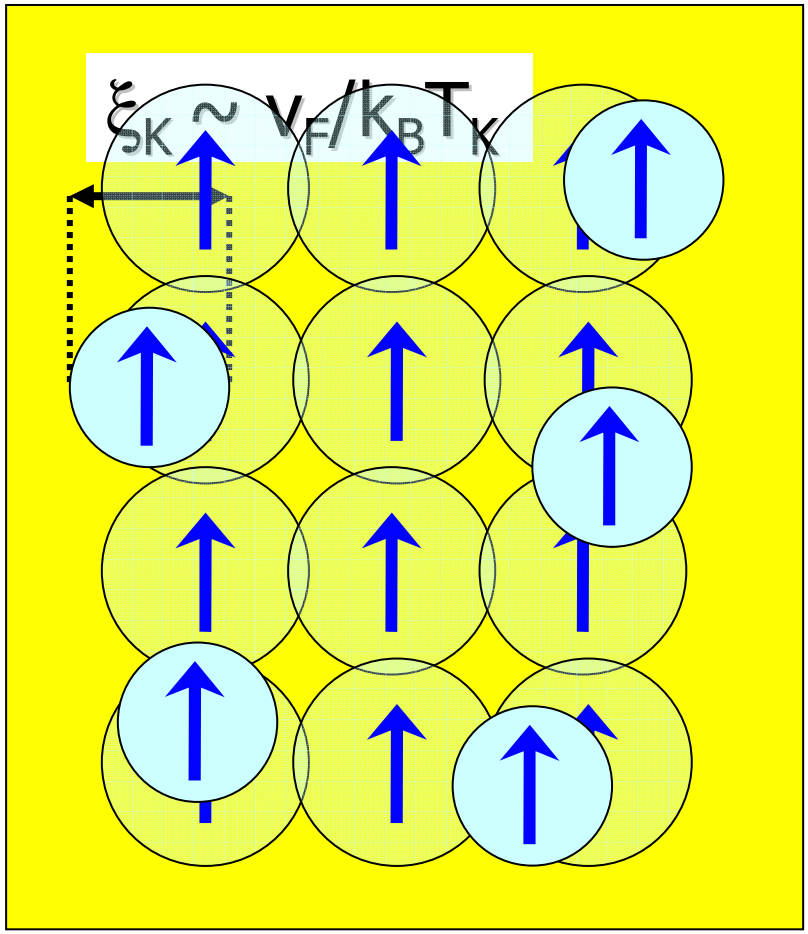
- Theory diverges *logarithmically* for T→0 or D→∞.
  (T<T_K → perturbation expasion no longer holds)
- Experiments show *finite* R as T→0 or D→∞.



Kondo Impurity and Lattice models

Diluted case (Kondo impurity model)

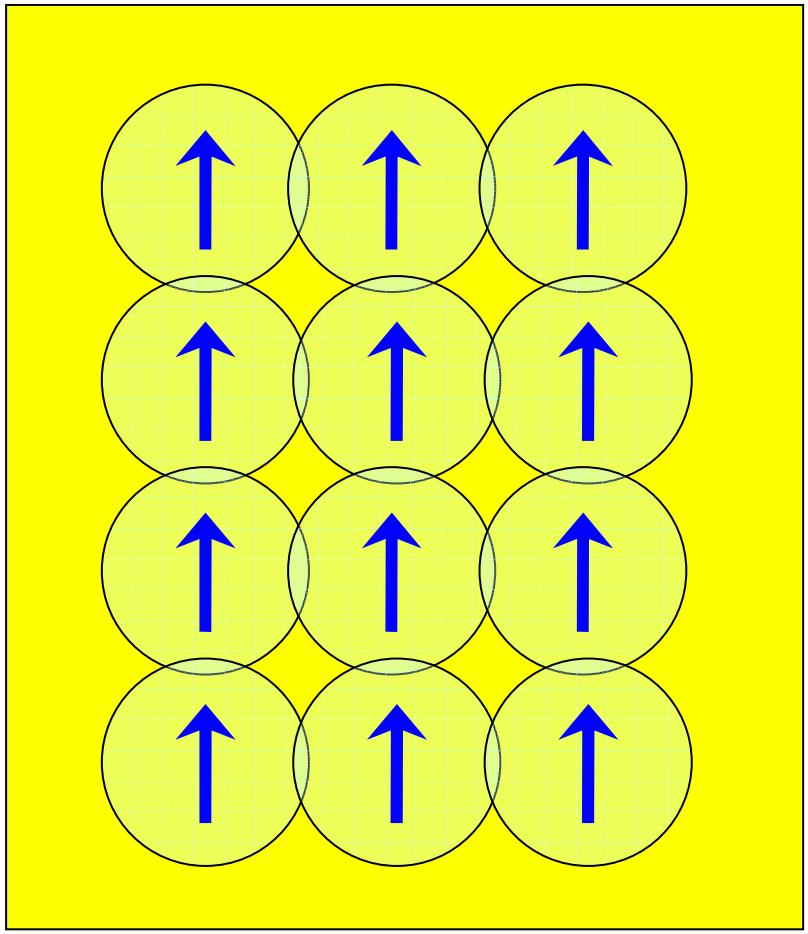
“Concentrated” case: Kondo Lattice (e.g., some heavy-Fermion materials)



- 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} ; etc).

Kondo Lattice models

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



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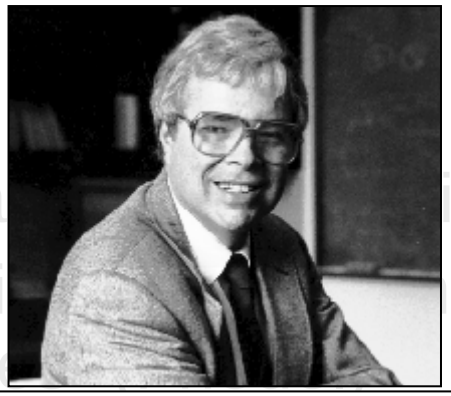
- This includes so called “heavy fermion” materials (e.g. Cerium and Uranium-based compounds $CeCu_2Si_2$, UBe_{13}).

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"

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

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

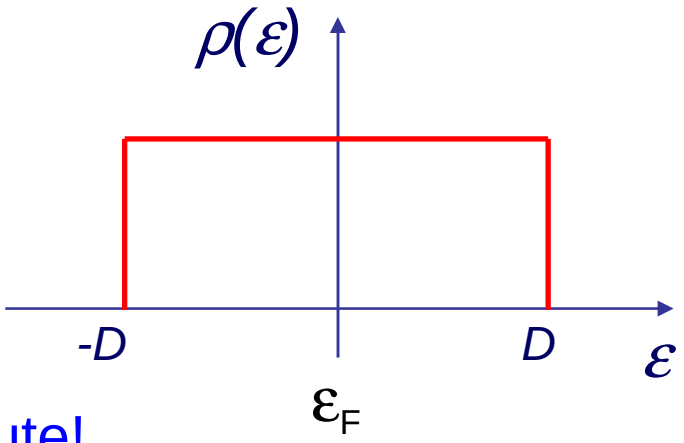
- Diverges *logarithmically* for $T \to 0$ or $D \to \infty$.

What is going on?

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

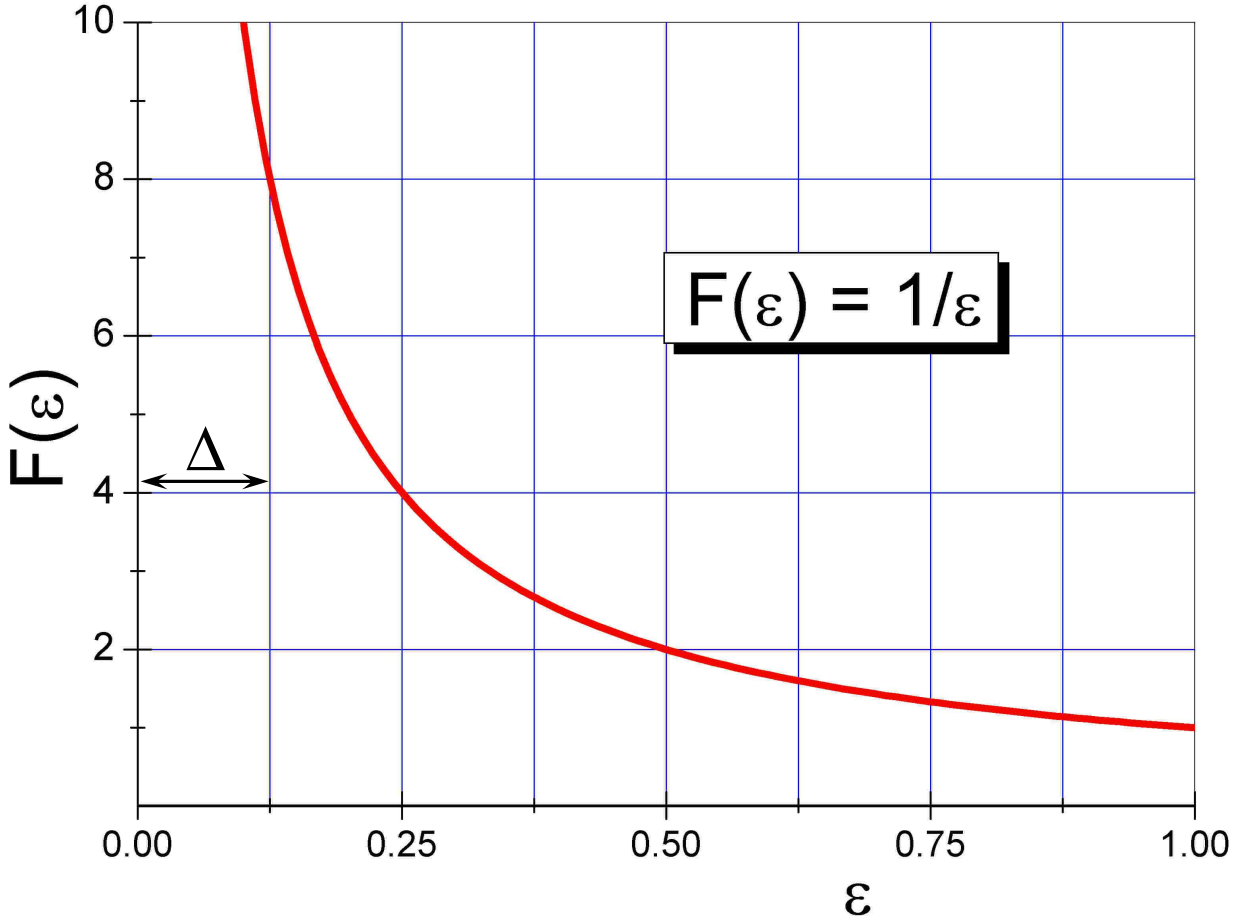
- Experiments show *finite* R as $T \to 0$ or $D \to \infty$.
- The log comes from something like:

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



- *All* energy scales contribute!

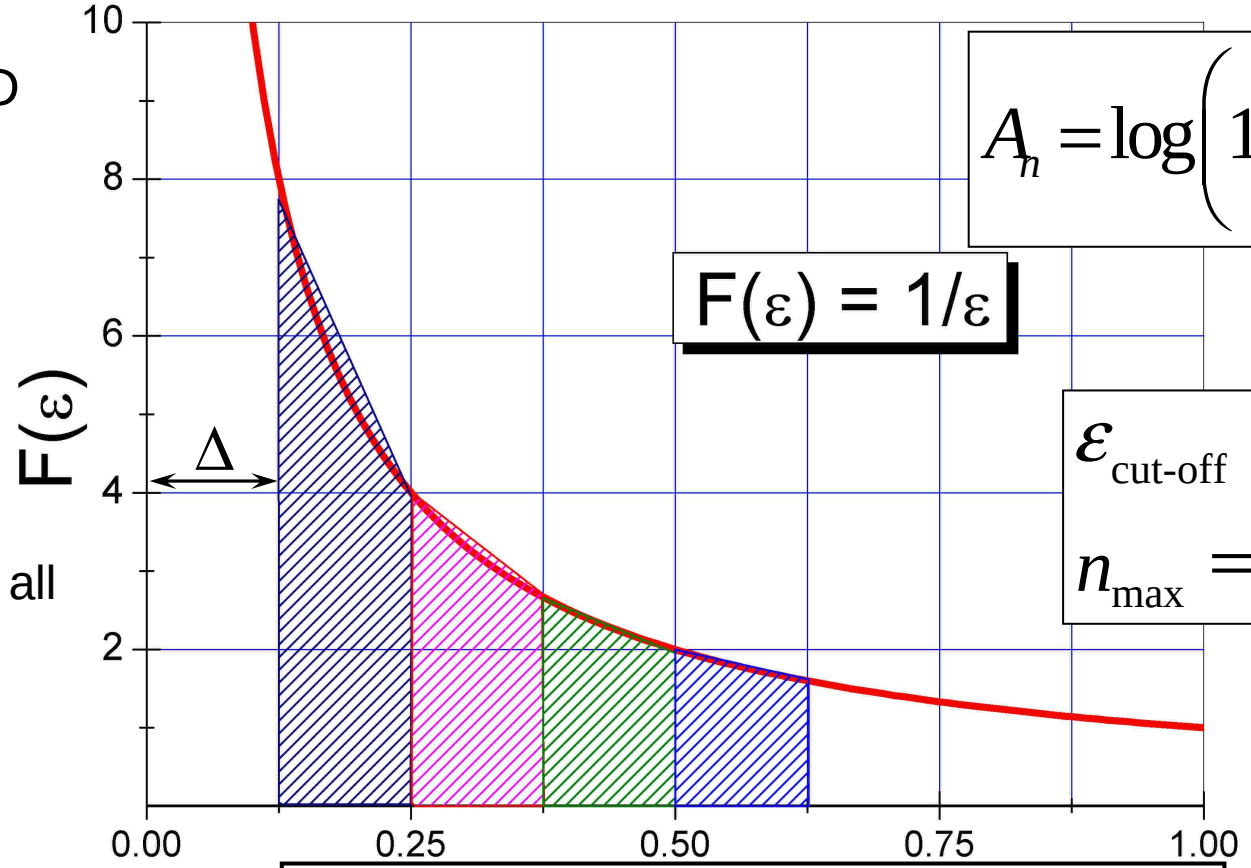
“Perturbative” Discretization of CB



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

“Perturbative” Discretization of CB

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



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

$F(\varepsilon) = 1/\varepsilon$

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

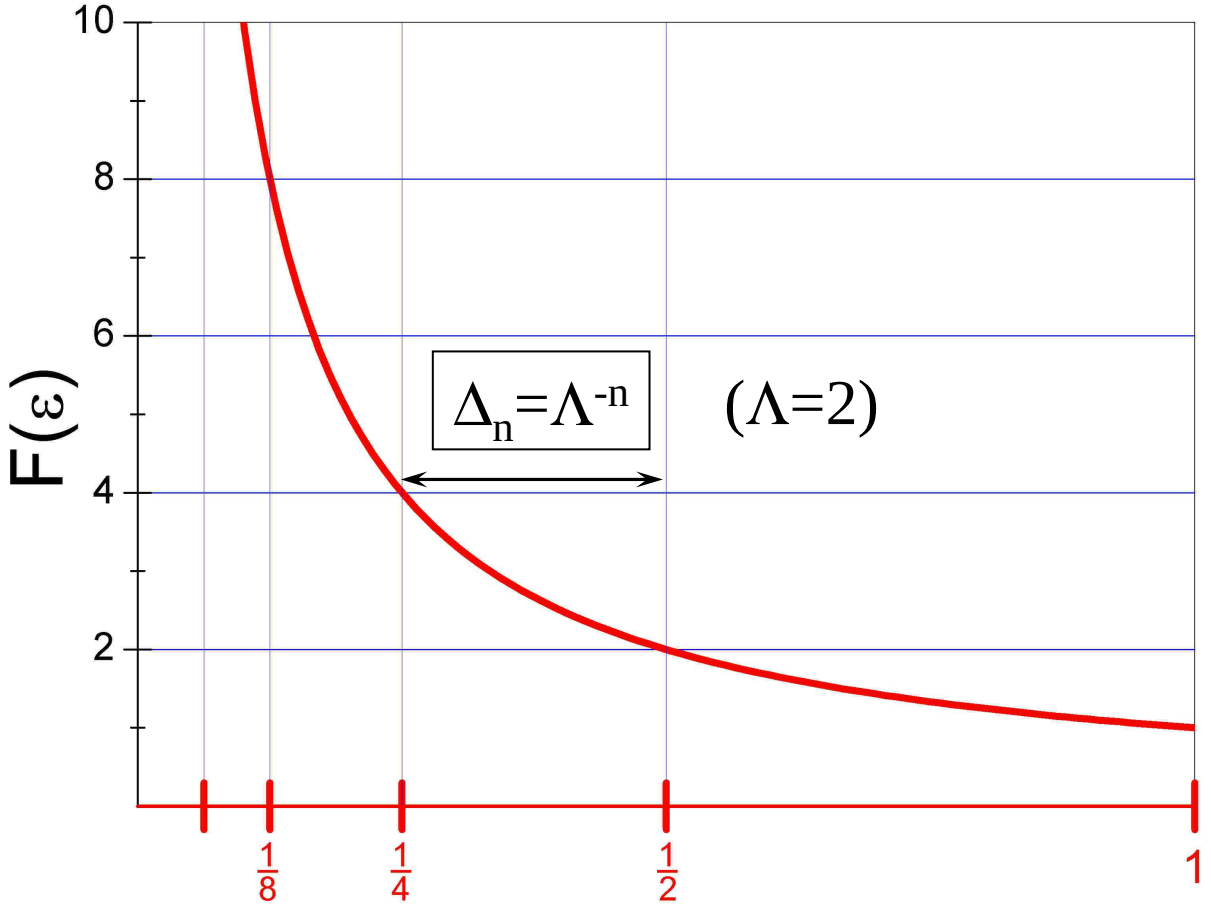
$$n_{\max} = \Delta^{-1} - 1$$

Want to keep all contributions for D⟶∞?

$\mathbf{A_7 > A_6 > A_5 > A_4 > A_3 > A_2 > A_1}$

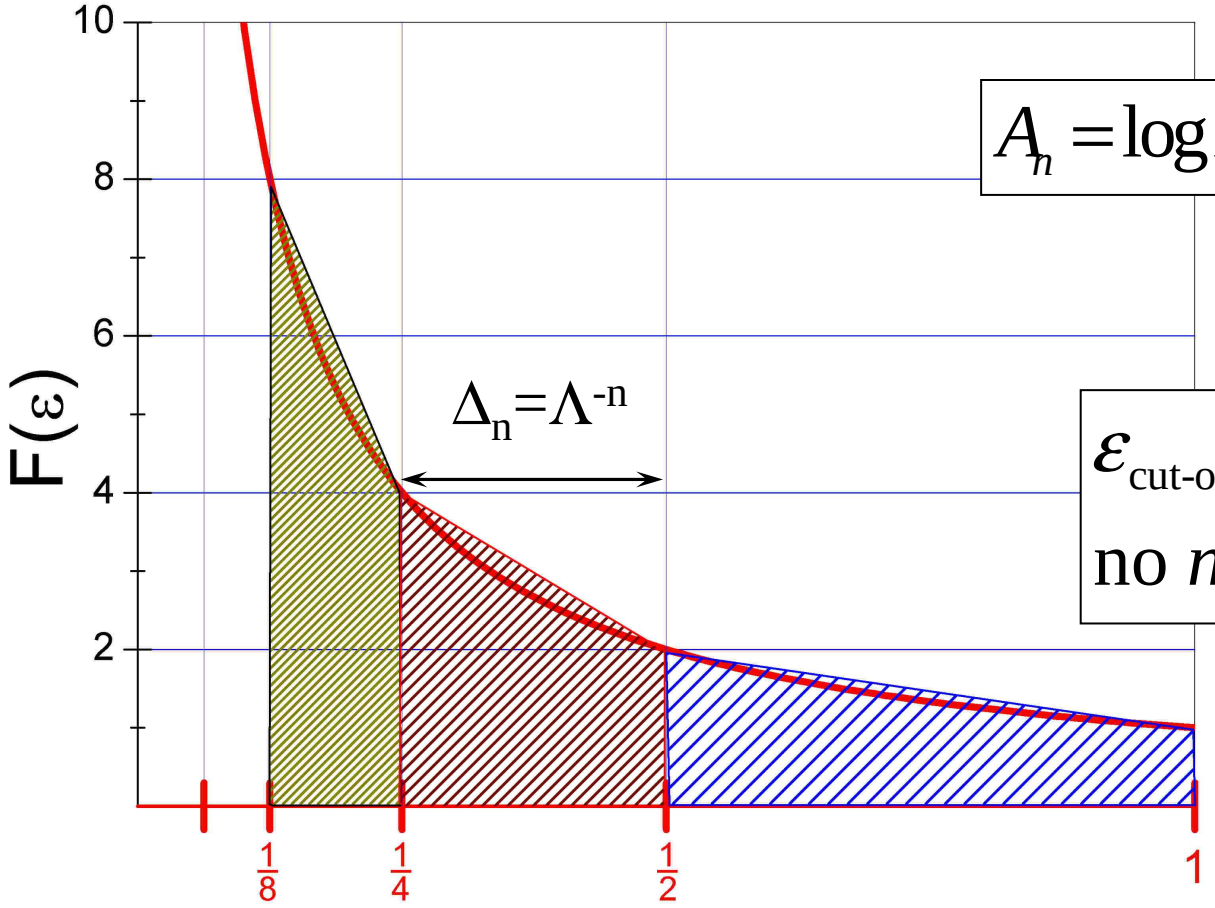
Not a good approach!

Wilson's CB Logarithmic Discretization



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

Wilson's CB Logarithmic Discretization



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

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

no $n_{\max}$

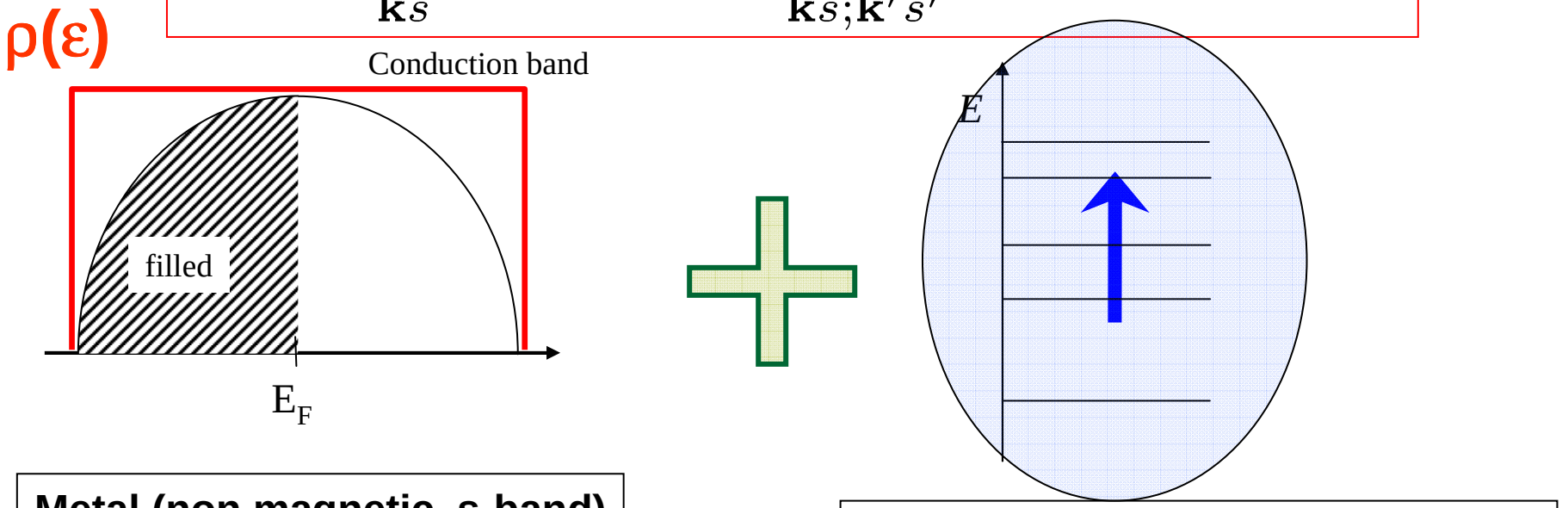
Now you're ok! ⬅

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

Kondo problem: s-d Hamiltonian

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

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

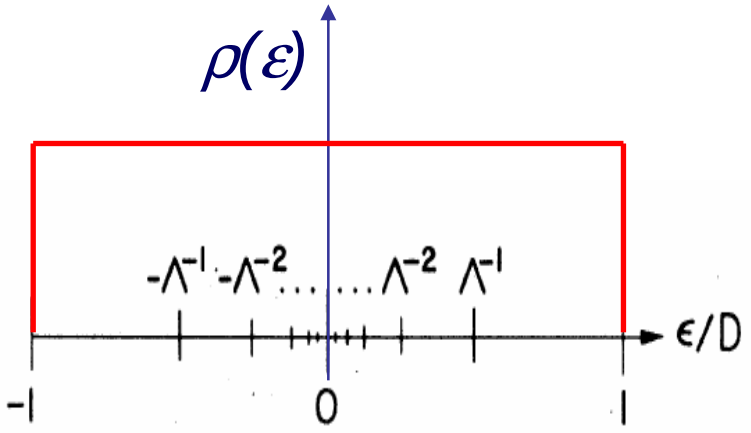


Metal (non magnetic, s-band)

Magnetic impurity (unfilled d-level)

Kondo s-d Hamiltonian

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

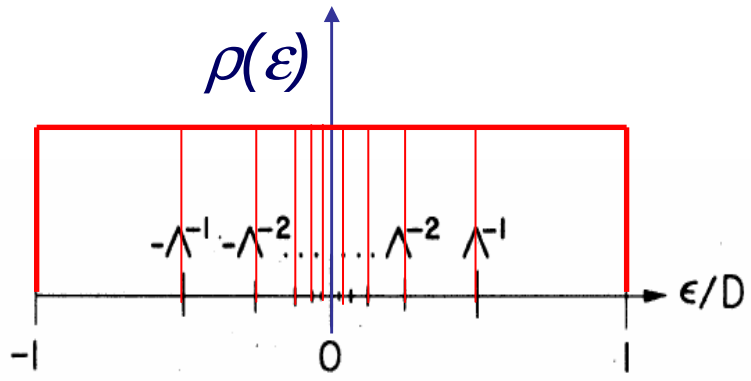


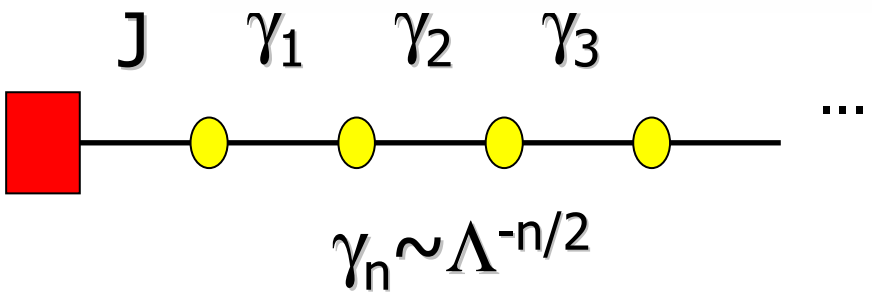
- From continuum *k* to a *discretized* band.
- Transform $H_{\text{s-d}}$ into a linear chain form (exact, as long as the chain is infinite):

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

“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

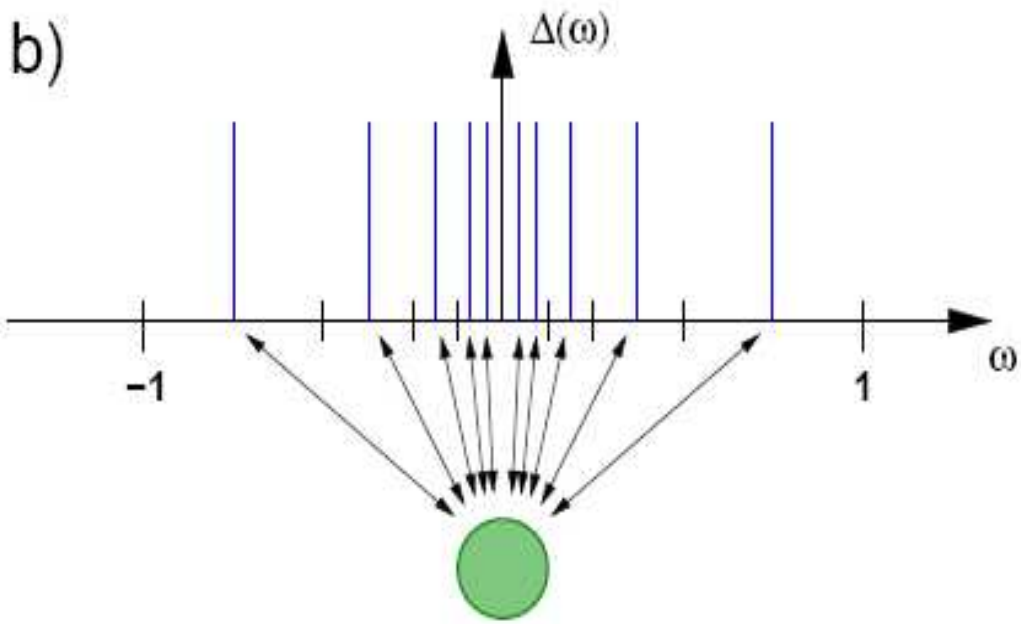


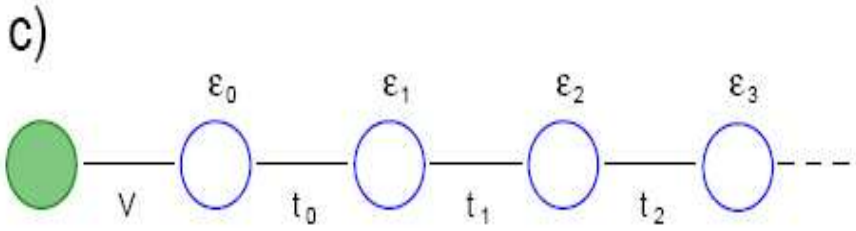


Logarithmic Discretization.

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.



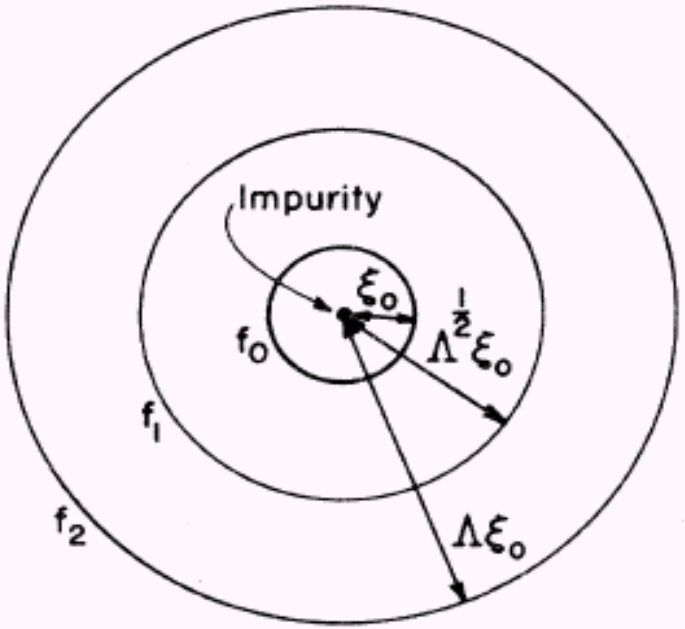


$t_n \sim \Lambda^{-n/2}$

Wilson's CB Logarithmic Discretization

- Logarithmic Discretization (in space):

$\Lambda>1$



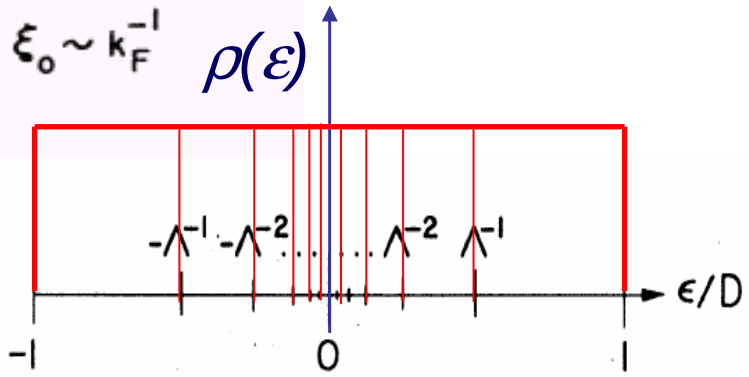


FIG. 4. Spherical shells in r space depicting the extents of the wave functions of f_n. Within their shells, every wave function has oscillations so that they are mutually orthogonal. Alternately one can show that, in the wave-vector space,

Wilson's CB Logarithmic Discretization

- Logarithmic Discretization (in energy):

$\Lambda>1$

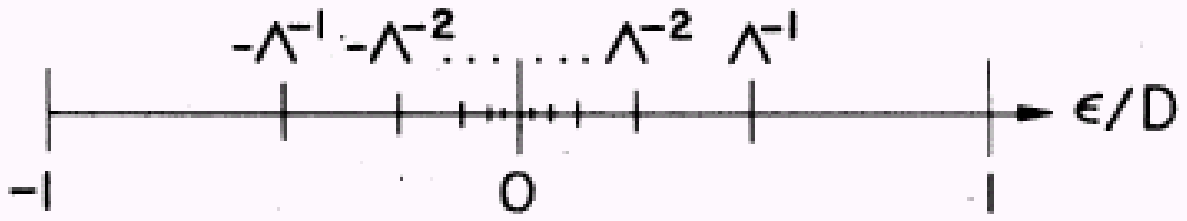
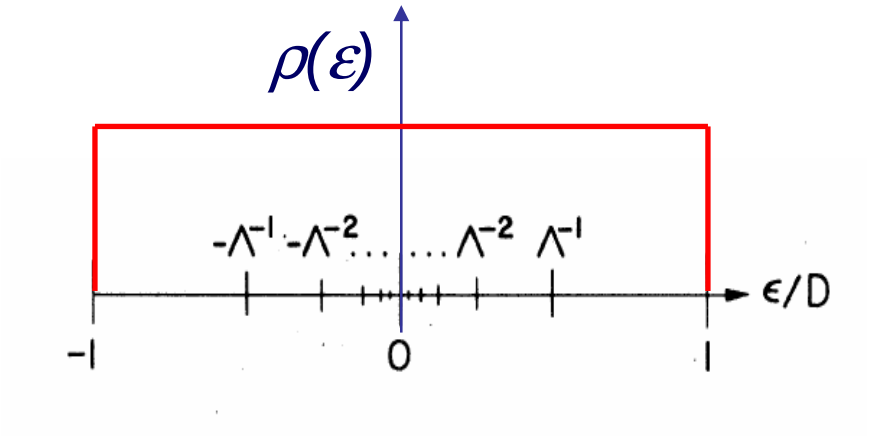


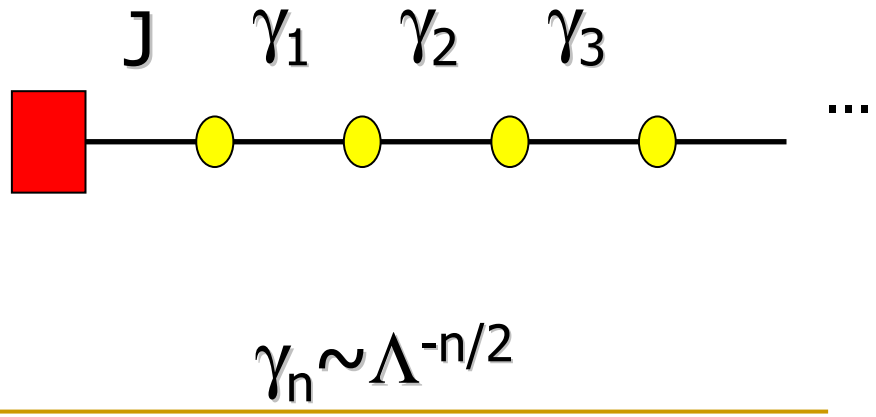
FIG. 1. Logarithmic discretization of the conduction bond. The Fermi energy is at zero and the top and bottom of the conduction bond at $k \equiv \epsilon/D = +1$ and -1, respectively.

“New” Hamiltonian (Wilson)

- Recurrence relation (Renormalization procedure).

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





“New” Hamiltonian (Wilson)

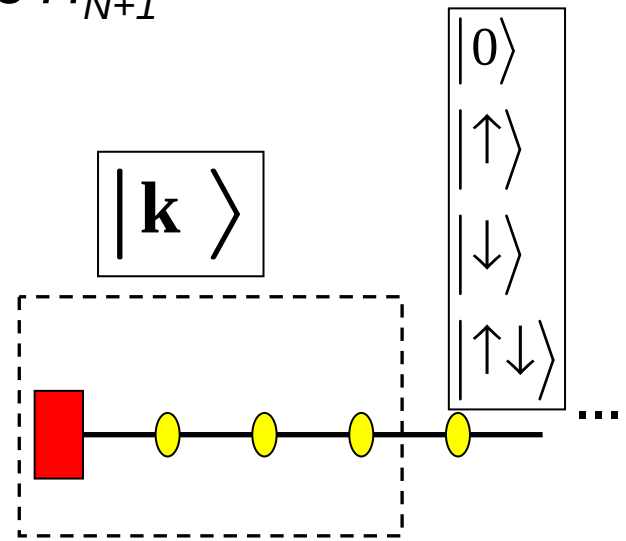
- Suppose you diagonalize H_N getting E_k and |k> and you want to diagonalize H_{N+1} using this basis.
- First, you expand your basis:

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

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

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

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

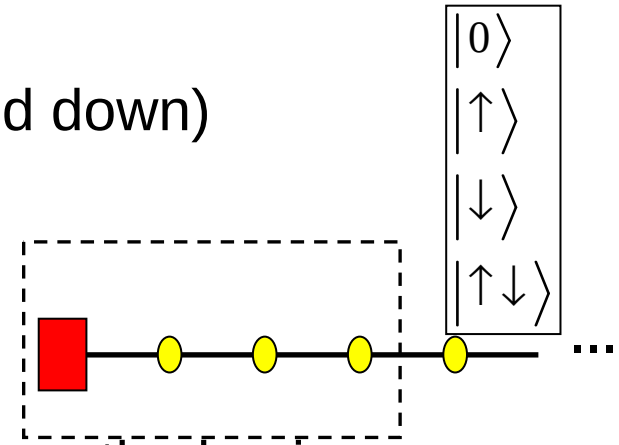


- Then you calculate <*k*,a|f^{+}_{N}|*k*’,a’>, <*k*,a|f_{N}|*k*’,a’>and you have the matrix elements for H_{N+1} (sounds easy, right?)

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?

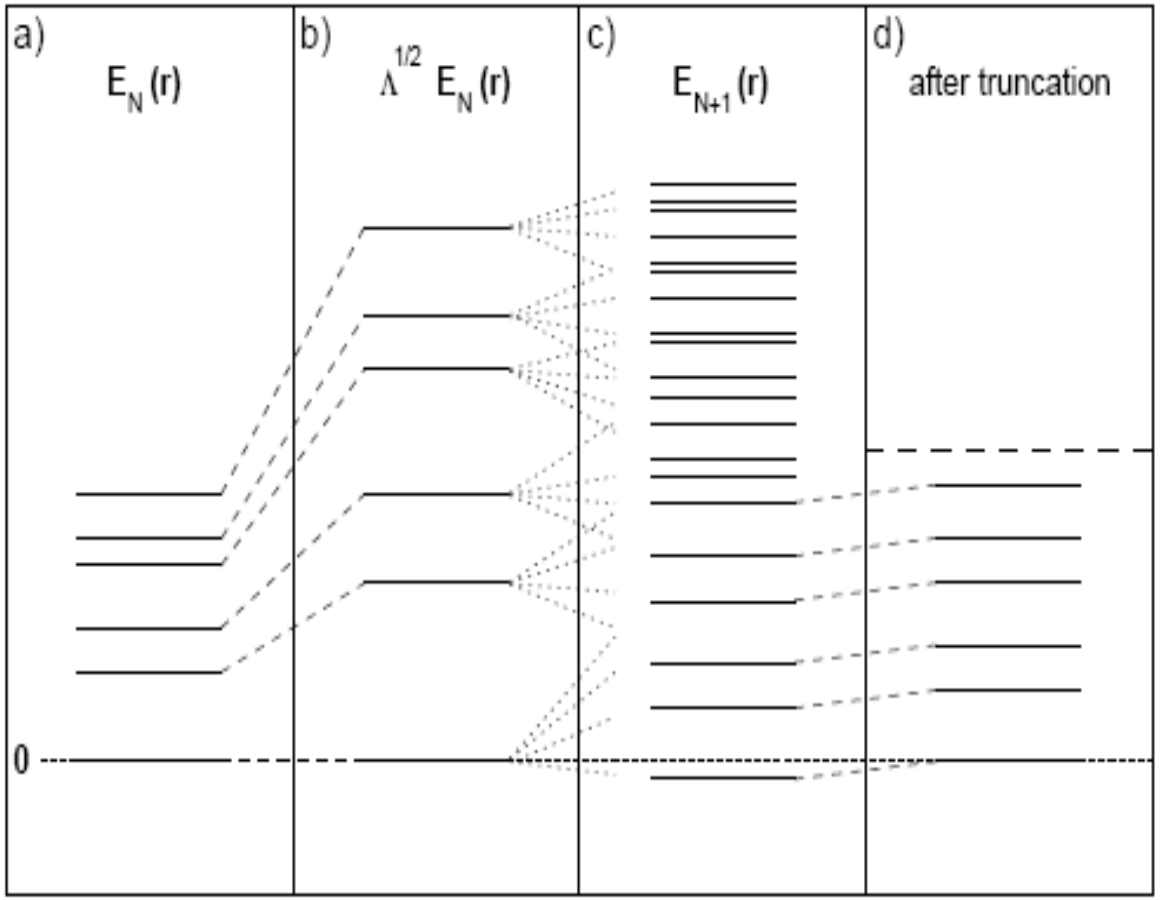
      (Hint: The number of atoms in the universe is ~ 10^{80})



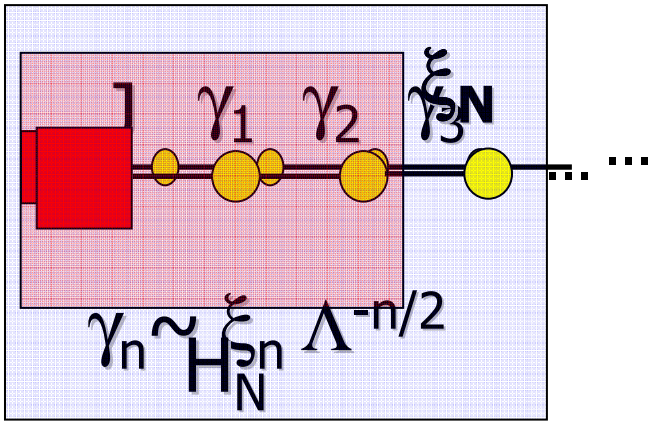
- Cut-off the basis $\rightarrow$ lowest ~1500 or so in the next round (Even then, you end up having to diagonalize a 4000x4000 matrix…).

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.



Renormalization Group Transformation

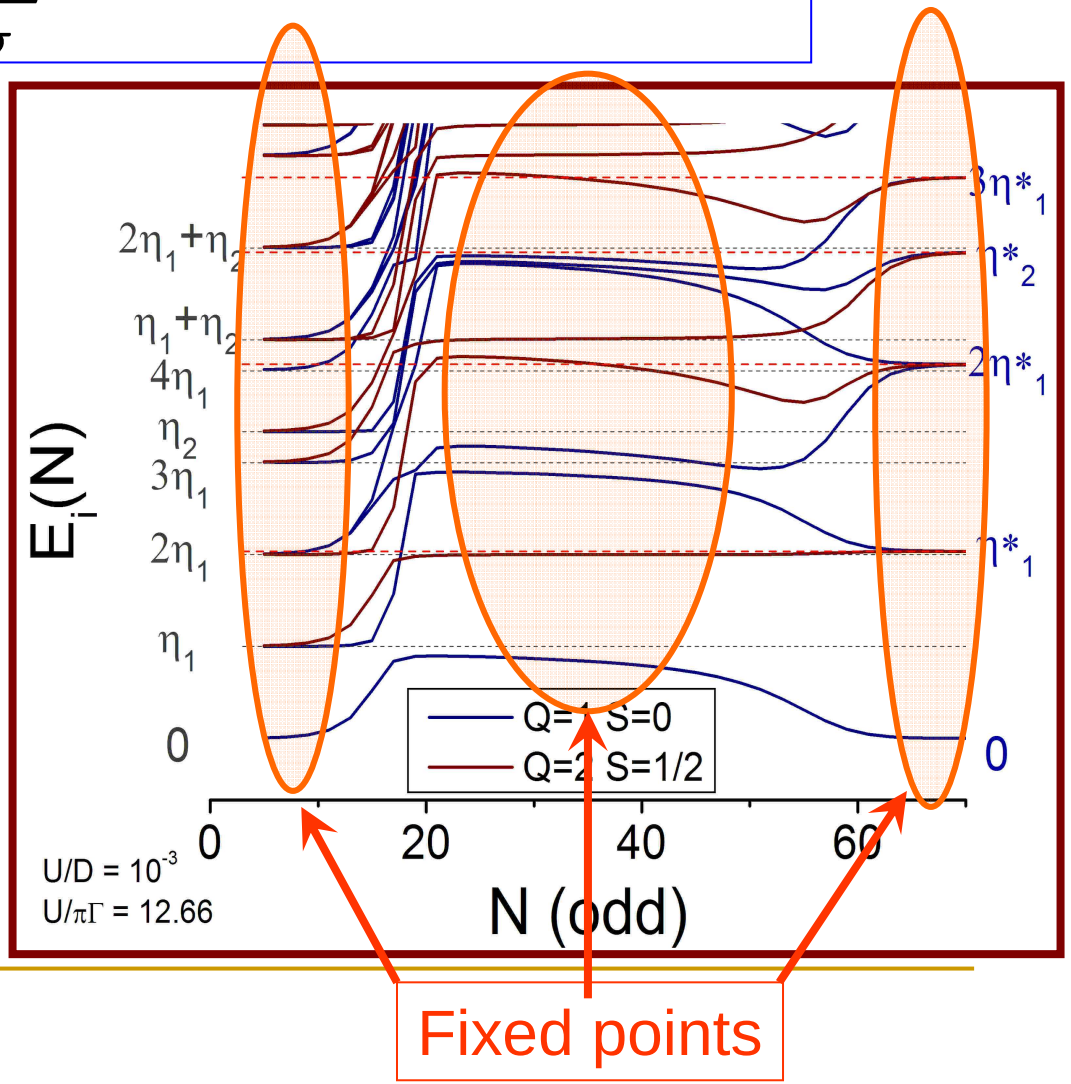
$$H_{N+1} = \sqrt{\Lambda} H_N + \xi_N \sum_\sigma f^\dagger_{N+1\sigma} f_{N\sigma} + f^\dagger_{N\sigma} f_{N+1\sigma}$$

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

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

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

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



Spectral function calculation

Local Density of states: Lehmann representation.

$$A_\sigma(\omega, T=0) = \frac{1}{Z(0)} \sum_r |M_{r,0}|^2 \delta(\omega + (E_r - E_0))$$

$$+ \frac{1}{Z(0)} \sum_{r'} |M_{0,r'}|^2 \delta(\omega - (E_{r'} - E_0), \qquad (6$$

At each NRG step, you define

$$A^N_\sigma(\omega, T=0) = \frac{1}{Z_N(0)} \sum_r |M^N_{r,0}|^2 \delta(\omega + E^N_r)$$

$$+ \frac{1}{Z_N(0)} \sum_{r'} |M^N_{0,r'}|^2 \delta(\omega - E^N_{r'}). \qquad (68)$$

$$H_N |r\rangle_N = E^N_r |r\rangle_N,$$

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

Spectral function

At each NRG step:

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

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

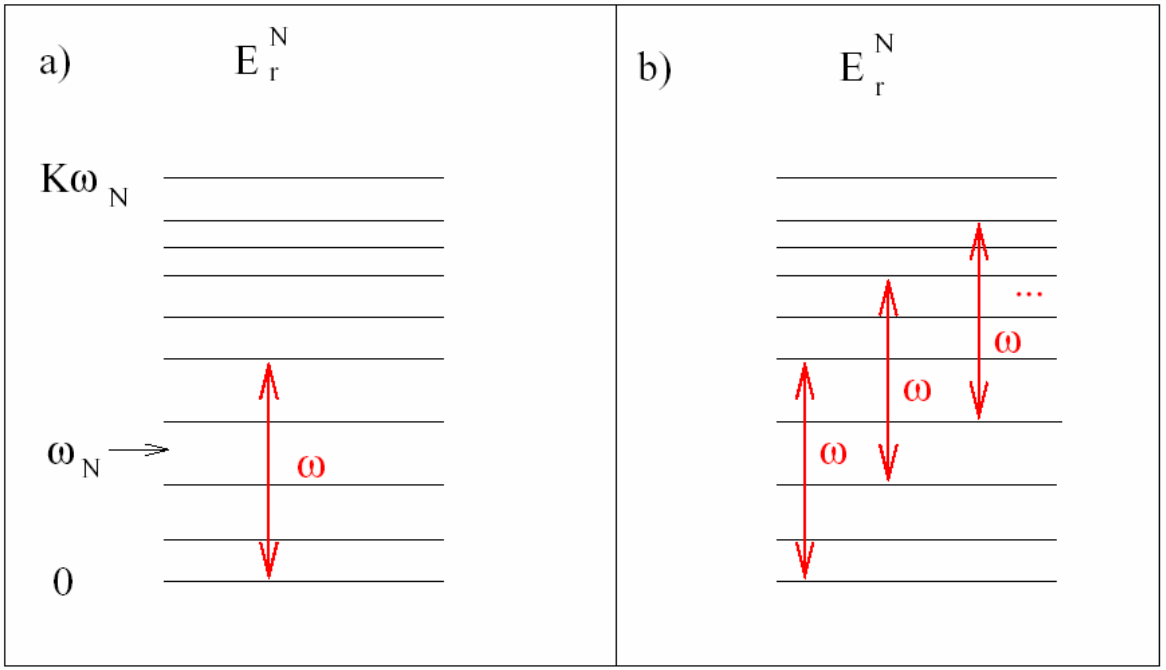


FIG. 9 Excitations of H_N contributing to the spectral function at frequency ω for, (a), $T = 0$, and, (b), $T > 0$.

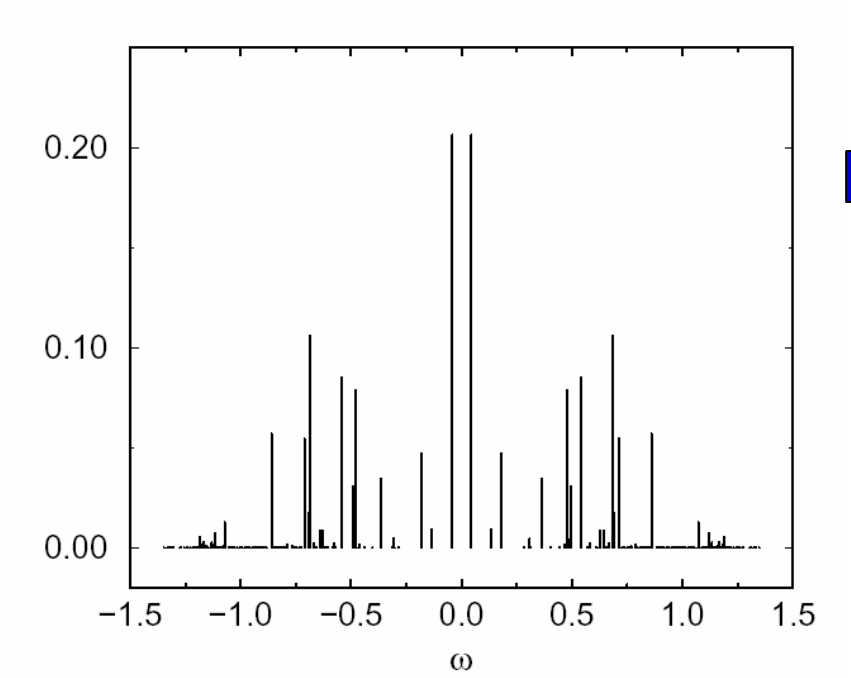
Spectral function calculation (Costi)

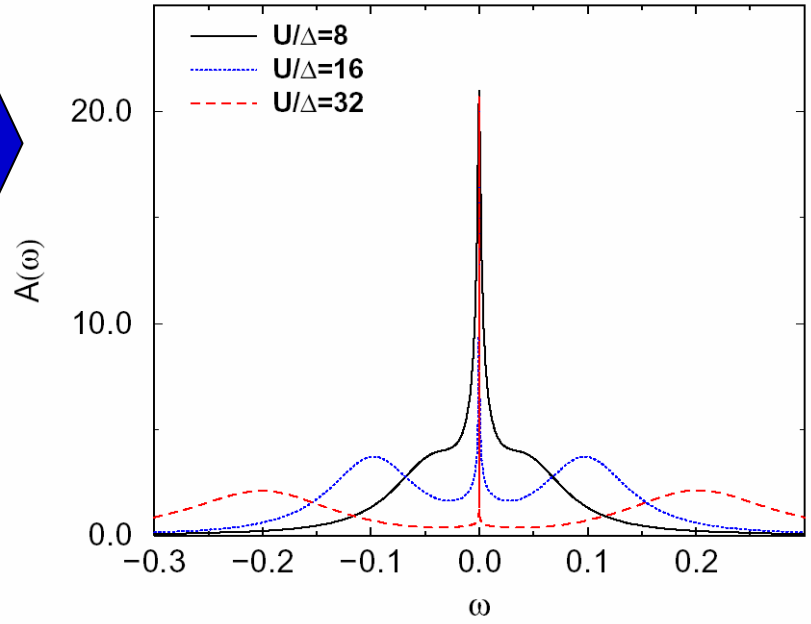
$$A_\sigma^N(\omega, T=0) = \frac{1}{Z_N(0)} \sum_r |M_{r,0}^N|^2 \delta(\omega + E_r^N)$$

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

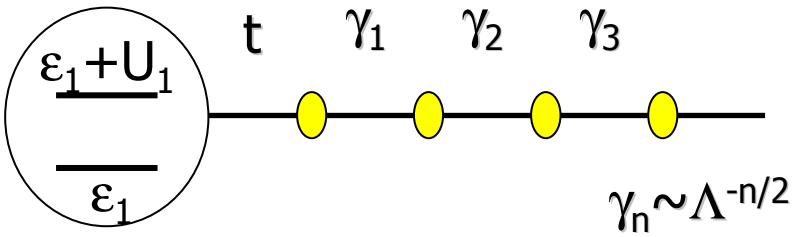
To get a continuos curve, need to broaden deltas. Best choice: log gaussian

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

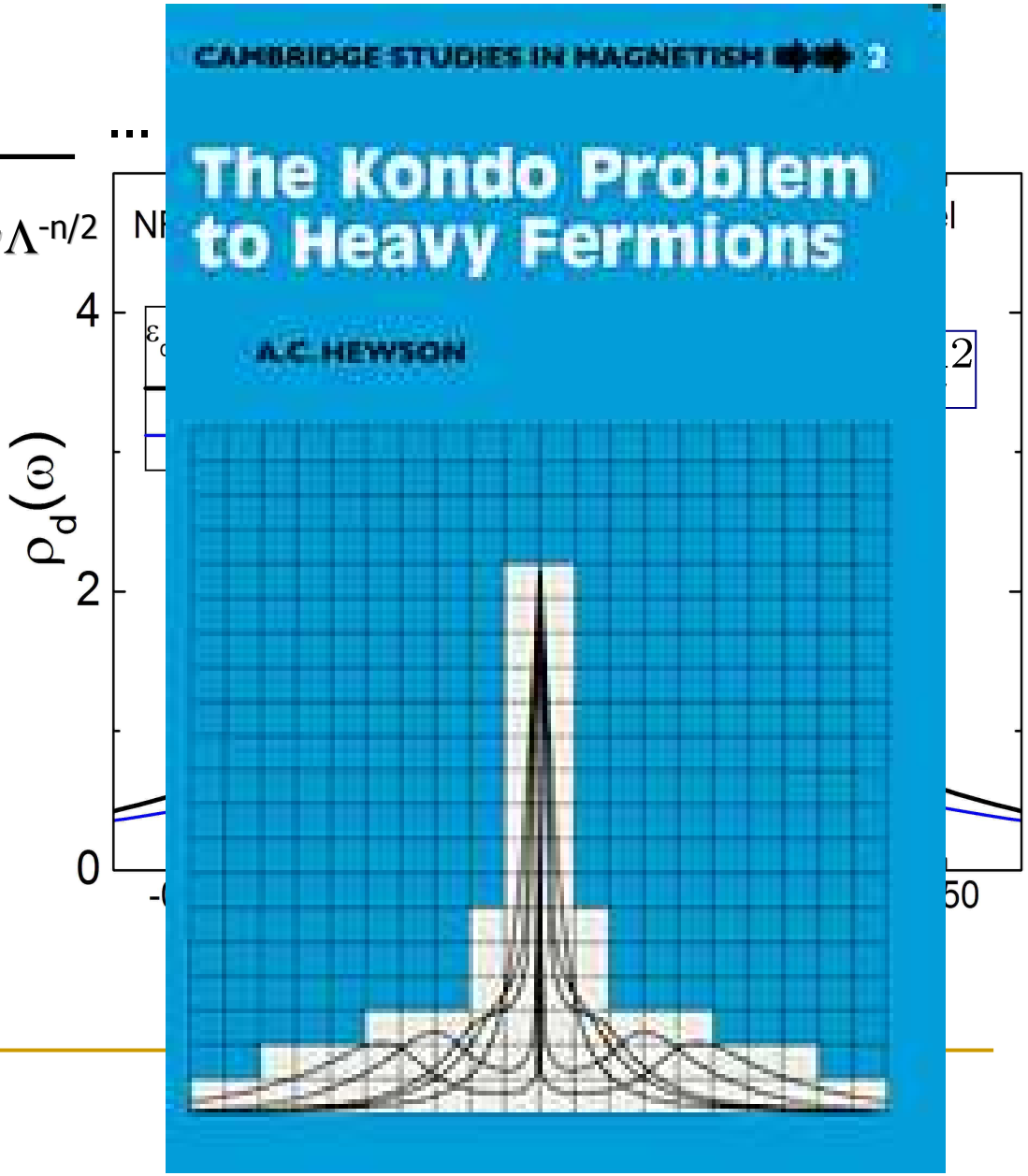




NRG on Anderson model: LDOS



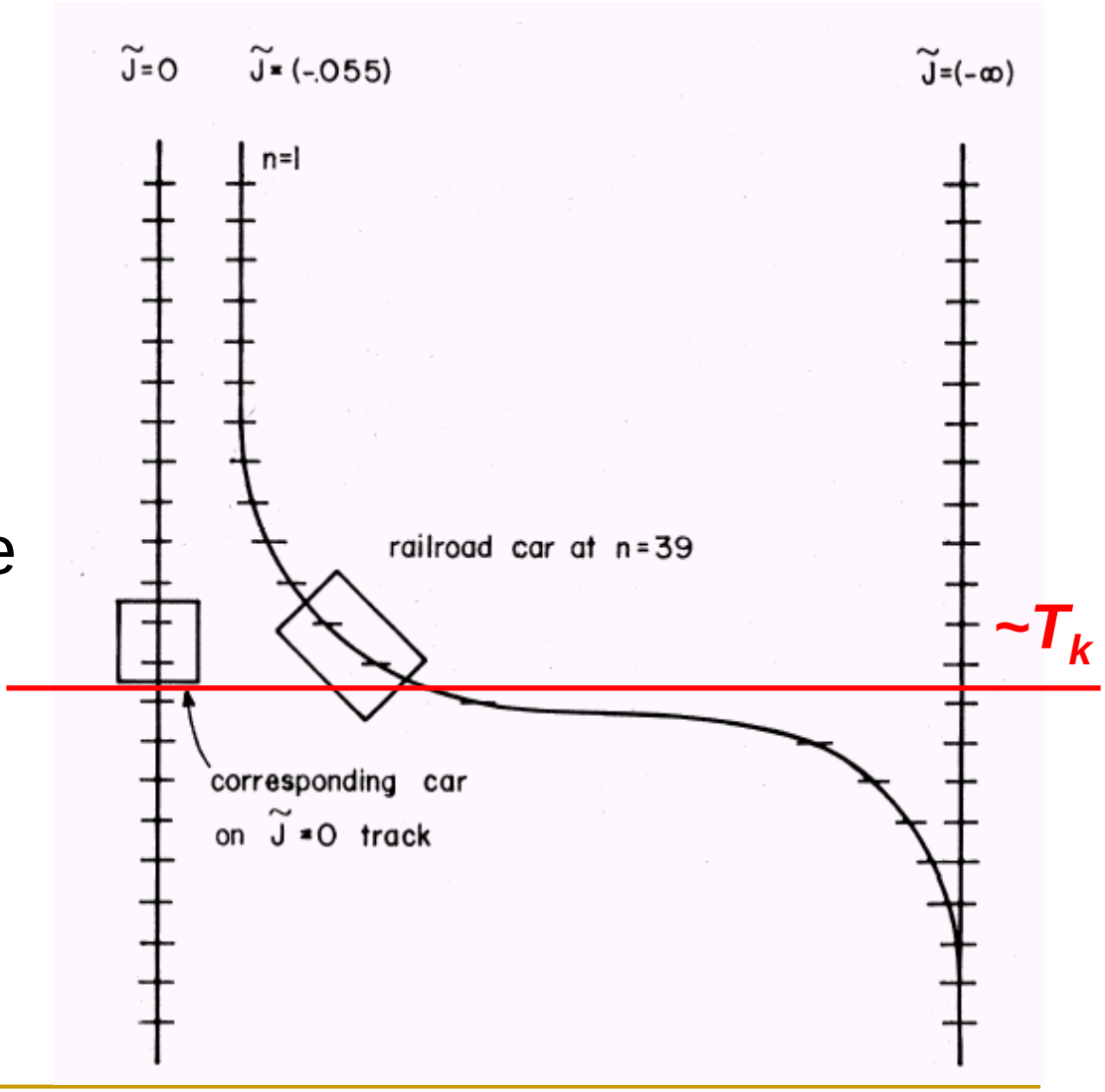
- Single-particle peaks at ε_d and ε_d+U.
- *Many-body* peak at the Fermi energy: ***Kondo resonance*** (width ~T_K).
- NRG: good resolution at low ω (log discretization).



Numerical Renormalization Group

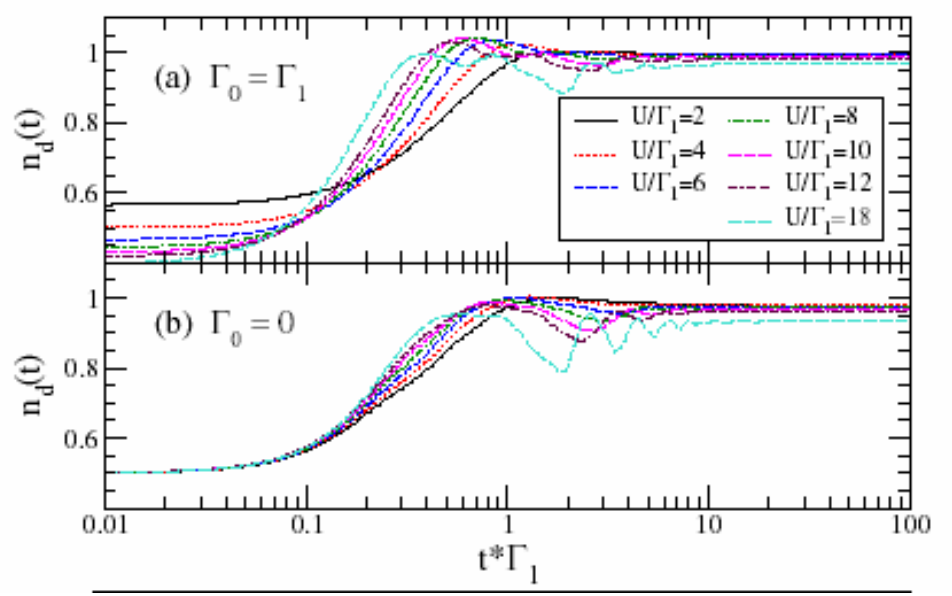
What can you do?

- Describe the physics at different energy scales for arbitrary *J.*
- Probe the parameter phase diagram.
- Crossing between the “free” and “screened” magnetic moment regimes.
- Energy scale of the transition is of order T_k



Recent Developments: TD-NRG

Application: time dependent impurity problems



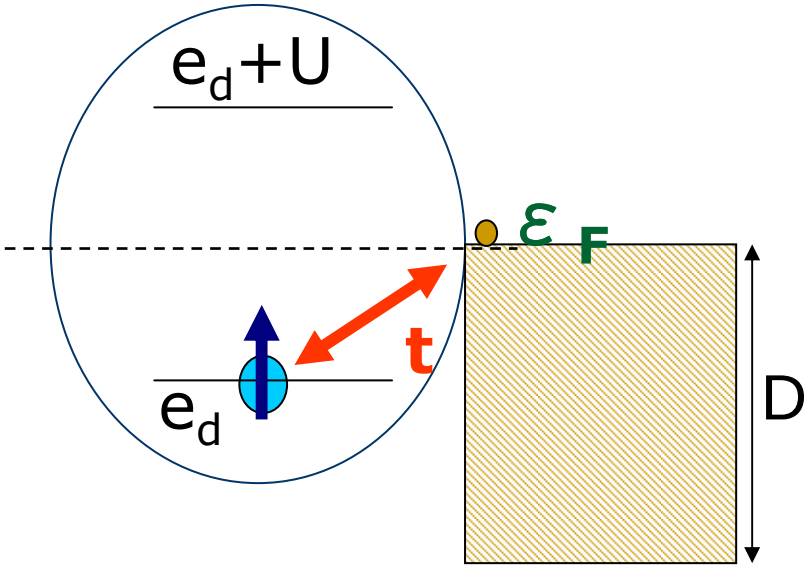
$$\mathcal{H} = \sum_{k,\sigma} \varepsilon_{k\sigma} c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{\sigma=\pm 1} \left[E_d(t) - \frac{\sigma}{2} H(t) \right] d^{\dagger}_{\sigma} d_{\sigma}$$

$$+ U \hat{n}^d_{\uparrow} \hat{n}^d_{\downarrow} + V(t) \sum_{k,\sigma} \{ d^{\dagger}_{\sigma} c_{k\sigma} + c^{\dagger}_{k\sigma} d_{\sigma} \}.$$

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

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

"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

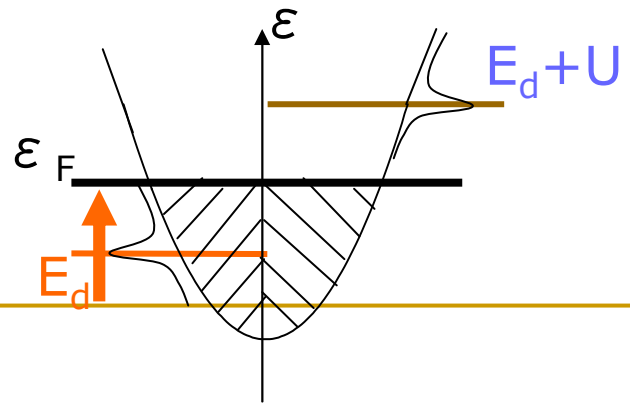
Schrieffer- Wolff Transformation

Anderson Model

Existence of localized moment

$$|V_{kd}| << U$$

Schrieffer-Wolff transformation



s-d Model

Schrieffer- Wolff Transformation

From: Anderson Model (single occupation)

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

with

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

$$J = t^2 \sum_{k,k'} \left\{ \frac{1}{U + \epsilon_d - \epsilon'_k} + \frac{1}{\epsilon_k - \epsilon_d} \right\}$$

To: s-d (Kondo) Model

$$\begin{aligned} H_{\text{s-d}} &= J \sum_{kk'} S^+ c^\dagger_{k\downarrow} c_{k'\uparrow} + S^- c^\dagger_{k\uparrow} c_{k'\downarrow} \\ &+ S_z \left(c^\dagger_{k\downarrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow} \right) \\ &+ \sum_k \epsilon_k \hat{n}_{k\sigma} \end{aligned}$$

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”)
- ...