Lectures: Condensed Matter II

1 – Electronic Transport in
Quantum dots

2 – Kondo effect: Intro/theory.

3 – Kondo effect in nanostructures

Luis Dias – UT/ORNL

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1 – Electronic Transport in Quantum dots

2 – Kondo effect: Intro/theory.

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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.

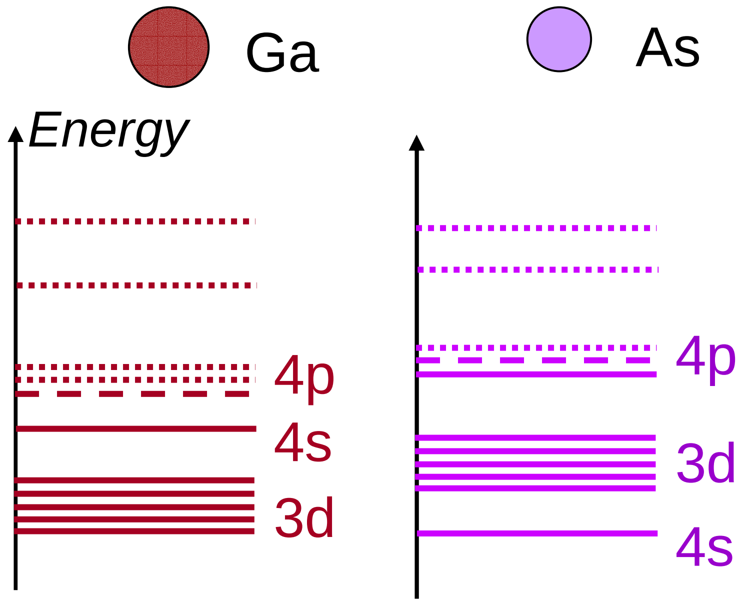
“More is Different”

“ 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)

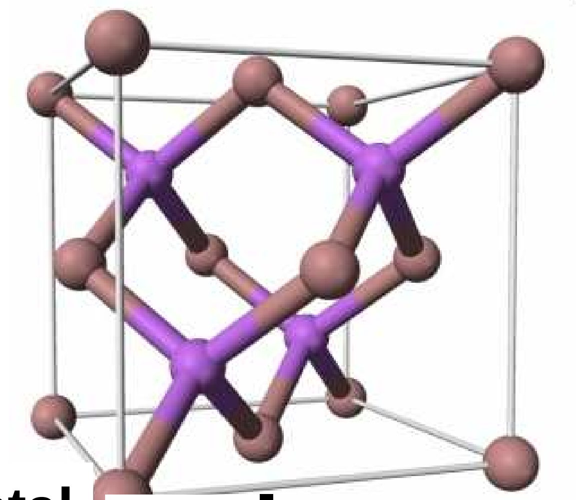
Can you make “atoms” out of atoms?



[Ar] $3d^{10}$ $4s^2$ $4p^1$ [Ar] $4s^2$ $3d^{10}$ $4p^3$

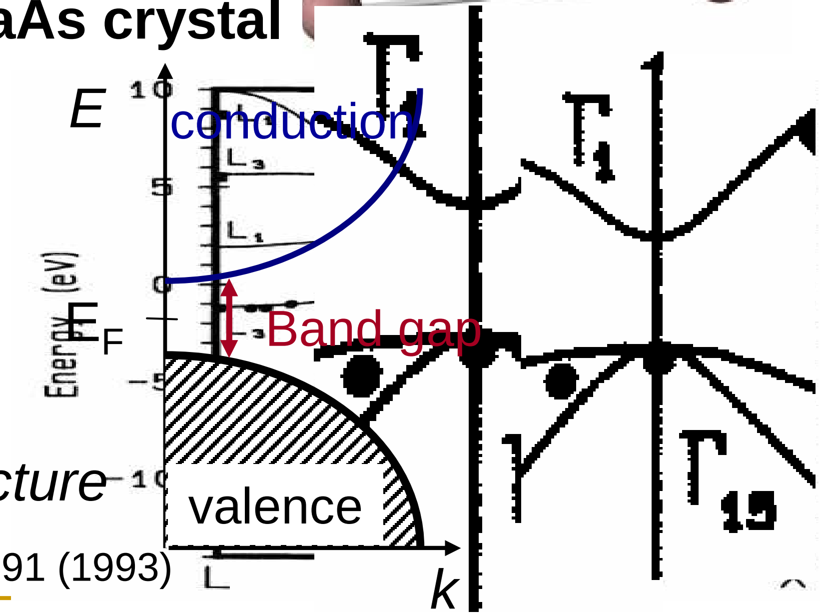
Atomic Energy levels

Many Atoms!



GaAs crystal

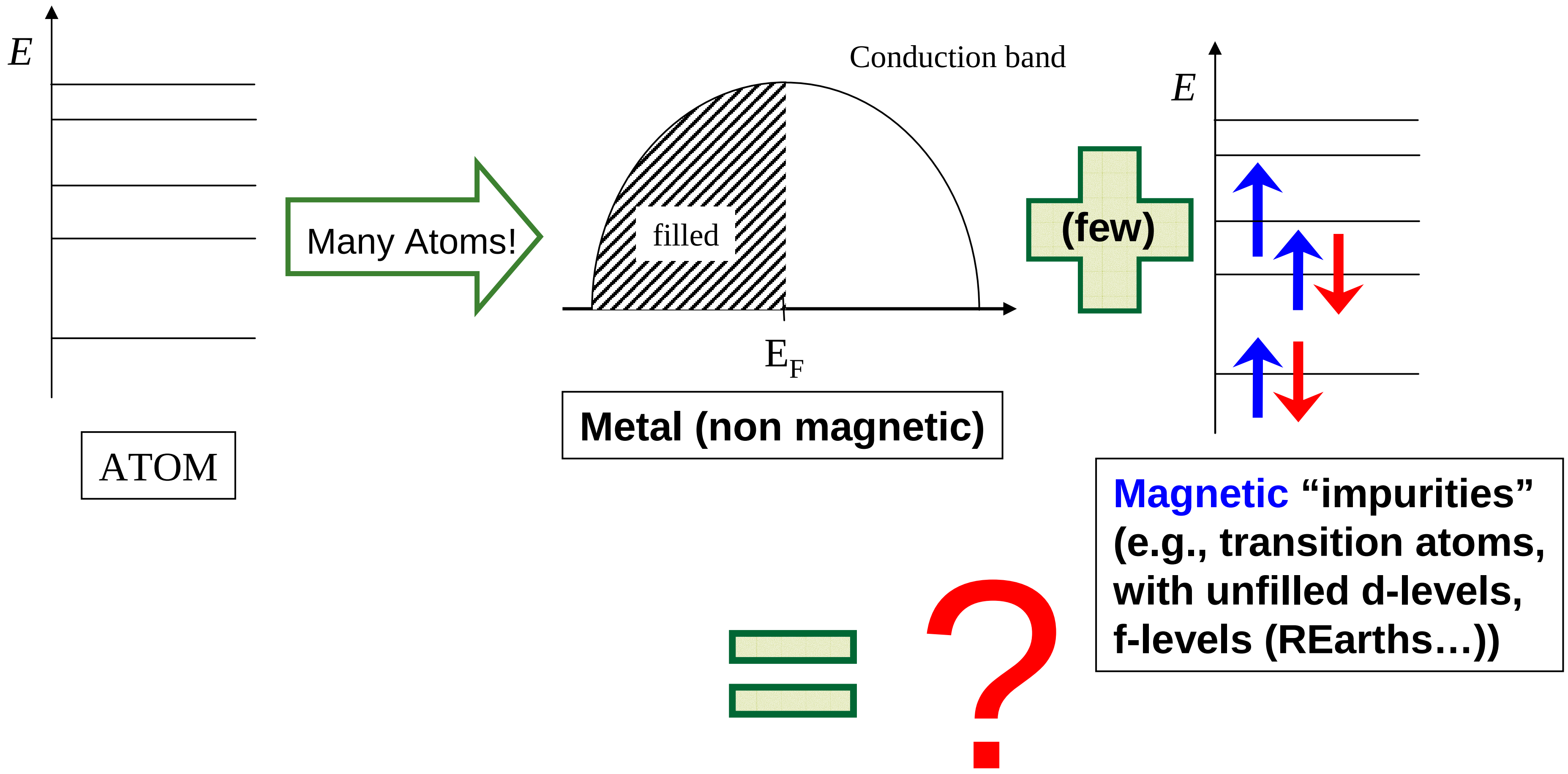
Many Atoms!



Band structure

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

From atoms to metals, plus atoms…

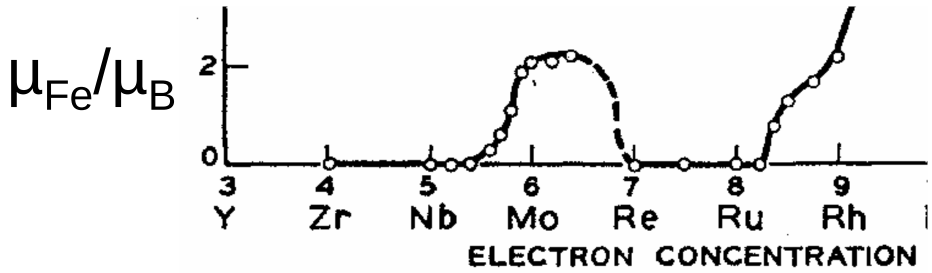


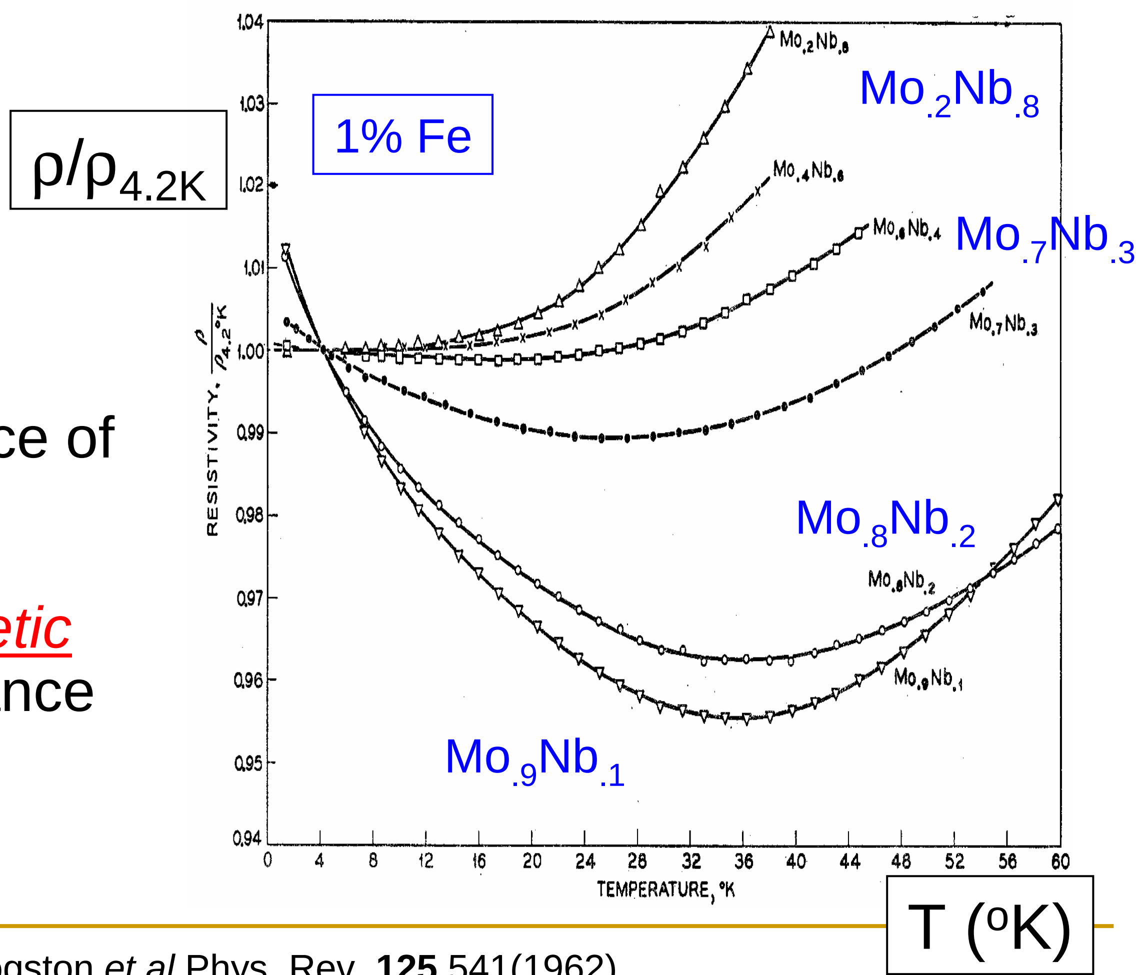
Is the resulting compound still a metal ?

Kondo effect

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

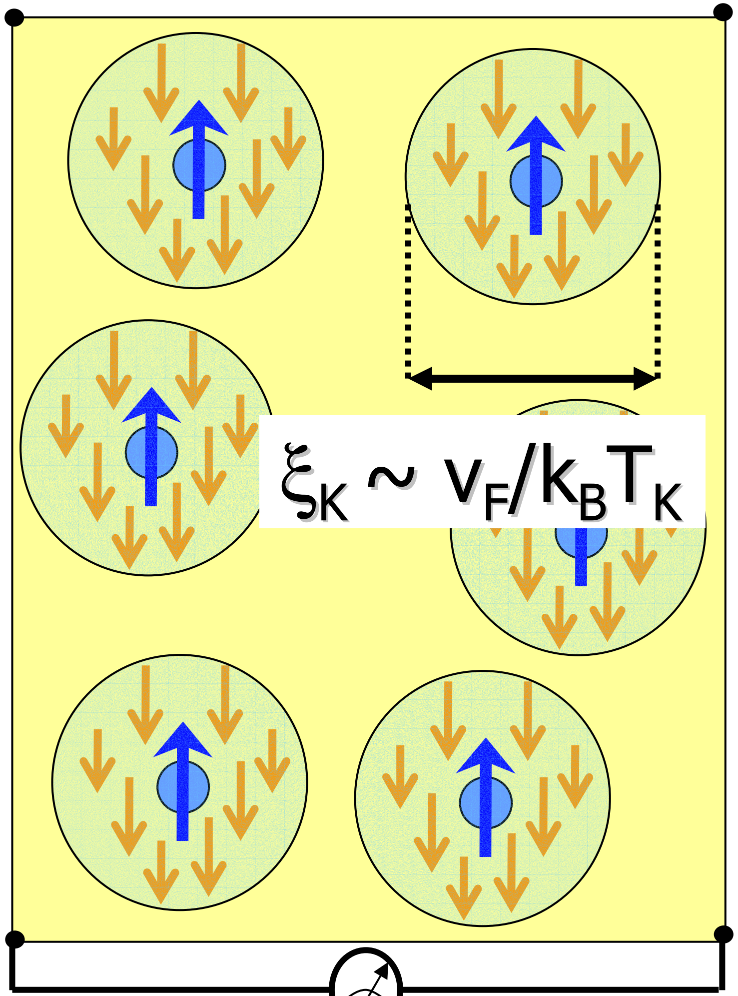
    T_{min} depends on $c_{imp.}$
  - 60's - Correlation between the existence of a Curie-Weiss component in the susceptibility (*magnetic moment*) and resistance minimum .





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

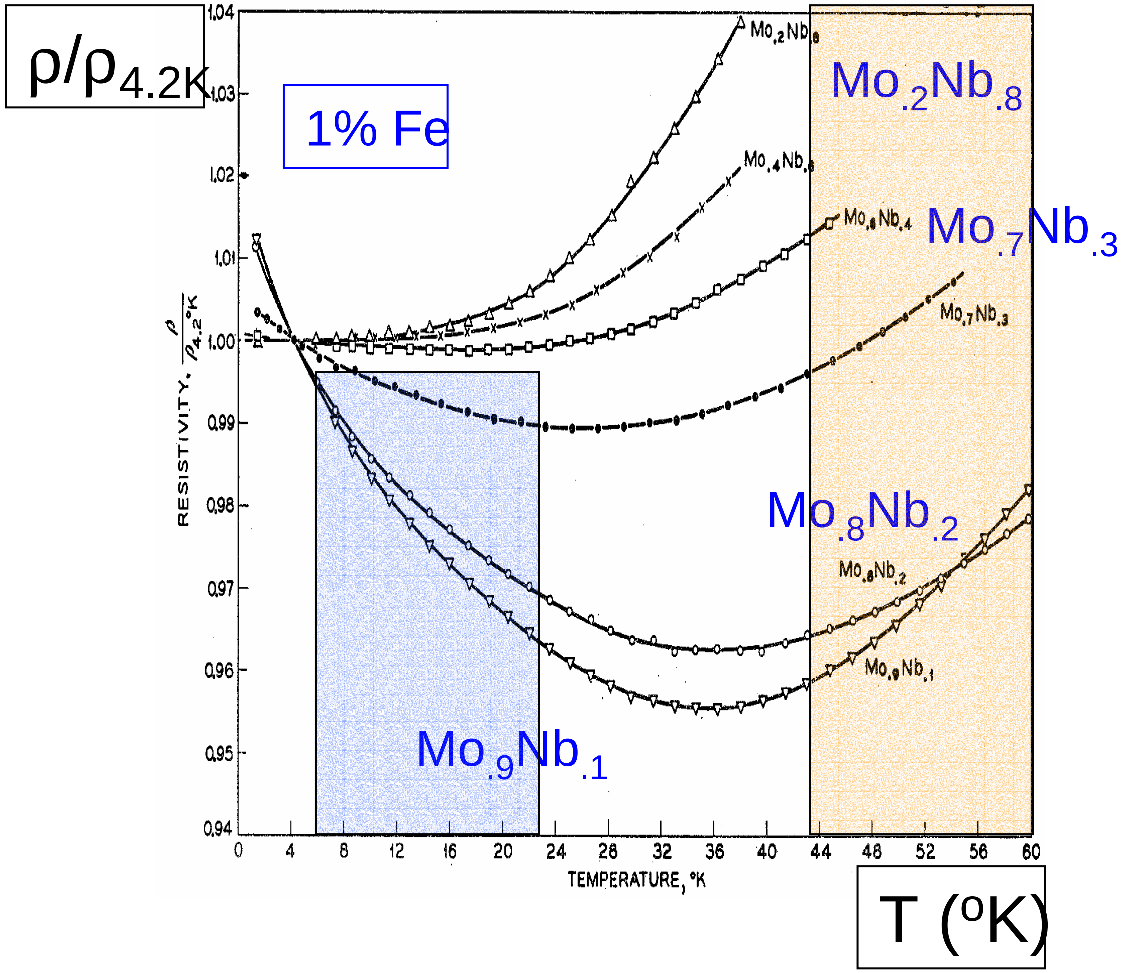
Kondo effect



ρ(T)

$T \ll T_K$

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



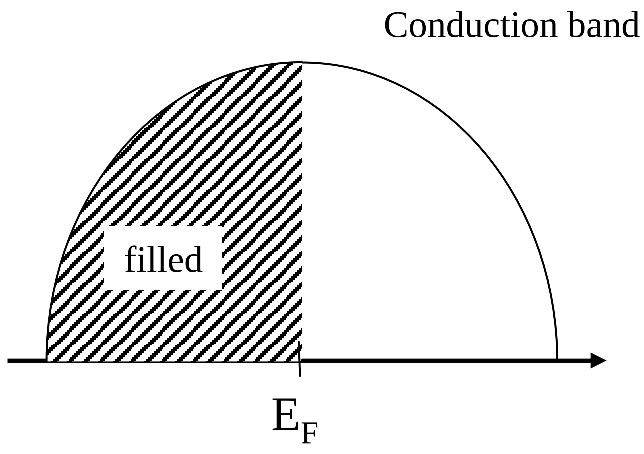
Resistivity decreases with decreasing temperature (usual)

Characteristic energy scale: the Kondo temperature T_K (Kondo effect)

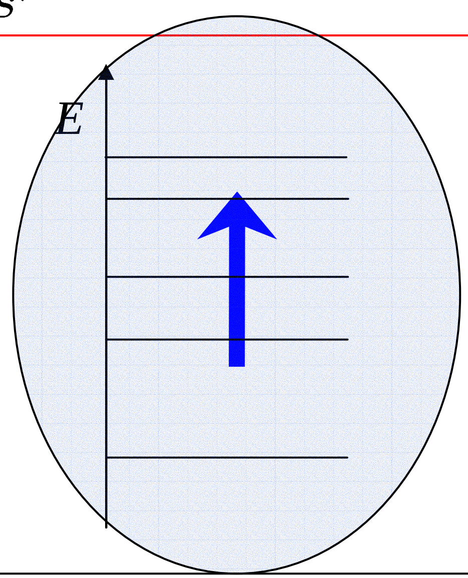
Kondo problem: s-d Hamiltonian

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

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



Metal (non magnetic, s-band)



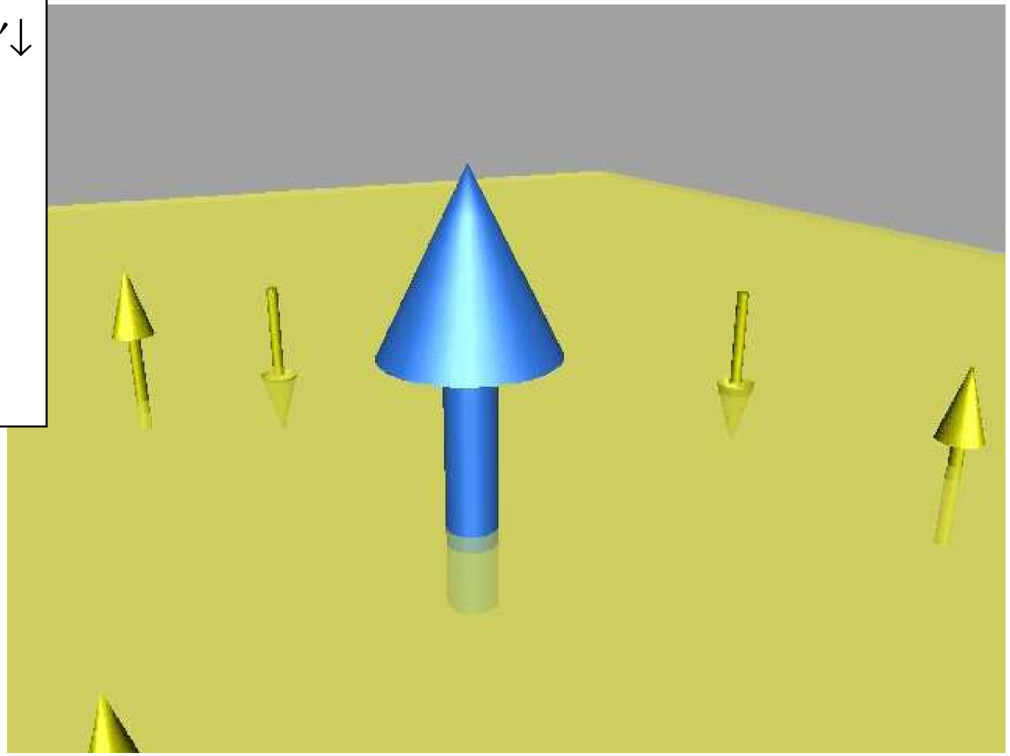
Magnetic impurity (unfilled d-level)

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

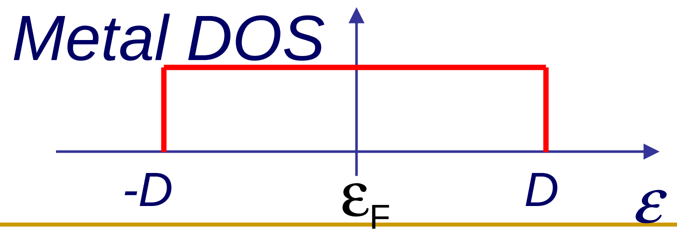
$$
\begin{aligned}
H_{\text{s-d}} = {} & J \sum_{k,k'} S^{+}\, c^{\dagger}_{k\downarrow} c_{k'\uparrow} + S^{-}\, c^{\dagger}_{k\uparrow} c_{k'\downarrow} \\
& + S_z \left(c^{\dagger}_{k\uparrow} c_{k'\uparrow} - c^{\dagger}_{k\downarrow} c_{k'\downarrow} \right) \\
& + \sum_{k} e_k\, c^{\dagger}_{k\sigma}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

Spin: J>0 AFM

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**):



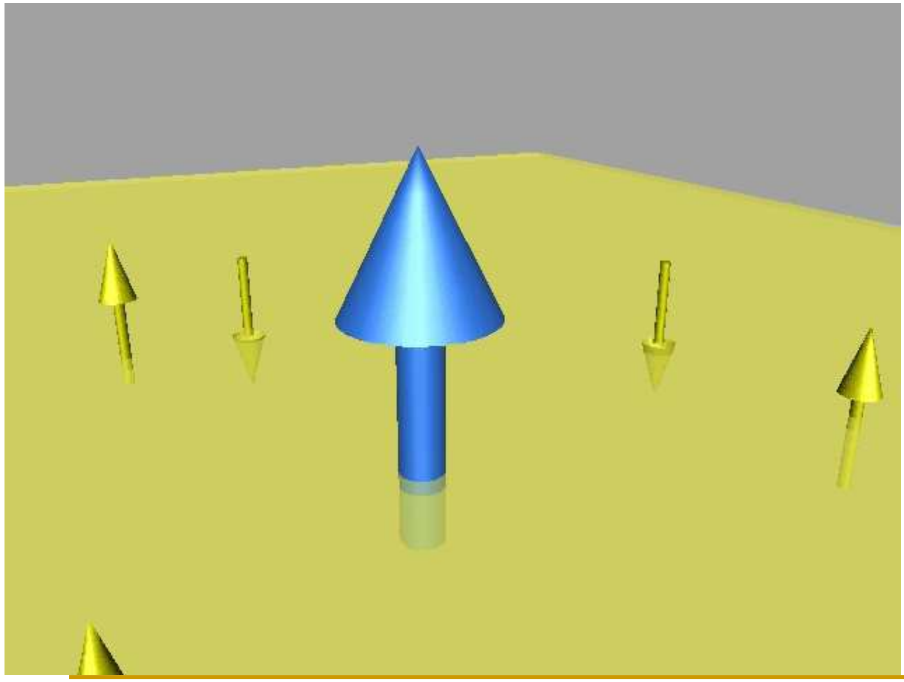
Kondo's explanation for T_{min} (1964)

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

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

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

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



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

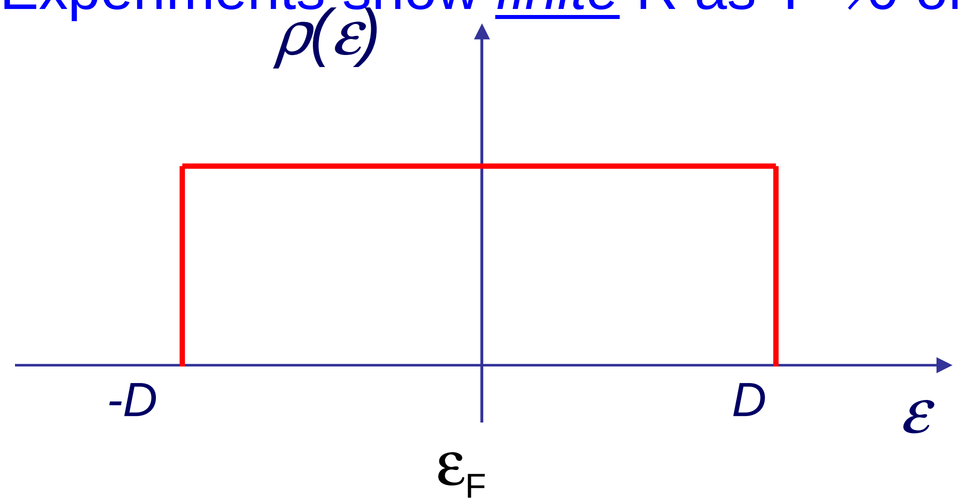
$$k_B T_K \sim D e^{-1/2J\rho_0}$$

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

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

What is going on?

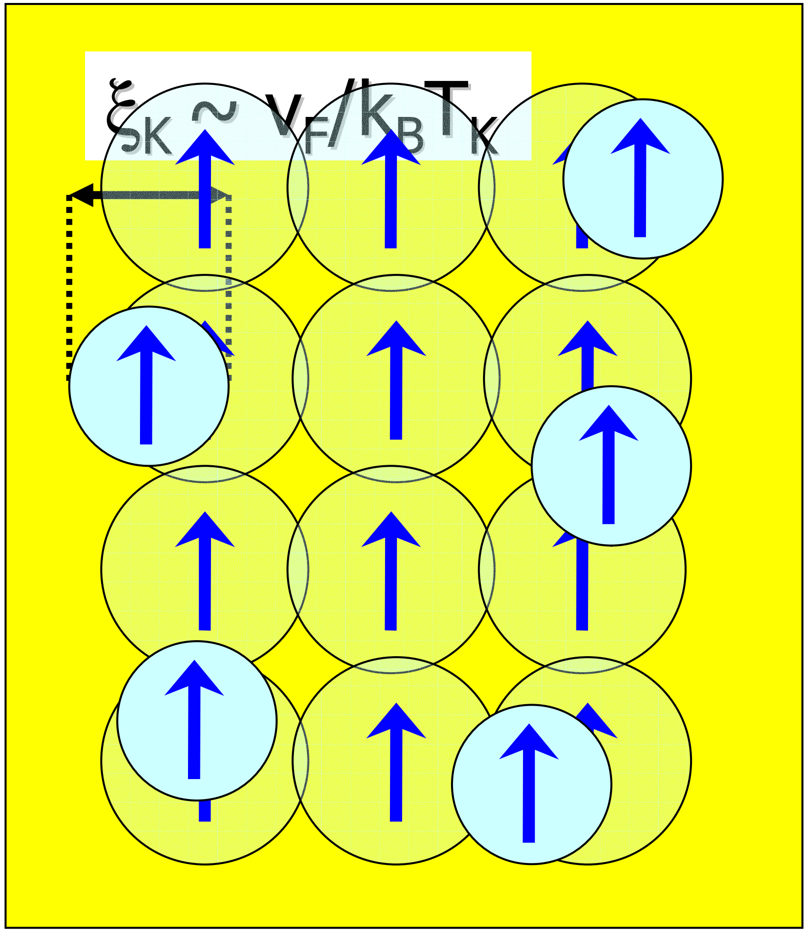
- Theory diverges *logarithmically* for $T \to 0$ or $D \to \infty$.
  ($T < T_K \to$ perturbation expasion no longer holds)
- Experiments show *finite* R as $T \to 0$ or $D \to \infty$.



Kondo Impurity and Lattice models

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

Diluted case (Kondo impurity model)

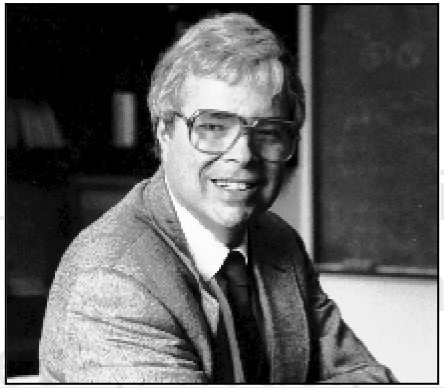


- Kondo impurity model suitable for diluted impurities in metals.
- Some rare-earth compounds (localized 4f or 5f shells) can be described as "Kondo lattices".
- This includes so called "heavy fermion" materials (e.g. Cerium and Uranium-based compounds: $CeCu_2Si_2$; UBe_{13} ; etc).

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:



- Early '30s : Resista... in some metals
- Early '50s : theoreti... purities in metals "Virtual Bound State..."
- 1961: An... in metals

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

- 1964: s-d model and Kon... solution (PT)
- 1970: Anderson "Poor's m...n scaling"
- **1974-75: Wilson's Numerical Renormalization Group (non PT)**
- 1980 : Andrei and Wiegmann's exact solution

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

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

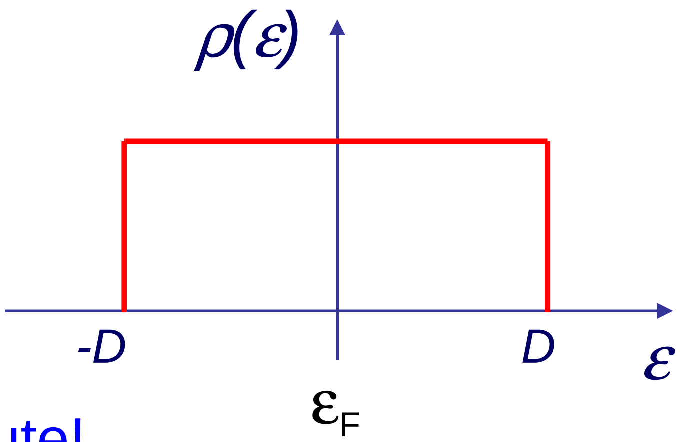
What is going on? {

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

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

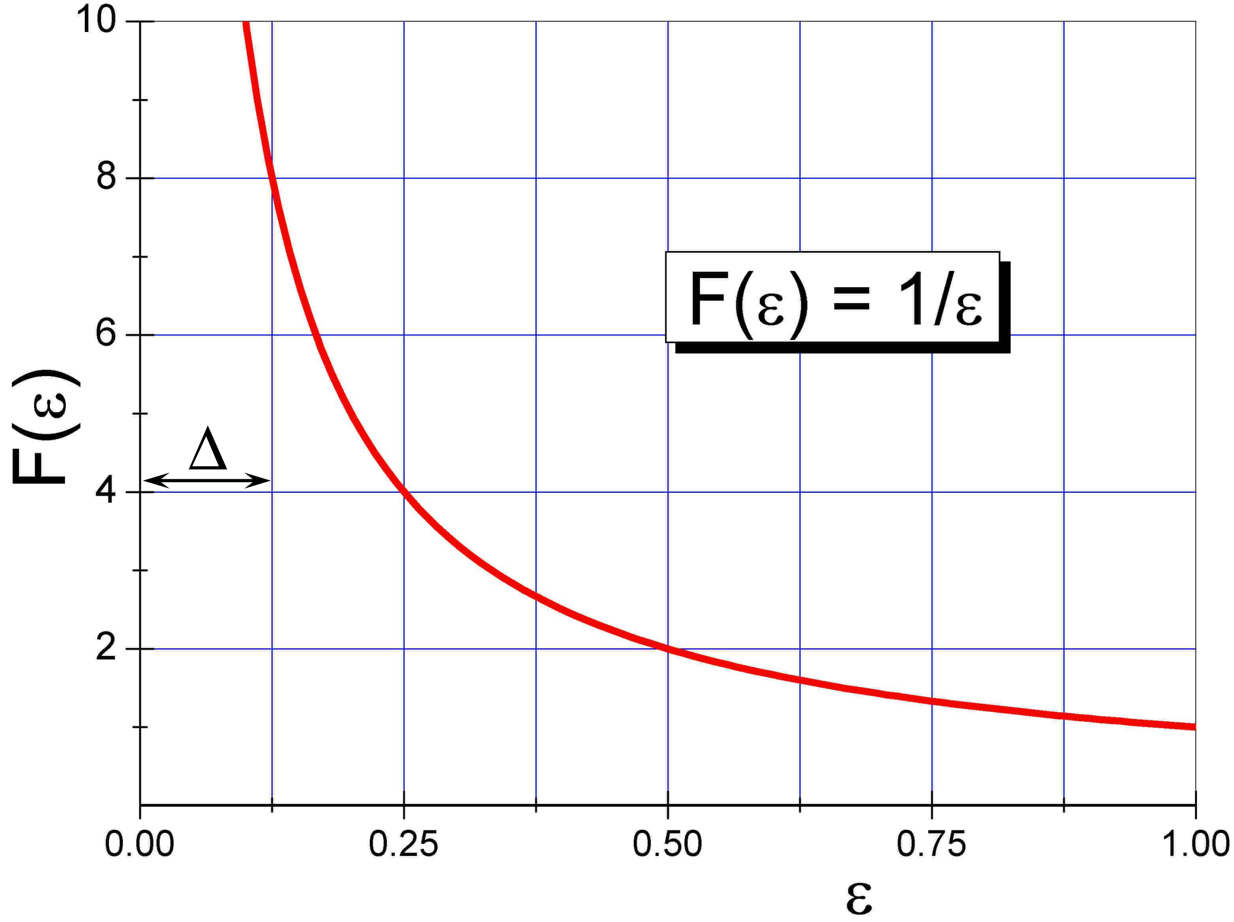
- Experiments show *finite* R as $T \to 0$ or $D \to \infty$.
- The log comes from something like:

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



- *All* energy scales contribute!

“Perturbative” Discretization of CB

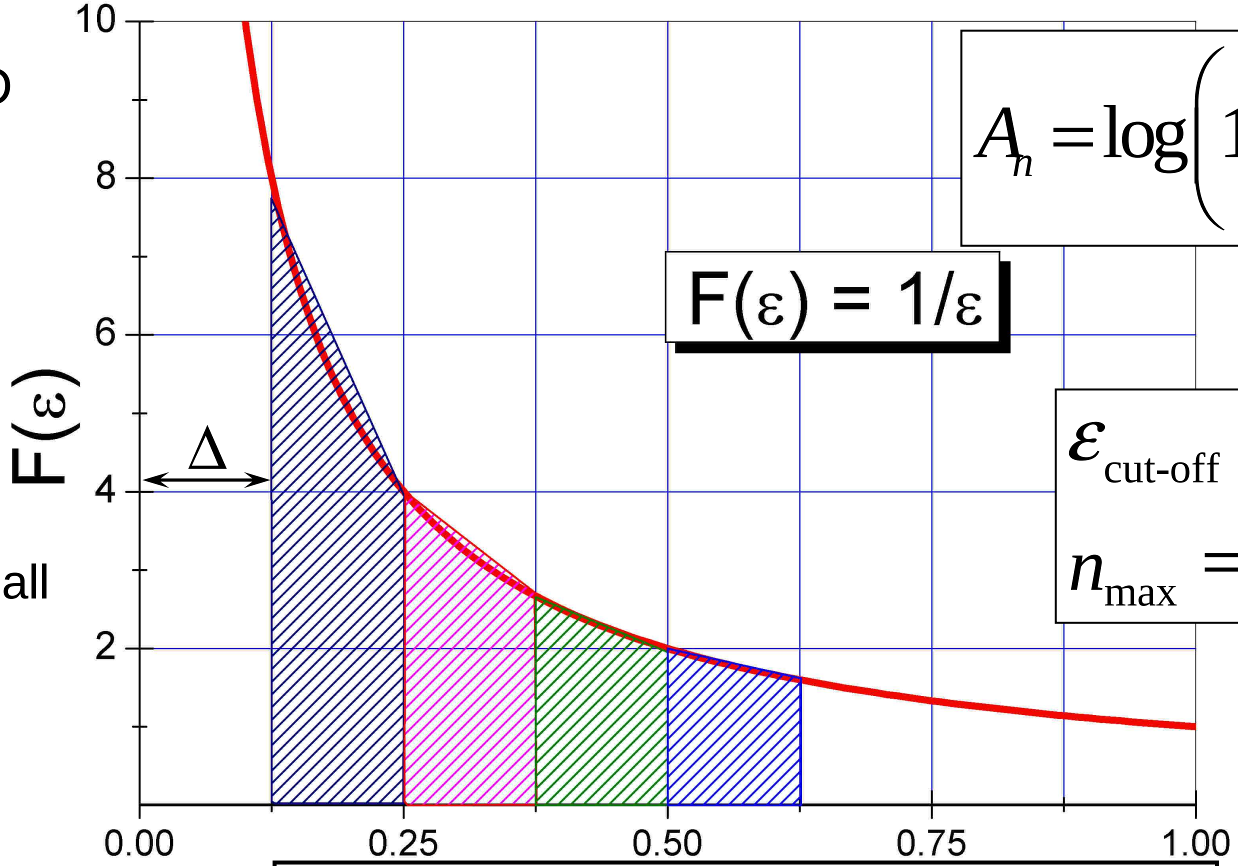


$\varepsilon = (E-E_F)/D$

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

"Perturbative" Discretization of CB

Δ = (ΔE)/D



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

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

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

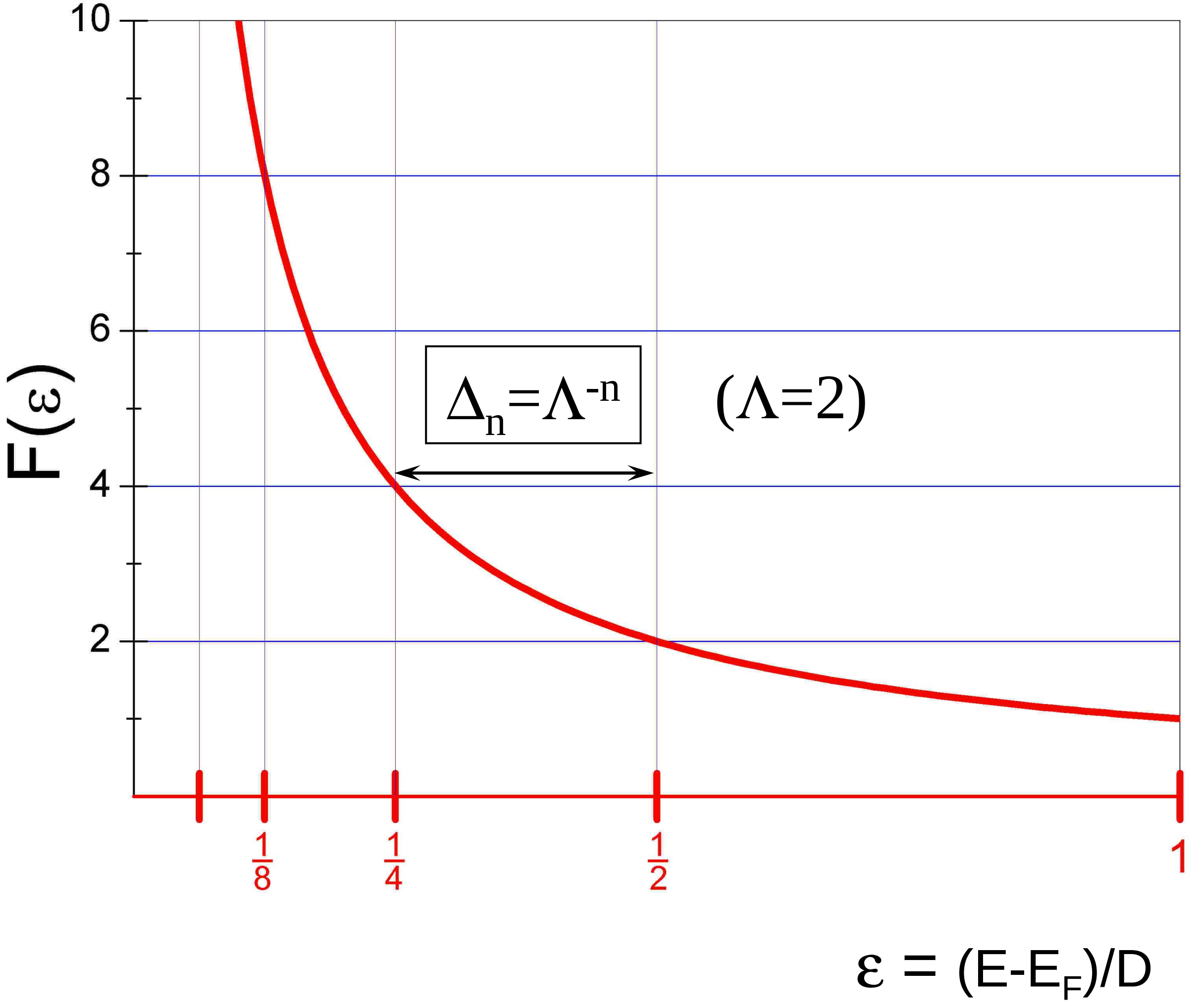
Want to keep all contributions

for D⟶∞?

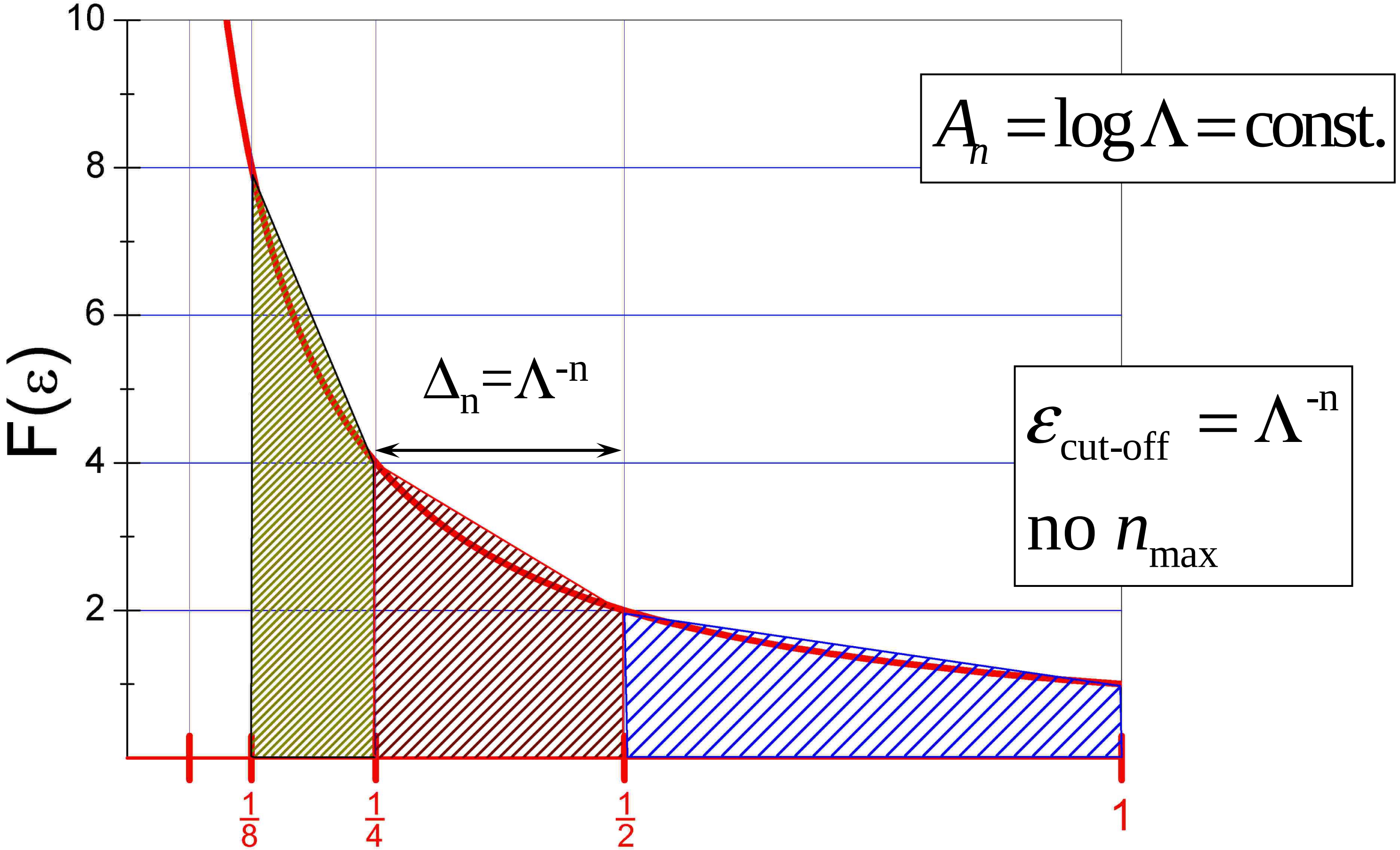
$$\mathbf{A_7} > \mathbf{A_6} > \mathbf{A_5} > \mathbf{A_4} > \mathbf{A_3} > \mathbf{A_2} > \mathbf{A_1}$$

Not a good approach!

Wilson's CB Logarithmic Discretization



Wilson's CB Logarithmic Discretization



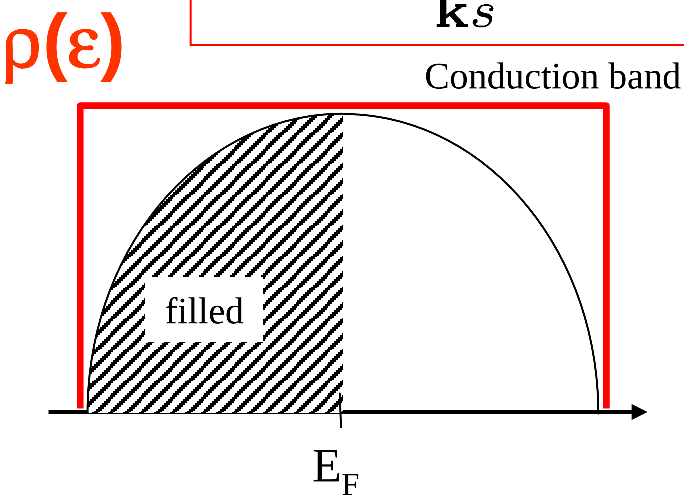
Now you're ok!

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

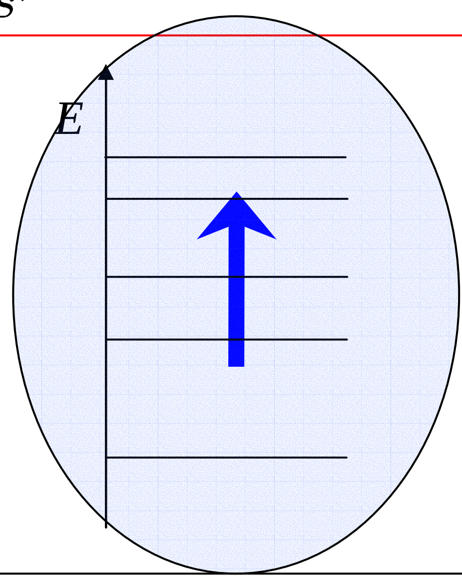
Kondo problem: s-d Hamiltonian

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

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



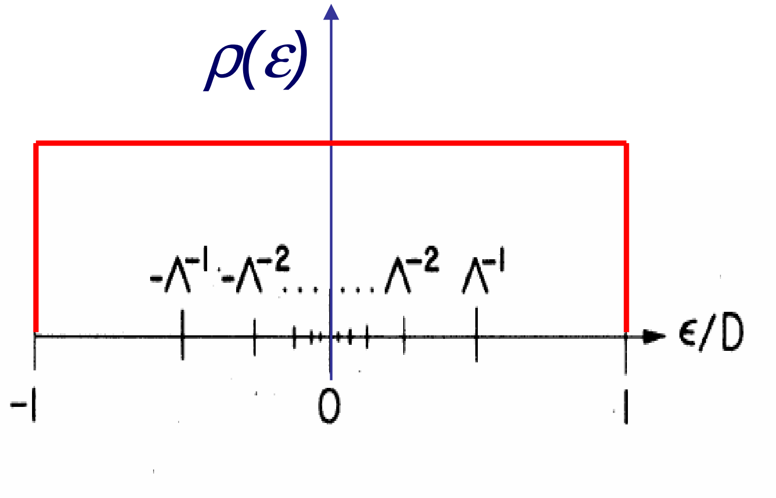
Metal (non magnetic, s-band)



Magnetic impurity (unfilled d-level)

Kondo s-d Hamiltonian

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

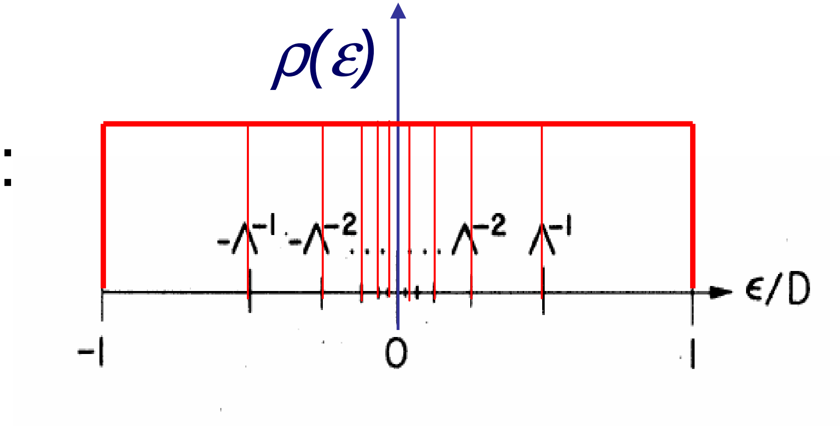


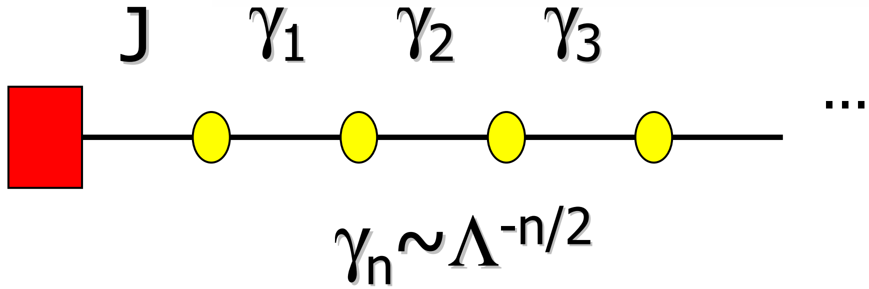
- From continuum *k* to a *discretized* band.
- Transform $H_{\text{s-d}}$ into a linear chain form (exact, as long as the chain is infinite):

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

"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

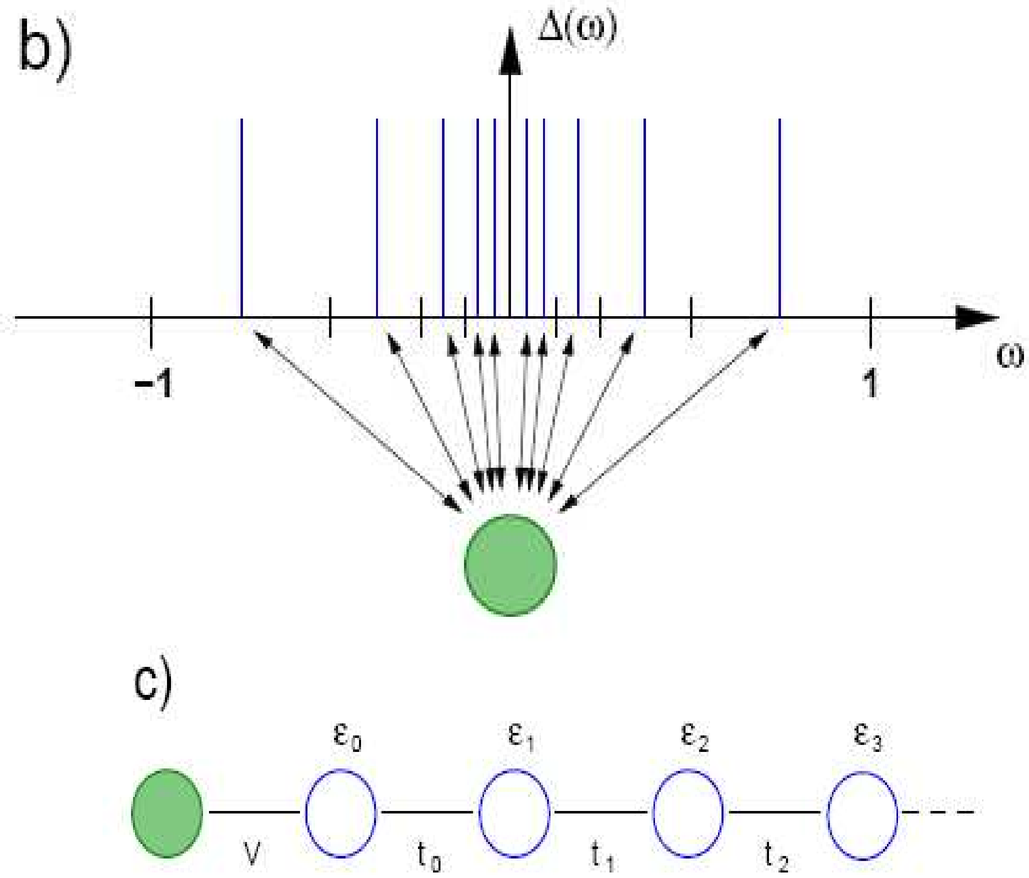




Logarithmic Discretization.

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):

$\Lambda > 1$

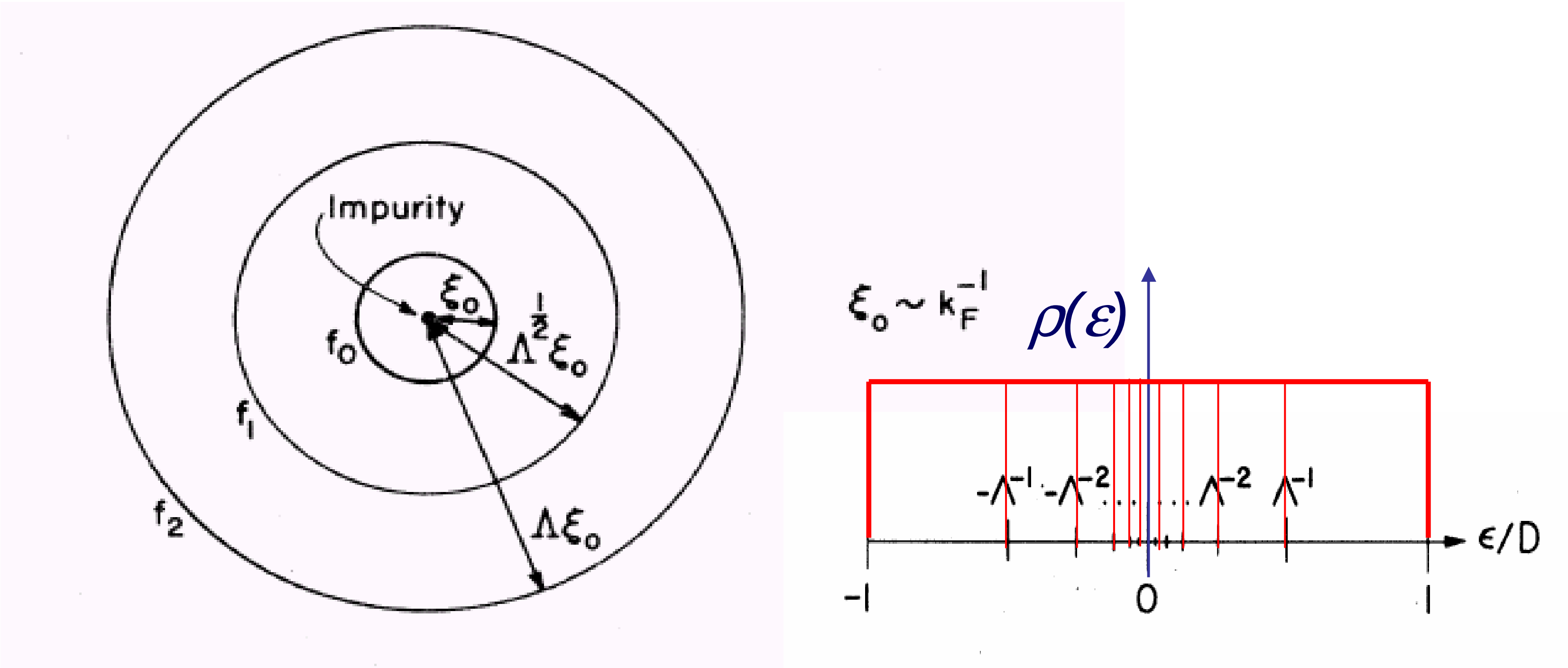


FIG. 4. Spherical shells in r space depicting the extents of the wave functions of f_n. Within their shells, every wave function has oscillations so that they are mutually orthogonal. Alternately one can show that, in the wave-vector space,

Wilson's CB Logarithmic Discretization

- Logarithmic Discretization (in energy):

$\Lambda > 1$

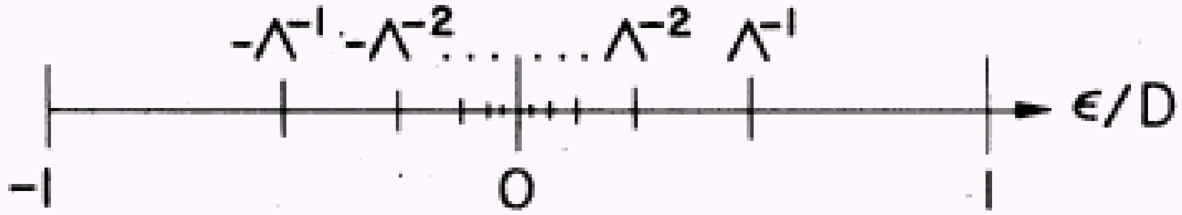
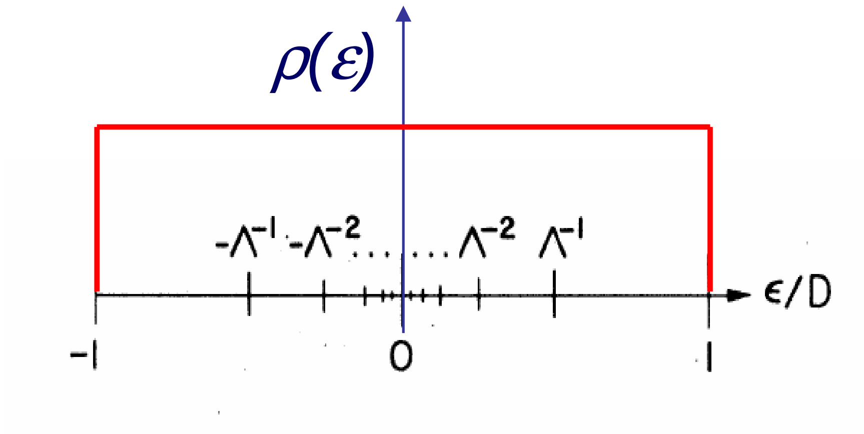


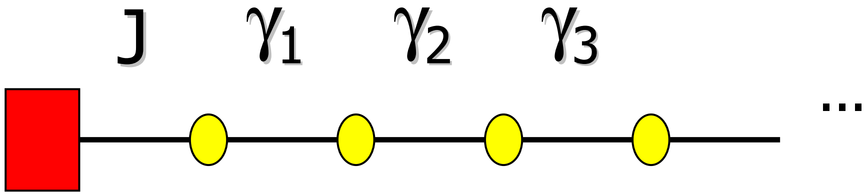
FIG. 1. Logarithmic discretization of the conduction bond. The Fermi energy is at zero and the top and bottom of the conduction bond at $k \equiv \epsilon/D = +1$ and -1, respectively.

“New” Hamiltonian (Wilson)

- Recurrence relation (Renormalization procedure).

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



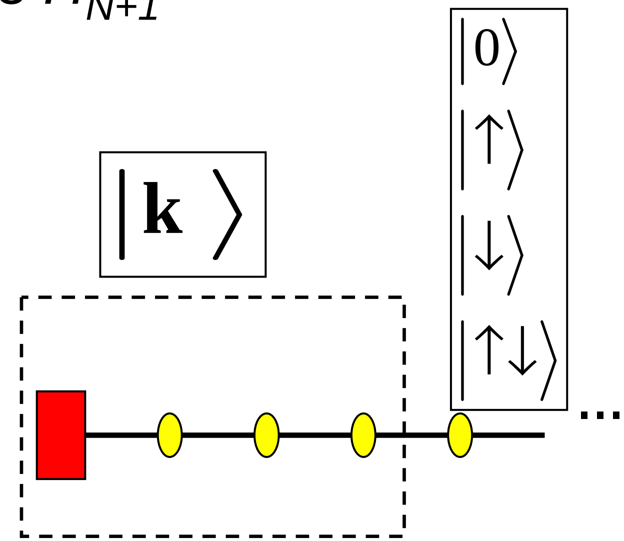


$\gamma_n \sim \Lambda^{-n/2}$

"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:

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

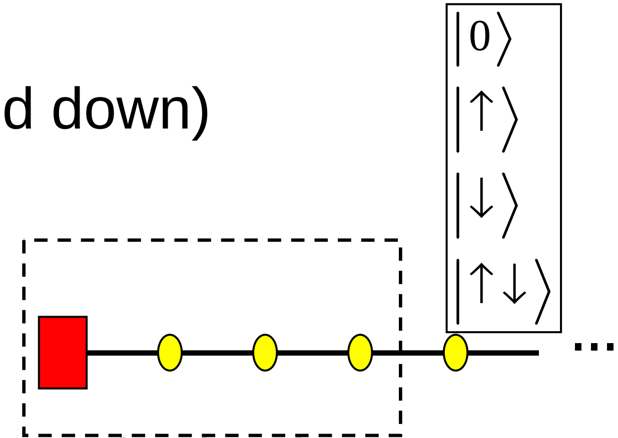


- Then you calculate $\langle k,a|f^{+}_{N}|k',a'\rangle$, $\langle k,a|f_{N}|k',a'\rangle$ and you have the matrix elements for H_{N+1} (sounds easy, right?)

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?

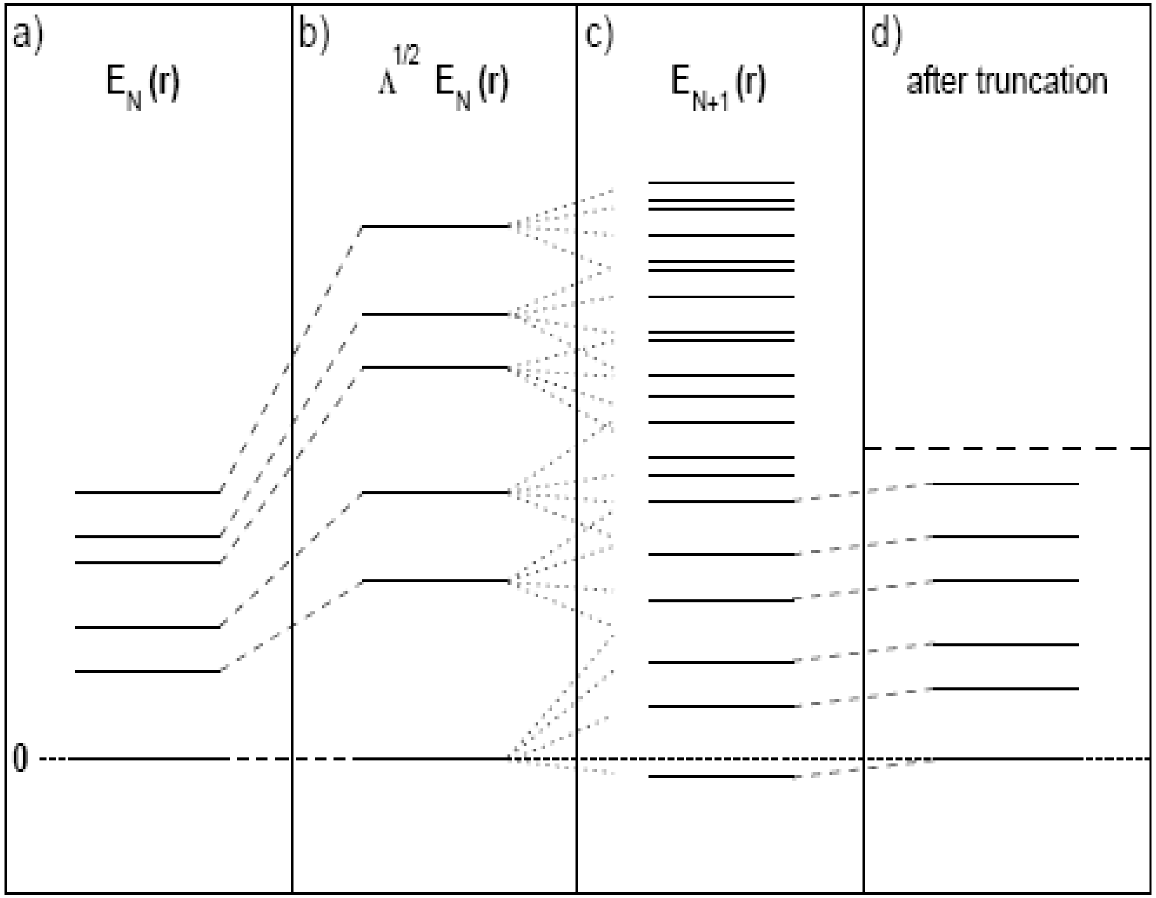
      (Hint: The number of atoms in the universe is ~ 10^{80})



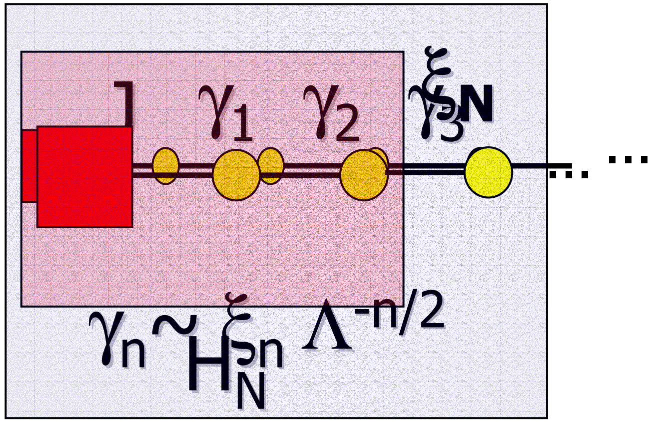
- Cut-off the basis $\rightarrow$ lowest ~1500 or so in the next round (Even then, you end up having to diagonalize a 4000x4000 matrix…).

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.



H_{N+1}

Renormalization Group Transformation

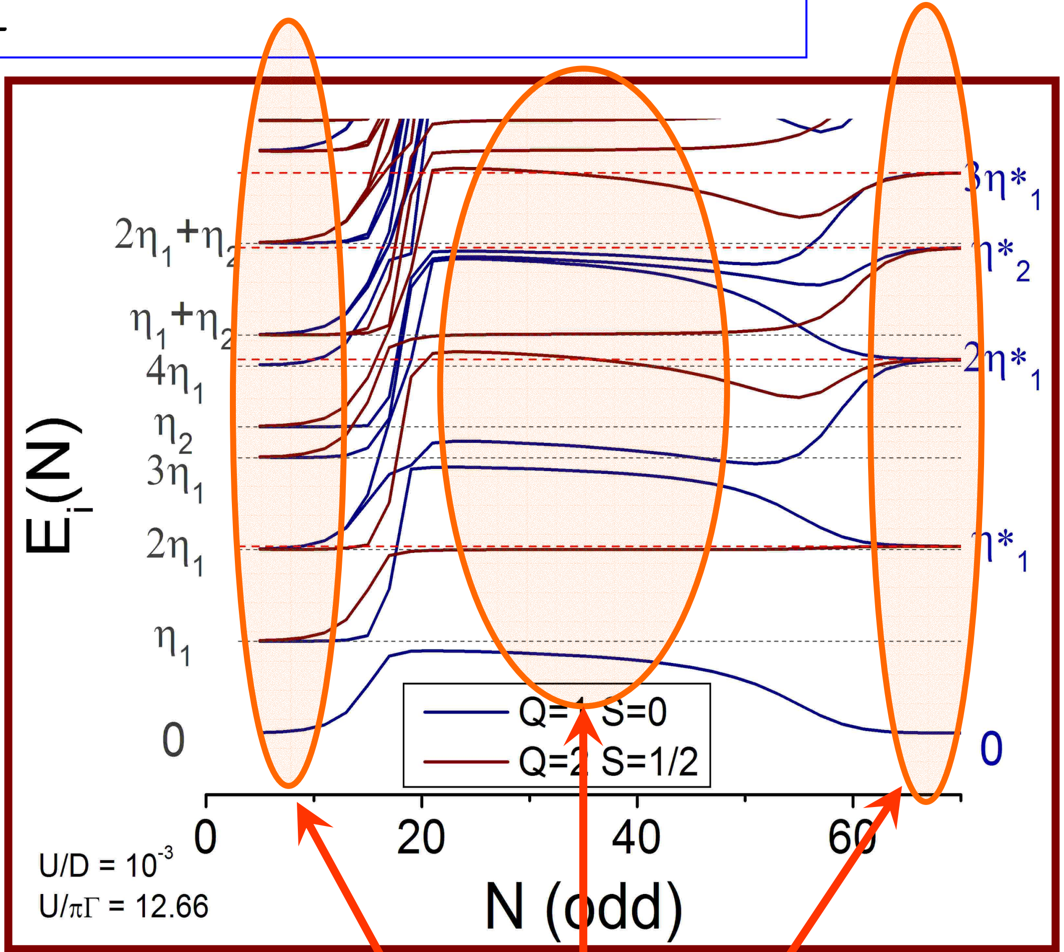
$$H_{N+1} = \sqrt{\Lambda} H_N + \xi_N \sum_{\sigma} f^{\dagger}_{N+1\sigma} f_{N\sigma} + f^{\dagger}_{N\sigma} f_{N+1\sigma}$$

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

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

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

$$\boxed{H^* = R^2(H^*)}$$

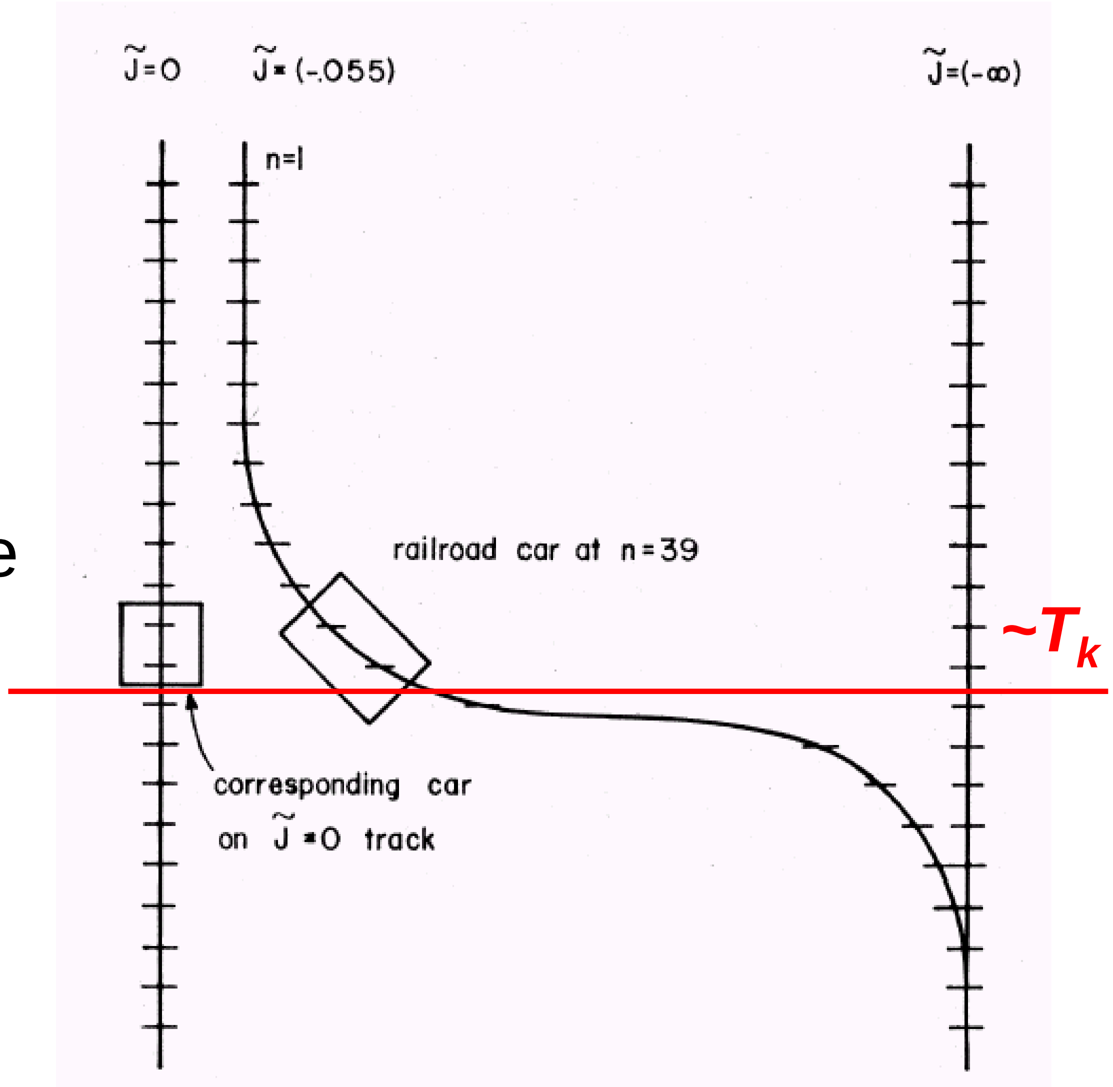


Fixed points

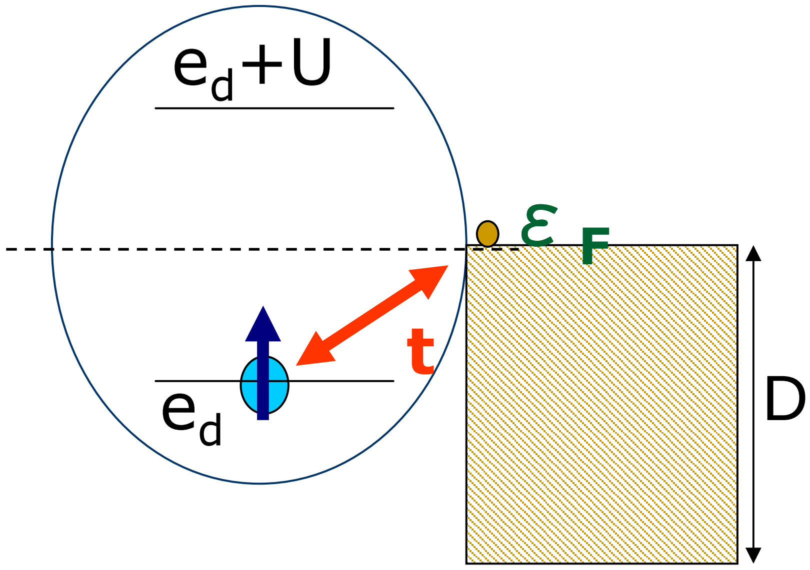
Numerical Renormalization Group

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



Anderson Model



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

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

- 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

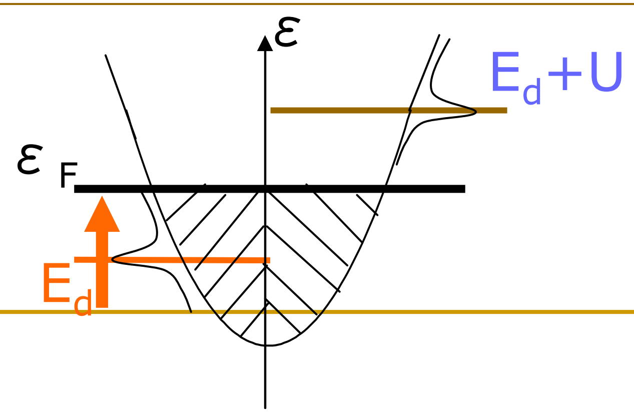
Schrieffer- Wolff Transformation

Anderson Model

Existence of localized moment

$$\left|V_{kd}\right| << U$$

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

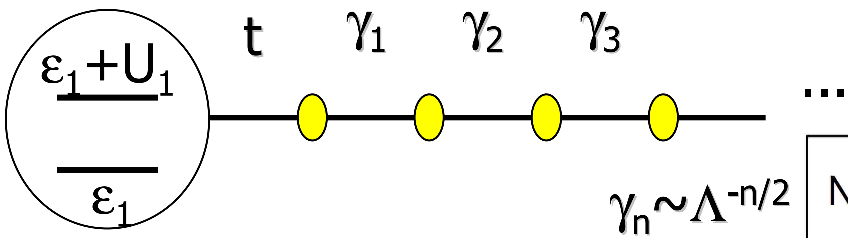
$$\begin{aligned} \hat{n}_{d\sigma} &= c^\dagger_{d\sigma} c_{d\sigma} \\ \hat{n}_{k\sigma} &= c^\dagger_{k\sigma} c_{k\sigma} \end{aligned}$$

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

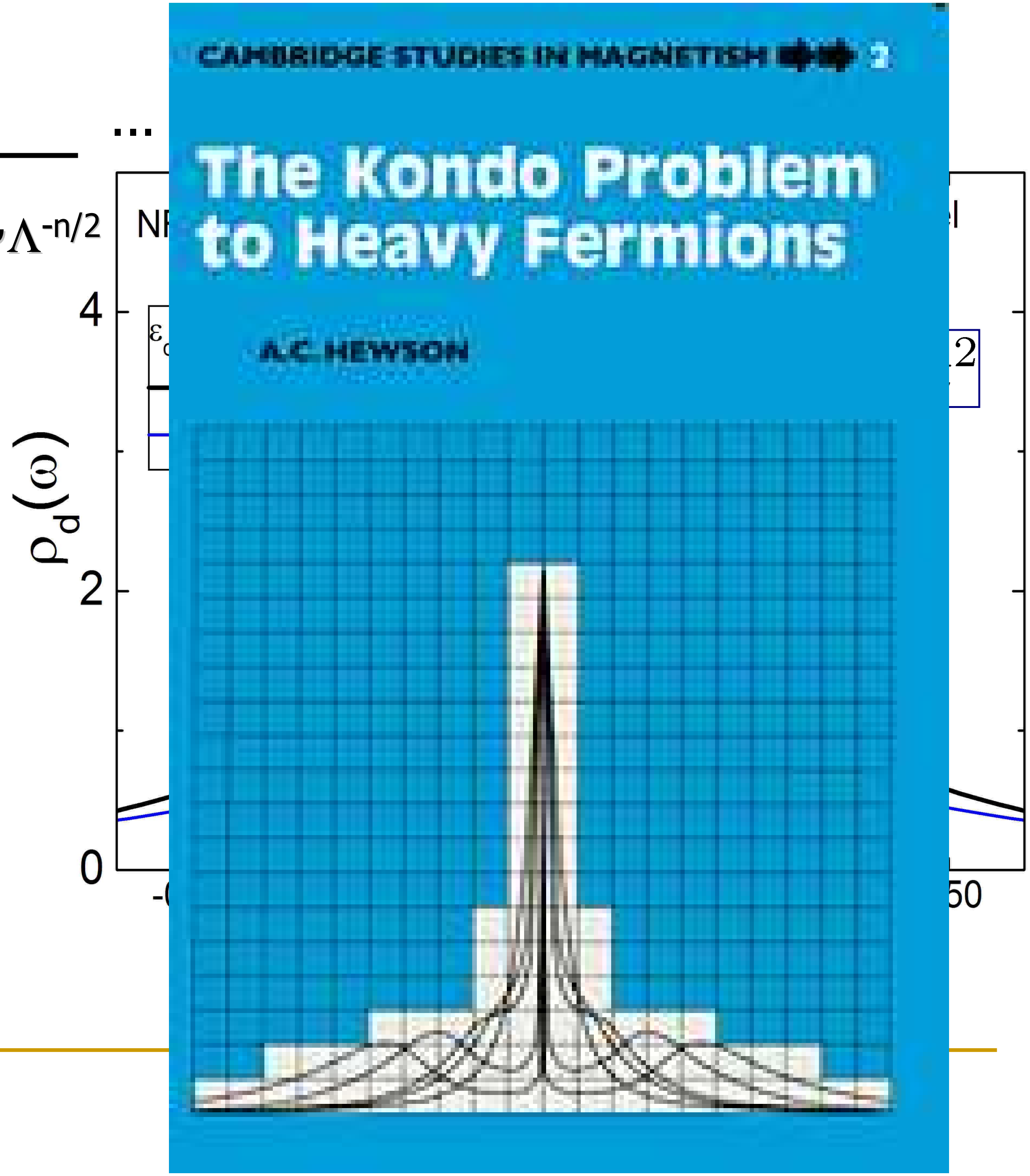
To: s-d (Kondo) Model

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

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).



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")
- ...

Lecture 3 (coming up)