Kondo effect in metals and nanostructures

Ramón Aguado ICMM-CSIC

Bibliography:

- A. C. Hewson “The Kondo problem to heavy fermions”, Cambridge University Press, 1997.

- P. Coleman, “Introduction to Many Body Physics” (chapters 16 and 17), Cambridge University Press , 2015

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Outline

- Historical introduction: first experimental puzzles.

- Theoretical developments that led to the understanding of the Kondo effect in metals:

  - the Anderson and Kondo models.
  - Kondo's calculation.
  - Anderson's scaling.
  - Non-perturbative approaches.
  - Strong coupling: the Kondo resonance.

- The two-impurity Kondo problem, generalization to the lattice (slave bosons and 1/N expansions) and relevance to heavy fermion materials.

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Lecture II

- The two-impurity Kondo problem, generalization to the lattice (slave bosons and 1/N expansions) and relevance to heavy fermion materials.

Outline

- Modern aspects of the Kondo effect in mesoscopic systems: quantum dots and nanotubes, non-equilibrium effects, etc.

- New developments: hybrid systems (competition between superconductivity and Kondo), Yu-Shiba-Rusinov, states, etc.

Lecture III

Local magnetic moments in metals

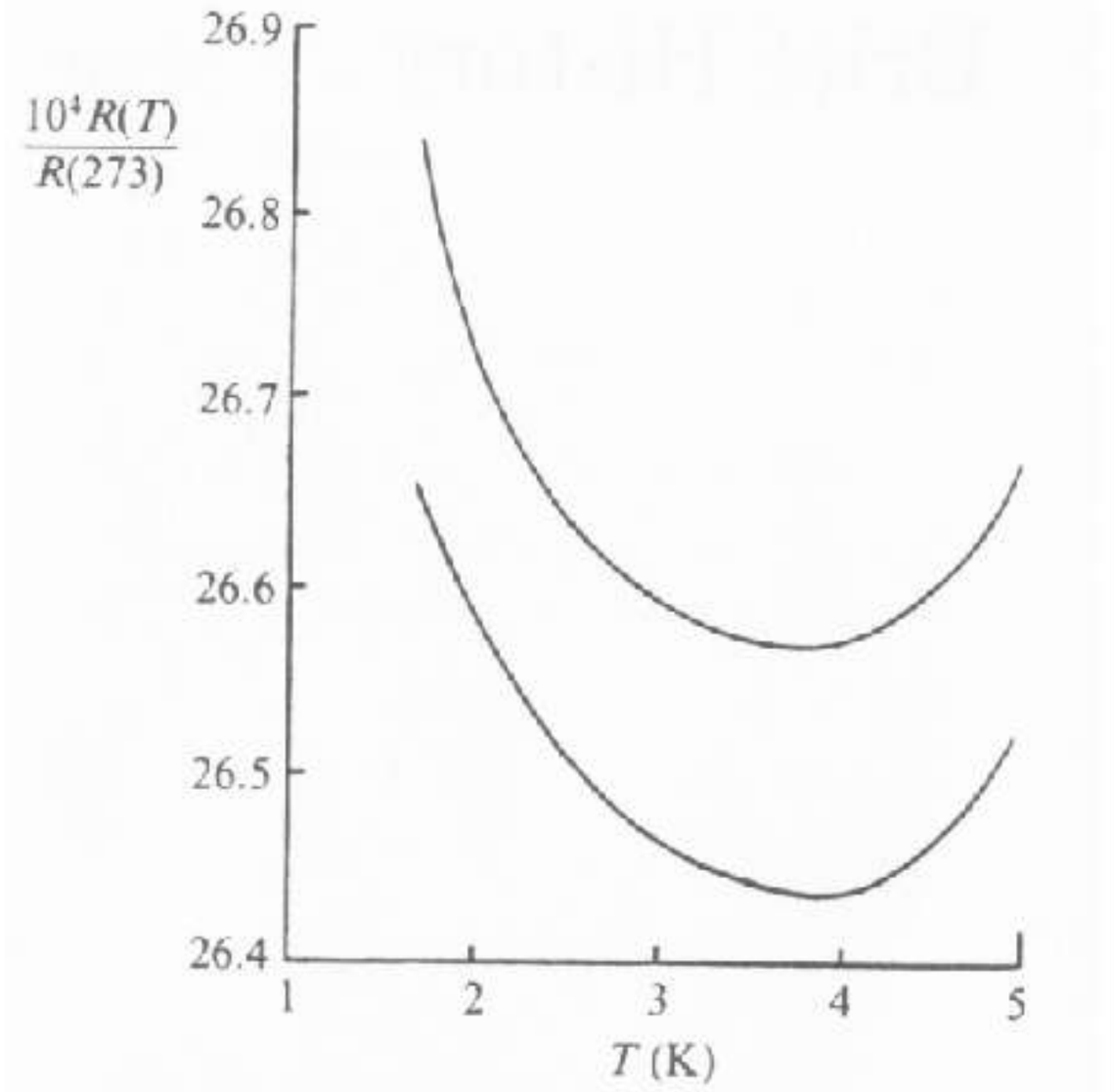
Some relevant questions:

- How does a magnetic moment survive in a metallic environment?

- How does it affect the conduction electrons of the host metal?

- What is the origin of various anomalous contributions to many metallic properties, particularly transport?

Early puzzles

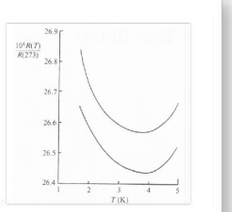


First experiments in Leiden (1934): de Haas et al discovered a “resistance minimum” that develops in the resistivity of copper, gold, silver and many other metals at low temperatures.

The phonon contribution becomes smaller as temperature decreases as

$$R(T) \sim T^5$$

but, somehow, the resistivity increases as low temperatures.
What is going on?



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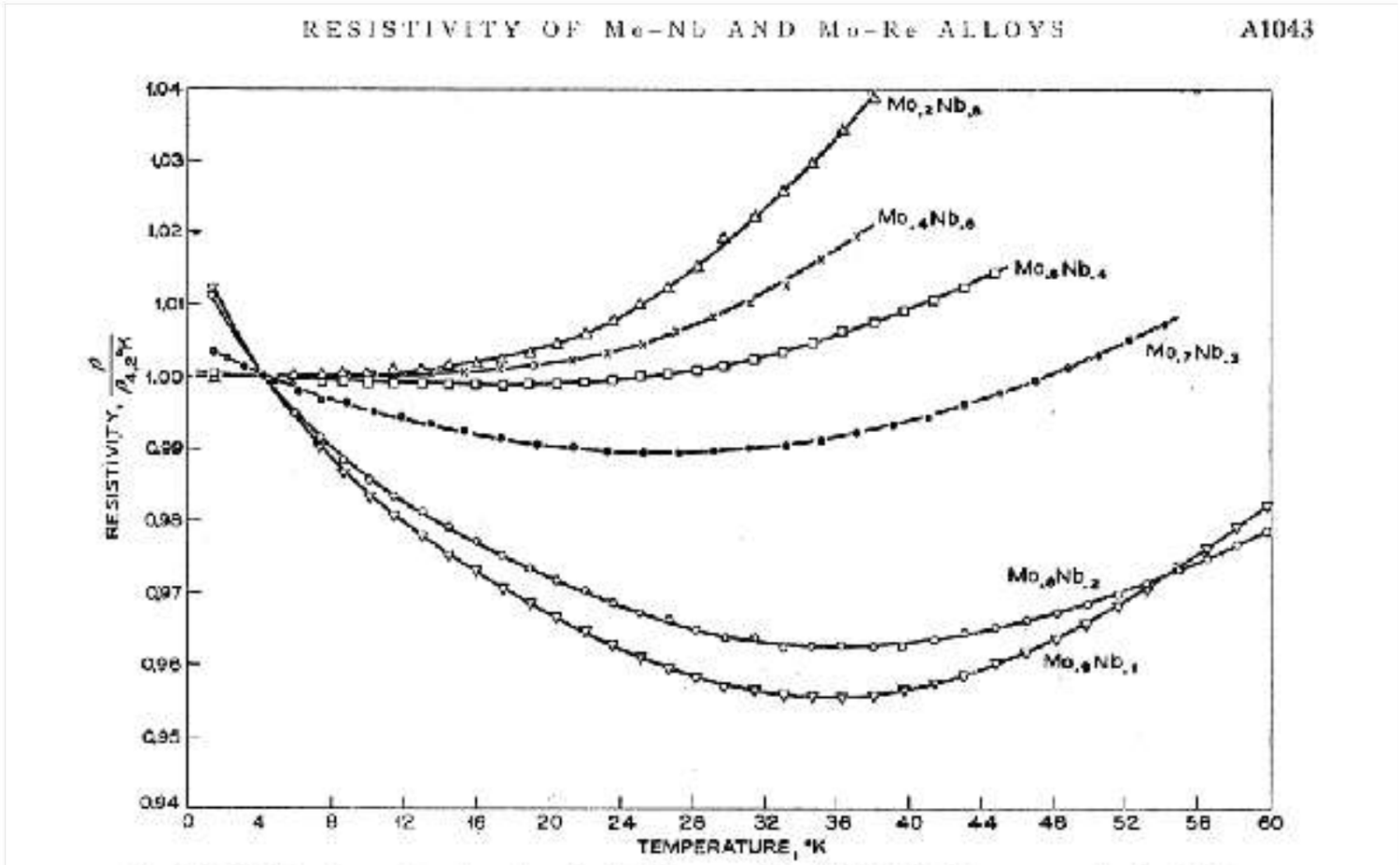
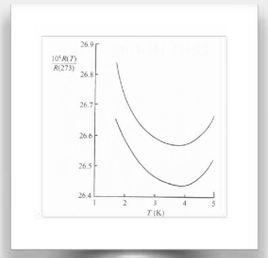
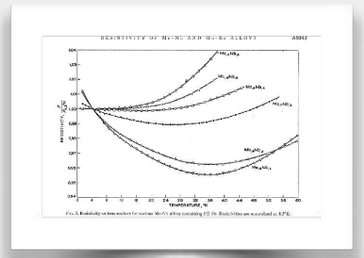


FIG. 3. Resistivity vs temperature for various Mo-Nb alloys containing 1% Fe. Resistivities are normalized at 4.2°K.

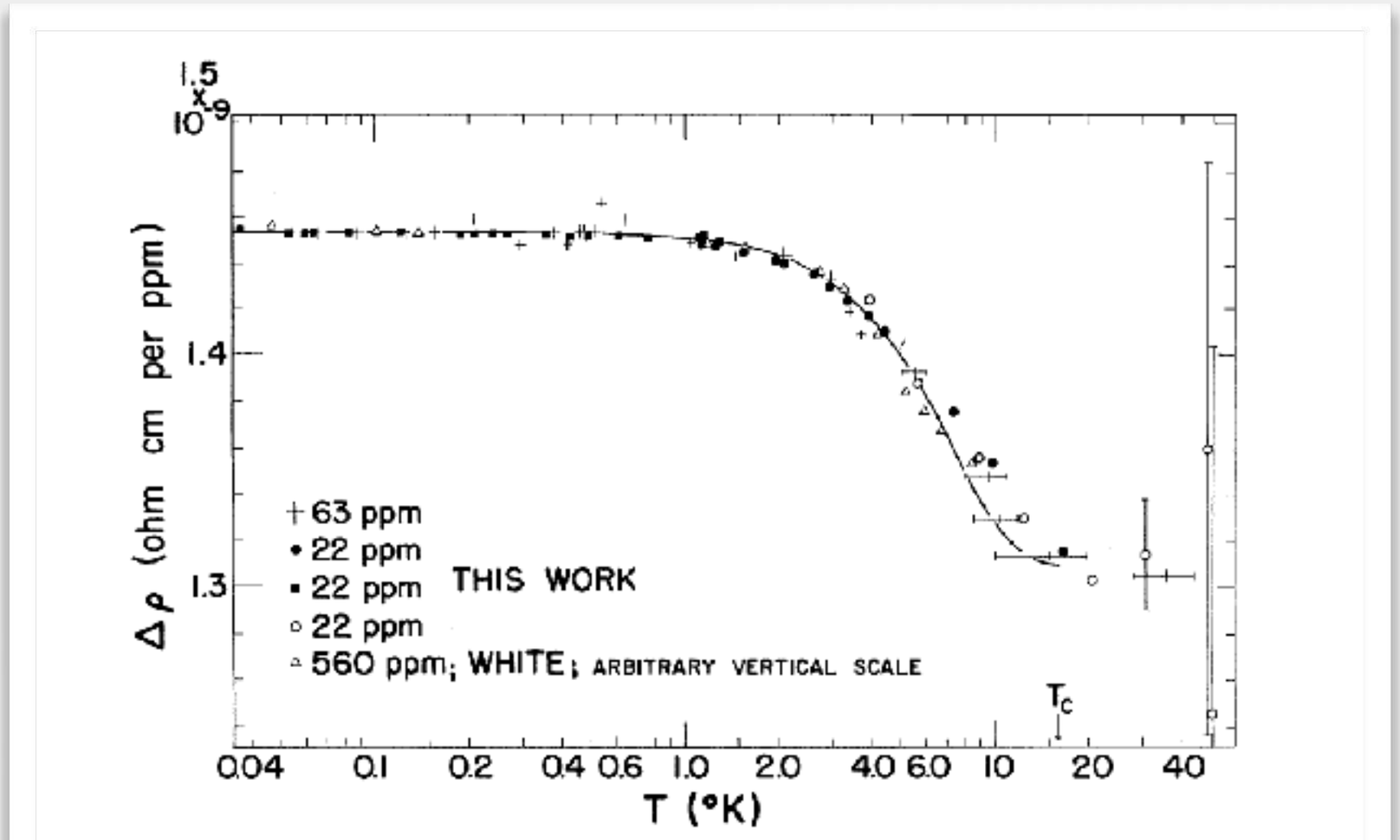
It took a further 30 years before the purity of metals and alloys improved to a point where the resistance minimum could be linked to the presence of magnetic impurities

Clogson et al, 1962;
Sarachik et al, 1964

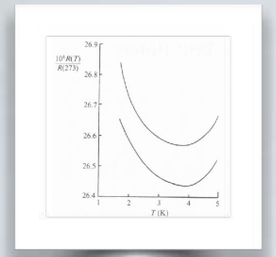


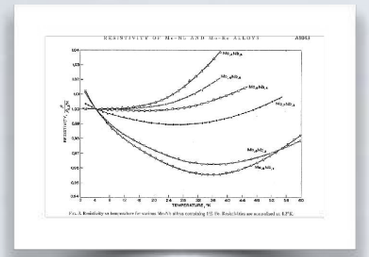


Early puzzles

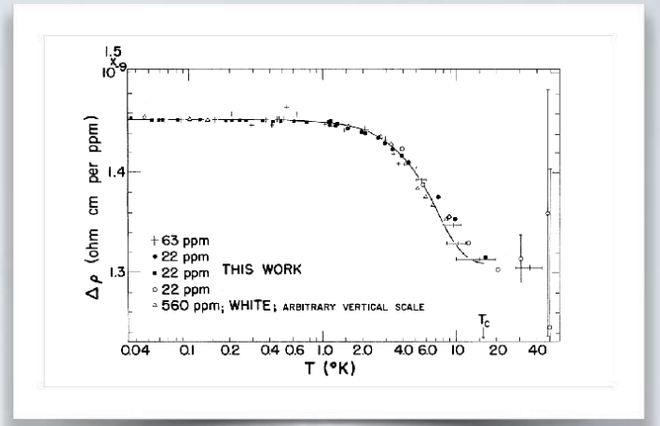


Such anomalous behavior of the electrical resistivity as a function of temperature challenged theorists for decades. The resistivity **increases logarithmically** as temperature decreases!!!



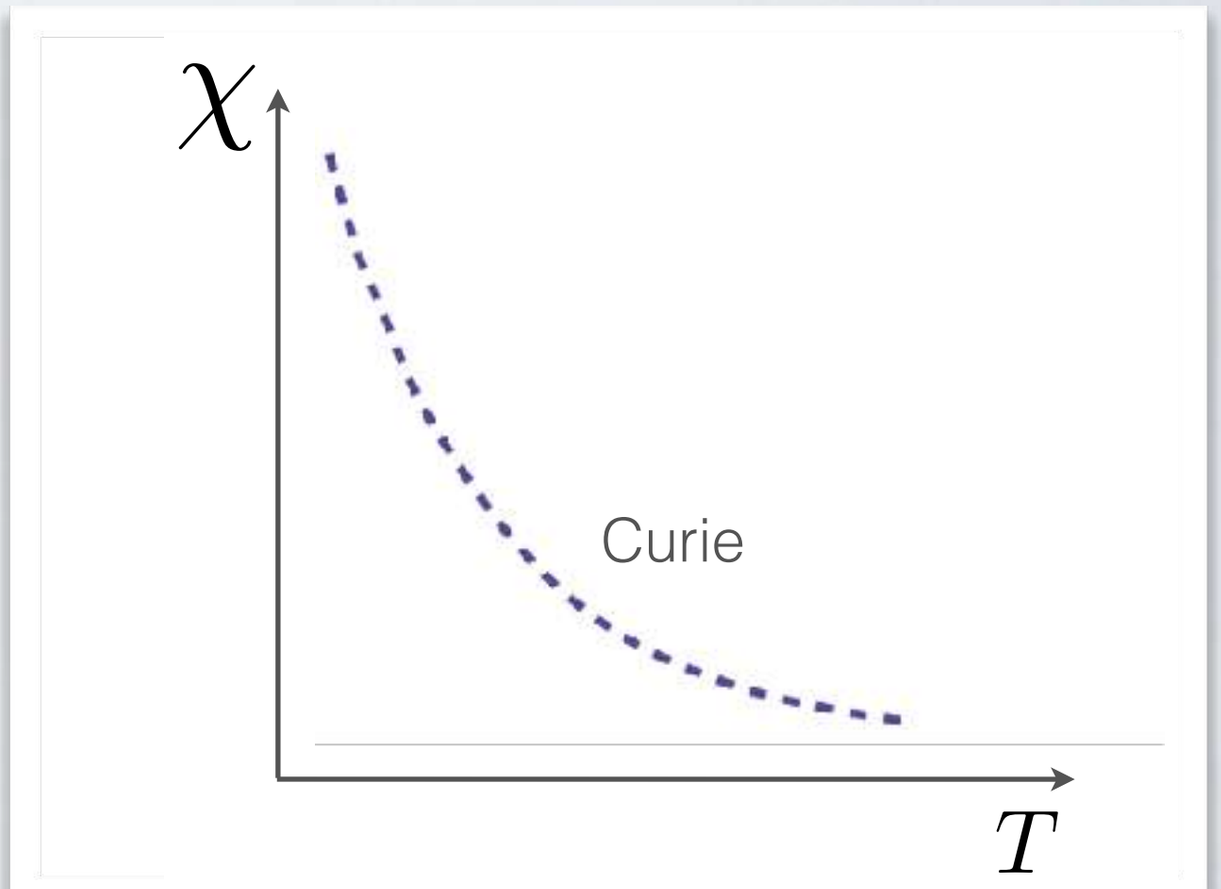


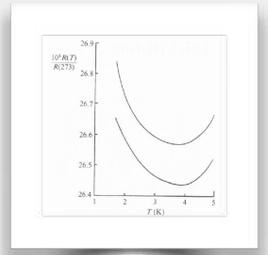
Early puzzles

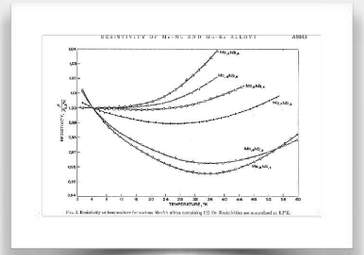


- Magnetic impurities contribute with a Curie-Weiss term in the spin susceptibility in addition to the temperature independent Pauli susceptibility of the host metal:

$$\chi = \frac{g^2 \mu_B^2 S(S+1)}{3k_B(T+T_0)}$$







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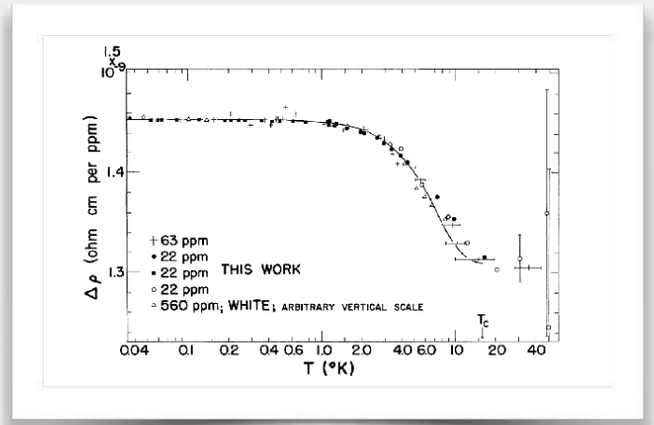
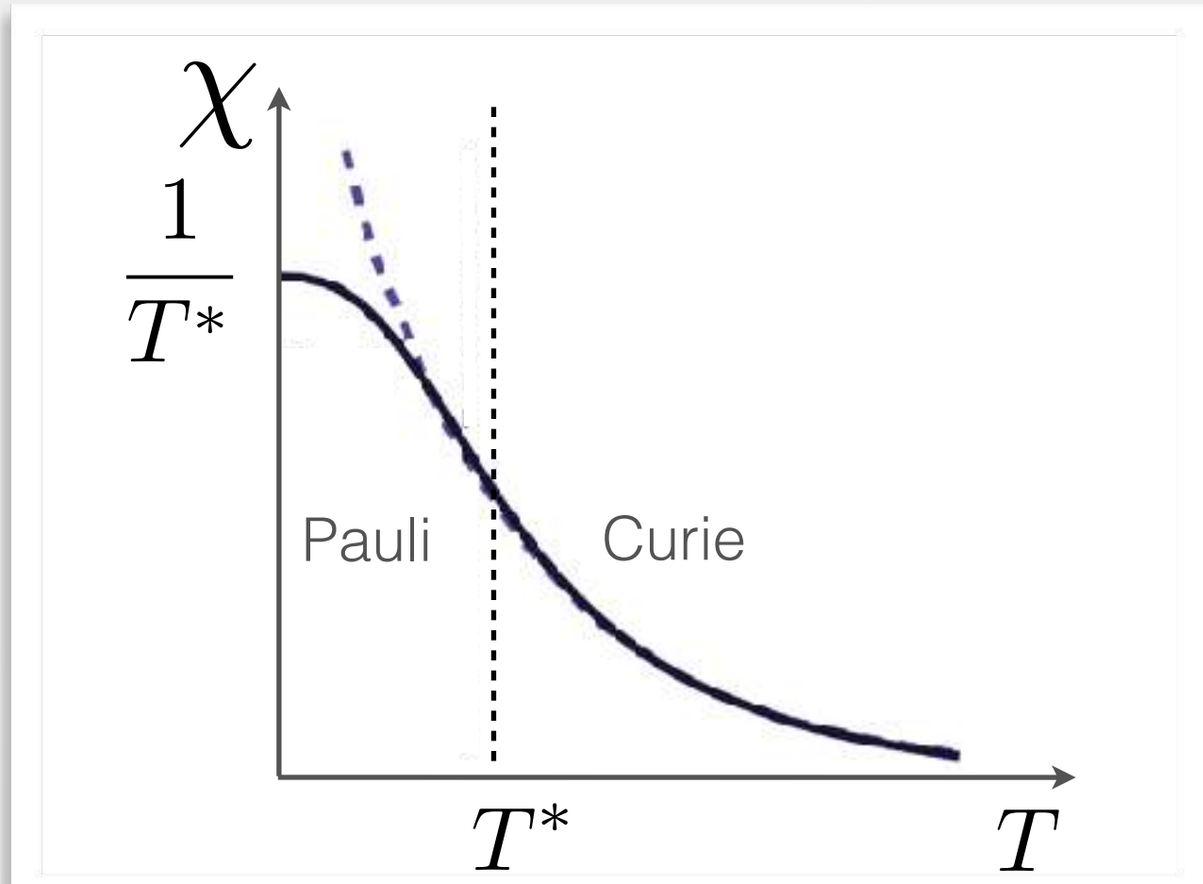


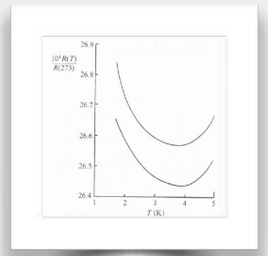
Apart from the minimum in resistivity many anomalous features:

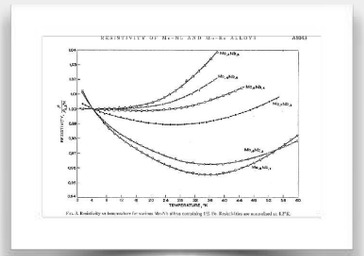
- The logarithmic increase saturates at a characteristic temperature T*.

- At this T*, the susceptibility changes from Curie to constant=Pauli (the local moment “disappears”!).

- Completely opposite to ferromagnetism: at low enough temperatures, traces of magnetism seem to disappear.







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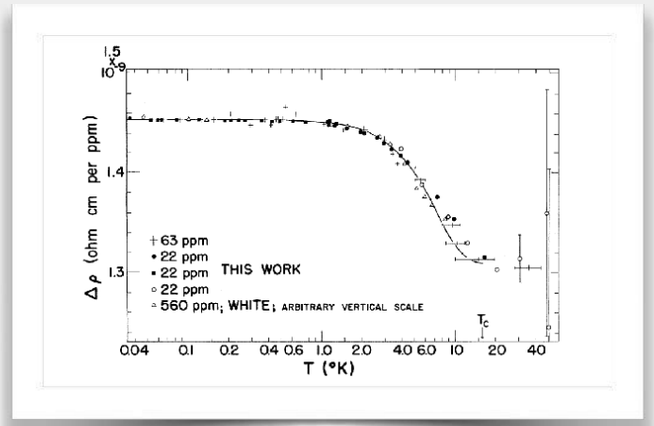
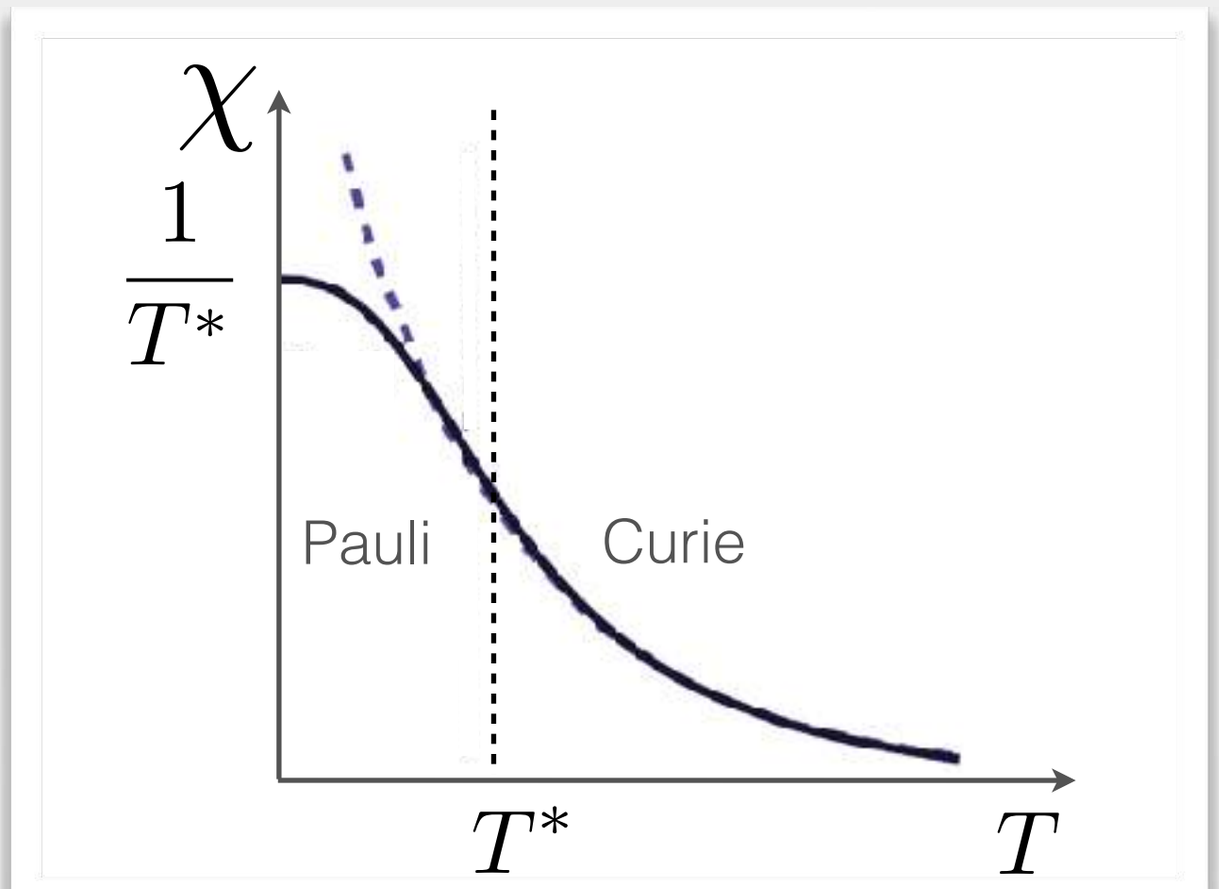
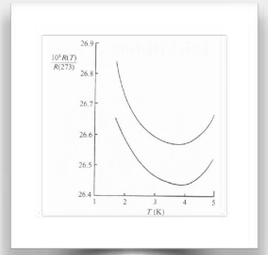


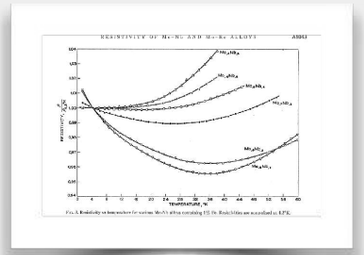
Key observation:

- A constant susceptibility at T=0 is characteristic of a <u>singlet</u> state.

- Since the logarithmic increase of resistivity vanishes once the impurities begin to condense into singlet states, the resistivity minimum <u>must be due to the interaction of the impurity spin with those of the host metal.</u>







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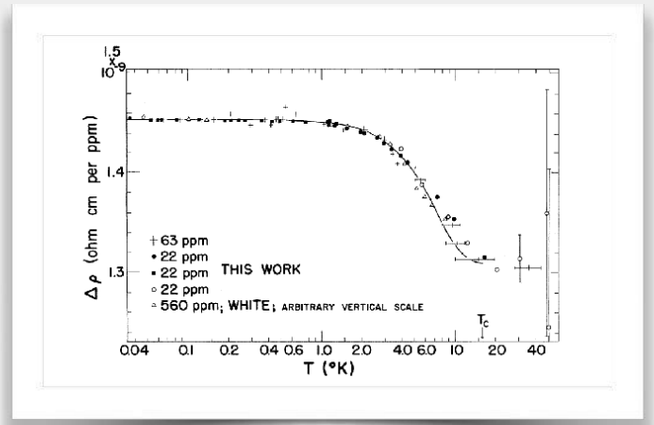
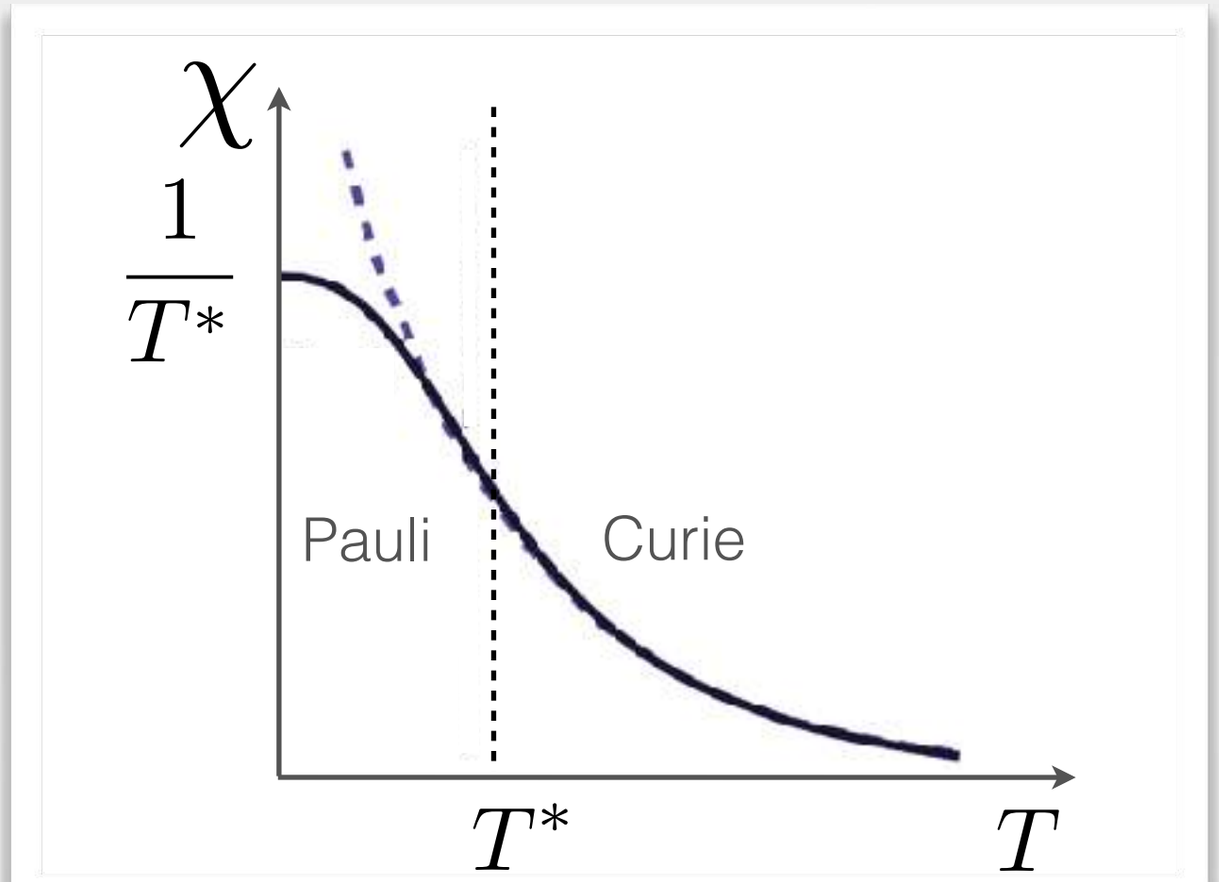
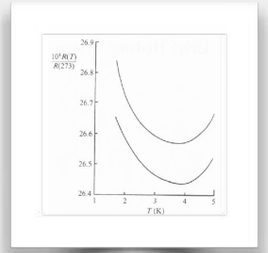
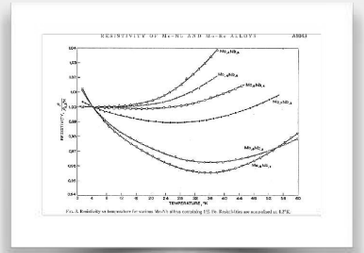


- Big puzzle: band theory (very successful at that time) **could not** explain these observations.

- The question was: **what a magnetic moment in a metal means?**







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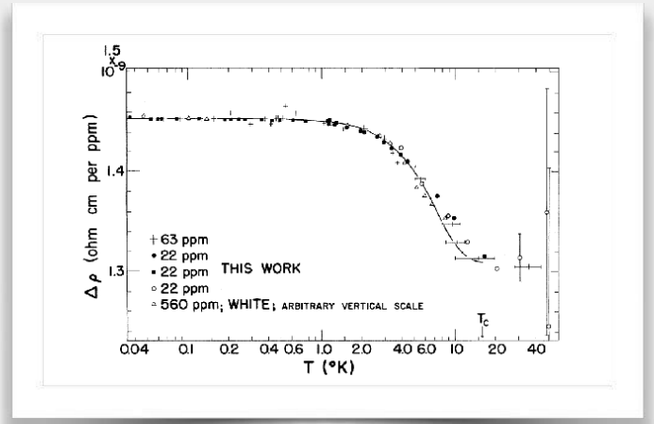


- First models describing magnetic impurities in metallic hosts appear in the 1950's (MJ Calderón's lecture).
- These models are essentially **ad-hoc Heisenberg-like models** between the impurity spins and conduction electrons.

$$\sum_{k\sigma} \varepsilon_k n_{k\sigma} + J\vec{S}.\vec{s}$$

PHYSICAL REVIEW VOLUME 81, NUMBER 4 FEBRUARY 1, 1951

Interaction Between the *d* Shells in the Transition Metals*

C. ZENER
Institute for the Study of Metals, University of Chicago, Chicago, Illinois
(Received October 9, 1950)

It is assumed (1) that the interaction between the incomplete *d* shells of the transition elements is insufficient to disrupt the coupling between the *d* electrons in the same shells, and (2) that the exchange interaction between adjacent *d* shells always has the same sign irrespective of distance of separation. The direct interaction between adjacent *d* shells then invariably leads to a tendency for an antiferromagnetic alignment of *d* spins. The body-centered cubic structure of the transition metals V, Cr, Cb, Mo, Ta, and W is thereby interpreted, as well as more complex lattices of certain alloys. It is demonstrated that the spin coupling between the incomplete *d* shells and the conduction electrons leads to a tendency for a ferromagnetic alignment of *d* spins. The occurrence of ferromagnetism is thereby interpreted in a much more straightforward manner than through the *ad hoc* assumption of a reversal in sign of the exchange integral. The occurrence of antiferromagnetism and of ferromagnetism in various systems is readily understood, and certain simple rules are deduced for deciding which type of magnetism will occur in particular alloys.

Also, Owen, Browne, Knight and Kittel, Phys. Rev. 102, 1501 (1956)
Yosida, Phys. Rev. 106, 893 (1957), etc.

Local magnetic moments in metals: some history

LOCAL MOMENTS AND LOCALIZED STATES

Nobel Lecture, 8 December, 1977

by
PHILIP W. ANDERSON
Bell Telephone Laboratories, Inc, Murray Hill, New Jersey, and Princeton University, Princeton, New Jersey, USA

first, they flew in the face of the overwhelming ascendancy. at the time of the band theory of solids, in emphasizing *locality* : how a magnetic moment, or an eigenstate, could be permanently pinned down in a given region. It is this fascination with the local and with the failures, not successes, of band theory,

1928 Felix Bloch's PhD Thesis "Quantum Mechanics of Electrons in Crystals and Developing the Theory of Metallic Conduction". First student of Werner Heisenberg just one year after his famous uncertainty principle was formulated.

Local magnetic moments in metals: basic phenomenology

Anderson's model combines two basic ideas:

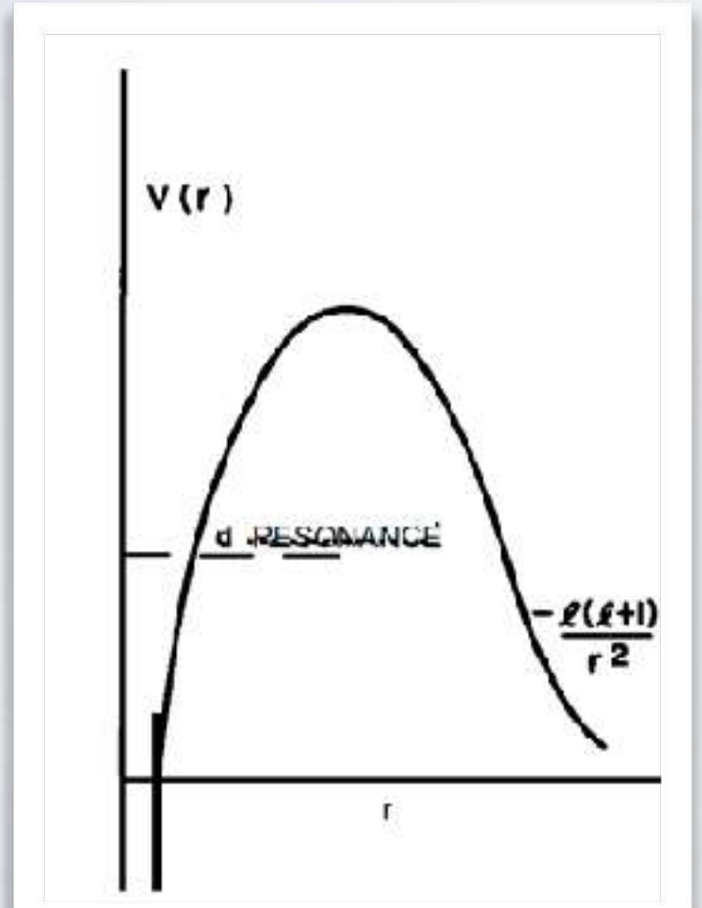
1. **The localizing influence of Coulomb interactions**. Peierls and Mott had reasoned in the 1940s that strong-enough Coulomb repulsion between electrons in an atomic state would blockade the passage of electrons, converting a metal into what is now called a "Mott insulator". These ideas were independently explored by Van Vleck and Hurvitz in an early attempt to understand magnetic ions in metals.

2. **The formation of an electronic resonance.** In the 1950's Friedel and Blandin proposed that electrons in the core states of magnetic atoms tunnel out into the conduction sea, forming a resonance. Revolutionary idea at that time: Impurities in a metal can be described as scattering processes.

Local magnetic moments in metals: some history

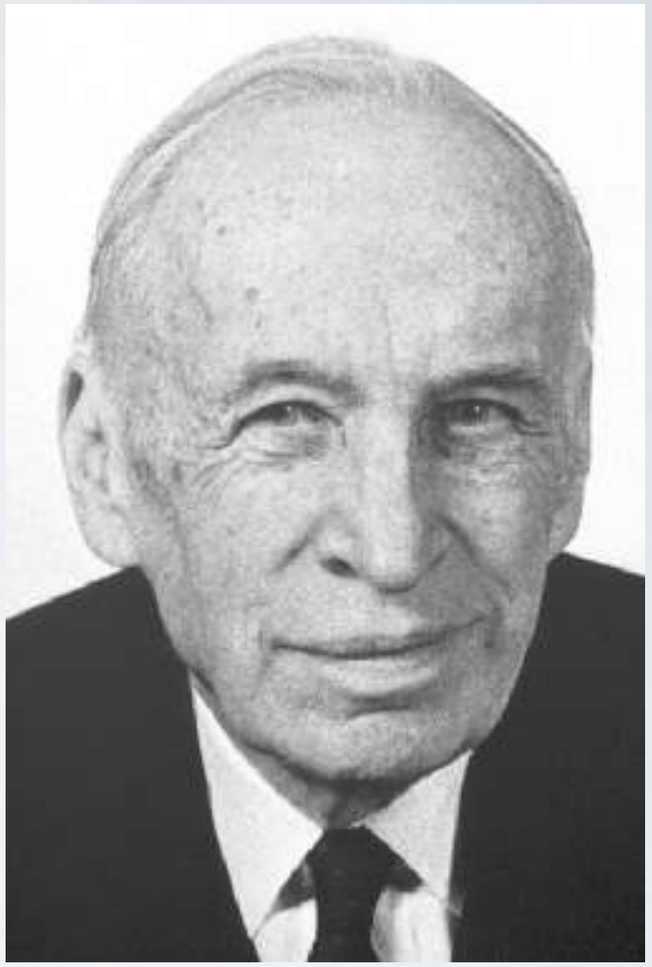
- An impurity in a nonmagnetic metal can give rise to a local moment if an electronic state on the impurity is singly occupied (Friedel, Nuovo Cimento Supp. VII 287, 1958).

- Friedel's model describes the effect of the impurity as an effective deep Coulombic core plus an angular momentum-dependent centrifugal barrier



- Such a potential can support bound states. Those occurring well below the Fermi energy will be doubly occupied and have no magnetic moments. A local magnetic moment can form, however, in a bound or resonant state of the impurity near the Fermi level if spins are nondegenerate.

Local magnetic moments in metals: some history



The Nobel Prize in Physics 1977 was awarded jointly to Philip Warren Anderson, Sir Nevill Francis Mott and John Hasbrouck Van Vleck "for their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems"

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The implications for magnetism in metals - as opposed to insulators - of this on-site Coulomb interaction U were first suggested by Van Vleck and elaborated in Hurwitz' thesis (3) during the war, and later in a seminal paper which. I heard in 1951, published in 1953 (4). Also, very influential for me was a small conference on magnetism in metals convened at Brasenose College, Oxford, September 1959, by the Oxford-Harwell group, where I presented some very qualitative ideas on how magnetism in the iron group might come about. More important was my first exposure to Friedel's and Blandin's ideas on resonant or virtual states (5, 6) at that conference. The essence of Friedel's ideas were 1) that impurities in metals were often best described not by atomic orbitals but by scattering phase shifts for the band electrons, which would in many cases be of resonant form; 2) that spins in the case of magnetic impurities might be described by spin-dependent scattering phase shifts.

Local magnetic moments in metals: some history

- Anderson, adopting the basic ideas of Friedel, developed a one-band model of local moment formation (Anderson, Phys. Rev. 124, 41, 1961).

magnetic atom had no effect, or raised T_c (as in Fig. 3b). A systematic study of the occurrence of moments was carried out by Clogston *et al* (8). As yet, no real thought (except see Ref. (6)) had been given to what a magnetic moment in a metal *meant:* the extensive investigations of Owen *et al* (9) and of Zimmermann (10), for instance, on Mn in Cu, and the Yosida calculation (11), essentially postulated a local atomic spin given by God and called S, connected to the free electrons by an empirical exchange integral J; precisely what we now call the "Kondo Hamiltonian":

$$H = \sum_{k\sigma} \varepsilon_k \, n_{k\sigma} + \mathcal{J} \, \vec{S} \cdot \vec{s} \qquad (3)$$

where $s = \sum c^{+}_{k\sigma} \, \vec{\sigma}_{\sigma\sigma'} \, c_{k'\sigma'}$

is the local spin density of free electrons at the impurity.

The "Anderson model" (12) is the simplest one which provides an electronic mechanism for the existence of such a moment. We insert the vital on-site exchange term *U*, and we characterize the impurity atom by an additional

Local magnetic moments in metals: basic phenomenology

- Anderson, adopting the basic ideas of Friedel, developed a one-band model of local moment formation (Anderson, Phys. Rev. 124, 41, 1961).

- The band in the non-metallic host is represented by a set of Bloch states with band energies:

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

Second quantization

$$H_{band} = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma}$$

Local magnetic moments in metals: basic phenomenology

- The impurity is treated as a **local site on which a single orbital level is placed**. While this simplification does not capture the five-fold degeneracy of the d-orbitals of typical impuritties, such as Fe, Ni, Co, this deficiency is not crucial as we will see.

- We denote the wave function of the orbital $\phi_d(\vec{r})$ and the energy required to place an electron on the impurity with spin either up or down is ε_d

- The orbital can be either singly occupied or occupied by two electrons. The latter case costs an energy U which physically arises from the Coulomb repulsion between electrons and is thus given by

$$U = \langle d|V_{ee}|d\rangle = \int dr_1 dr_2 |\phi_d(r_1)|^2 \frac{e^2}{|r_1 - r_2|} |\phi_d(r_2)|^2$$

Local magnetic moments in metals: basic phenomenology

- The Anderson model only includes on-site interactions which is, a priori, a strong approximation. In general, an electron localized on a d-level interacts with localized electrons on other sites. These additional interactions where estimated by Hubbard (Proc. Roy Soc. Lond. A, 276, 238, 1964) in a lattice model for d-electrons

$$\langle ij|V_{ee}|kl\rangle = \int dr_1 dr_2 \phi_i^*(r_1)\phi_j^*(r_2)\frac{e^2}{|r_1 - r_2|}\phi_l(r_1)\phi_k(r_2)$$

on-site	$U = \langle ii\|V_{ee}\|ii\rangle \approx 20eV$
nearest neighbor	$V = \langle ij\|V_{ee}\|ij\rangle \approx 2eV$
exchange	$Y = \langle ij\|V_{ee}\|ji\rangle \approx 0.02eV$

Local magnetic moments in metals: basic phenomenology

- The final ingredient in the Anderson model is a spin-conserving coupling between the impurity level and the band states in the metal, described by a matrix element $V_{k,d}$ this interaction causes a hybridization of the band states and the impurity level. The final Anderson hamiltonian reads:

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_{\sigma} \varepsilon_d n_{d\sigma}$$

$$+ \sum_{k,\sigma} V_{kd}(a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma}) + U n_{d\uparrow} n_{d\downarrow}$$

$n_{d\sigma} = a^\dagger_{d\sigma} a_{d\sigma}$ is the number operator for a localized spin σ

Local magnetic moments in metals: basic phenomenology

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_\sigma \varepsilon_d n_{d\sigma}$$

$$+ \sum_{k,\sigma} V_{kd}(a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma}) + U n_{d\uparrow} n_{d\downarrow}$$

- Paradigm model of strong correlations
- Despite its apparent simplicity, extremely nontrivial: strong on-site interactions+quantum fluctuations

Anderson, Phys. Rev. 124, 41, 1961

Physics of the Anderson model

1. The Coulomb interaction favors the formation of local moments because it tends to inhibit double occupation of a site.

2. On the other hand, quantum fluctuations of charge on the impurity caused by strong hybridization of the impurity level with the band states tends to wash out local moments. These fluctuations are governed by an energy scale

$$\frac{1}{\tau} = \frac{2\Gamma}{\hbar} = \frac{2\pi}{\hbar}|V_{kd}|^2\rho(\varepsilon_d)$$

Density of electron k-states per volume and per spin evaluated at the impurity energy

Physics of the Anderson model

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_{\sigma} \varepsilon_d n_{d\sigma}$$

$$+ \sum V_{kd} (a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma}) + U n_{d\uparrow} n_{d\downarrow}$$

$$k,\sigma$$

Physics of the Anderson model

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_\sigma \varepsilon_d n_{d\sigma}$$

$$+ \sum_{k,\sigma} V_{kd}(a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma}) + U n_{d\uparrow} n_{d\downarrow}$$

Atomic limit

Non-magnetic

$|2\rangle \quad E_{|2\rangle} = 2\epsilon_d + U$

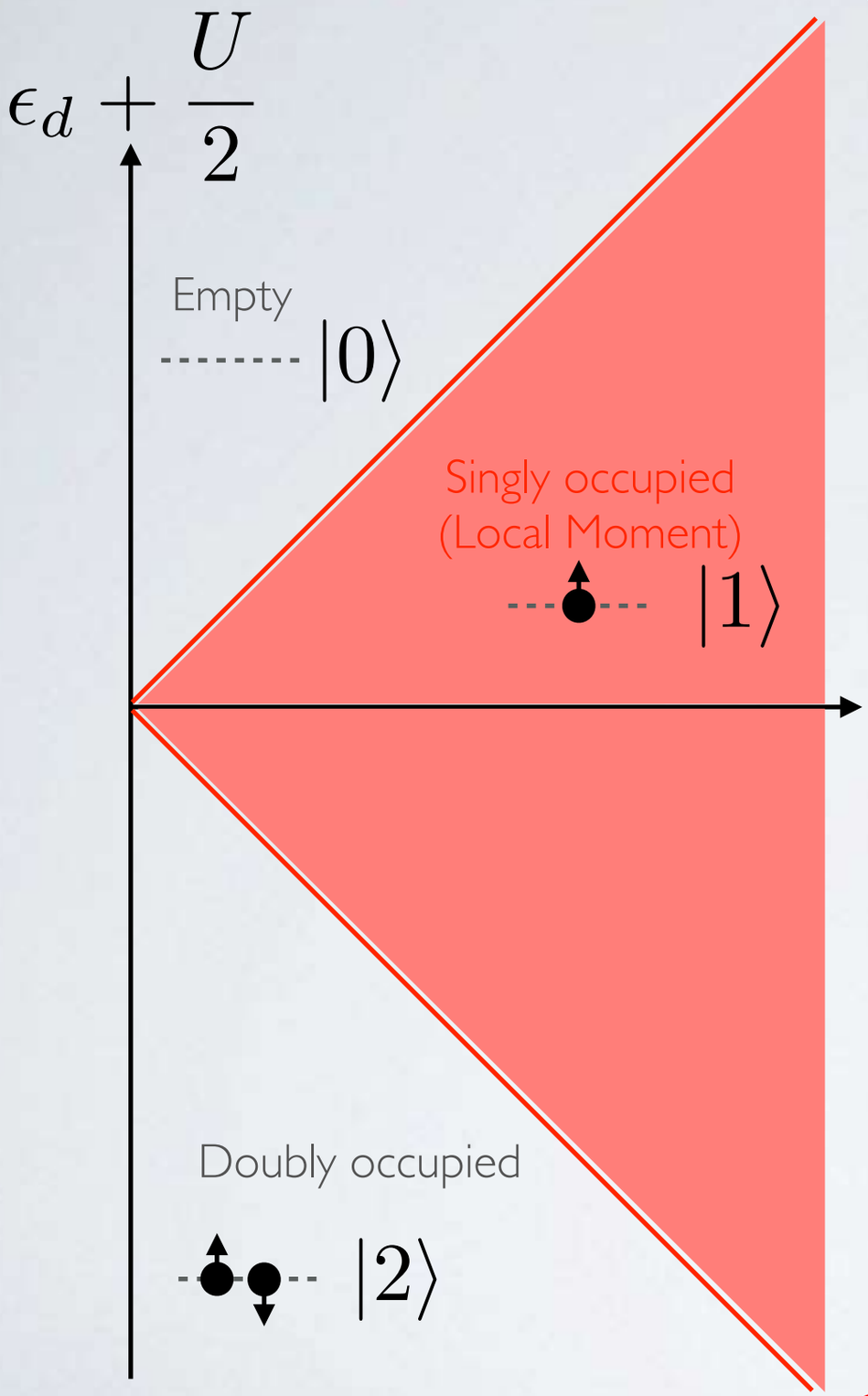
$|0\rangle \quad E_{|0\rangle} = 0$

Magnetic

$|\uparrow\rangle$

$|\downarrow\rangle$

$E_{|1\rangle} = \epsilon_d$



$$\epsilon_d + \frac{U}{2} = U$$

Non-magnetic

$$|2\rangle \quad E_{|2\rangle} = 2\epsilon_d + U$$

$$|0\rangle \quad E_{|0\rangle} = 0$$

Magnetic

$$|\uparrow\rangle \qquad |\downarrow\rangle$$

$$E_{|1\rangle} = \epsilon_d$$

$$\epsilon_d + \frac{U}{2} = -U$$

Physics of the Anderson model

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_\sigma \varepsilon_d n_{d\sigma}$$

$$+ \sum_{k,\sigma} V_{kd}(a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma}) + U n_{d\uparrow} n_{d\downarrow}$$

Hartree-Fock solution

$$U n_{d\uparrow} n_{d\downarrow} \rightarrow U n_{d\uparrow} \langle n_{d\downarrow} \rangle + U \langle n_{d\uparrow} \rangle n_{d\downarrow} - U \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle$$

Anderson, Phys. Rev. 124, 41, 1961

Physics of the Anderson model

Hartree-Fock solution

$$U n_{d\uparrow} n_{d\downarrow} \rightarrow U n_{d\uparrow} \langle n_{d\downarrow} \rangle + U \langle n_{d\uparrow} \rangle n_{d\downarrow} - U \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle$$

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_{\sigma} E_{d\sigma} n_{d\sigma}$$

$$+ \sum_{k,\sigma} V_{kd} (a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma})$$

$$E_{d\sigma} = \varepsilon_d + U \langle n_{d-\sigma} \rangle$$ effective level

Anderson, Phys. Rev. 124, 41, 1961

Physics of the Anderson model

Hartree-Fock solution

$$E_{d\sigma} = \varepsilon_d + U\langle n_{d-\sigma}\rangle$$ effective level

The exact Green's function of the problem can be solved formally as:

$$G^r_\sigma(\omega) = \frac{1}{\omega - \varepsilon_d - U\langle n_{d-\sigma}\rangle - \Sigma^r(\omega)}$$

$$\Sigma^r(\omega) = \sum_k \frac{|V_k|^2}{\omega - \varepsilon_k + i\eta}$$

Anderson, Phys. Rev. 124, 41, 1961

Physics of the Anderson model

$$\langle n_{d-\sigma}\rangle = -\frac{1}{\pi}\int d\omega Im G^r_{-\sigma}(\omega) f_{FD}(\omega)$$

$$G^r_\sigma(\omega) = \frac{1}{\omega - \varepsilon_d - U\langle n_{d-\sigma}\rangle - \Sigma^r(\omega)}$$

$$\Sigma^r(\omega) = \sum_k \frac{|V_k|^2}{\omega - \varepsilon_k + i\eta} = \int \rho(\epsilon)\frac{|V(\epsilon)|^2}{\omega - \epsilon + i\eta}$$

Anderson, Phys. Rev. 124, 41, 1961

Physics of the Anderson model

$$\Sigma^r(\omega) = \sum_k \frac{|V_k|^2}{\omega - \varepsilon_k + i\eta} = \int \rho(\epsilon) \frac{|V(\epsilon)|^2}{\omega - \epsilon + i\eta}$$

$$\int \rho(\epsilon) \frac{|V(\epsilon)|^2}{\omega - \epsilon + i\eta} = P \int \rho(\epsilon) \frac{|V(\epsilon)|^2}{\omega - \epsilon} - i\pi\delta(\omega)|V(\omega)|^2$$

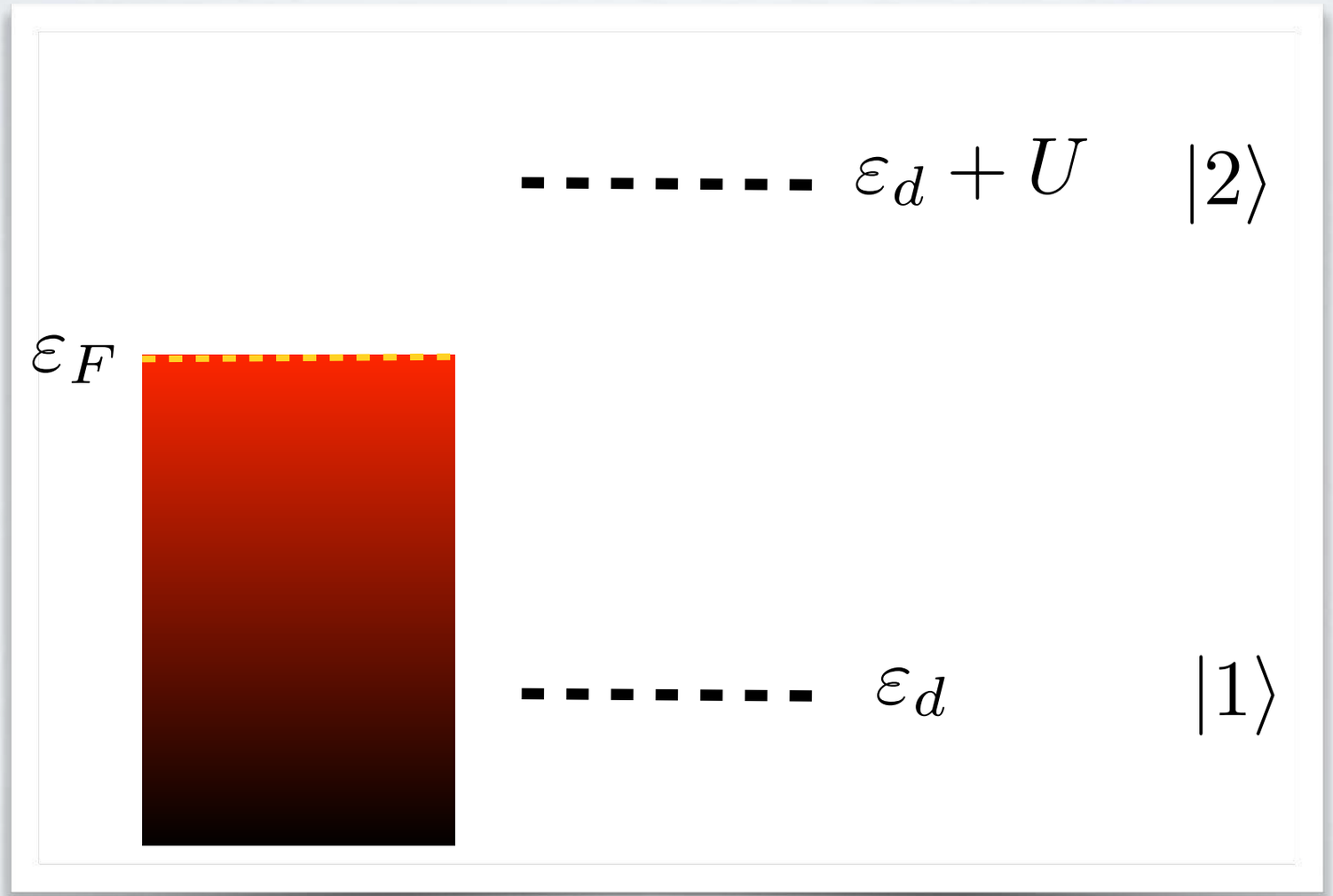
level shift width

$$\Sigma^r(\omega) \approx \frac{\Gamma}{\pi} \int_{-D}^{D} \frac{1}{\omega - \epsilon} - i\Gamma = -\frac{\Gamma}{\pi} ln|\frac{D+\omega}{D-\omega}| - i\Gamma$$

Anderson, Phys. Rev. 124, 41, 1961

Physics of the Anderson model

As a result of quantum fluctuations the energy levels of the impurity become broadened. the width of these levels is governed by Γ



Physics of the Anderson model

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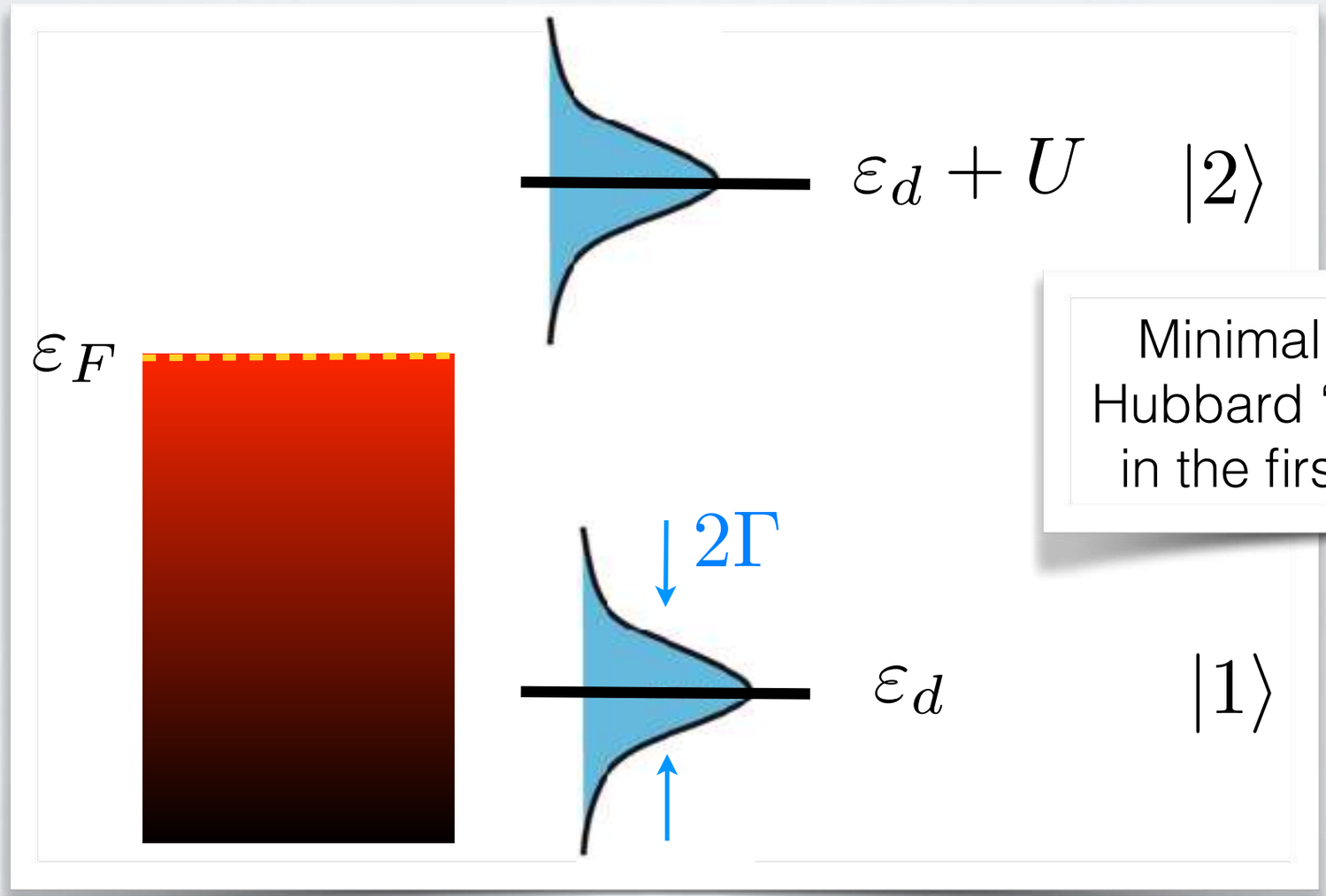


Minimal realization of the Hubbard “bands” discussed in the first lectures by Leni

Mean field phase diagram of the Anderson model

$$\langle n_{d\sigma}\rangle = -\frac{1}{\pi}\int d\omega Im G^r_\sigma(\omega) f_{FD}(\omega)$$

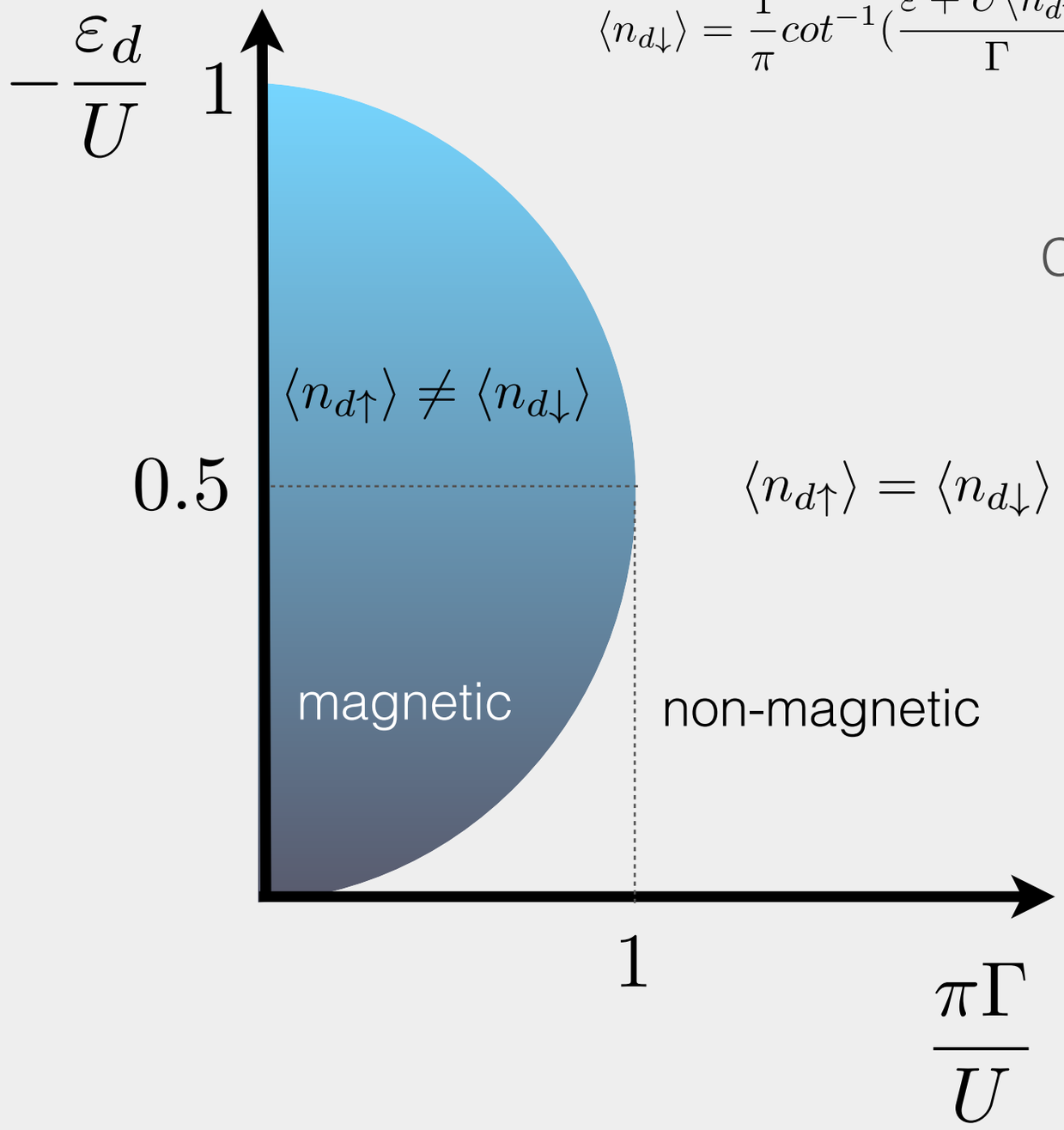
$$\langle n_{d\sigma}\rangle \approx \int_{-\infty}^{0} \frac{d\omega}{2\pi} \frac{2\Gamma}{(\omega - \tilde{\varepsilon} - U\langle n_{d-\sigma}\rangle)^2 + \Gamma^2}$$

selfconsistent solution

$$\begin{cases} \langle n_{d\uparrow}\rangle = \frac{1}{\pi} cot^{-1}\left(\frac{\tilde{\varepsilon} + U\langle n_{d\downarrow}\rangle}{\Gamma}\right) \\ \langle n_{d\downarrow}\rangle = \frac{1}{\pi} cot^{-1}\left(\frac{\tilde{\varepsilon} + U\langle n_{d\uparrow}\rangle}{\Gamma}\right) \end{cases}$$

Mean field phase diagram of the Anderson model

$$\langle n_{d\uparrow}\rangle = \frac{1}{\pi} cot^{-1}\left(\frac{\tilde{\varepsilon} + U\langle n_{d\downarrow}\rangle}{\Gamma}\right)$$
$$\langle n_{d\downarrow}\rangle = \frac{1}{\pi} cot^{-1}\left(\frac{\tilde{\varepsilon} + U\langle n_{d\uparrow}\rangle}{\Gamma}\right)$$

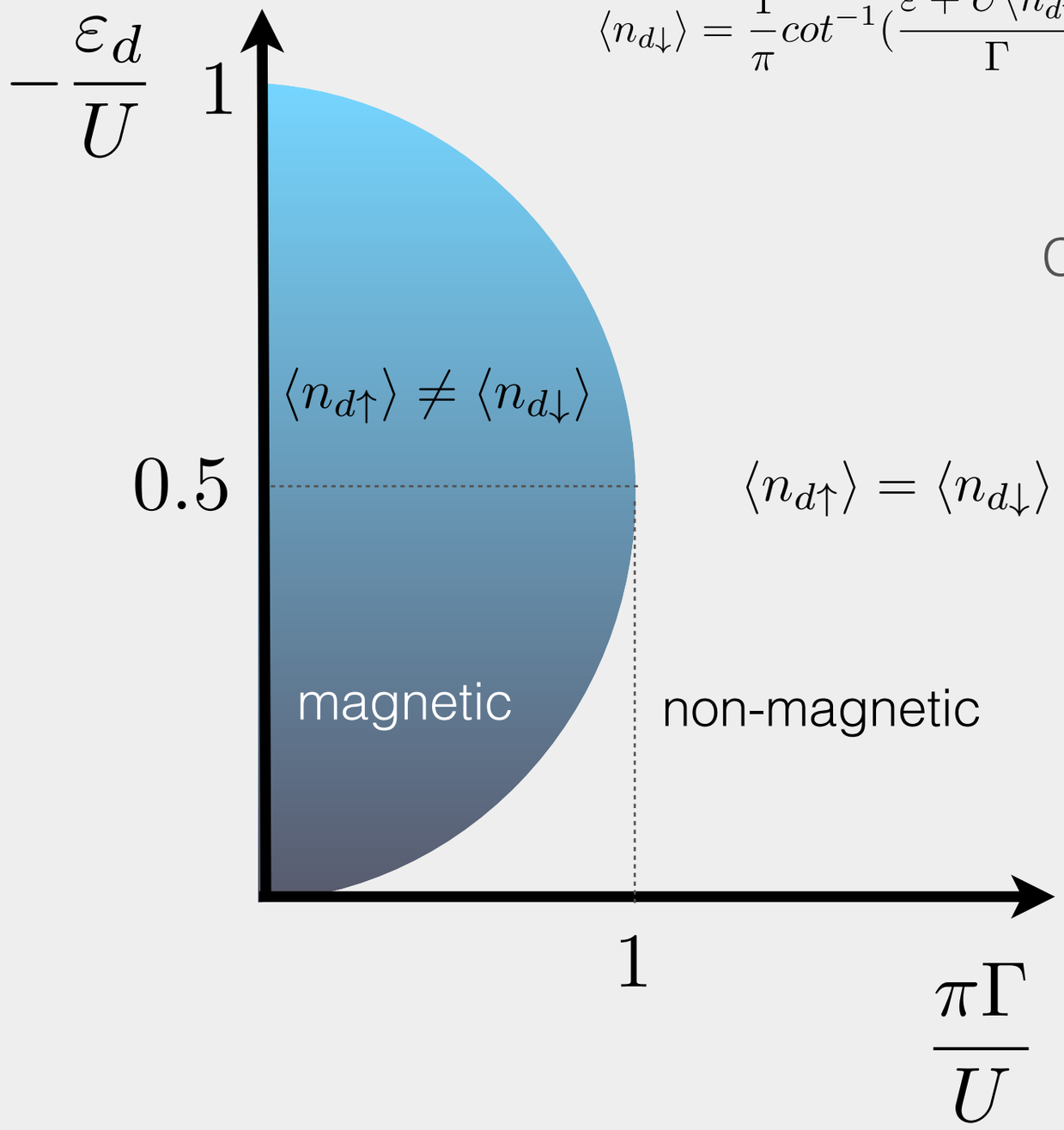


Criterion for local moment formation at half-filling

$$\frac{\pi\Gamma}{U} < 1$$

Mean field phase diagram of the Anderson model

$$\langle n_{d\uparrow}\rangle = \frac{1}{\pi} cot^{-1}\left(\frac{\tilde{\varepsilon} + U\langle n_{d\downarrow}\rangle}{\Gamma}\right)$$
$$\langle n_{d\downarrow}\rangle = \frac{1}{\pi} cot^{-1}\left(\frac{\tilde{\varepsilon} + U\langle n_{d\uparrow}\rangle}{\Gamma}\right)$$

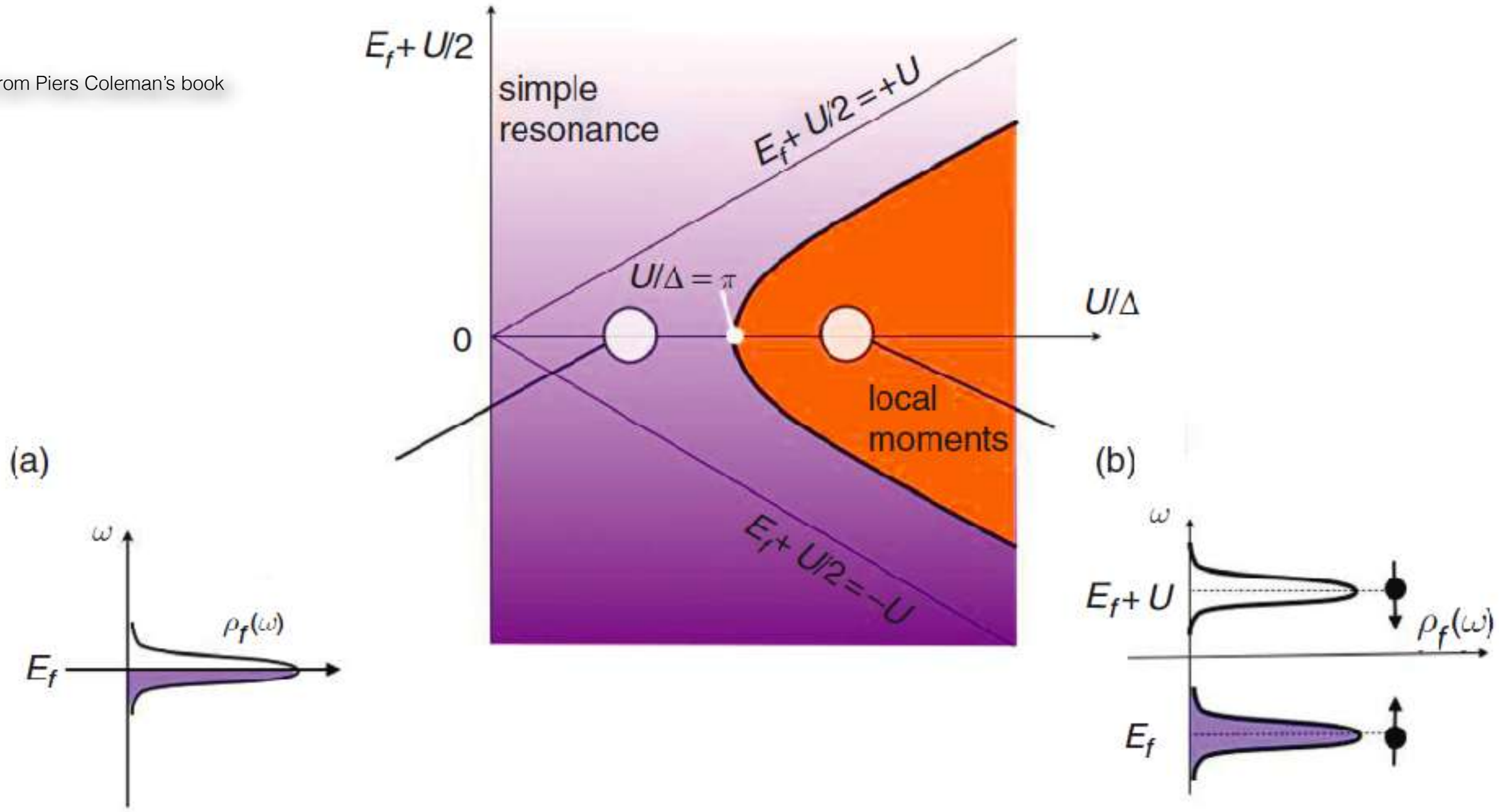


Criterion for local moment formation in general

$$U\rho(\varepsilon_F) > 1$$

Similar to Stoner's criterion for ferromagnetism

Image from Piers Coleman's book



Deep physical meaning in terms of scattering phase shifts

$$G^{\sigma}_{kk'} = \frac{\delta_{kk'}}{\omega - \varepsilon_k + i\eta} + \frac{V_k}{\omega - \varepsilon_k + i\eta} G^r_{\sigma}(\omega) \frac{V^*_{k'}}{\omega - \varepsilon_{k'} + i\eta}$$

T-matrix

$$T^{\sigma}_{kk'}(\omega) = V_k G^r_{\sigma}(\omega) V^*_{k'} \sim e^{2i\delta^{\sigma}(\omega)} - 1$$

$$ImT^{\sigma}_{kk}(\omega) = -\pi |V_k|^2 \rho^{\sigma}(\omega)$$

Phase shift induced by the impurity

$$\delta^{\sigma}(\omega) = cot^{-1}\left(\frac{\varepsilon_d + U\langle n_{d-\sigma}\rangle - \omega}{\Gamma}\right)$$

Deep physical meaning in terms of scattering phase shifts

$$\delta^{\sigma}(\omega) = cot^{-1}(\frac{\varepsilon_d + U\langle n_{d-\sigma}\rangle - \omega}{\Gamma})$$

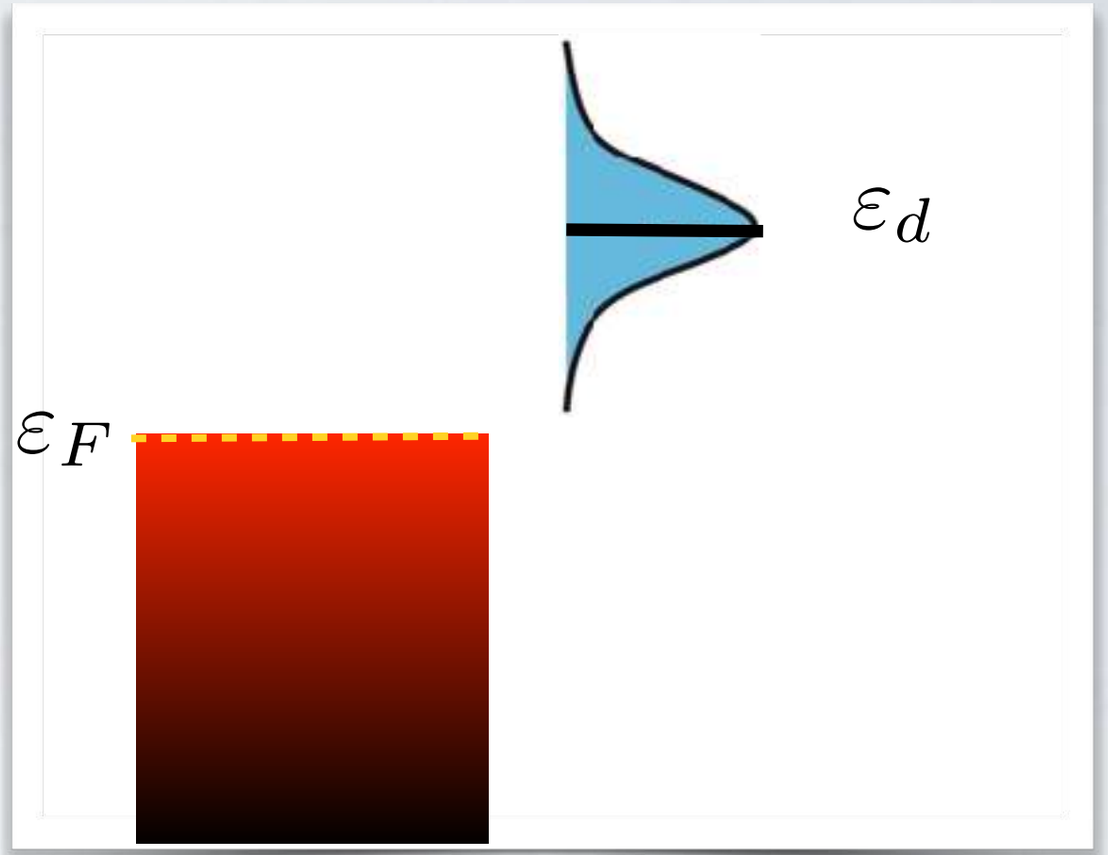
$$\langle n_{d\downarrow}\rangle = \frac{1}{\pi} cot^{-1}(\frac{\tilde{\varepsilon} + U\langle n_{d\uparrow}\rangle}{\Gamma}) = \frac{\delta^{\downarrow}(0)}{\pi}$$

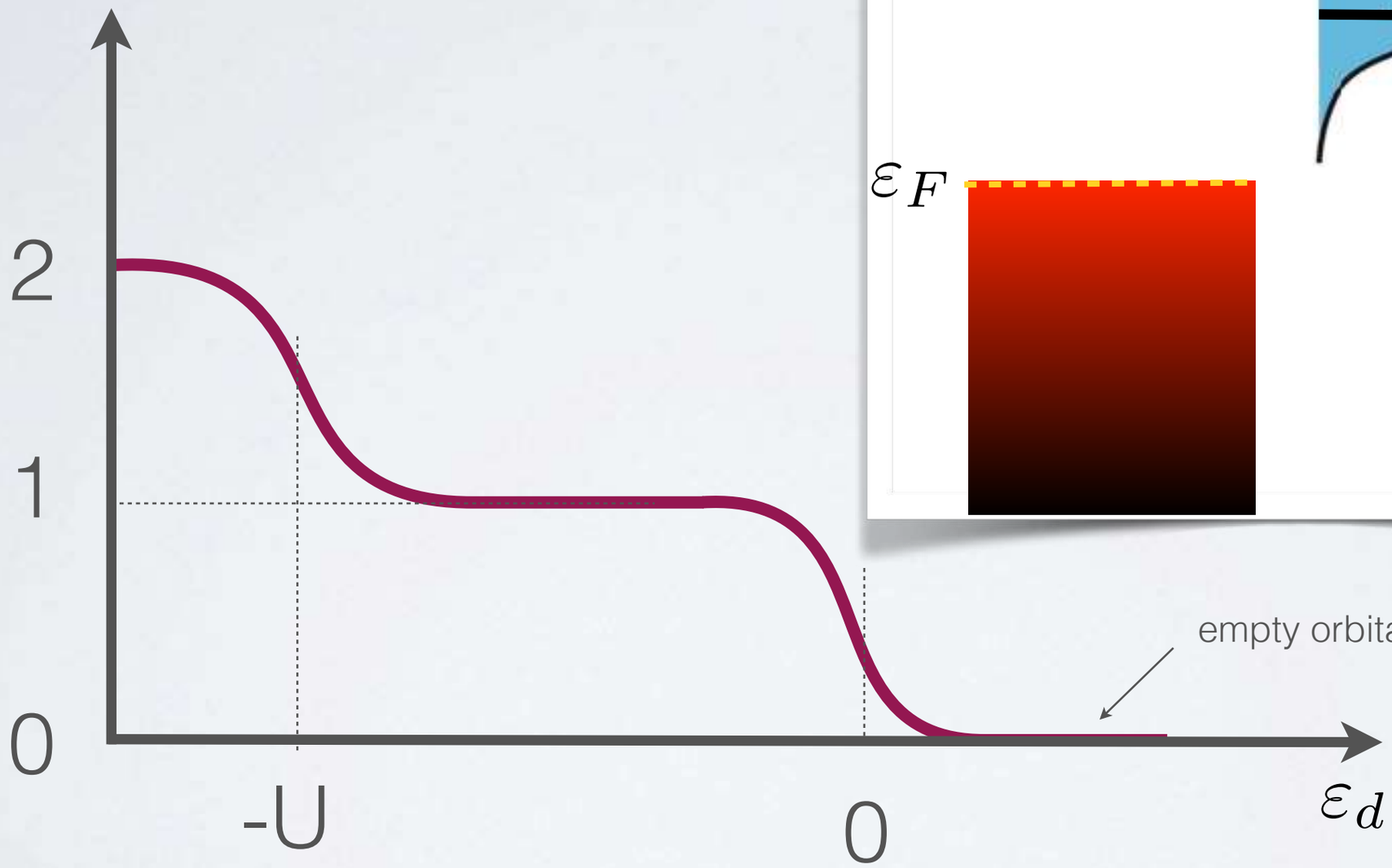
$$\langle n_{d\uparrow}\rangle = \frac{1}{\pi} cot^{-1}(\frac{\tilde{\varepsilon} + U\langle n_{d\downarrow}\rangle}{\Gamma}) = \frac{\delta^{\uparrow}(0)}{\pi}$$

Friedel's sum rule that relates the occupancy of the impurity site and the phase shifts of conduction electrons at the Fermi energy scattering on the impurity.

Physics of the Anderson model

$$n_d \equiv \langle n_{d\uparrow} + n_{d\downarrow} \rangle$$





Physics of the Anderson model

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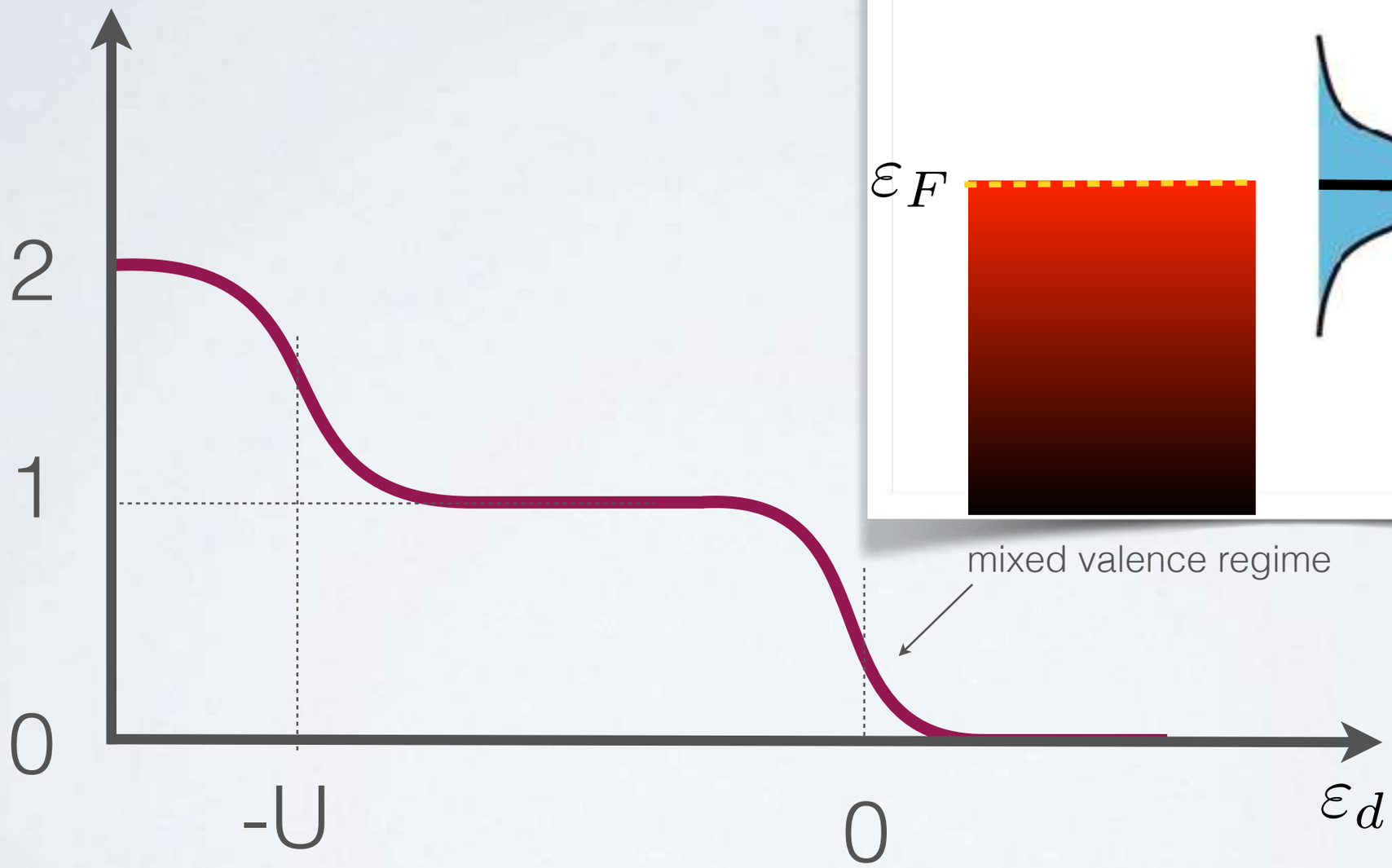
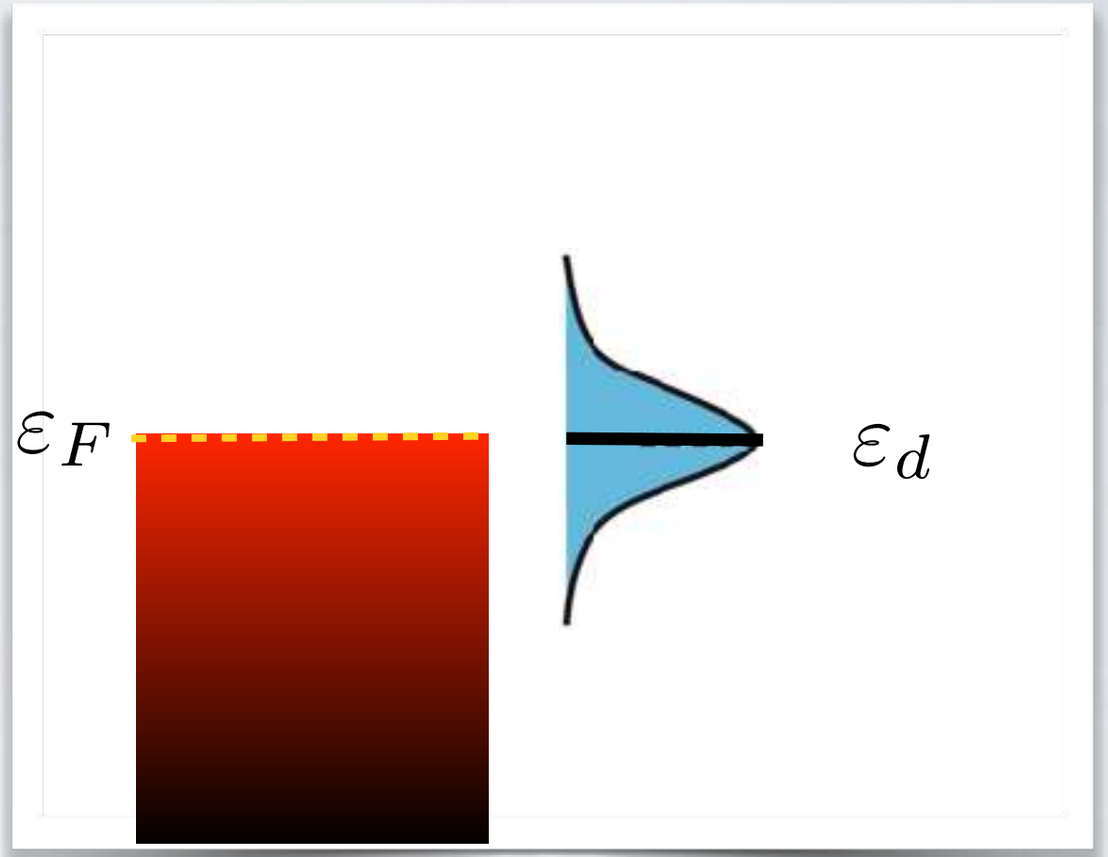
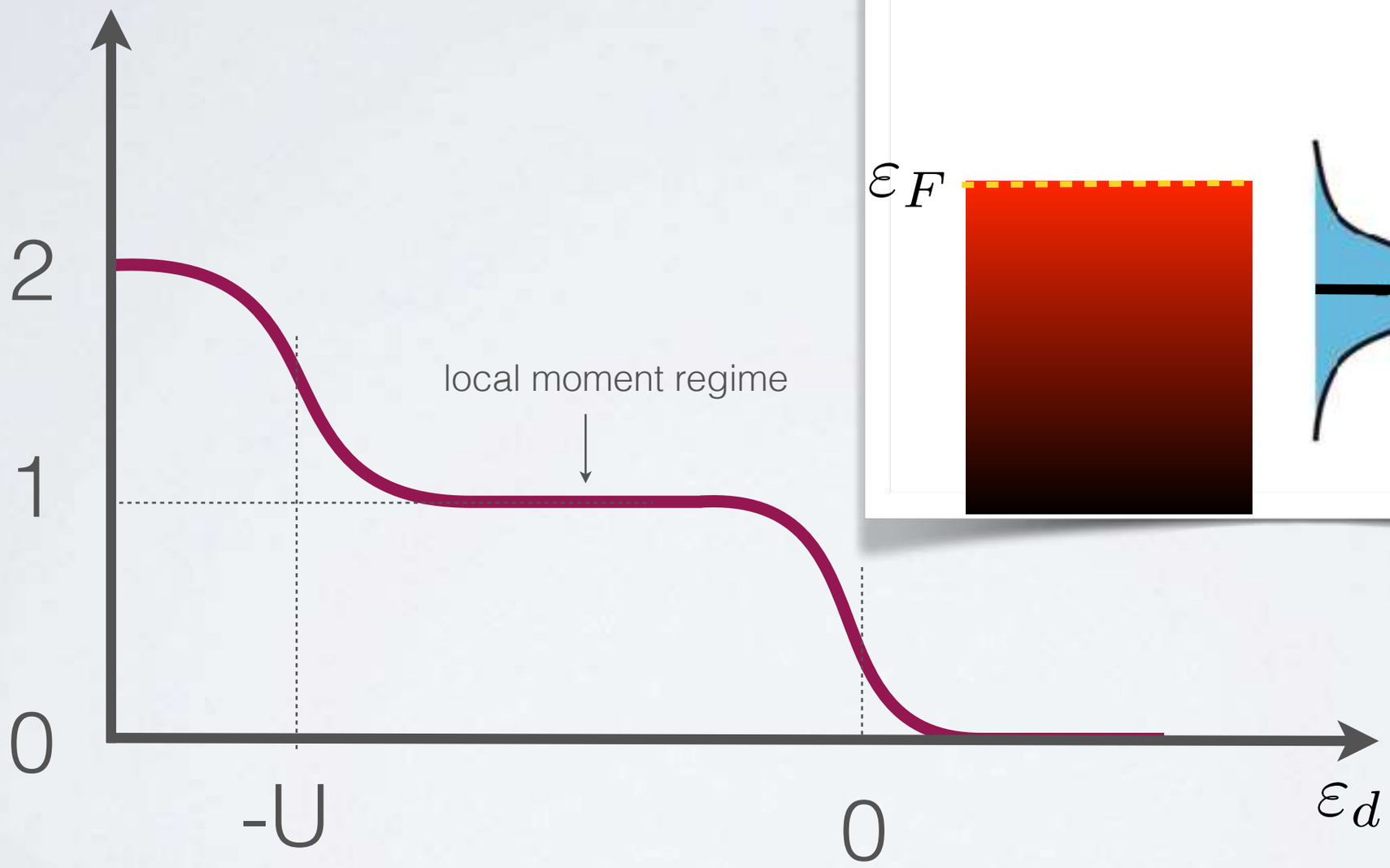
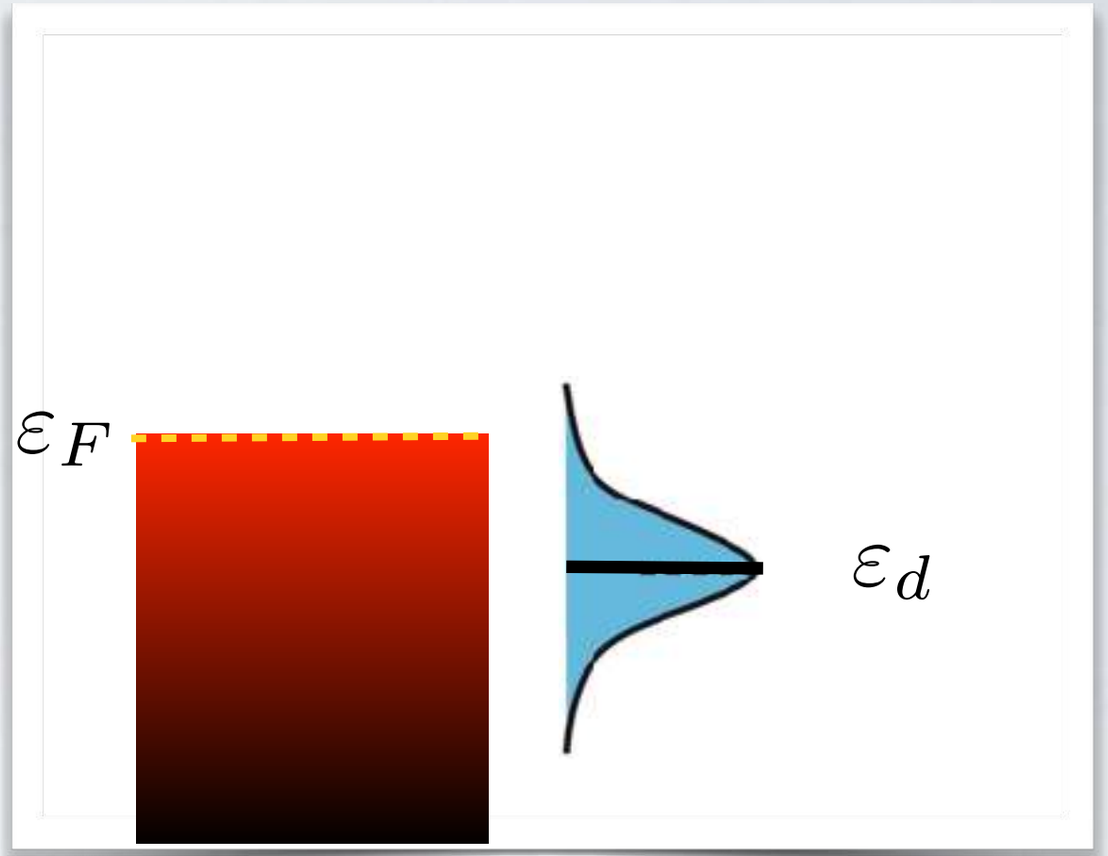




Physics of the Anderson model

$$n_d \equiv \langle n_{d\uparrow} + n_{d\downarrow} \rangle$$





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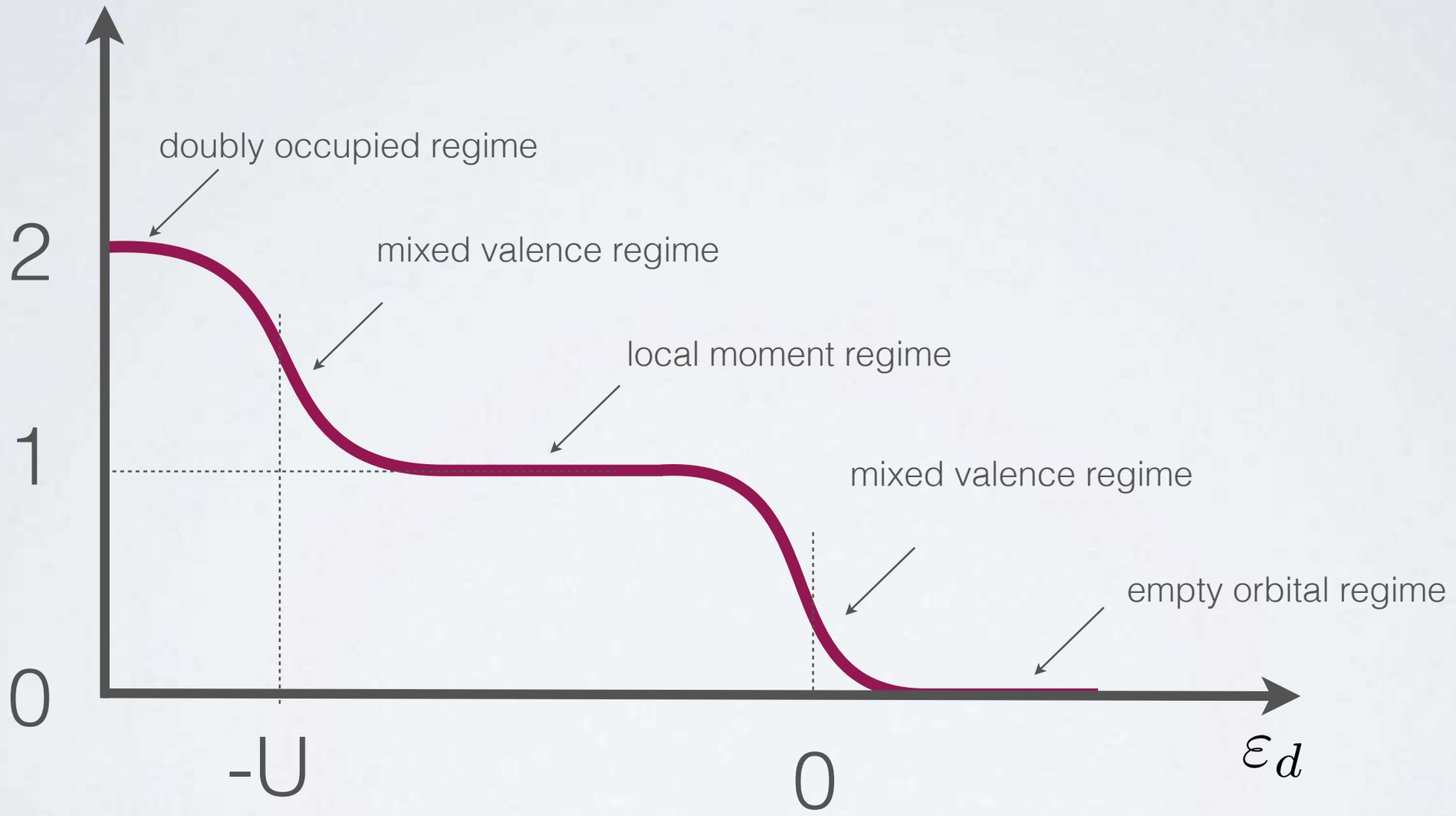


Quenching of local moments: Kondo's calculation

As we mentioned, the first models describing the interaction of local spins with conduction electrons date back the 1950's. The essence of these models is that an exchange interaction J exists between the local impurity spin and the conduction electrons.

$$H = \sum_{k\sigma} \varepsilon_k n_{k\sigma} + J\vec{S}.\vec{s}$$

Quenching of local moments: Kondo's calculation

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_{\sigma} \varepsilon_d n_{d\sigma}$$

$$+ \sum_{k,\sigma} V_{kd}(a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma}) + U n_{d\uparrow} n_{d\downarrow}$$

versus

$$H = \sum_{k\sigma} \varepsilon_k n_{k\sigma} + J\vec{S}.\vec{s}$$

It turns out that both models can be related. The Kondo model is a limiting case of the Anderson model when charge fluctuations are integrated out.

Quenching of local moments: Kondo's calculation

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_\sigma \varepsilon_d n_{d\sigma} + \sum_{k,\sigma} V_{kd}(a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma}) + U n_{d\uparrow} n_{d\downarrow}$$

$$\Rightarrow \quad H = \sum_{k\sigma} \varepsilon_k n_{k\sigma} + J\vec{S}.\vec{s}$$

The basic idea is the following: second-order virtual processes in the Anderson model that lead to scattering of a conduction electron with a local moment. Such processes have amplitudes

$$V_{kd} \frac{1}{E_i - E_{int}} V^*_{k'd}$$

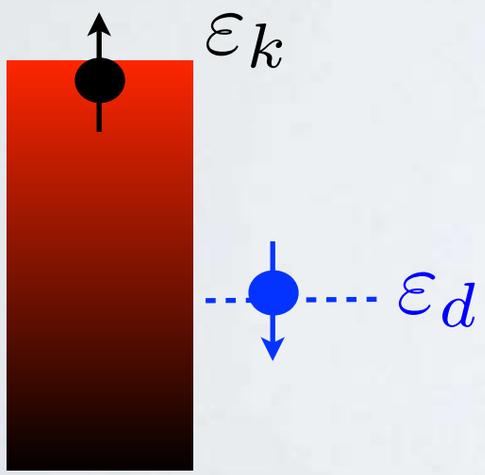
initial

intermediate

Quenching of local moments: Kondo's calculation

$$V_{kd}\frac{1}{E_i - E_{int}}V^*_{k'd}$$

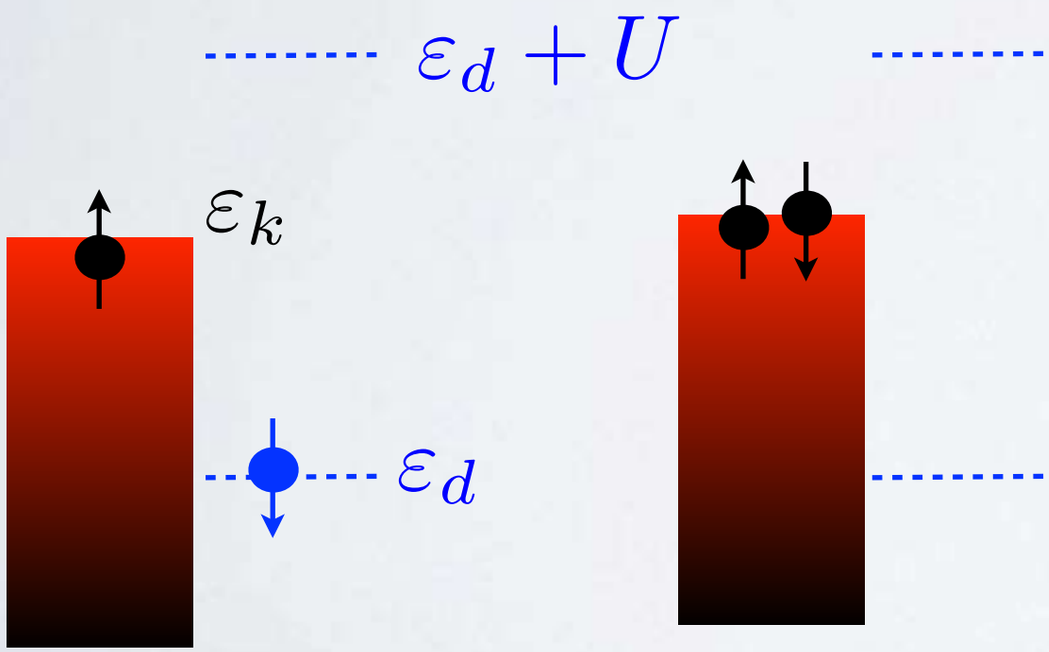
$\varepsilon_d + U$



initial

Quenching of local moments: Kondo's calculation

$$V_{kd}\frac{1}{E_i - E_{int}}V^*_{k'd}$$

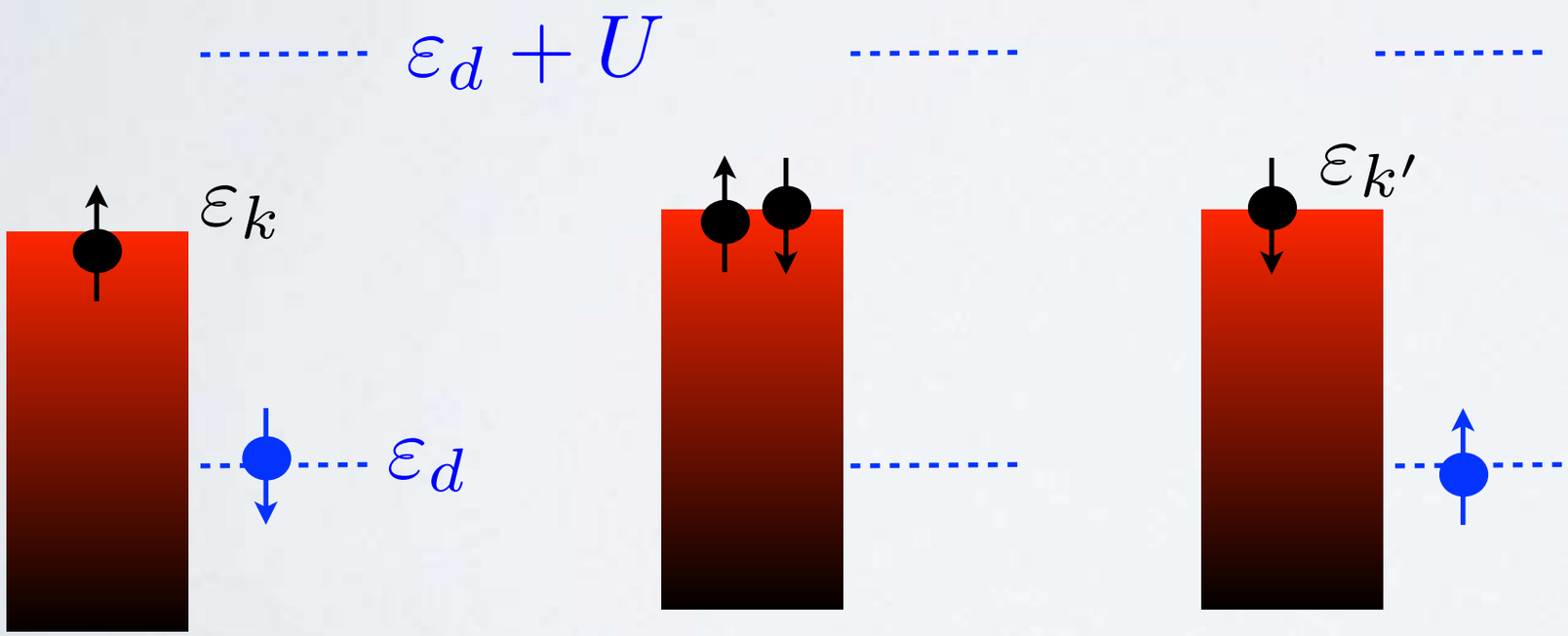


Quenching of local moments: Kondo's calculation

$$T_{k\uparrow,d\downarrow\rightarrow k'\downarrow,d\uparrow} \sim -V_{kd}\frac{1}{\varepsilon_d}V^*_{k'd}$$

we have exchanged two fermions

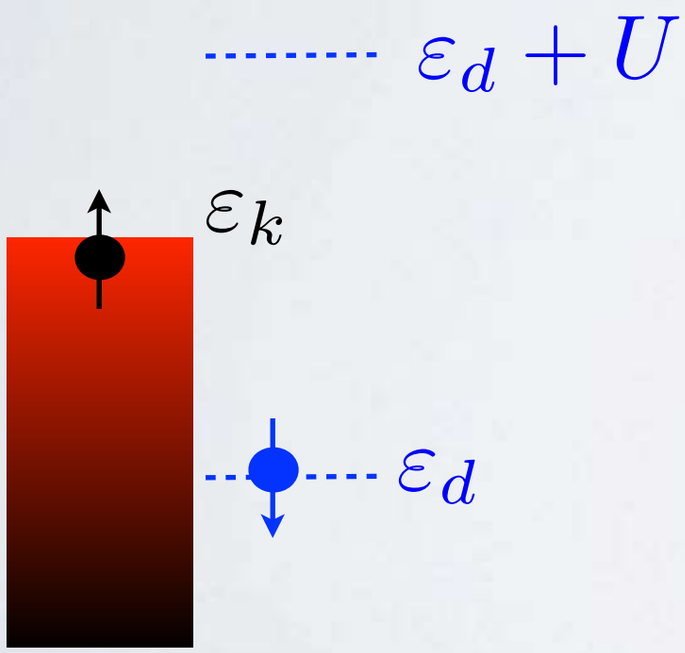
$\varepsilon_k \approx \varepsilon_{k'} \approx 0$



Spin-flip.

Quenching of local moments: Kondo's calculation

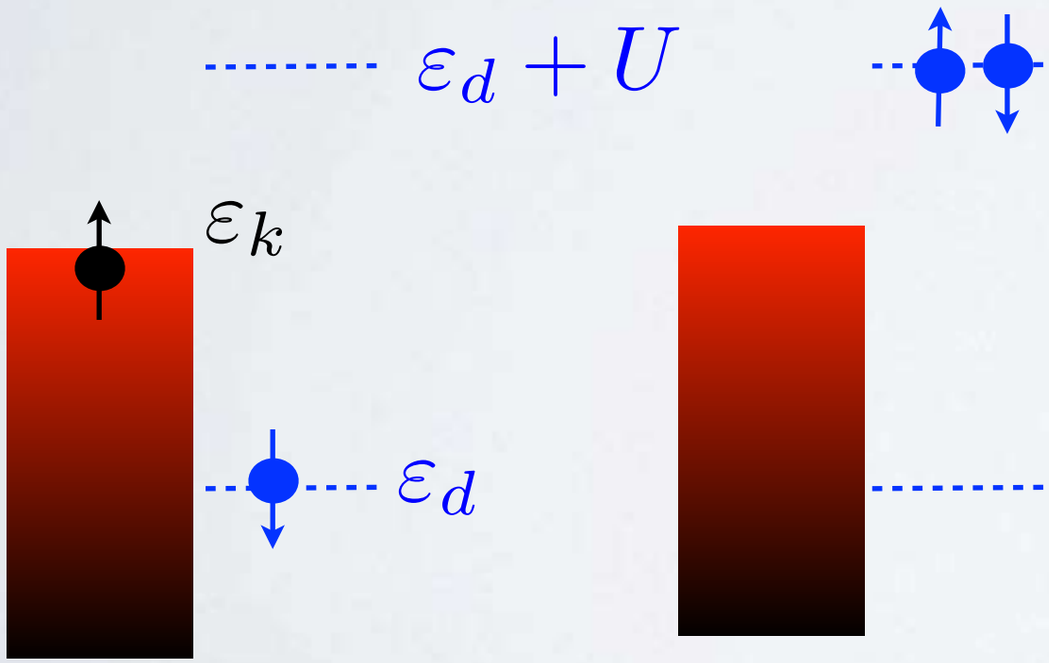
$$V_{kd}\frac{1}{E_i - E_{int}}V^*_{k'd}$$



initial

Quenching of local moments: Kondo's calculation

$$V_{kd}\frac{1}{E_i - E_{int}}V^*_{k'd}$$

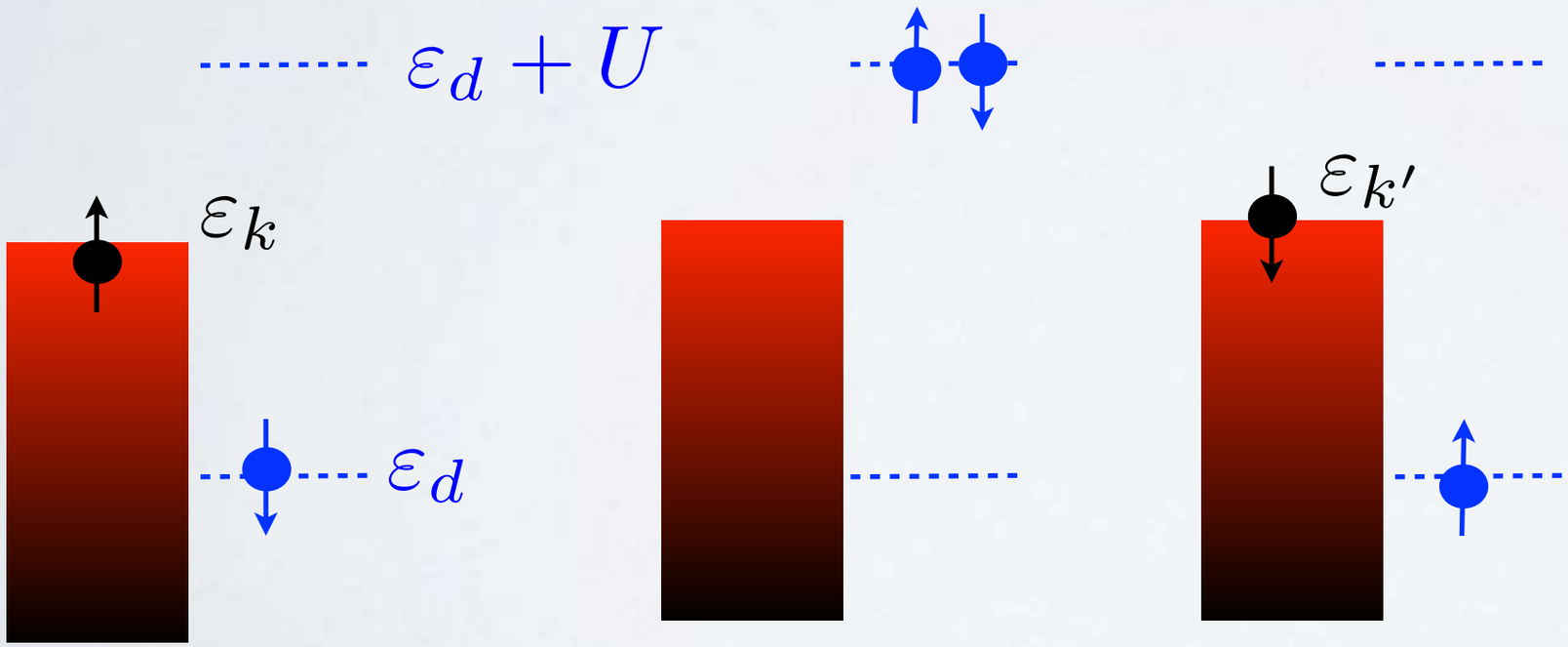


Quenching of local moments: Kondo's calculation

$$T_{k\uparrow,d\downarrow\rightarrow k'\downarrow,d\uparrow} \sim -V_{kd}\frac{1}{-\varepsilon_d - U}V^*_{k'd}$$

$\varepsilon_k \approx \varepsilon_{k'} \approx 0$

we have exchanged two fermions



Spin-flip.

Quenching of local moments: Kondo's calculation

Such processes can be formally traced out by a unitary transformation (Schrieffer-Wolff)

$$\tilde{H} = e^{S} H e^{-S}$$

$$S = \sum_{k\sigma} \frac{V_k}{\varepsilon_k - \varepsilon_d - U} n_{-\sigma} (c^{\dagger}_{k\sigma} d_\sigma - d^{\dagger}_\sigma c_{k\sigma}) + \frac{V_k}{\varepsilon_k - \varepsilon_d} (1 - n_{-\sigma}) (c^{\dagger}_{k\sigma} d_\sigma - d^{\dagger}_\sigma c_{k\sigma})$$

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Relation between the Anderson and Kondo Hamiltonians

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(Received 24 March 1966)

A canonical transformation is used to relate the Anderson model of a localized magnetic moment in a dilute alloy to that of Kondo. In the limit of small *s-d* mixing, which is the most favorable case for the occurrence of a moment, the two models are shown to be equivalent. The Anderson model thus has low-temperature anomalies similar to those previously discussed for the Kondo model.

Quenching of local moments: Kondo's calculation

$$J_{kk'} = 2V_{kd}V^*_{k'd}(\frac{1}{\varepsilon_k - \varepsilon_d - U} + \frac{1}{\varepsilon_d - \varepsilon_{k'}})$$

$$\varepsilon_k \approx \varepsilon_{k'} \approx 0$$

$$J_{eff} = 2|V_{kd}|^2(\frac{1}{\varepsilon_d} - \frac{1}{\varepsilon_d + U}) = \frac{2\Gamma}{\pi}(\frac{1}{\varepsilon_d} - \frac{1}{\varepsilon_d + U})$$

Quenching of local moments: Kondo's calculation

Kondo showed that a logarithmic correction appears in a perturbative expansion in terms of J (Prog. Theor. Phys. **32**, 37, 1964).

$$H_K = \sum_{k,\sigma} \varepsilon_k n_{k,\sigma} - \sum_{k,k'} \frac{J_{kk'}}{\hbar^2} (\Psi^\dagger_{k'} S \Psi_k).(\Psi^\dagger_d S \Psi_d)$$

Quenching of local moments: Kondo's calculation

$$\Psi_k = \begin{pmatrix} a_{k\uparrow} \\ a_{k\downarrow} \end{pmatrix} \quad \Psi_d = \begin{pmatrix} a_{d\uparrow} \\ a_{d\downarrow} \end{pmatrix}$$

Conduction electrons

$$H_K = \sum_{k,\sigma} \varepsilon_k n_{k,\sigma} - \sum_{k,k'} \frac{J_{kk'}}{\hbar^2} (\Psi^\dagger_{k'} S \Psi_k)(\Psi^\dagger_d S \Psi_d)$$

Impurity

Quenching of local moments: Kondo's calculation

$$H_K = \sum_{k,\sigma} \varepsilon_k n_{k,\sigma} - \sum_{k,k'} \frac{J_{kk'}}{\hbar^2} (\Psi^\dagger_{k'} S \Psi_k).(\Psi^\dagger_d S \Psi_d)$$

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$xx = \frac{\hbar^2}{4} \sum_{k,k'} (c^\dagger_{k'\uparrow} c_{k\downarrow} + c^\dagger_{k'\downarrow} c_{k\uparrow})(a^\dagger_{d\uparrow} a_{d\downarrow} + a^\dagger_{d\downarrow} a_{d\uparrow})$$

$$yy = \frac{-\hbar^2}{4} \sum_{k,k'} (c^\dagger_{k'\uparrow} c_{k\downarrow} - c^\dagger_{k'\downarrow} c_{k\uparrow})(a^\dagger_{d\uparrow} a_{d\downarrow} - a^\dagger_{d\downarrow} a_{d\uparrow})$$

$$zz = \frac{\hbar^2}{4} \sum_{k,k'} (c^\dagger_{k'\uparrow} c_{k\downarrow} - c^\dagger_{k'\downarrow} c_{k\uparrow})(a^\dagger_{d\uparrow} a_{d\downarrow} - a^\dagger_{d\downarrow} a_{d\uparrow})$$

Quenching of local moments: Kondo's calculation

$$H_K = \sum_{k,\sigma} \varepsilon_k n_{k,\sigma} - \sum_{k,k'} \frac{J_{kk'}}{\hbar^2} (\Psi^\dagger_{k'} S \Psi_k).(\Psi^\dagger_d S \Psi_d)$$

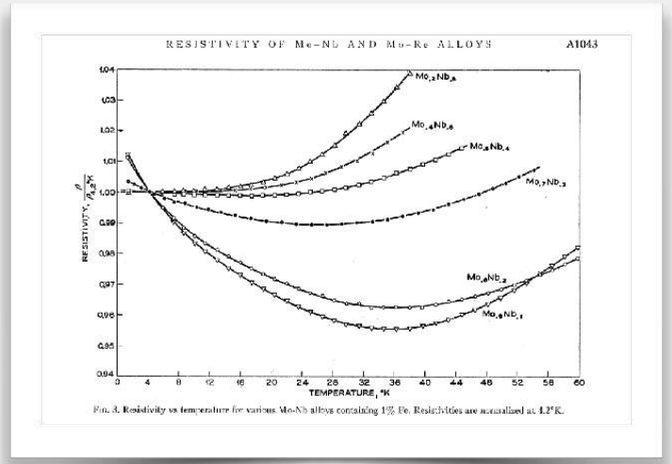


FIG. 3. Resistivity vs temperature for various Mo-Nb alloys containing 1% Fe. Resistivities are normalized at 4.2°K.

Remember: the goal was to calculate the resistivity minimum.
Linear response theory tells us that we need essentially the T-matrix of the problem

$$\sigma = \frac{ne^2}{m} \tau(k_F)$$

$$\frac{1}{\tau(k)} = \sum_{\mathbf{k'}} W_{\mathbf{kk'}} (1 - cos\theta_{\mathbf{kk'}}) \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k'}})$$

$$W_{\mathbf{kk'}} = \frac{2\pi N_{imp}}{\hbar} |T_{\mathbf{kk'}}|^2$$

Quenching of local moments: Kondo's calculation

Compact notation

$$H = \sum_{\mathbf{k},\mathbf{k}'} J_{\mathbf{k}\mathbf{k}'} (S^+ a^\dagger_{\mathbf{k},\downarrow} a_{\mathbf{k}',\uparrow} + S^- a^\dagger_{\mathbf{k},\uparrow} a_{\mathbf{k}',\downarrow} + S^z (a^\dagger_{\mathbf{k},\uparrow} a_{\mathbf{k}',\uparrow} - a^\dagger_{\mathbf{k},\downarrow} a_{\mathbf{k}',\downarrow}))$$

Lowest order (Born approximation)

$$\langle \mathbf{k},\uparrow |T| \mathbf{k}',\uparrow \rangle_{(1)} = \langle \mathbf{k},\uparrow |H| \mathbf{k}',\uparrow \rangle = J_{\mathbf{k}\mathbf{k}'} S^z$$

$$\langle \mathbf{k},\uparrow |T| \mathbf{k}',\downarrow \rangle_{(1)} = \langle \mathbf{k},\uparrow |H| \mathbf{k}',\downarrow \rangle = J_{\mathbf{k}\mathbf{k}'} S^-$$

$$\langle \mathbf{k},\downarrow |T| \mathbf{k}',\downarrow \rangle_{(1)} = \langle \mathbf{k},\downarrow |H| \mathbf{k}',\downarrow \rangle = -J_{\mathbf{k}\mathbf{k}'} S^z$$

$$\langle \mathbf{k},\downarrow |T| \mathbf{k}',\uparrow \rangle_{(1)} = \langle \mathbf{k},\downarrow |H| \mathbf{k}',\uparrow \rangle = J_{\mathbf{k}\mathbf{k}'} S^+$$

$$|T_{\mathbf{k}\mathbf{k}'}|^2 = |J_{\mathbf{k}\mathbf{k}'}|^2 (2S_z^2 + S^+ S^- + S^- S^+)$$

Quenching of local moments: Kondo's calculation

$$|T_{\mathbf{kk'}}|^2 = |J_{\mathbf{kk'}}|^2(2S_z^2 + S^+S^- + S^-S^+)$$

$$W_{\mathbf{kk'}} = \frac{2\pi N_{imp}}{\hbar}|T_{\mathbf{kk'}}|^2 = \frac{2\pi N_{imp}}{\hbar}\frac{J^2}{N_s^2}(2S_z^2 + S^+S^- + S^-S^+)$$

$$\frac{1}{\tau(k)} = \sum_{\mathbf{k'}} W_{\mathbf{kk'}}(1 - cos\theta_{\mathbf{kk'}})\delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k'}})$$

Temperature independent

$$\frac{1}{\tau(k_F)} = \frac{3\pi c_{imp} n J^2}{2\varepsilon_F \hbar} S(S+1)$$

$$c_{imp} = \frac{N_{imp}}{N_s} \qquad n = \frac{p_F^3}{3\pi^2\hbar^3}$$

Quenching of local moments: Kondo's calculation

Compact notation

$$H = \sum_{\mathbf{k},\mathbf{k}'} J_{\mathbf{k}\mathbf{k}'} (S^+ a^\dagger_{\mathbf{k},\downarrow} a_{\mathbf{k}',\uparrow} + S^- a^\dagger_{\mathbf{k},\uparrow} a_{\mathbf{k}',\downarrow} + S^z (a^\dagger_{\mathbf{k},\uparrow} a_{\mathbf{k}',\uparrow} - a^\dagger_{\mathbf{k},\downarrow} a_{\mathbf{k}',\downarrow}))$$

The next order generates many contributions

$$\langle \mathbf{k},\sigma | T | \mathbf{k}',\sigma' \rangle_{(2)} = \langle \mathbf{k},\sigma | H \frac{1}{\varepsilon - H_0 + i\eta} H | \mathbf{k}',\sigma' \rangle$$

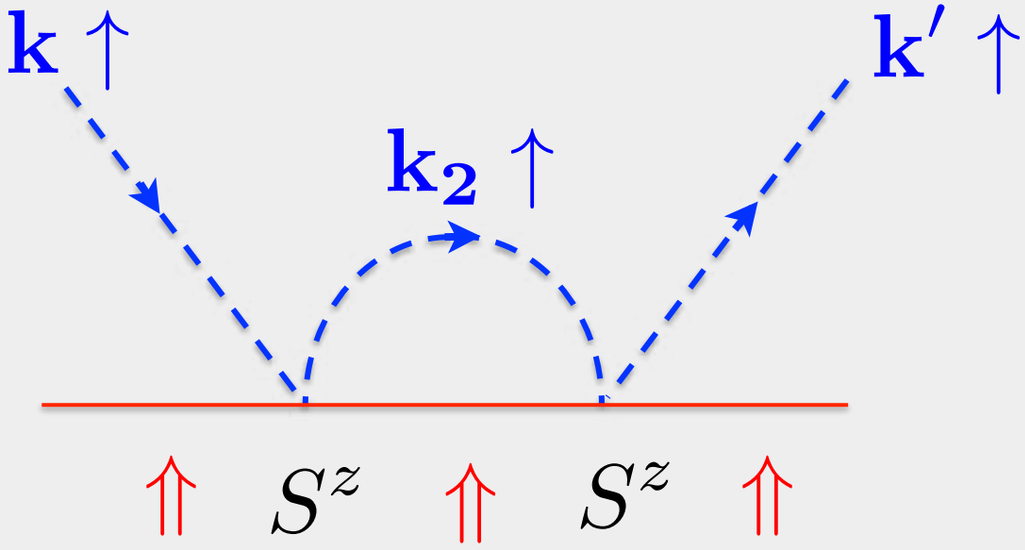
Quenching of local moments: Kondo's calculation

Longitudinal terms

$$J^2 \sum_{\mathbf{k_1},\mathbf{k_1'},\mathbf{k_2},\mathbf{k_2'}} \langle \mathbf{k}',\uparrow | S^z a^\dagger_{\mathbf{k_1}\uparrow} a_{\mathbf{k_1'}\uparrow} \frac{1}{\varepsilon - H_0 + i\eta} S^z a^\dagger_{\mathbf{k_2}\uparrow} a_{\mathbf{k_2'}\uparrow} | \mathbf{k},\uparrow \rangle$$

$$\mathbf{k}' = \mathbf{k_1}, \mathbf{k} = \mathbf{k_2'}, \mathbf{k_1'} = \mathbf{k_2}$$

$$J^2 \sum_{\mathbf{k_2}} S^z S^z \frac{(1 - f(\varepsilon_{\mathbf{k_2}}))}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)}$$



$\mathbf{k},\uparrow$ Electron scatters into an unoccupied hole state $\mathbf{k_2},\uparrow$

$\mathbf{k_2},\uparrow$ electron then scatters into the final $\mathbf{k}',\uparrow$

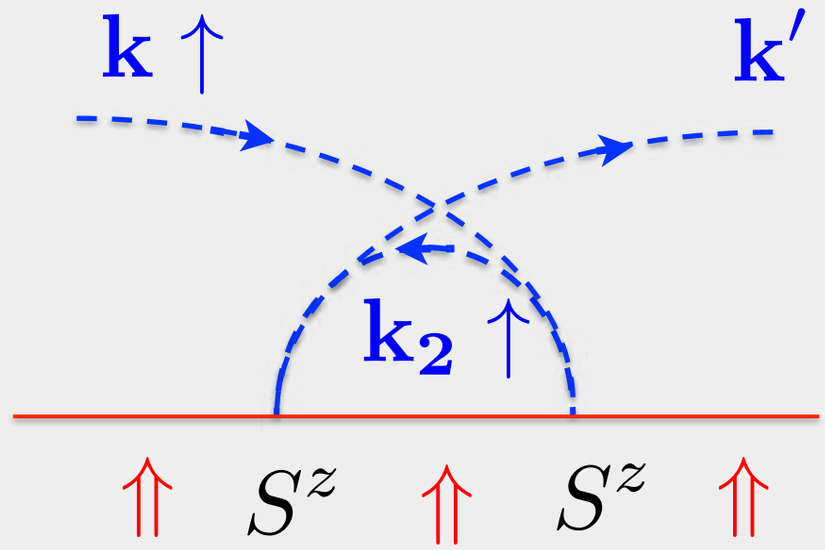
Quenching of local moments: Kondo's calculation

Longitudinal terms

$$J^2 \sum_{\mathbf{k_1},\mathbf{k_1'},\mathbf{k_2},\mathbf{k_2'}} \langle \mathbf{k}',\uparrow | S^z a^\dagger_{\mathbf{k}_2,\uparrow} a_{\mathbf{k}_2',\uparrow} \frac{1}{\epsilon - H_0 + i\eta} S^z a^\dagger_{\mathbf{k}_1,\uparrow} a_{\mathbf{k}_1',\uparrow} | \mathbf{k},\uparrow \rangle$$

$$\mathbf{k_2'} = \mathbf{k}', \mathbf{k_2} = \mathbf{k_1'}, \mathbf{k_2} = \mathbf{k}$$

$$J^2 \sum_{\mathbf{k_2}} S^z S^z \frac{f(\varepsilon_{\mathbf{k_2}})}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)}$$

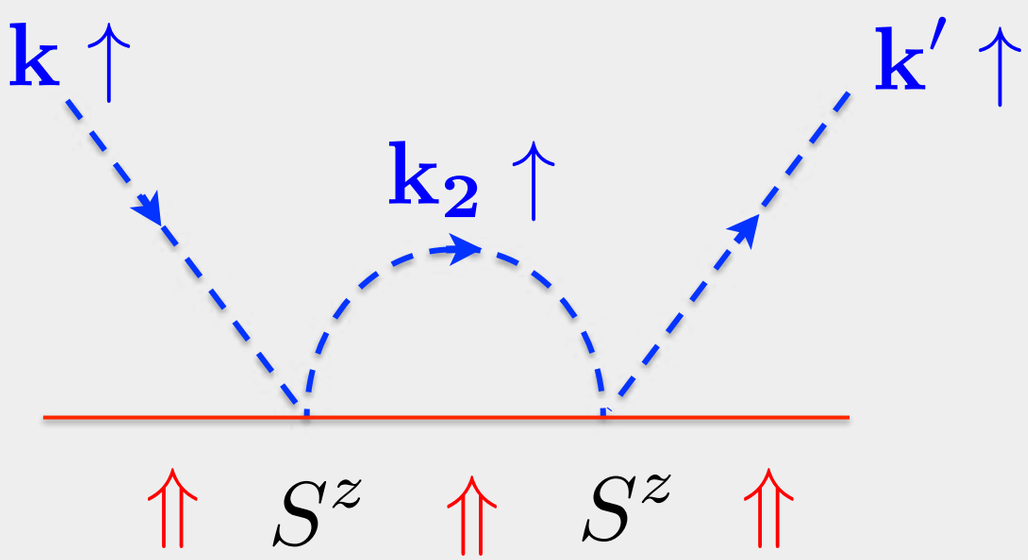


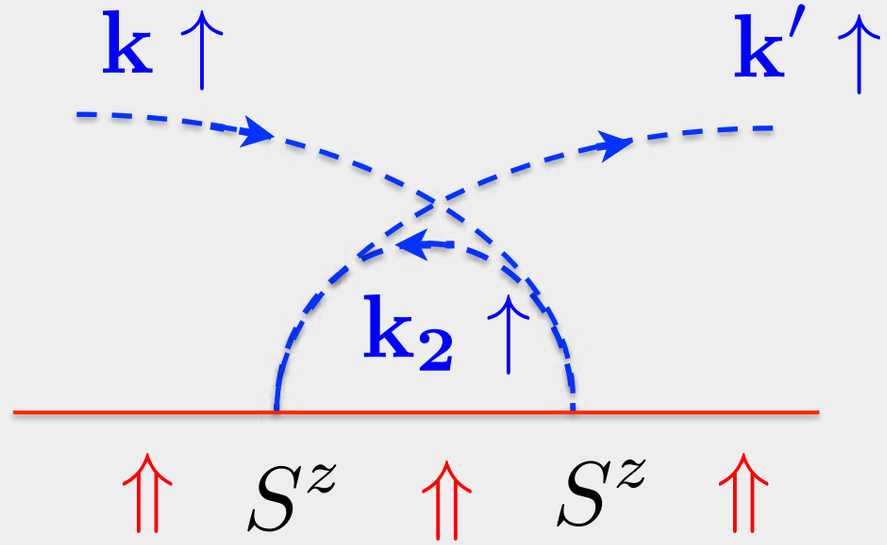
Electron in an occupied state $\mathbf{k_2},\uparrow$ is scattered into $\mathbf{k}',\uparrow$

The remaining hole $\mathbf{k_2},\uparrow$ is annihilated by the initial $\mathbf{k},\uparrow$

Quenching of local moments: Kondo's calculation

Longitudinal terms





$$J^2 \sum_{\mathbf{k_2}} S^z S^z \frac{(1 - f(\varepsilon_{\mathbf{k_2}}))}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)} + J^2 \sum_{\mathbf{k_2}} S^z S^z \frac{f(\varepsilon_{\mathbf{k_2}})}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)}$$

When we add both terms the fermi distribution cancels out: the final probability does not depend on the occupation of intermediate states and hence on temperature.

$$J^2 \sum_{\mathbf{k_2}} S^z S^z \frac{1}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)}$$

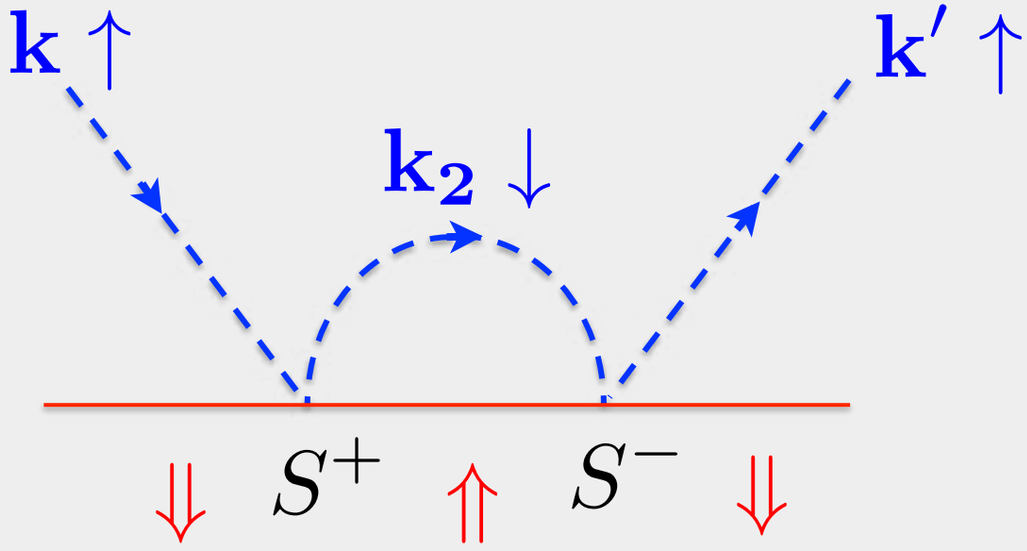
Quenching of local moments: Kondo's calculation

Transverse terms

$$J^2 \sum_{\mathbf{k_1},\mathbf{k_1'},\mathbf{k_2},\mathbf{k_2'}} \langle \mathbf{k'},\uparrow | S^- a^\dagger_{\mathbf{k_1}\uparrow} a_{\mathbf{k_1'}\downarrow} \frac{1}{\varepsilon - H_0 + i\eta} S^+ a^\dagger_{\mathbf{k_2}\downarrow} a_{\mathbf{k_2'}\uparrow} | \mathbf{k},\uparrow \rangle$$

$$\mathbf{k'} = \mathbf{k_1}, \mathbf{k} = \mathbf{k_2'}, \mathbf{k_1'} = \mathbf{k_2}$$

$$J^2 \sum_{\mathbf{k_2}} S^- S^+ \frac{(1 - f(\varepsilon_{\mathbf{k_2}}))}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)}$$



Quenching of local moments: Kondo's calculation

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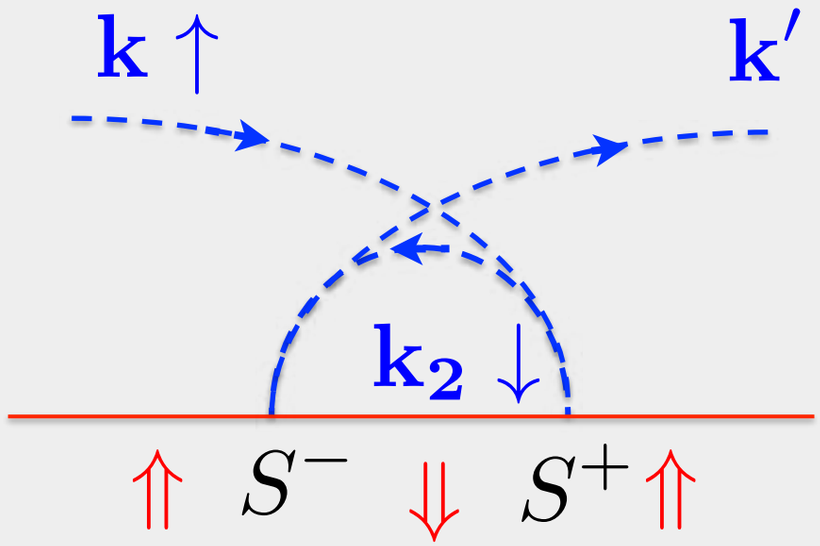


Quenching of local moments: Kondo's calculation

$$J^2 \sum_{\mathbf{k_2}} S^- S^+ \frac{(1 - f(\varepsilon_{\mathbf{k_2}}))}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)} \quad + \quad J^2 \sum_{\mathbf{k_2}} S^+ S^- \frac{f(\varepsilon_{\mathbf{k_2}})}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)}$$

Very important: spin flips DO NOT commute

$$S^+ S^- = S^- S^+ + 2S_z$$

Quenching of local moments: Kondo's calculation

$$J^2 \sum_{\mathbf{k_2}} S^- S^+ \frac{(1 - f(\varepsilon_{\mathbf{k_2}}))}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)} \quad + \quad J^2 \sum_{\mathbf{k_2}} S^+ S^- \frac{f(\varepsilon_{\mathbf{k_2}})}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)}$$

Very important: spin flips DO NOT commute

$$S^+ S^- = S^- S^+ + 2S_z$$

$$(S^2 - S_z) J^2 \sum_{\mathbf{k_2}} \frac{1}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)} + 2S_z J^2 \sum_{\mathbf{k_2}} \frac{f(\varepsilon_{\mathbf{k_2}})}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)}$$

Quenching of local moments: Kondo's calculation

$$(S^2 - S_z)J^2 \sum_{\mathbf{k_2}} \frac{1}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)} + 2S_z J^2 \sum_{\mathbf{k_2}} \frac{f(\varepsilon_{\mathbf{k_2}})}{(\varepsilon - \varepsilon_{\mathbf{k_2}} + i\eta)}$$

This lack of commutativity , combined with the restriction of the allowed occupancy of the intermediate states arising from Pauli principle, leads to a nontrivial temperature dependence of the scattering amplitudes.

Quenching of local moments: Kondo's calculation

$$\sum_{\mathbf{p}'} \frac{f(\varepsilon_{\mathbf{p}'}) - \frac{1}{2}}{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'}} = \int d\varepsilon \rho(\varepsilon) \frac{f(\varepsilon) - \frac{1}{2}}{\varepsilon_{\mathbf{p}} - \varepsilon} = \frac{1}{2}\rho(0) \int_{-D}^{D} d\varepsilon \frac{tanh(\frac{\varepsilon}{2k_B T})}{\varepsilon - \varepsilon_{\mathbf{p}}}$$

$$\varepsilon_{\mathbf{p}} << k_B T \rightarrow \approx \rho(0) \int_{k_B T}^{D} \frac{d\varepsilon}{\varepsilon} = \rho(0) ln \frac{D}{k_B T}$$

Logarithmic divergences

Quenching of local moments: Kondo's calculation

$$\frac{1}{\tau(k_F)} = \frac{3\pi c_{imp} n J^2}{2\varepsilon_F \hbar} S(S+1)$$

$$\frac{1}{\tau(p)} = \frac{3\pi c_{imp} n J^2}{2\varepsilon_F \hbar} S(S+1)\left(1 + \frac{4J}{N_s}\sum_{\mathbf{p}'} \frac{f(\varepsilon_{\mathbf{p}'}) - \frac{1}{2}}{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'}}\right) + O(J^4)$$

Logarithmic divergences

Quenching of local moments: Kondo's calculation

$$R = \frac{3\pi c_{imp} m J^2}{2e^2\hbar\varepsilon_F} S(S+1)(1 - 4J\rho(0) ln\frac{k_B T}{D}) + O(J^4)$$

Quenching of local moments: Kondo's calculation

$$R = \frac{3\pi c_{imp} m J^2}{2e^2\hbar\varepsilon_F} S(S+1)(1 - 4J\rho(0) ln\frac{k_B T}{D}) + O(J^4)$$

$$R(T) = AT^5 - Bln\frac{k_B T}{D}$$

If we add the phonon term, Kondo's calculation explains the resistance minimum.

Progress of Theoretical Physics, Vol. 32, No. 1, July 1964

Resistance Minimum in Dilute Magnetic Alloys

Jun KONDO

Electro-technical Laboratory
Nagatacho, Chiyodaku, Tokyo

(Received March 19, 1964)

Based on the *s-d* interaction model for dilute magnetic alloys we have calculated the scattering probability of the conduction electrons to the second Born approximation. Because of the dynamical character of the localized spin system, the Pauli principle should be taken into account in the intermediate states of the second order terms. Thus the effect of the Fermi sphere is involved in the scattering probability and gives rise to a singular term in the resistivity which involves $c \log T$ as a factor, where c is the concentration of impurity atoms. When combined with the lattice resistivity, this gives rise to a resistance minimum, provided the *s-d* exchange integral J is negative. The temperature at which the minimum occurs is proportional to $c^{1/5}$

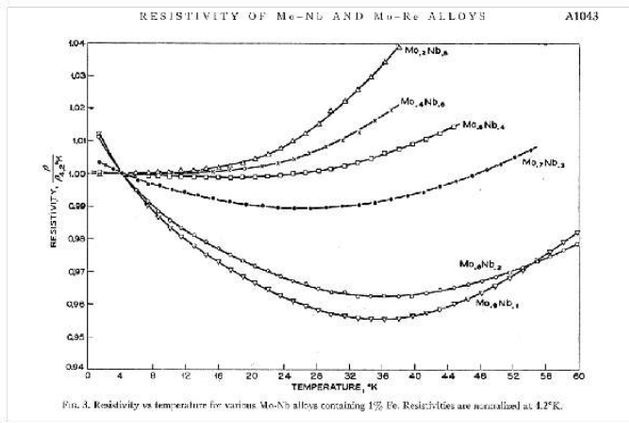


Fig. 3. Resistivity vs temperature for various Mo-Nb alloys containing 1% Fe. Resistivities are normalized at 4.2°K.

Quenching of local moments: the Kondo problem

$$\frac{1}{\tau(p)} = \frac{3\pi c_{imp} n J^2}{2\varepsilon_F \hbar} S(S+1)(1 + 4J\rho(0) ln \frac{D}{max(|\varepsilon_p|, k_B T}))$$

Physics behind the divergence at low temperatures:

- the magnetic impurity causes a dramatic increase of the scattering rate near the Fermi energy. This is remarkable as the Fermi energy is not an energy scale associated with the impurity.

- **Emergent scale at low energies**

Quenching of local moments: Kondo's calculation

$$R = \frac{3\pi m J^2}{2e^2\hbar\varepsilon_F} S(S+1)(1 - 4J\rho(0) ln \frac{k_B T}{D})$$

- More relevant: the resistivity diverges as $T \to 0$

The solution of this Non-perturbative problem is what is known as the **Kondo problem**. More than three decades of theory work towards solving this problem helped to develop a great deal of strongly correlated electron techniques.

- Scaling: Anderson 60's
- Numerical renormalization group: Wilson 70's, Nobel prize.
- Fermi liquid: Langreth, Nozieres, 70's
- Exact solutions by Bethe Anstaz: Andrei, Wiegman, 80's
- 1/N expansions 80's, 90's
- Non-equilibrium properties, 2000-present

Quenching of local moments: the Kondo problem

$$\frac{1}{\tau(p)} = \frac{3\pi c_{imp} n J^2}{2\varepsilon_F \hbar} S(S+1)(1 + 4J\rho(0) ln \frac{D}{max(|\varepsilon_p|, k_B T)})$$

Physics behind the divergence at low temperatures:

- the magnetic impurity causes a dramatic increase of the scattering rate near the Fermi energy. This is remarkable as the Fermi energy is not an energy scale associated with the impurity.

- The fact that such anomalous enhancement of the scattering rate is tied to the Fermi energy plays a key role in the analysis of the Kondo problem.

Quenching of local moments: the Kondo problem

$$\frac{1}{\tau(p)} = \frac{3\pi c_{imp} n J^2}{2\varepsilon_F \hbar} S(S+1)(1 + 4J\rho(0) ln \frac{D}{max(|\varepsilon_p|, k_B T}))$$

We will discuss how this enhanced scattering rate is tied to a non-trivial energy dependence of the phase shift (optical theorem) and, hence, via the Friedel sum rule to **an enhanced density of states near the Fermi energy**.

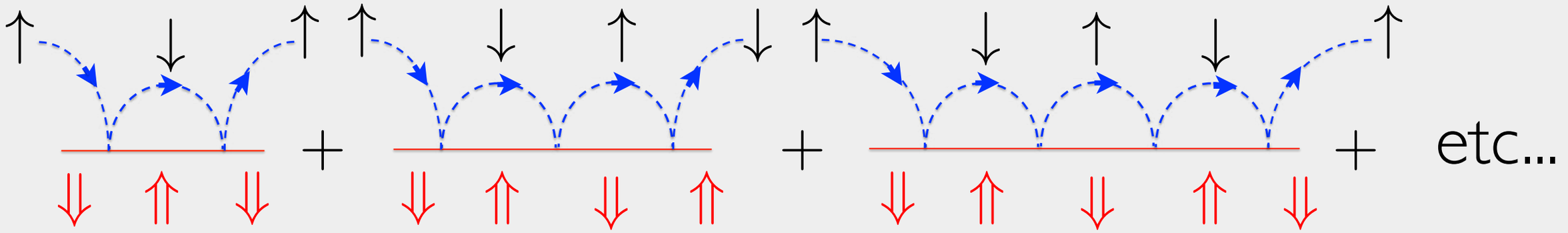
Kondo resonance

Quenching of local moments: the Kondo problem

First non-perturbative calculations Abrikosov Physics 2, 5, 1965

(resummation of so-called parquet diagrams to leading logartihmic order: terms that at order n diverge as

$$(ln(\frac{D}{k_B T}))^{n-1}$$



Quenching of local moments: the Kondo problem

Theoretical challenge, spins do no commute so standard Wick's decoupling in diagrammatics can NOT be applied.

Trick: represent spins as fermions+constraint (Abrikosov Fermions), first use of slave particles.

$$\vec{S} = f^{\dagger}_{\alpha}(\frac{\vec{\sigma}}{2})_{\alpha\beta} f_{\beta}$$

$$|\sigma\rangle = f^{\dagger}_{\sigma}|0\rangle$$

However, unwanted expansion of the Hilbert space (empty and doubly occupied states need to be eliminated).

$$n_f = 1$$

Quenching of local moments: the Kondo problem

However, unwanted expansion of the Hilbert space (empty and doubly occupied states need to be eliminated).

$$n_f = 1$$

The projection can be performed by using the Popov-Fedatov complex chemical potential

$$\mu = -i\pi \frac{T}{2}$$

$$G(i\omega_n) = \frac{1}{i\omega_n + \mu} \rightarrow \frac{1}{i\omega_n - i\pi\frac{T}{2}} = \frac{1}{2\pi i T(n + \frac{1}{4})}$$

$$\omega_n = \frac{(2n+1)\pi}{\beta}$$ Matsubara frequency

Quenching of local moments: the Kondo problem

First non-perturbative calculations Abrikosov Physics 2, 5, 1965

(resummation of so-called parquet diagrams to leading logartihmic order: terms that at order n diverge as

$$(ln(\frac{D}{k_B T}))^{n-1}$$

$$R = \frac{3\pi m J^2}{2e^2\hbar\varepsilon_F} S(S+1)(1 - 4J\rho(0) ln \frac{k_B T}{D})$$

$$R = \frac{3\pi c_{imp} m J^2}{2e^2\hbar\varepsilon_F} S(S+1) \frac{1}{(1 + 2J\rho(0) ln \frac{k_B T}{D})^2}$$

The logarithm is now in the denominator due to the summation of a geometric series (infinite subset of diagrams)

Quenching of local moments: the Kondo problem

First non-perturbative calculations Abrikosov Physics 2, 5, 1965

(resummation of so-called parquet diagrams to leading logartihmic order: terms that at order n diverge as

$$(ln(\frac{D}{k_B T}))^{n-1}$$

Spin susceptibility

$$\chi = \frac{(g\mu_B)^2 S(S+1)}{3k_B T}[1 - \frac{2J\rho(0)}{1+2J\rho(0)ln\frac{k_B T}{D}}]$$

For ferromagnetic coupling J<0, the zero temperature limit is well defined and we recover the Curie limit of a free impurity

$$\chi = \frac{(g\mu_B)^2 S(S+1)}{3k_B T}$$

Quenching of local moments: the Kondo problem

First non-perturbative calculations Abrikosov Physics 2, 5, 1965

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Spin susceptibility

$$\chi = \frac{(g\mu_B)^2 S(S+1)}{3k_B T}[1 - \frac{2J\rho(0)}{1+2J\rho(0)ln\frac{k_B T}{D}}]$$

For antiferromagnetic coupling J>0, this expression diverges now at finite temperature!

$$k_B T = De^{-\frac{1}{2J\rho(0)}}$$

Quenching of local moments: the Kondo problem

resolve these difficulties we must investigate higher order terms. Suhl[2] and Nagaoka[3] have undertaken such investigations. They have set up fairly rigorous equations. Although they have not yet reached the exact self-consistent solutions, Suhl has pointed out that the logarithmic divergence is replaced by a resonance scattering.

Non-divergent summations beyond Abrikosov's were done essentially at the same time by Suhl and Nagaoka in 1965.

Progress of Theoretical Physics, Vol. 34, No. 2, August 1965

s-d Scattering at Low Temperatures

Jun KONDO

Electro-Technical Laboratory, Tanashi, Tokyo

(Received April 20, 1965)

Based on a simple model which can be solved exactly, the electrical resistivity due to the s-d interaction in dilute alloys has been found to be expressed by

$$[\pi^3 S(S+1)ch/ze^2k_F][\{\log(T/T_c)\}^2+(\pi/2)^2]^{-1},$$

where $kT_c \sim \varepsilon_F e^{1/2zJ_F}$, for both signs of J. From this we draw four conclusions as follows;

PHYSICAL REVIEW VOLUME 138, NUMBER 2A 19 APRIL 1965

Dispersion Theory of the Kondo Effect

H. SUHL*
Physics Department, University of California, San Diego, La Jolla, California
(Received 30 November 1964)

According to recent work by Kondo, the scattering cross section of an electron in exchange interaction with a paramagnetic impurity immersed in a Fermi sea of electrons has a logarithmic infinity as the electron energy approaches the Fermi energy. We examine this problem by means of the Chew-Low method first devised for meson-nucleon scattering. It is found that the singularity is replaced by a resonant scattering close to the Fermi level.

PHYSICAL REVIEW VOLUME 138, NUMBER 4A 17 MAY 1965

Self-Consistent Treatment of Kondo's Effect in Dilute Alloys*

YOSUKE NAGAOKA†
Department of Physics, University of California, San Diego, La Jolla, California
(Received 7 December 1964)

We investigate how conduction electrons in dilute alloys are affected by the exchange interaction with localized spins of impurities. It is shown that, if the interaction is antiferromagnetic, the perturbational treatment breaks down below a critical temperature, and that near the Fermi surface there appears a quasi-bound state between the conduction-electron spin and the localized spin. Because of the appearance of this quasibound state, the resistivity increases with decreasing temperature, but has a finite value at $T=0$. There is no logarithmic term in the resistivity at low temperatures, in contrast to Kondo's theory of the resistance minimum. There also appears an anomaly in the specific heat at low temperatures.

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Quenching of local moments: the Kondo problem

- An interesting physical picture starts to emerge: non-perturbative effects give rise to resonant scattering near the Fermi energy.

- Strictly speaking, the **“Kondo resonance”** should be called Abrikosov-Suhl-Nagaoka resonance!!

Quenching of local moments: the Kondo problem

The nature of the ground state of the problem was first worked out by Yosida (Physical Review 147, 223, 1966) who understood, using a variational wave function approach, that **this resonance comes from a singlet ground state between the impurity and the conduction electrons.**

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

- Essentially, the idea of Anderson's "poor man's scaling" is to integrate out degrees of freedom far away from the Fermi level, thereby reducing the bandwidth D.

J. Phys. C: Solid St. Phys., 1970, Vol. 3. Printed in Great Britain

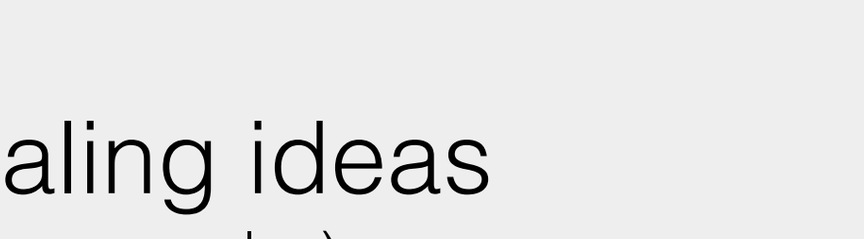

Figure 1.

A poor man's derivation of scaling laws for the Kondo problem

P. W. ANDERSON
Cavendish Laboratory,† Cambridge, England
and
Bell Telephone Laboratories, Murray Hill, New Jersey, USA

MS. received 28*th April* 1970

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

- Essentially, the idea of Anderson's "poor man's scaling" is to integrate out degrees of freedom far away from the Fermi level, thereby reducing the bandwidth D.

- In this way, the argument k_BT/D of the divergent logarithm will be reduced, and the divergence becomes weaker. Upon integrating out these degrees of freedom, one has to adapt, or "renormalize" the important coupling parameters of the theory.

- This is essentially an equivalent way of re-arranging perturbation theory similar to Abrikosov's non-perturbative result.

- **First use of renormalisation ideas (before they became successful in high energy physics).**

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$T(\varepsilon) = V + V\frac{1}{\varepsilon - H_0}V + ... = V + V\frac{1}{\varepsilon - H_0}T(\varepsilon) \qquad -D < \varepsilon < D$$

What is the goal?

$T(\varepsilon)$ remains invariant when $\begin{matrix} V \to \tilde{V} \\ H_0 \to \tilde{H}_0 \end{matrix}$ as high-energy states are removed

$$D \to \tilde{D} = D - \delta D$$

$$T(\varepsilon) = \tilde{V} + \tilde{V}\frac{1}{\varepsilon - \tilde{H}_0}T(\varepsilon)$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$H = J(D) \sum_{|\epsilon_k|,|\epsilon'_k|<D} c^\dagger_{k\alpha} \vec{\sigma}_{\alpha\beta} c_{k'\beta} \cdot \vec{S}$$

$$T_{ab}(E) = \sum_{\lambda \in [D', D]} \frac{H_{a\lambda} H_{\lambda b}}{E - E_\lambda}$$

Breakthrough: Anderson's scaling ideas

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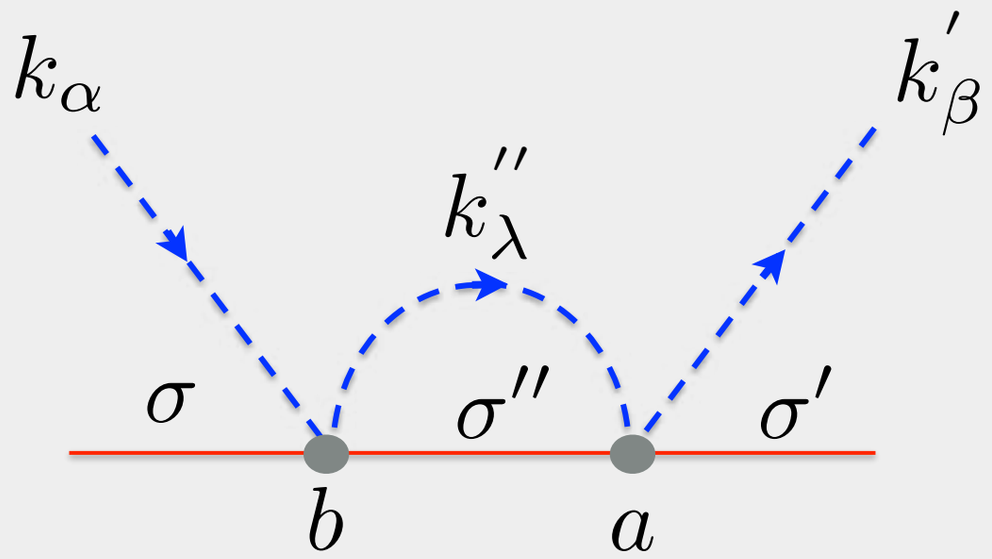


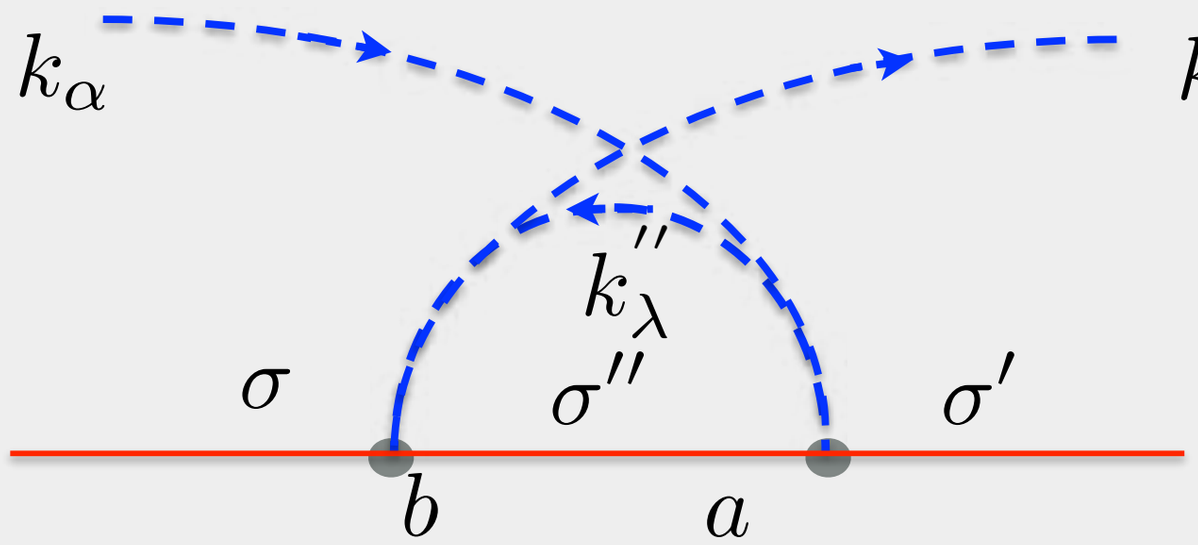
Scattering into a high energy electron state

$$T(E)_{k'\beta\sigma',k\alpha\sigma} = J^2 \sum_{\epsilon_{k''}\in[D-\delta D,D]} [\frac{1}{E-\epsilon_{k''}}](\sigma\sigma^b)_{\beta\alpha}(S^a S^b)_{\sigma'\sigma}$$

$$T(E)_{k'\beta\sigma',k\alpha\sigma} \approx J^2\rho\delta D[\frac{1}{E-D}](\sigma\sigma^b)_{\beta\alpha}(S^a S^b)_{\sigma'\sigma}$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)



Scattering into a high energy hole state

$$T(E)_{k'\beta\sigma',k\alpha\sigma} = -J^2 \sum_{\epsilon''_k \in [-D,-D+\delta D]} [\frac{1}{E-(\epsilon_k+\epsilon'_k-\epsilon''_k)}](\sigma^b\sigma^a)_{\beta\alpha}(S^aS^b)_{\sigma'\sigma}$$

$$T(E)_{k'\beta\sigma',k\alpha\sigma} = -J^2\rho\delta D[\frac{1}{E-D}](\sigma^b\sigma^a)_{\beta\alpha}(S^aS^b)_{\sigma'\sigma}$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

adding both terms

$$T(E)_{k'\beta\sigma',k\alpha\sigma} = -J^2\rho\frac{|\delta D|}{D}[\sigma^a,\sigma^b]_{\beta\alpha}(S^aS^b)_{\sigma'\sigma}$$

$$T(E)_{k'\beta\sigma',k\alpha\sigma} = 2J^2\rho\frac{|\delta D|}{D}\vec{\sigma}_{\beta\alpha}\cdot\vec{S}_{\sigma,\sigma'}$$

$$J(D-|\delta D|) = J(D) + \mathbf{2}J^2\boldsymbol{\rho}\frac{|\delta D|}{D} = J(D) - 2J^2\rho\frac{\delta D}{D}$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$J(D - |\delta D|) = J(D) + 2J^2\rho\frac{|\delta D|}{D} = J(D) - 2J^2\rho\frac{\delta D}{D}$$

The virtual emission of a high-energy electron and hole generates an **antiferromagnetic correction** to the original Kondo exchange since we have reduced the bandwidth

$$\delta D = -|\delta D|$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$J(D-|\delta D|) = J(D) + \mathbf{2}J^{\mathbf{2}}\boldsymbol{\rho}\frac{|\delta D|}{D} = J(D) - 2J^2\rho\frac{\delta D}{D}$$

$$\frac{\partial J\rho}{\partial lnD} = -2(J\rho)^2$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$\frac{\partial J\rho}{\partial lnD} = -2(J\rho)^2$$

$$g = \rho J \quad \text{(Dimensionless coupling)}$$

$$\frac{\partial g}{\partial lnD} = \beta(g) = -2g^2 + O(g^3)$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$\frac{\partial g}{\partial ln D} = \beta(g) = -2g^2 + O(g^3)$$

$g = 0$ is a fixed point since $\beta(g = 0) = 0$

(Scaling comes to a halt at this fixed point)

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$\frac{\partial g}{\partial ln D} = \beta(g) = -2g^2 + O(g^3)$$

$g = 0$ is a fixed point

$$\frac{\partial ln g}{\partial ln(D_0/D)} = 2g + O(g^2)$$

The direction of scaling depends **on the sign of** g

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$\frac{\partial lng}{\partial ln(D_0/D)} = 2g + O(g^2)$$

$$\int_{g_0}^{g(D)} \frac{dg'}{g'^2} = -2 \int_{lnD_0}^{lnD'} dlnD''$$

$$\frac{1}{g_0} - \frac{1}{g(D')} = -2ln(D'/D_0)$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$\frac{\partial lng}{\partial ln(D_0/D)} = 2g + O(g^2)$$

$$g(D') = \frac{g_0}{1 - 2g_0 ln(D_0/D')}$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

Ferromagnetic case

$$g(D') = -\frac{|g_0|}{1 + 2|g_0| ln(D_0/D')}$$

Very gradual decreasing of the effective coupling of the local moment to the surrounding conduction sea. Irrelevant since the interaction scales to zero (the problem remains perturbative).

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

Antiferromagnetic case

$$g(D') = \frac{g_0}{1 - 2g_0 ln(D_0/D')} = \frac{1}{2} \frac{1}{ln[\frac{D'}{D_0 exp(-1/2g_0)}]}$$

$$2g(D') = \frac{1}{ln(D'/T_K)}$$

$$T_K = D_0 exp[-1/2g_0]$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

Antiferromagnetic case

$$2g(D') = \frac{1}{ln(D'/T_K)}$$

The effective coupling diverges at a **dynamically generated scale**: the Kondo temperature.

$$T_K = D_0 exp[-1/2g_0]$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

- The Kondo interaction can only be treated perturbatively at energies larger compared with the Kondo temperature.

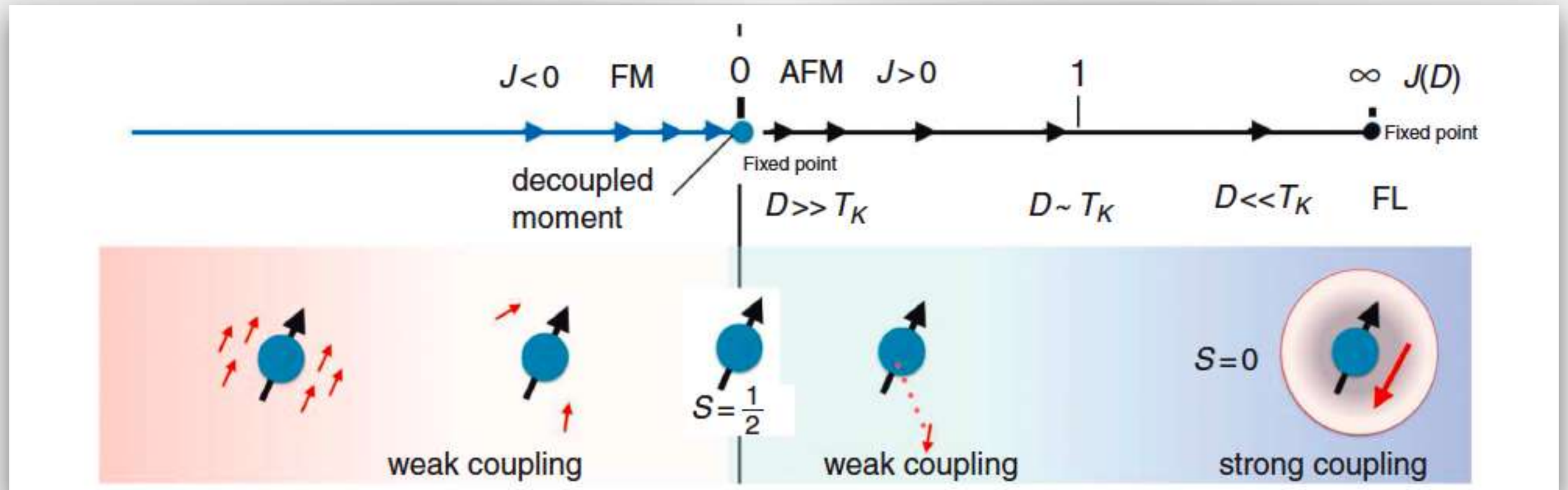
- The Kondo problem does not depend on the high-energy details of the model but rather on one relevant energy scale, the Kondo temperature

$$T_K = D_0 exp[-1/2g_0]$$

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$T_K = D_0 exp[-1/2g_0]$$



Scaling of the Anderson model (Haldane's PhD thesis 1977) gives:

$$T_K \sim D\sqrt{\frac{2\Gamma U}{\pi}} e^{\frac{\pi\varepsilon_d(\varepsilon_d+U)}{2\Gamma U}}$$

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The Nobel Prize in Physics 2016 was awarded with one half to David J. Thouless, and the other half to F. Duncan M. Haldane and J. Michael Kosterlitz "for theoretical discoveries of topological phase transitions and topological phases of matter"

Breakthrough: Anderson's scaling ideas

(the art of projecting out unwanted high-energy scales)

$$T_K = D_0 exp[-1/2g_0]$$

Remember $\frac{1}{g_0} - \frac{1}{g(D')} = -2ln(D'/D_0)$

$$\frac{1}{g_0} - 2lnD_0 = \frac{1}{g(D')} - 2lnD'$$

The Kondo temperature is a <u>scaling invariant</u> quantity.

Anderson's scaling ideas

$$g(D') = \frac{g}{1 - 2gln(\frac{D}{D'})}$$

$$\chi = \frac{(g\mu_B)^2 S(S+1)}{3k_B T}[1-g]$$

Anderson's scaling ideas

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$$\chi = \frac{(g\mu_B)^2 S(S+1)}{3k_B T}[1 - \frac{g}{1 - 2gln\frac{D}{k_B T}}]$$

Non-perturbative

Anderson's scaling ideas

All logarithmic corrections vanish when the high-energy cutoff equals the thermal energy:

$$g(k_B T) = \frac{g}{1 - 2g ln(\frac{D}{k_B T})}$$

$$T_K = D e^{-\frac{1}{2g}}$$

$$2g = \frac{1}{ln(T/T_K)}$$

All physical quantities depend on temperature only through this logarithm

Still, this kind of scaling analysis breaks down below the Kondo temperature so a good description of the strong coupling limit at zero temperature was needed. This led to many theoretical approaches trying to describe such strong coupling limit.

I am indebted to a London Times article about Idi Amin for learning that in Swahili "Kondoism" means "robbery with violence." This is not a bad description of this mathematical wilderness of models; H. Suhl has been heard to say that no Hamiltonian so incredibly simple has ever previously done such violence to the literature and to national science budgets.

Extracted from Anderson's Nobel lecture 1977