COLLÈGE DE FRANCE
1530

Chaire de Physique
de la Matière Condensée
Antoine Georges

Fermions en interaction: Introduction à la théorie de Champ Moyen Dynamique(DMFT)

Cours 4 & 5

Un atome dans un bain : introduction au modèle d'impureté d'Anderson dans la perspective de la théorie de champ moyen dynamique

Cycle 2018-2019
28 mai 2019

COLLÈGE DE FRANCE
1530

Chaire de Physique
de la Matière Condensée
Antoine Georges

Interacting Fermions: Introduction to Dynamical Mean-Field Theory (DMFT)

Lectures 4 & 5

Atom in a bath: introduction to the single-impurity Anderson model with a DMFT perspective

Slides will be in English

Please don't hesitate to ask questions in French or English

2018-2019 Lectures
May 28, 2019

Today's menu (lectures 4+5)

- Derivation of the DMFT equations: the cavity method (follow-up from lecture 3)

→ On blackboard

- Atom in a bath: introduction to the single-impurity Anderson model

Reminder: next session Tuesday June 11 (no session on June 4)

- 9:30-11:00: A.G. (last lecture)
- 11:30-12:30: Seminar by Olivier Parcollet

- 14:00-18:30 Mini-workshop on `Dynamical Mean-Field Theory and Beyond – Recent Developments' (Salle 2)

Mini-Workshop June,11

14:00-14:45 Manuel Zingl (CCQ, Flatiron Institute). ***Recent insights on Sr_2RuO_4: High-resolution photoemission and Hall effect***

14:45-15:30 Jernej Mravlje (Jožef Stefan Institute, Ljubljana). ***Hund's metals: overview, NRG insights, and the role of spin-orbit coupling***

15:30-16:15 Hugo Strand (CCQ, Flatiron Institute). ***Magnetic response of a Hund's metal within DMFT: Sr_2RuO_4***

16:15-17:00 Break

17:00-17:45 Alessandro Toschi (IFP – TU Wien). ***Fluctuation diagnostics of many-electron systems: how to read between the lines of single-particle spectra***

17:45-18:30 Leonid Pourovskii (CPHT, Ecole Polytechnique and Collège de France).
A DMFT insight into the Earth's core: many-electron effects in iron under extreme conditions

Reminder: Derivation of DMFT equations

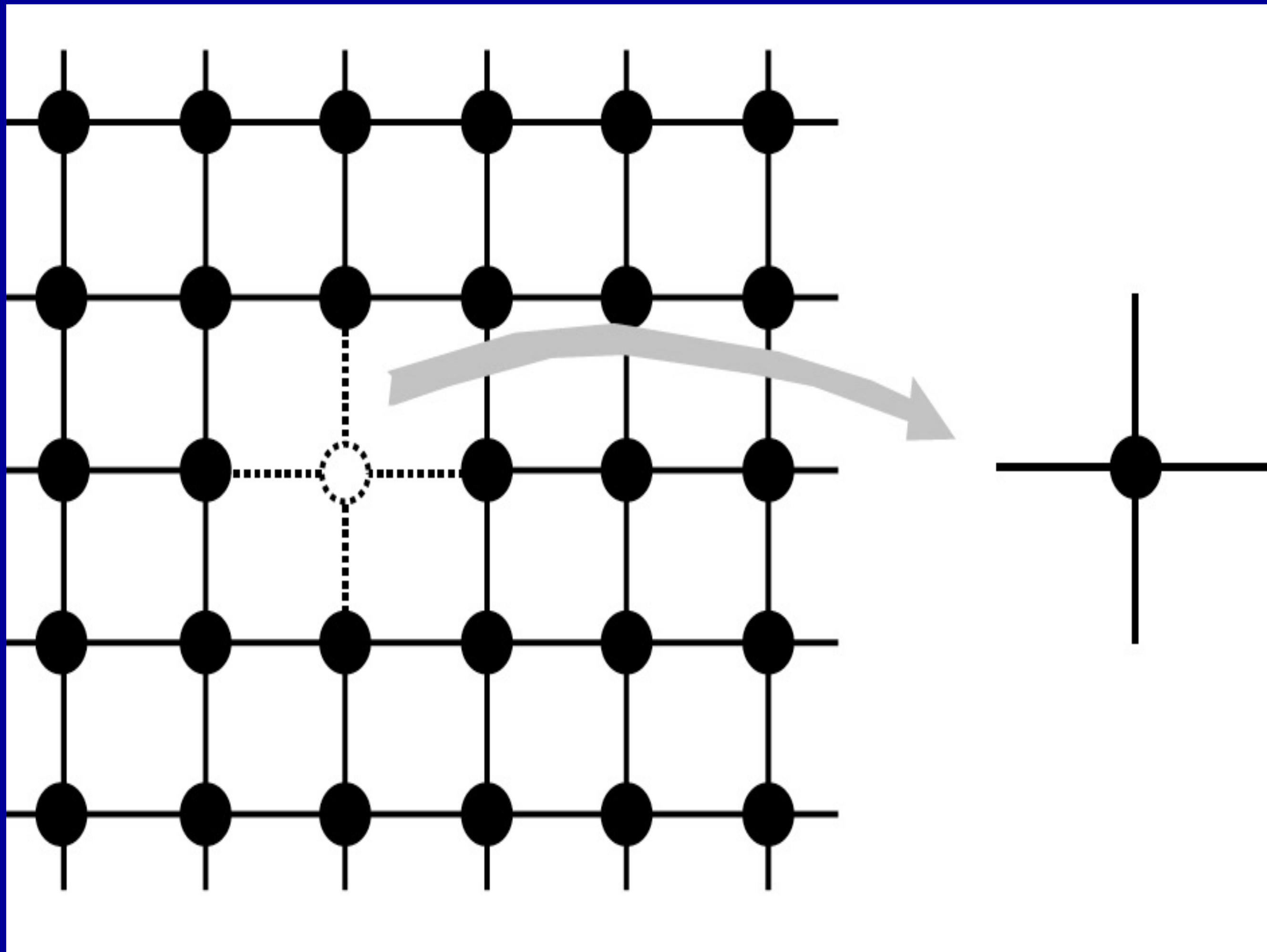
Locality of the Luttinger-Ward functional:

$$\Omega_{BK}[G,\Sigma] = -Tr\ln\left[(i\omega_n+\mu)\delta_{ij} - t_{ij} - \Sigma_{ij}\right] - \\ -Tr\left[\Sigma\cdot G\right] + \\ +\sum_i \phi_{atom}\left[G_{ii}\right]$$

$$\frac{\delta\Omega}{\delta\Sigma} = 0 \rightarrow \hat{G}^{-1} = \hat{G}_0^{-1} - \hat{\Sigma} \quad \text{(Dyson)}$$

$$\boxed{\frac{\delta\Omega}{\delta G_{ij}} = 0 \rightarrow \Sigma_{ij} = \delta_{ij}\,\Sigma_{atom}\left[G_{ii}\right]}$$

Cavity method (on blackboard)



Classical StatMech Models in which an infinite series of terms must be summed in d=infty: fully frustrated Ising

J. Phys. A: Math. Gen. **23** (1990) 2165–2171. Printed in the UK

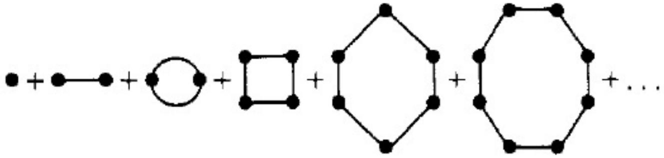
The fully frustrated Ising model in infinite dimensions

Jonathan S Yedidia† and Antoine Georges‡

† Department of Physics, Jadwin Hall, Princeton University, Princeton, NJ 08544, USA
‡ Laboratoire de Physique Théorique, Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France

Received 28 September 1989

Abstract. We solve, subject to the validity of some reasonable assumptions, the 'fully frustrated' Ising model in the limit of infinite dimensions using an extension of the TAP theory for spin glasses. In contrast to the TAP theory of the infinite-range spin glass, an infinite summation of diagrams is required to recover the Gibbs free energy for this model. The model undergoes a first-order transition. The method used to solve the model should have many applications to other physical problems.

$-\beta G =$  $+ \dots$

$$= -\sum_i \left(\frac{1+m_i}{2}\right)\ln\left(\frac{1+m_i}{2}\right) + \left(\frac{1-m_i}{2}\right)\ln\left(\frac{1-m_i}{2}\right)$$

$$+\beta \sum_{(ij)} J_{ij} m_i m_j + \frac{\beta^2}{2}\sum_{(ij)} J_{ij}^2 (1-m_i^2)(1-m_j^2)$$

$$+\beta^4 \sum_{(ijkl)} J_{ij} J_{jk} J_{kl} J_{li} (1-m_i^2)(1-m_j^2)(l-m_k^2)(1-m_l^2) + \dots .$$

Figure 1. The Gibbs free energy of the 'fully frustrated' Ising model on a hypercubic lattice in the limit of infinite dimensions.

Atom in a bath: Introduction to the single-impurity Anderson model with a DMFT perspective

`Anderson – Friedel- Wolff' model

J.Friedel, Can.J.Phys 34, 1190 (1956)

P.W.Anderson, Phys Rev 124, 41 (1961)

P.A.Wolff, Phys. Rev. 124, 1030 (1961)

See also lecture in 2009-2010 cycle

The simplest `atom'

$$H_{\rm at} \;=\; \varepsilon_d \sum_\sigma d^\dagger_\sigma d_\sigma + U\, n^d_\uparrow n^d_\downarrow$$

Eigenstates:

- $|0\rangle \;\;,\;\; E=0$
- $|\uparrow\rangle$ and $|\downarrow\rangle$, $E=\varepsilon_d$, *doubly degenerate* (in zero-field).
- $|\uparrow\downarrow\rangle$, $E=2\varepsilon_d+U$

Level crossings:

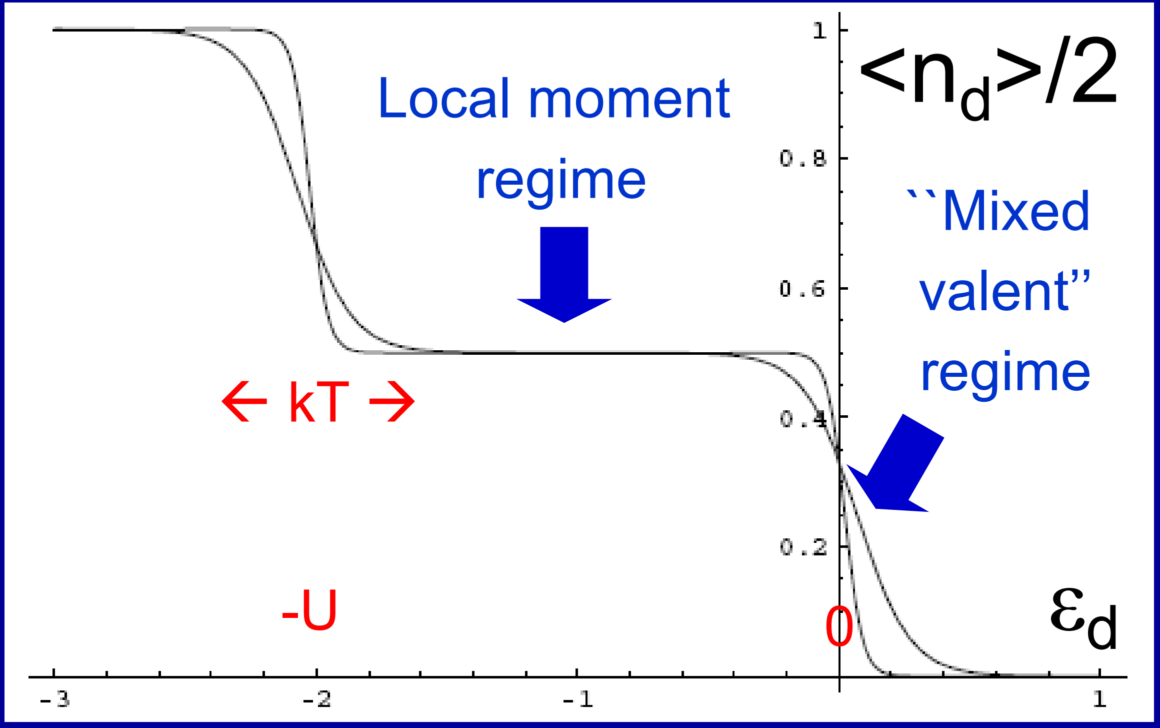
- Between |n=0> and |n=1> at $\varepsilon = 0$

- Between |n=1> and |n=2> at $\varepsilon = -U$

Occupancy of the isolated atom :

$$n_{d\sigma} \equiv \langle d_\sigma^\dagger d_\sigma \rangle = \frac{n_d}{2} = \frac{1}{Z}\left(1 \times e^{-\beta\varepsilon_d} + 1 \times e^{-\beta(2\varepsilon_d+U)}\right)$$

$$Z = 1 + 2e^{-\beta\varepsilon_d} + e^{-\beta(2\varepsilon_d+U)}$$



Plot of $n_d/2$ vs. ε_d for $U = 2$ at $\beta = 30$ and $\beta = 10$.

``Coulomb staircase'': Blocking of charge by repulsive interactions, Except at points of level-crossing (charge degeneracy)

Spectroscopy of the isolated atom

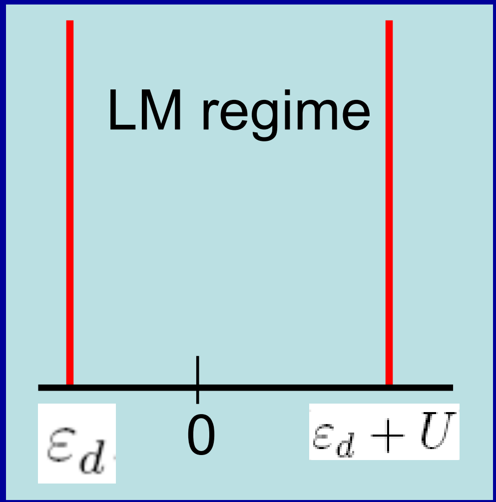
One-particle spectral function, at T=0:

$$
\begin{aligned}
A_d(\omega) &\equiv \sum_A |\langle \Psi_A | d_\sigma^\dagger | \Psi_0 \rangle|^2 \, \delta(\omega + E_0 - E_A) \quad (\omega > 0) \\
&\equiv \sum_B |\langle \Psi_B | d_\sigma | \Psi_0 \rangle|^2 \, \delta(\omega + E_B - E_0) \quad (\omega < 0)
\end{aligned}
$$

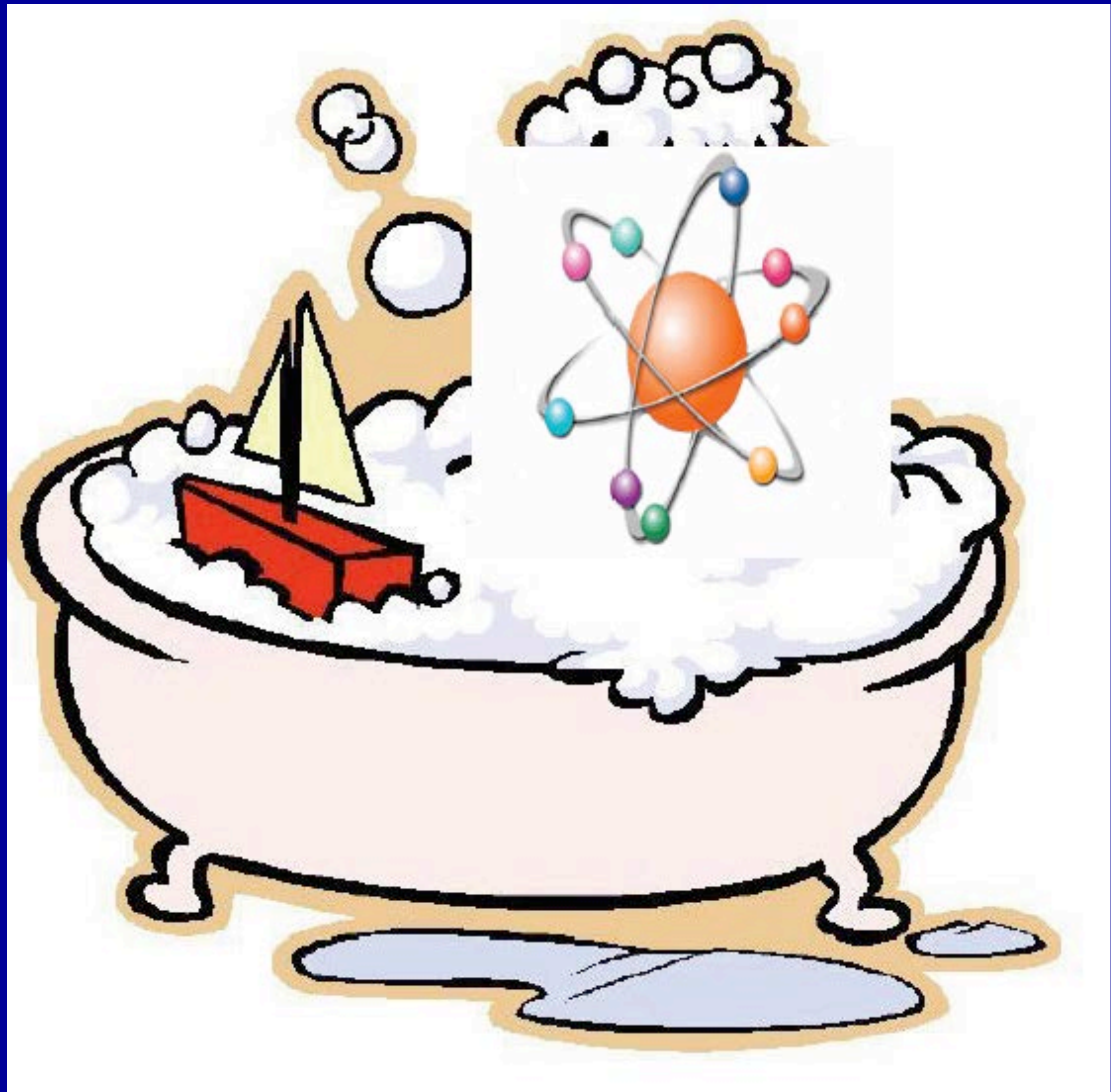
and, at finite temperature:

$$
A_d(\omega) \equiv \frac{1}{Z} \sum_{A,B} |\langle \Psi_A | d_\sigma^\dagger | \Psi_B \rangle|^2 \, \left(e^{-\beta E_A} + e^{-\beta E_B}\right) \delta(\omega + E_B - E_A)
$$

$$
\begin{aligned}
A_d(\omega) &= \frac{e^{-\beta\varepsilon_d} + e^{-\beta(2\varepsilon_d + U)}}{Z} \delta(\omega - \varepsilon_d - U) + \frac{1 + e^{-\beta\varepsilon_d}}{Z} \delta(\omega - \varepsilon_d) \\
&= \frac{n_d}{2} \delta(\omega - \varepsilon_d - U) + (1 - \frac{n_d}{2}) \delta(\omega - \varepsilon_d) \\
&\quad [|\sigma\rangle \leftrightarrow |\uparrow\downarrow\rangle \text{ transition}] + [|\sigma\rangle \leftrightarrow |0\rangle \text{ transition}]
\end{aligned}
$$



``Atom in a bath''



Hamiltonian formulation: Anderson impurity model

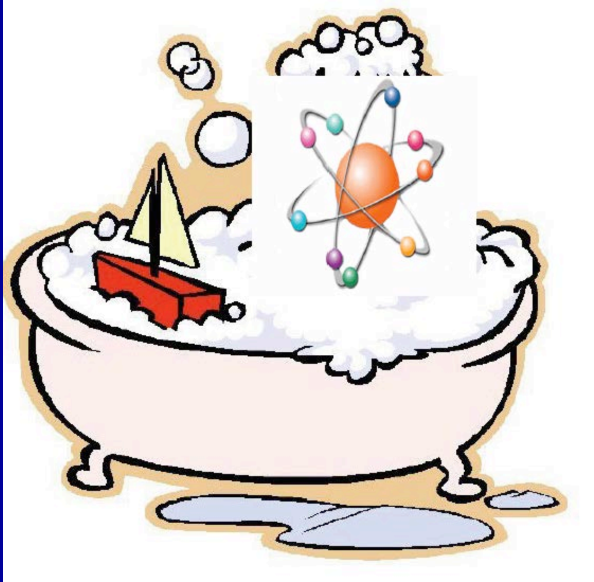
$$H_c = \sum_{l\sigma} E_l a^+_{l\sigma} a_{l\sigma}$$

$$H = H_c + H_{at} + H_{hyb}$$

Conduction electron host (``bath'', environment)

$$H_{at} = \varepsilon_d \sum_\sigma d^\dagger_\sigma d_\sigma + U\, n^d_\uparrow n^d_\downarrow$$

Single-level ``atom''



$$H_{hyb} = \sum_{l\sigma} [V_l a^+_{l\sigma} d_\sigma + \mathrm{h.c.}]$$

Transfers electrons between bath
and atom – Hybridization, tunneling

Shakespeare's anticipation of DMFT: Correlation effects `in a nutshell'

"O God! I could be bounded in a nutshell,
and count myself king of infinite space,
were it not that I have bad dreams !"

William Shakespeare (in: Hamlet)

Bibliography (some)

- Kondo and Anderson models:

- I.Affleck *Quantum impurity problems in condensed matter physics Lecture notes at Les Houches, arXiv:0809.3474*
- A.Hewson *The Kondo problem to heavy fermions, Cambridge UP*
- G.Grüner and A.Zawadowski *Rep Prog Phys 37 (1974) 1497*
- D. Cox Lectures at Boulder school, 2003 http://sexton.ucdavis.edu/CondMatt/cox/
- D. Cox and A. Zawadovski Adv. Phys. **47**, 599 (1998)
- + Many other references…

C. R. Physique 17 (2016) 430–446

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Condensed matter physics in the 21st century: The legacy of Jacques Friedel

The beauty of impurities: Two revivals of Friedel's virtual bound-state concept

La beauté des impuretés : nouveaux contextes pour le concept d'état lié virtuel

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https://www.sciencedirect.com/journal/comptes-rendus-physique/vol/17/issue/3

Relevance to physical systems

- 1. Magnetic impurities in metals

- Low concentration of magnetic atoms, with quite localized orbitals, into metallic host

- e.g. 3d transition metals (Mn, Cr, Fe) into Au or Cu or Al
4f dilute rare-earth compounds e.g. $Ce_xLa_{1-x}\ Cu_6$ ($x << 1$)

In some cases, all range of solid solution can be studied,
from dilute to dense system (Kondo alloy to Heavy-Fermion regime)

PHYSICAL REVIEW VOLUME 124, NUMBER 1 OCTOBER 1, 1961

Localized Magnetic States in Metals

P. W. Anderson
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received May 31, 1961)

The conditions necessary in metals for the presence or absence of localized moments on solute ions containing inner shell electrons are analyzed. A self-consistent Hartree-Fock treatment shows that there is a sharp transition between the magnetic state and the nonmagnetic state, depending on the density of states of free electrons, the s-d admixture matrix elements, and the Coulomb correlation integral in the d shell; that in the magnetic state the d polarization can be reduced rather severely to nonintegral values, without appreciable free electron polarization because of a compensation effect; and that in the nonmagnetic state the virtual localized d level tends to lie near the Fermi surface. It is emphasized that the condition for the magnetic state depends on the Coulomb (i.e., exchange self-energy) integral, and that the usual type of exchange alone is not large enough in d-shell ions to allow magnetic moments to be present. We show that the susceptibility and specific heat due to the inner shell electrons show strongly contrasting behavior even in the nonmagnetic state. A calculation including degenerate d orbitals and d-d exchange shows that the orbital angular momentum can be quenched, even when localized spin moments exist, and even on an isolated magnetic atom, by kinetic energy effects.

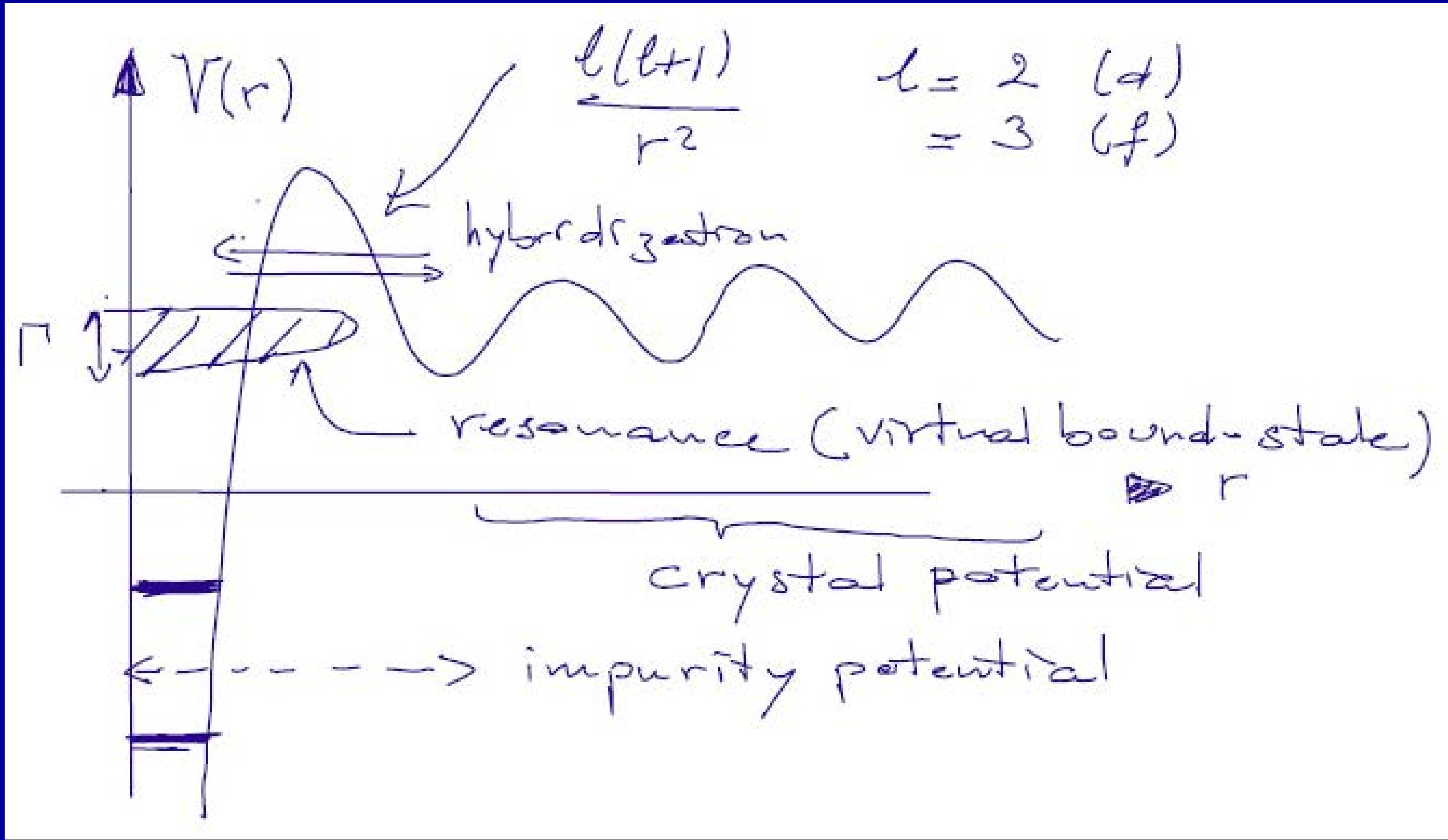
PHYSICAL REVIEW VOLUME 124, NUMBER 4 NOVEMBER 15, 1961

Localized Moments in Metals

P. A. Wolff
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received July 14, 1961)

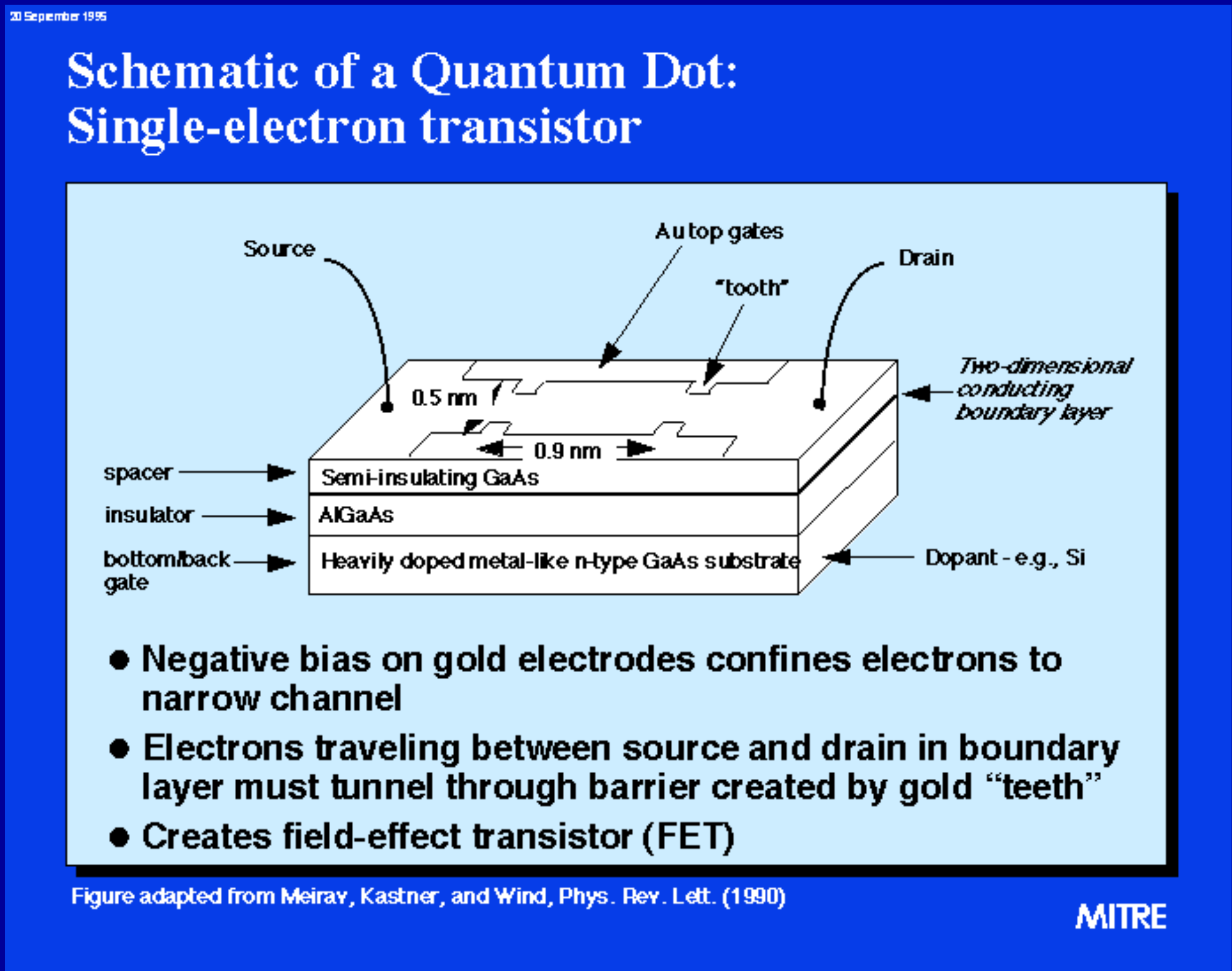
A simple model is used to study the occurrence of localized magnetic moments in dilute alloys. The phenomenon is treated as a scattering problem in which conduction electrons scatter from impurity potentials. Under appropriate circumstances the scattering amplitude may show a resonance—corresponding to a virtual level of the impurity. It is shown that if such a level is sufficiently sharp and lies close enough to the Fermi level, the impurity atom will develop an exchange potential that polarizes neighboring electrons. The potentials for spin-up and spin-down electrons are determined by a pair of coupled equations, whose solutions are discussed in a number of interesting cases.

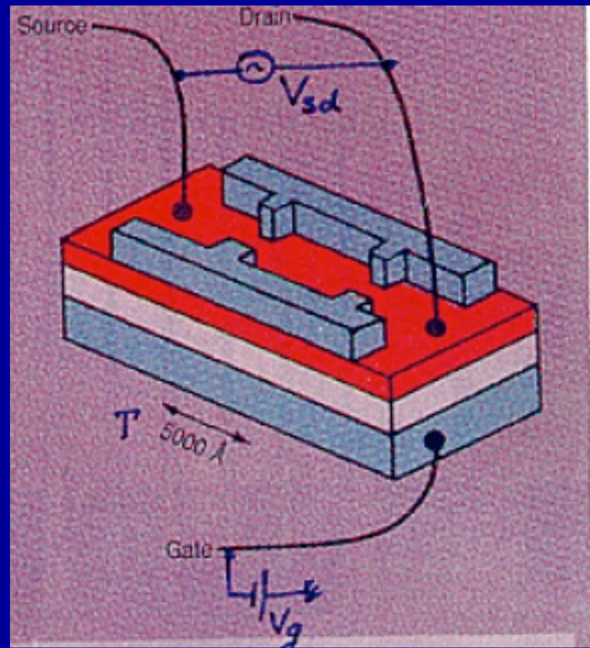
Friedel's virtual bound-state concept



Cf. Jacques Friedel Can.J.Phys 34, p. 1190 (1956)
Nuov Cim Supp 7, p.287 (1958)
Varenna school XXXVII, 1966

• <u>2. Nanostructures: Many-Body effects on the Coulomb blockade</u>





$$U \simeq \frac{e^2}{C}$$

Coulomb repulsion on the dot <u>increases</u> as the size (capacitance) decreases

Extremely simplified model: a slight modification of the Anderson single-impurity model (w/ 2 baths)

$$H = H_{\text{dot}}[d_\sigma, d_\sigma^\dagger] + \sum_{p=L,R} \sum_\sigma \left[V_p\, d_\sigma^\dagger a_{p\sigma} + h.c + E_p\, a_{p\sigma}^\dagger a_{p\sigma} \right]$$

Hybridization to the leads

Leads

$$H_{\text{dot}} = \varepsilon_d \sum_\sigma n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}$$

Coulomb blockade on the dot

Valid for widely separated energy levels on the dot, considering a single level (NOT correct for a metallic island, OK for 2DEG dots).

Integrate out the bath: Effective action

$$S \;=\; S_{at} + S_{hyb}$$

$$S_{at} = \int_0^\beta d\tau \sum_\sigma d_\sigma^+(\tau)\left(\frac{\partial}{\partial\tau} + \varepsilon_d\right) d_\sigma(\tau) + U\int_0^\beta d\tau\, n_\uparrow(\tau) n_\downarrow(\tau)$$

$$S_{hyb} = \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma d_\sigma^+(\tau)\Delta(\tau-\tau')d_\sigma(\tau')$$

$$\boxed{\Delta(i\omega_n) \;=\; \sum_l \frac{|V_l|^2}{i\omega_n - E_l}}$$

$$\mathcal{G}_0^{-1}(i\omega_n) \;=\; i\omega_n - \varepsilon_d - \Delta(i\omega_n)$$

Effective `bare propagator'.

The non-interacting case (U=0)

- A different point of view, offered by the Anderson model (not available for Kondo model)
- In contrast to the V-expansion, small U and large U are smoothly connected.

$$H_{U=0} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \varepsilon_d \sum_{\sigma} d^\dagger_\sigma d_\sigma + \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} (c^\dagger_{\mathbf{k}\sigma} d_\sigma + d^\dagger_\sigma c_{\mathbf{k}\sigma})$$

$$G^{-1}_{d0}(i\omega_n) = i\omega_n - \varepsilon_d - \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{i\omega_n - \varepsilon_{\mathbf{k}}}$$

``Integrating out'' c-electrons, or simple diagrammatics, or eqs of motion

Key quantity: hybridization function

$$\Delta(i\omega_n) \equiv \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{i\omega_n - \varepsilon_{\mathbf{k}}}$$

$$\Gamma(\varepsilon) \equiv \pi \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2\, \delta(\varepsilon - \varepsilon_{\mathbf{k}}) = -\,\mathrm{Im}\,\Delta(\varepsilon + i0^+) = \pi\Delta(\varepsilon)$$

Case of a broad band w/ structureless d.o.s:

(Note: the integrable case, by Bethe ansatz, for arbitrary U)

$$\Gamma(\varepsilon) = \Gamma = \pi\Delta(0) \quad , \quad \text{for}\, \varepsilon \in [-\mathrm{D}, +\mathrm{D}]$$

$$\Delta(i\omega_n) = -\frac{\Gamma}{\pi} \ln \frac{D - i\omega_n}{-D - i\omega_n} \rightarrow -i\Gamma \mathrm{sign}(\omega_n) \quad (D \rightarrow \text{infinity})$$

$$\Delta(\omega + i0^+) = \frac{\Gamma}{\pi} \ln \left| \frac{\omega + D}{\omega - D} \right| - i\Gamma \rightarrow -i\Gamma$$

$$\Gamma = \pi V^2 \rho_c$$

`Virtual bound-state' resonance
Width given by Fermi's Golden rule

In this limit:

$$A_d^0(\omega) = \frac{1}{\pi} \frac{\Gamma}{(\omega - \varepsilon_d)^2 + \Gamma^2}$$

$$\frac{n_d}{2} = \int_{-\infty}^{+\infty} d\omega\, A_d^0(\omega) = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\varepsilon_d}{\Gamma}$$

No Coulomb blockade. of course
Goes smoothly from n=0 to n=2

The atomic limit (V=0) is SINGULAR

(when the bath has states at low-energy, as in a metal)

The ground-state is actually modified as soon as $V \neq 0$ and becomes a singlet state (S=0) in which the local moment has been `swallowed' (screened out) by the conduction electron bath

→ Kondo effect

Exact solution for a single site in the bath:

$$H = H_{\text{at}} + V \sum_{\sigma} \left(c_{\sigma}^{\dagger} d_{\sigma} + d_{s}^{\dagger} c_{\sigma} \right)$$

Conserved quantum numbers:
N, S, S^z

1+4+6+4+1=16 states

- $N = 0$: one state $|0\rangle$ $(S = S^z = 0)$
- $N = 1$: 4 states, $S = 1/2, S^z = \pm 1/2$
- $N = 2$: $S = 1$ a triplet of states
- $N = 2$: $S = 0$ three singlet states
- $N = 3$: 4 states
- $N = 4$: one states: $|\uparrow\downarrow, \uparrow\downarrow\rangle$

Focus on N=2 (ground-state) sector in LM regime:

- The $N=2$, $S=1$ triplet sector has eigenstates: $|\uparrow,\uparrow\rangle$, $|\downarrow,\downarrow\rangle$ and $\frac{1}{\sqrt{2}}[|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle]$. These states are insensitive to the hybridization V because the Pauli principle does not allow for hopping an electron through. Hence their energy is ε_d.

The $N=2$, $S=0$ sector is more interesting.

Basis set: $|\uparrow\downarrow,0\rangle$, $\frac{1}{\sqrt{2}}[|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle]$ $|0,\uparrow\downarrow\rangle$.

The matrix reads: $\begin{pmatrix} 2\varepsilon_d+U & \sqrt{2}V & 0 \\ \sqrt{2}V & \varepsilon_d & \sqrt{2}V \\ 0 & \sqrt{2}V & 0 \end{pmatrix}$

Symmetric case ε_d=-U/2

$$E = 0 \ , \ E_{\pm} = -\frac{U}{4} \pm \frac{1}{2}\sqrt{\frac{U^2}{4} + 16V^2}$$

The *ground-state* has energy E_-. For $V \ll U$, this reads:

$$E_0 = E_- \simeq -\frac{U}{2} - \frac{8V^2}{U} + \cdots$$

Energy in SINGLET SECTOR is lowered by virtual hops

Double occupancy in intermediate state → energy denominator ~ U

Ground-state wave-function:

$$|\Psi_0\rangle = \sqrt{1-\eta^2}\,|\mathcal{S}\rangle + \eta\,|\mathcal{D}\rangle$$

$$|\mathcal{S}\rangle \equiv \frac{1}{\sqrt{2}}\left[|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right]$$

$$|\mathcal{D}\rangle \equiv \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right]$$

with $\eta \sim \frac{V}{U} \ll 1.$

Key points:

- Because of virtual hopping and the Pauli principle, a spin-singlet ground-state has been stabilized, in which the impurity spin is screened out by a conduction electron.
- Virtual hopping has induced a (small) admixture of states with $n_d = 0$ and $n_d = 2$ in the wave-function, hence allowing for charge fluctuations on the atom.

- The atomic limit V=0 is SINGULAR in the LM regime
- A non-zero V lifts the ground-state degeneracy
- The ground-state becomes a singlet: the impurity moment is ``screened'' by binding w/ a conduction electron

$$G(z) = \sum_{j=1}^{2} \left(\frac{a_j}{z - \epsilon_j} + \frac{a_j}{z + \epsilon_j} \right),$$

$$\epsilon_1 = \frac{1}{4} \left(\sqrt{U^2 + 64V^2} - \sqrt{U^2 + 16V^2} \right),$$

$$\epsilon_2 = \frac{1}{4} \left(\sqrt{U^2 + 64V^2} + \sqrt{U^2 + 16V^2} \right),$$

$$a_1 = \frac{1}{4} \left(1 - \frac{U^2 - 32V^2}{\sqrt{(U^2 + 64V^2)(U^2 + 16V^2)}} \right),$$

E.Lange
Mod Phys Lett B 12, 915 (1998)
arXiv:9810208
See also Appendix in
Alex Hewson's book

Spectral function for
1site in the bath,
½ filling

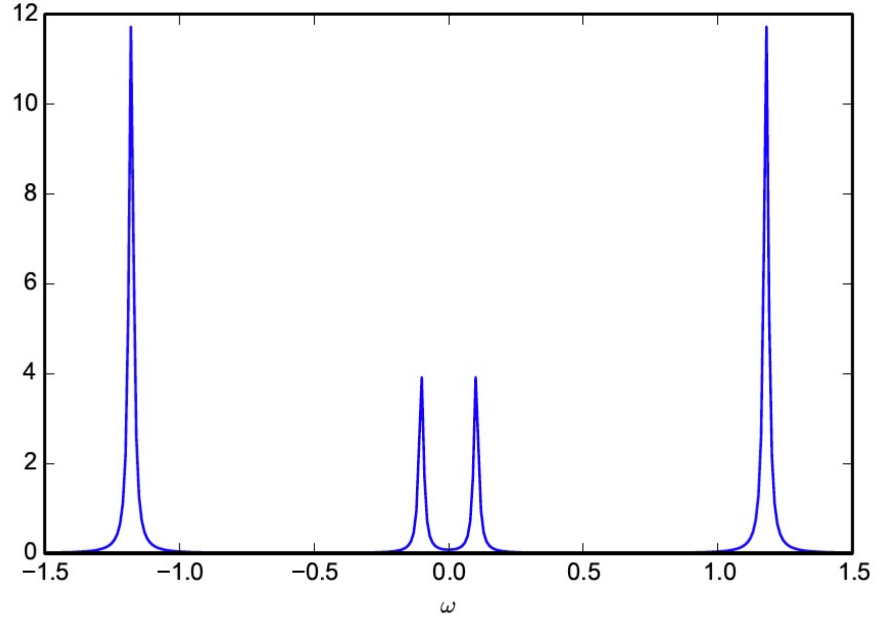


Figure 3: Spectral function for $U = 2.0$, $V = 0.2$

The Kondo effect from the small V ($\Gamma << U$) perspective

Effective Hamiltonian at small V: the Kondo model

1-site: low-energy Hilbert space ={ground-state + triplet S=1}

$$H_K = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^{+}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J_K \vec{S}_d \cdot \vec{S}_c(0) \;\;,\;\; J_K = \frac{8V^2}{U}$$

Sd, Sc: spin operators

Can be generalized to a full conduction electron band:

(Schrieffer-Wolff transformation –eliminating states w/ nd=0,2) -1966-

$$H_{\mathrm{eff}} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \vec{S}_d \cdot \sum_{\mathbf{k}\mathbf{k}'\alpha\alpha'} J_{\mathbf{k}\mathbf{k}'} \frac{1}{2} c^{\dagger}_{\mathbf{k}'\alpha'} \vec{\sigma}_{\alpha\alpha'} c_{\mathbf{k}\alpha} + \sum_{\mathbf{k}\mathbf{k}'\alpha} V^{\mathrm{pot}}_{\mathbf{k}\mathbf{k}'} c^{\dagger}_{\mathbf{k}'\alpha} c_{\mathbf{k}\alpha}$$

$$J_{\mathbf{k}\mathbf{k}'} = 2V_{\mathbf{k}}V_{\mathbf{k}'}\left[\frac{1}{\varepsilon_{\mathbf{k}'} - \varepsilon_d} + \frac{1}{\varepsilon_d + U - \varepsilon_{\mathbf{k}}}\right] \rightarrow 2V_{\mathbf{k}}V_{\mathbf{k}'}\frac{U}{|\varepsilon_d(\varepsilon_d+U)|}$$

$$V^{\mathrm{pot}}_{\mathbf{k}\mathbf{k}'} = \frac{1}{2}V_{\mathbf{k}}V_{\mathbf{k}'}\left[\frac{1}{\varepsilon_{\mathbf{k}'} - \varepsilon_d} - \frac{1}{\varepsilon_d + U - \varepsilon_{\mathbf{k}}}\right]$$

→ 0 in symmetric case

``No Hamiltonian so incredibly simple has ever previously done such violence to the literature and to national science budgets''

Attributed to Harry Suhl by P.W. Anderson
in his 1978 Nobel lecture
[Rev Mod Phys 50 (1978) 191 p. 195]

[Although the Ising model is surely a serious competitor…]

The Kondo effect as an history of spin-flips

(on blackboard, time permitting)

FLUCTUATION THEORY OF DILUTE MAGNETIC ALLOYS

D. R. Hamann
Bell Telephone Laboratories, Incorporated, Murray Hill, New Jersey 07974
(Received 6 May 1969)

A simple explanation of the Kondo effect is shown to follow from a functional integral form of Anderson's dilute-alloy model.

D.R. Hamann Phys Rev 23 (1969) 95
PW Anderson and G Yuval Phys Rev Lett 23 (1969) 89
Yuval and Anderson Phys Rev B 1 (1970) 1522
Anderson, Yuval, Hamann Phys Rev B (1970) 4464

From small U/Γ to large U/Γ
- a smooth evolution -

- In contrast to the expansion in the hybridization (Γ), the expansion in U is perfectly fine and smooth.
- Local Fermi liquid theory naturally emerges
- Pioneers: Yamada and Yosida

- How does one interpolate from $U/\Gamma=0$ limit

(1 broadened atomic level centered at ε_d)

to atomic limit $\Gamma/U=0$?

(2 sharp peaks corresponding to atomic transitions,
Doubly degenerate local-moment ground-state)

General many-body theory and (local) Fermi-liquid considerations

Focus on dynamics of impurity orbital: integrate out conduction electrons

→ Effective action for impurity orbital:

$$S = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma d^\dagger_\sigma(\tau') G^{-1}_{d0}(\tau-\tau') d_\sigma(\tau) + U \int_0^\beta d\tau n_\uparrow n_\downarrow$$

also reads:

$$S = S_{at} + S_{hyb}$$

$$S_{at} = \int_0^\beta d\tau \sum_\sigma d^+_\sigma(\tau)\left(\frac{\partial}{\partial\tau} + \varepsilon_d\right) d_\sigma(\tau) + U \int_0^\beta d\tau\, n_\uparrow(\tau) n_\downarrow(\tau)$$

$$S_{hyb} = \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma d^+_\sigma(\tau)\Delta(\tau-\tau') d_\sigma(\tau')$$

Feynman rules associated with this action (involving only time):

- A vertex U (local in time)
- A `bare' propagator (retarded): $G_{d0}(\tau-\tau') \sim \rho_c/(\tau-\tau') + \cdots$

The interaction leads to a self-energy for the d-orbital:

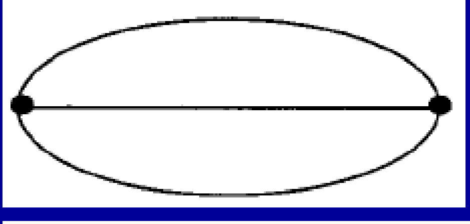
$$G_d(i\omega_n)^{-1} = G_{d0}(i\omega_n)^{-1} - \Sigma(i\omega_n)$$

(Local) Fermi-liquid form of self-energy, at T=0:

$$\Sigma'(\omega) = \Sigma(0) + \left(1 - \frac{1}{Z}\right)\omega + \cdots$$

$$\Sigma''(\omega) = -A\,\omega^2 + \cdots$$

First non-trivial diagram O(U²):



$$\sim U^2 \frac{1}{\tau^3} \rightarrow \Sigma'' \propto \omega^2$$

d-level spectral function, wide bandwidth limit, Fermi-liquid considerations:

$$A_d(\omega) = \frac{1}{\pi} \frac{\Gamma - \Sigma''(\omega)}{[\omega - \varepsilon_d - \Sigma'(\omega)]^2 + [\Gamma - \Sigma''(\omega)]^2}$$

Hence, at low-frequency:

$$\Sigma'(\omega) = \Sigma(0) + \left(1 - \frac{1}{Z}\right)\omega + \cdots$$

$$\Sigma''(\omega) = -A\,\omega^2 + \cdots$$

$$A_d(\omega \simeq 0) = \frac{Z}{\pi} \frac{\widetilde{\Gamma}}{(\omega - \widetilde{\varepsilon}_d)^2 + \widetilde{\Gamma}^2}$$

Resonance with renormalized level position and width, <u>overall spectral weight Z:</u>

$$\widetilde{\varepsilon}_d = Z\,[\varepsilon_d + \Sigma(0)] \quad , \quad \widetilde{\Gamma} = Z\,\Gamma$$

In particular, in particle-hole symmetric case (LM regime) $\varepsilon_d = -\frac{U}{2}$

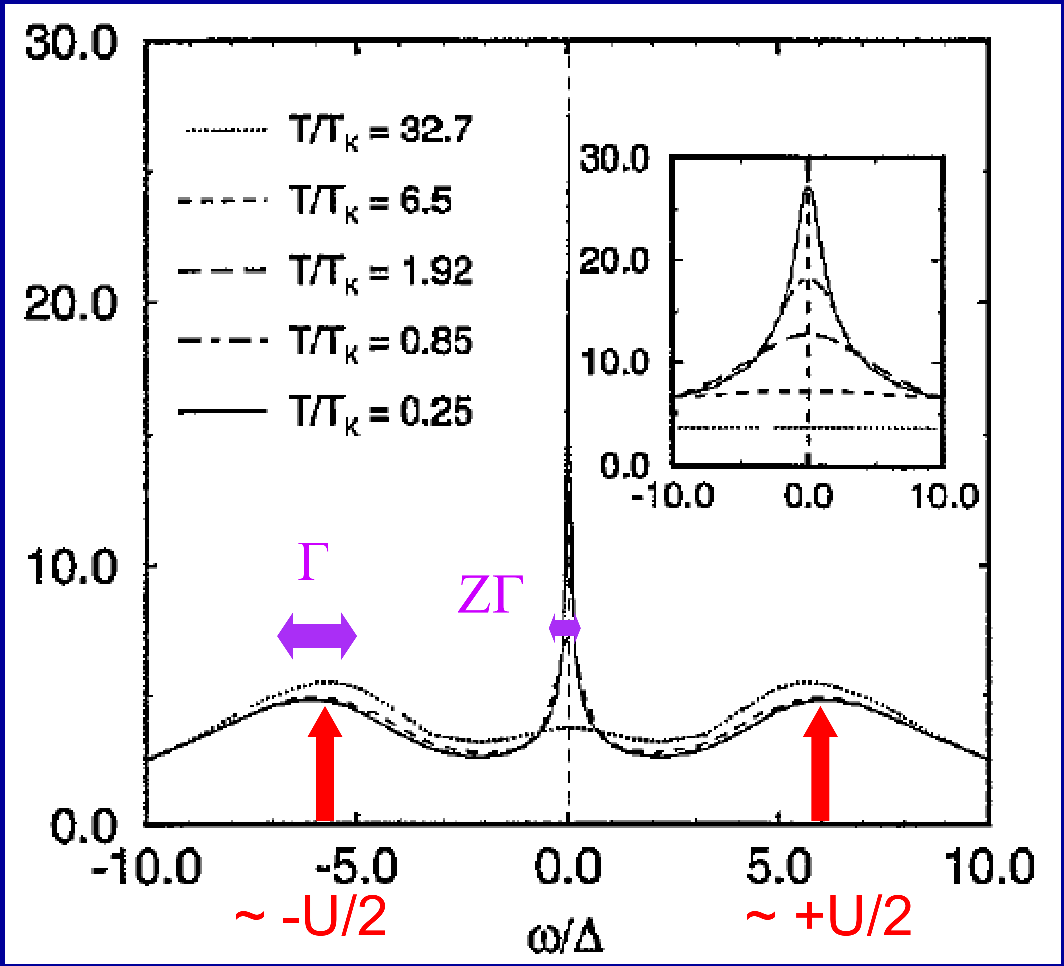
$$A_d(\omega \simeq 0) = \frac{Z}{\pi} \frac{Z\Gamma}{\omega^2 + (Z\Gamma)^2} \qquad A_d(\omega = 0) = \frac{1}{\pi\Gamma}$$

Width, Weight ~ Z

Height unchanged !

Numerical Renormalization Group (NRG) calculation

T.Costi and A.Hewson, J. Phys Cond Mat 6 (1994) 2519



Low energy associated with
the resonance and quasiparticle excitations:

$$Z \sim T_K/\Gamma \sim \exp -\frac{8\Gamma}{\pi U}$$

The T-matrix, at T=0 and ω=0 (wide bandwidth):

$$G_d(i0^+) = \frac{1}{-(\varepsilon_d + \Sigma'(0)) + i\Gamma}$$ → $$\tan\delta = \frac{\Gamma}{\varepsilon_d + \Sigma'(0)}$$

phase shift at T=ω=0

Hence :

$$|G_d|^2 = \frac{1}{\Gamma^2}\frac{1}{1+(\varepsilon_d+\Sigma_0)^2/\Gamma^2} = \frac{1}{\Gamma^2}\sin^2\delta$$

So that, finally:

$$G_d(i0^+) = -\frac{1}{\Gamma}\sin\delta\, e^{i\delta}$$

$$A_d(\omega=0) = \frac{\sin^2\delta}{\pi\Gamma}$$

$A_d(0)$ pinned at its U=0 value in symmetric case !

Im T takes maximal value

→ Unitary limit scattering

Local d.o.s of conduction electrons at ω=0:

$$G_c = G_{c0} + [G_{c0}]^2 V^2 G_d$$

$$A_c(\omega=0, T=0) \equiv -\frac{1}{\pi}\mathrm{Im}\sum_{\mathbf{kk}'} G_c^{\mathbf{kk}'} = \rho_c\,(1-\sin^2\delta)$$

d.o.s vanishes in symmetric case → Kondo screening `hole'

More complex atoms: Multiplets

… and more complex
Kondo-like
screening processes

Interactions: Kanamori hamiltonian:

[J.Kanamori, Prog. Theor. Phys. 30 (1963) 275]

$$H_{\mathrm{K}} = U \sum_{m} \hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U' \sum_{m\neq m'} \hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} + (U'-J) \sum_{m<m',\sigma} \hat{n}_{m\sigma}\hat{n}_{m'\sigma} + \\ -J \sum_{m\neq m'} d^{+}_{m\uparrow}d_{m\downarrow}\, d^{+}_{m'\downarrow}d_{m'\uparrow} + J \sum_{m\neq m'} d^{+}_{m\uparrow}d^{+}_{m\downarrow}\, d_{m'\downarrow}d_{m'\uparrow}$$

EXACT for a t_{2g} shell

Useful reference: Sugano, Tanabe & Kamimura,
Multiplets of transition-metal ions in crystals
Academic Press, 1970

Assuming furthermore ~ spherical symmetry of the screened interaction V_c , one can show that: U' = U-2J
[Deviations in Sr2RuO4 are on the 10% scale – GW/cRPA]
In this case, the hamiltonian can be written:

$$H_{t_{2g}} = (U-3J)\,\frac{\hat{N}(\hat{N}-1)}{2} - 2J\,\vec{S}^2 - \frac{J}{2}\vec{L}^2 + \frac{5}{2}J\,\hat{N}$$

$$\hat{N} = \sum_{m\sigma} \hat{n}_{m\sigma} \;\;,\;\; \vec{S} = \frac{1}{2}\sum_{m}\sum_{\sigma\sigma'} d^{\dagger}_{m\sigma}\vec{\tau}_{\sigma\sigma'}d_{m\sigma'} \;\;,\;\; L_m = i\sum_{m'm''}\sum_{\sigma}\epsilon_{mm'm''}d^{\dagger}_{m'\sigma}d_{m''\sigma},$$

Total charge, spin and orbital iso-spin operators

$U(1)_c \otimes SU(2)_s \otimes SO(3)_o$ symmetry

Spectrum of atomic t_{2g} hamiltonian with U'=U-2J (no spin-orbit)

N	S	L	Degeneracy $= (2S+1)(2L+1)$	Energy
0,[6]	0	0	$\boxed{1}$	0
1,[5]	1/2	1	$\boxed{6}$	$-5J/2,[10\mathcal{U}-5J/2]$
2,[4]	1	1	$\boxed{9}$	$\mathcal{U}-5J,[6\mathcal{U}-5J]$
2,[4]	0	2	5	$\mathcal{U}-3J,[6\mathcal{U}-3J]$
2,[4]	0	0	1	$\mathcal{U},[6\mathcal{U}]$
3	3/2	0	$\boxed{4}$	$3\mathcal{U}-15J/2$
3	1/2	2	10	$3\mathcal{U}-9J/2$
3	1/2	1	6	$3\mathcal{U}-5J/2$

Table 1: Eigenstates and eigenvalues of the t_{2g} Hamiltonian $\mathcal{U}\hat{N}(\hat{N}-1)/2 - 2J\vec{S}^2 - J\vec{T}^2/2$ in the atomic limit ($\mathcal{U} \equiv U - 3J$). The boxed numbers identifies the ground-state multiplet and its degeneracy, for $J > 0$.

- Hund's rule ground-state in each particle-number sector
- Symmetry broken by J from SU(6) to U(1)c × SU(2)s × SO(3)o
- → Degeneracies lifted by J: from 15-fold to 9-fold

Hund's metals (e.g. Sr_2RuO_4) : distinct crossover scales for orbital and spin degrees of freedom

~ 1000K

Fermi
Liquid

Metal with fluctuating spins
No orbital fluctuations

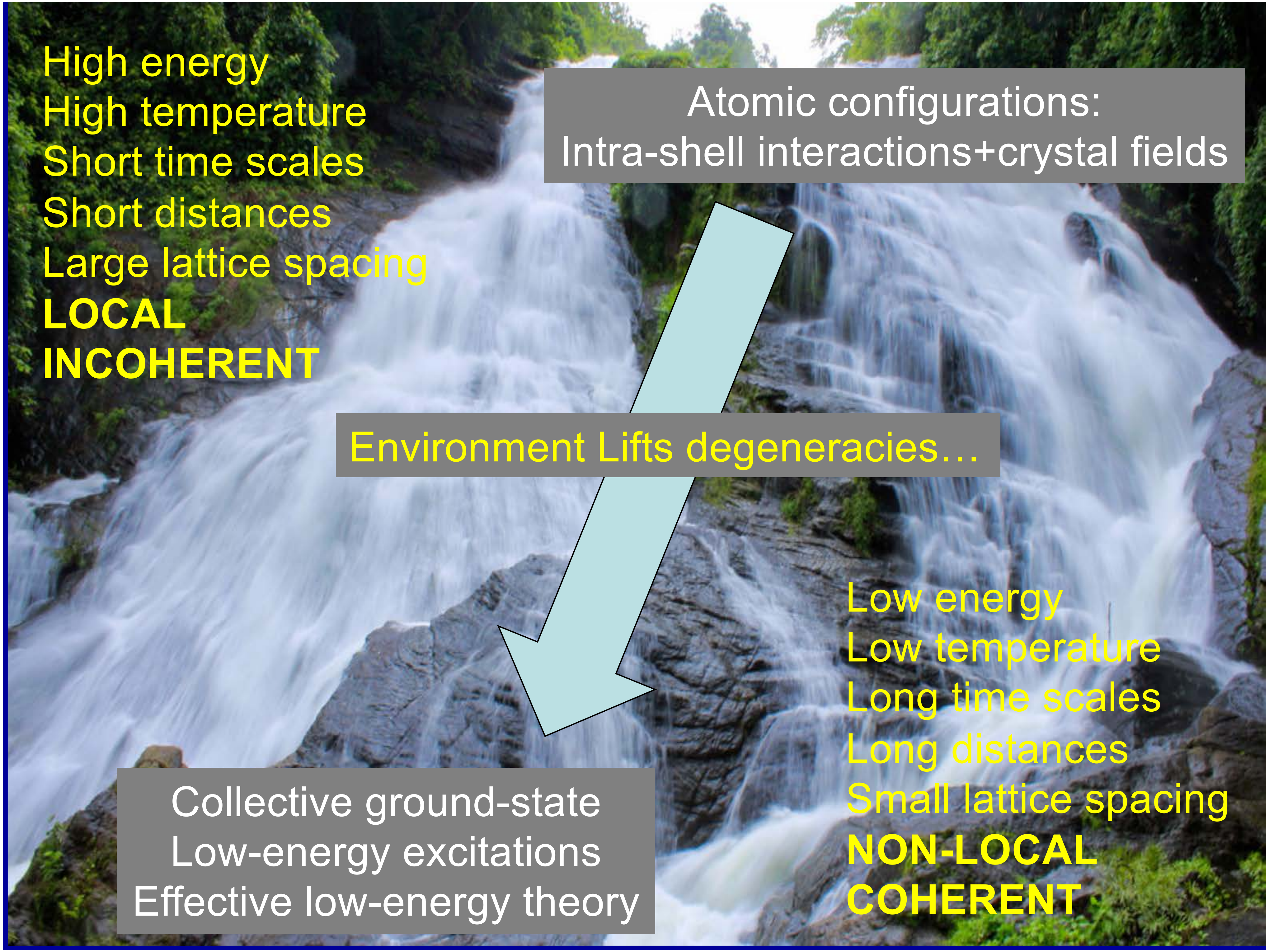
Now fully understood from a renormalization-group perspective, cf. work by von Delft, Kotliar, Aron et al. and Mravlje et al.

Following the flow to low energy…

Atomic configurations:
Intra-shell interactions+crystal fields

Insulators:
Kugel-Khomskii
Low-energy models
Magnons, Orbitons etc.

Metals
Fermi liquids
Quasiparticles
Collective modes



High energy
High temperature
Short time scales
Short distances
Large lattice spacing
LOCAL
INCOHERENT
Atomic configurations:
Intra-shell interactions+crystal fields
Environment Lifts degeneracies…
Collective ground-state
Low-energy excitations
Effective low-energy theory
Low energy
Low temperature
Long time scales
Long distances
Small lattice spacing
NON-LOCAL
COHERENT

This is very much how we think about materials

In DMFT:

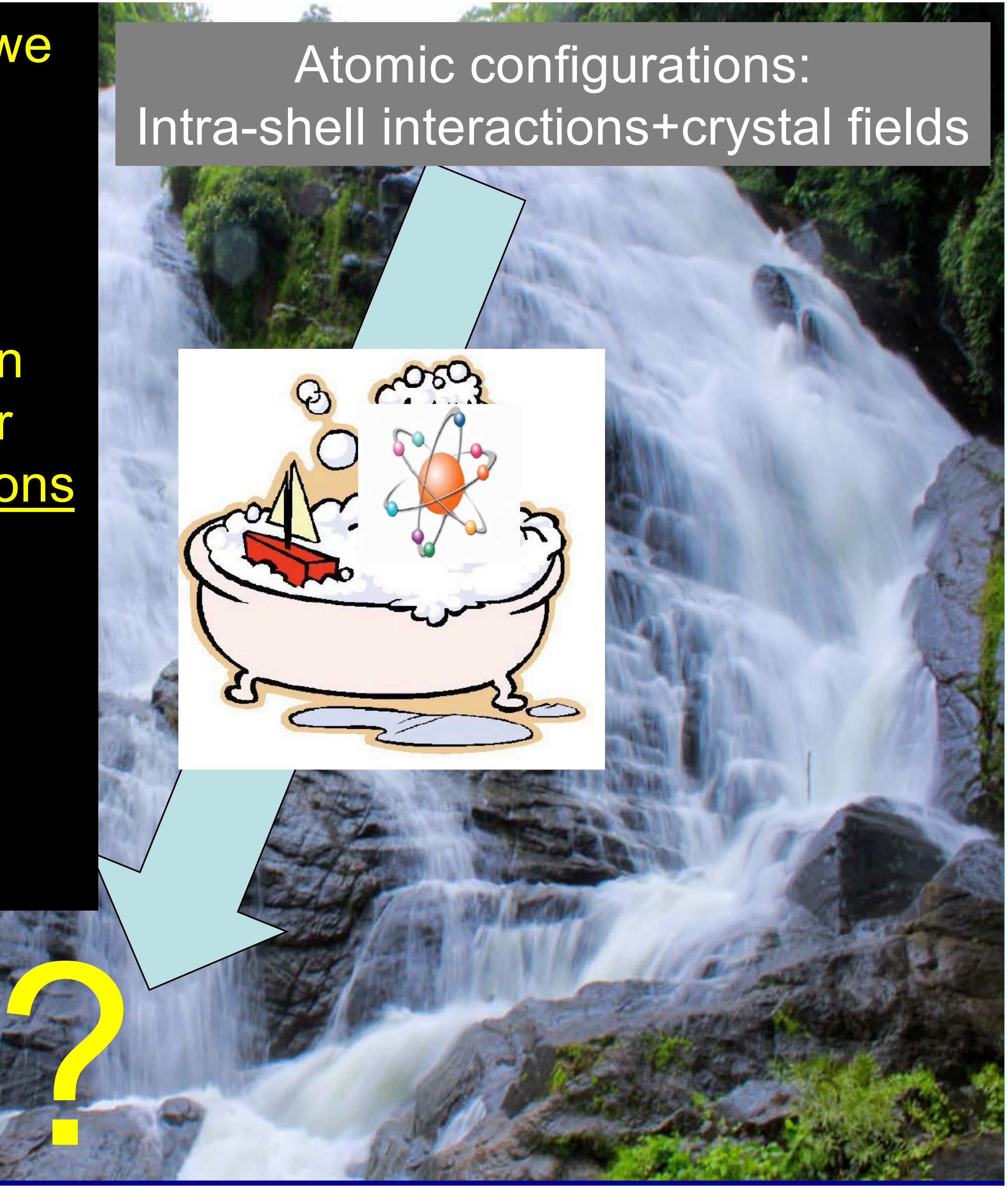
Start from local atomic configurations

and follow the flow down into collective behaviour

<u>Initially, spatial correlations are short-range</u>

At lower energy, spatial correlations build up

→ Cluster extensions of DMFT



Impurity Solvers: Brief Overview

- Solvers directly using an action form of the impurity problem – typically Quantum Monte Carlo
- Solvers requiring a Hamiltonian form

- e.g. ED, NRG

- Approximation Schemes – e.g. IPT, NCA,…

QMC algorithmic breakthroughs

entering a new age for DMFT approaches
(and extensions) …

Early days: Hirsch-Fye (1986)

Continuous-time quantum Monte Carlo
(CT-QMC) 2005 →

*****Rubtsov 2005 Interaction expansion(CT-INT)
*****P. Werner, M.Troyer, A.Millis et al 2006
Hybridization expansion (CT-HYB)
*****E**.**Gull O.Parcollet 2008 Auxiliary field (CT-AUX)

Review: Gull et al. Rev Mod Phys 83, 349 (2011)

REVIEWS OF MODERN PHYSICS, VOLUME 83, APRIL–JUNE 2011

Continuous-time Monte Carlo methods for quantum impurity models

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(Received 15 April 2010; published 5 May 2011)

$$Z = \mathrm{Tr} T_\tau e^{-\beta H_a} \exp\left[-\int_0^\beta d\tau H_b(\tau)\right]$$
$$= \sum_k (-1)^k \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \mathrm{Tr}[e^{-\beta H_a} H_b(\tau_k)$$
$$\times H_b(\tau_{k-1}) \cdots H_b(\tau_1)].$$

cf. Prokof'ev Svistunov, 1998

Need for efficient and sutainable open-source software libraries

TRIQS (@CCQ) (O.Parcollet, M.Ferrero, N.Wentzell, H.Strand et al.)

https://github.com/TRIQS/triqs

triqs
a Toolbox for Research on Interacting Quantum Systems

Install | Reference | Tutorials | Applications | Issues | About TRIQS

Welcome

TRIQS (**T**oolbox for **R**esearch on **I**nteracting **Q**uantum **S**ystems) is a scientific project providing a set of C++ and Python libraries to develop new tools for the study of interacting quantum systems.

TRIQS 2.0
This is the homepage TRIQS Version 2.0 For the changes in 2.0, Cf changelog page

The goal of this toolkit is to provide high level, efficient and simple to use libraries in C++ and Python, and to promote the use of modern programming techniques.

TRIQS is free software distributed under the GPL license.

TRIQS applications

Based on the TRIQS toolkit, several full-fledged applications are also available. They allow for example to solve a generic quantum impurity model or to run a complete LDA+DMFT calculation.

Developed in a collaboration between IPhT Saclay and Ecole Polytechnique since 2005, the TRIQS library and applications have allowed us to address questions as diverse as:

- Momentum-selective aspects on cuprate superconductors (with various cluster DMFT methods)
- Degree of correlation in iron-based superconductors (within an LDA+DMFT approach)
- Fermionic Mott transition and exploration of Sarma phase in cold-atoms

Python & C++

The libraries exist at two complementary levels: on the one hand, C++ libraries allow to quickly develop high-performance low-level codes; on the other hand python libraries implement the most common many-body objects, like Green's functions, that can be manipulated easily in python scripts.

This duality is a real advantage in the development of new many-body tools. Critical parts where performance is essential can be written in C++ (e.g. a quantum impurity solver) while the data analysis, preparation of the inputs or interface with other programs can be done at the very user-friendly python level.

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E.Gull et al.

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ALPSCore

Applications and Libraries for Physics Simulations Core libraries

The ALPS Core libraries aim to provide a set of well tested, robust, and standardized components for numerical simulations of condensed matter systems, in particular systems with strongly correlated electrons. They consist of a set of components that are used in state of the art high performance codes. The ALPSCore libraries are a spinoff of the ALPS libraries available from alps.comp-phys.org

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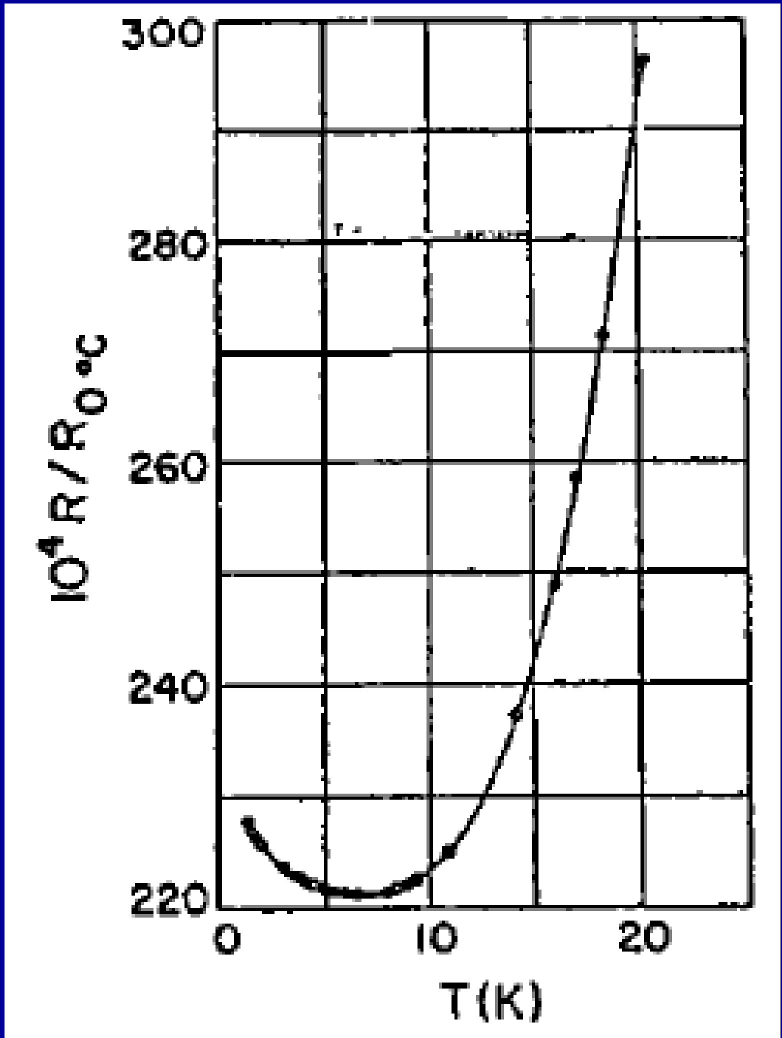
Methods using a Hamiltonian representation of the bath

- Exact Diagonalisation
- Wilson Numerical RG (NRG)
- DMRG/Tensor Network
- NB: Many possible representations of the bath - `Star', 1D chain/Continous Fraction [Possibly log-scale as in NRG], etc…

ADDITIONAL SLIDES

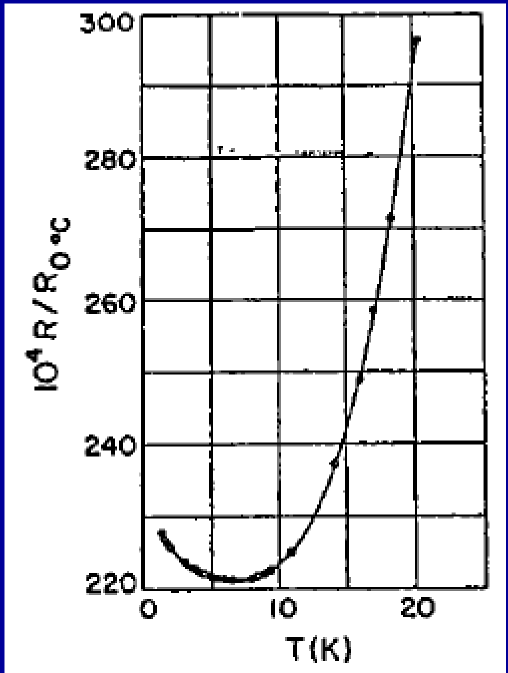
See also lectures of previous years

Magnetic impurities in metals: resistivity minimum



De Haas, de Boer
and van den Berg,
Physica 1 (1934) 1115

``The resistivity of the gold wires measured (not very pure) has a minimum."

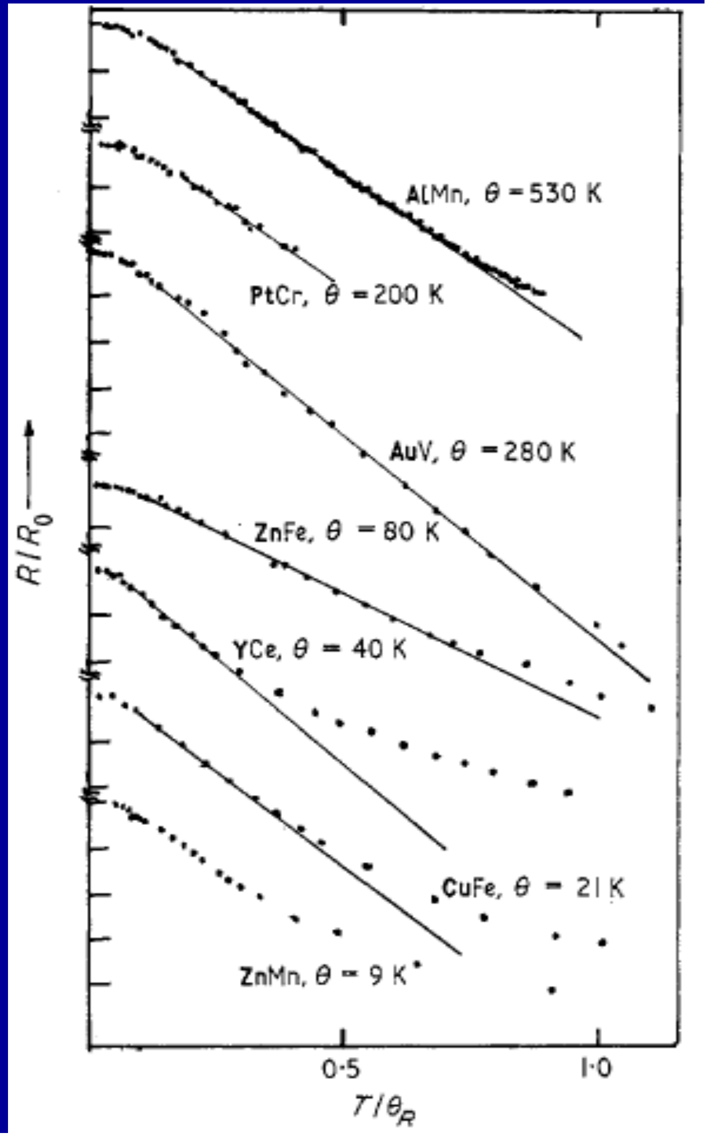


The Kondo effect :

contribution of magnetic impurities to resistivity increases as T is lowered !

De Haas, de Boer and van den Berg, Physica 1 (1934) 1115

``The resistivity of the gold wires Measured (not very pure) has a Minimum."



Impurity contribution to resistivity of different alloys, plotted against reduced temperature scale.

[After Rizzuto et al. J. Phys F 3, p.825 (1973)]

Note wide range of θ, defined from low-T:

$$\rho/\rho_0 = 1 - (T/\theta)^2 + \cdots$$

An experiment contemporary to Kondo's paper and demonstrating that the effect comes from Fe-moments :

PHYSICAL REVIEW VOLUME 135, NUMBER 4A 17 AUGUST 1964

Resistivity of Mo-Nb and Mo-Re Alloys Containing 1% Fe

M. P. SARACHIK, E. CORENZWIT, AND L. D. LONGINOTTI
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received 19 March 1964)

The resistivity of a series of Mo-Nb and Mo-Re alloys, with and without 1% Fe, has been measured at room temperature, and between 1.5 and 77°K. Large effects are observed near the alloy composition where the iron acquires a localized magnetic moment. These effects appear both as an excess temperature-independent scattering and in the form of large anomalies at low temperatures. Interpreted in the light of current theories of localized moments, the resistivity results confirm the existence of virtual bound states near the Fermi level. In addition, the anomalous behavior of the resistivity at low temperatures has been directly related to the existence of a localized magnetic moment.

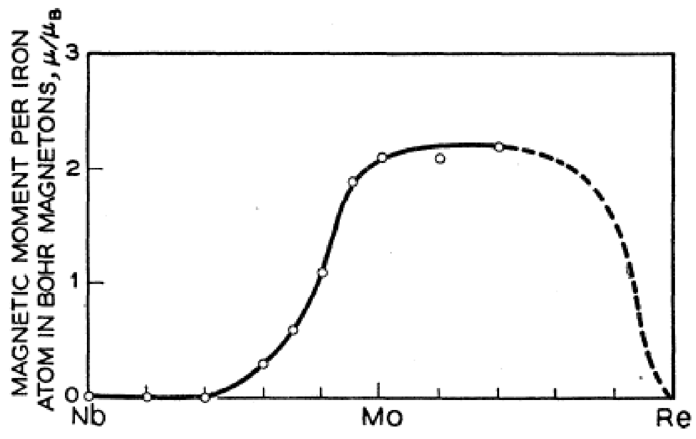


FIG. 1. Magnetic moment of an iron atom dissolved in various Mo-Nb and Mo-Re alloys as a function of alloy composition, according to Clogston *et al.*

Note added in proof. A recent theory by J. Kondo [Progr. Theoret. Phys. (Kyoto) (to be published)] predicts that a minimum exists whenever there is a negative $s-d$ exchange integral. This theory gives the observed linear dependence on concentration, and apparently gives the correct temperature dependence. I would like to thank Dr. Kondo for sending a preprint of his work prior to publication.

Kondo's

Resistance minimum:

$$\rho(T) = aT^5 + c_{\text{imp}}\rho_0 - c_{\text{imp}}\rho_1 \ln\frac{T}{D}$$

$$\Rightarrow T_{\text{min}} \sim c_{\text{imp}}^{1/5}$$

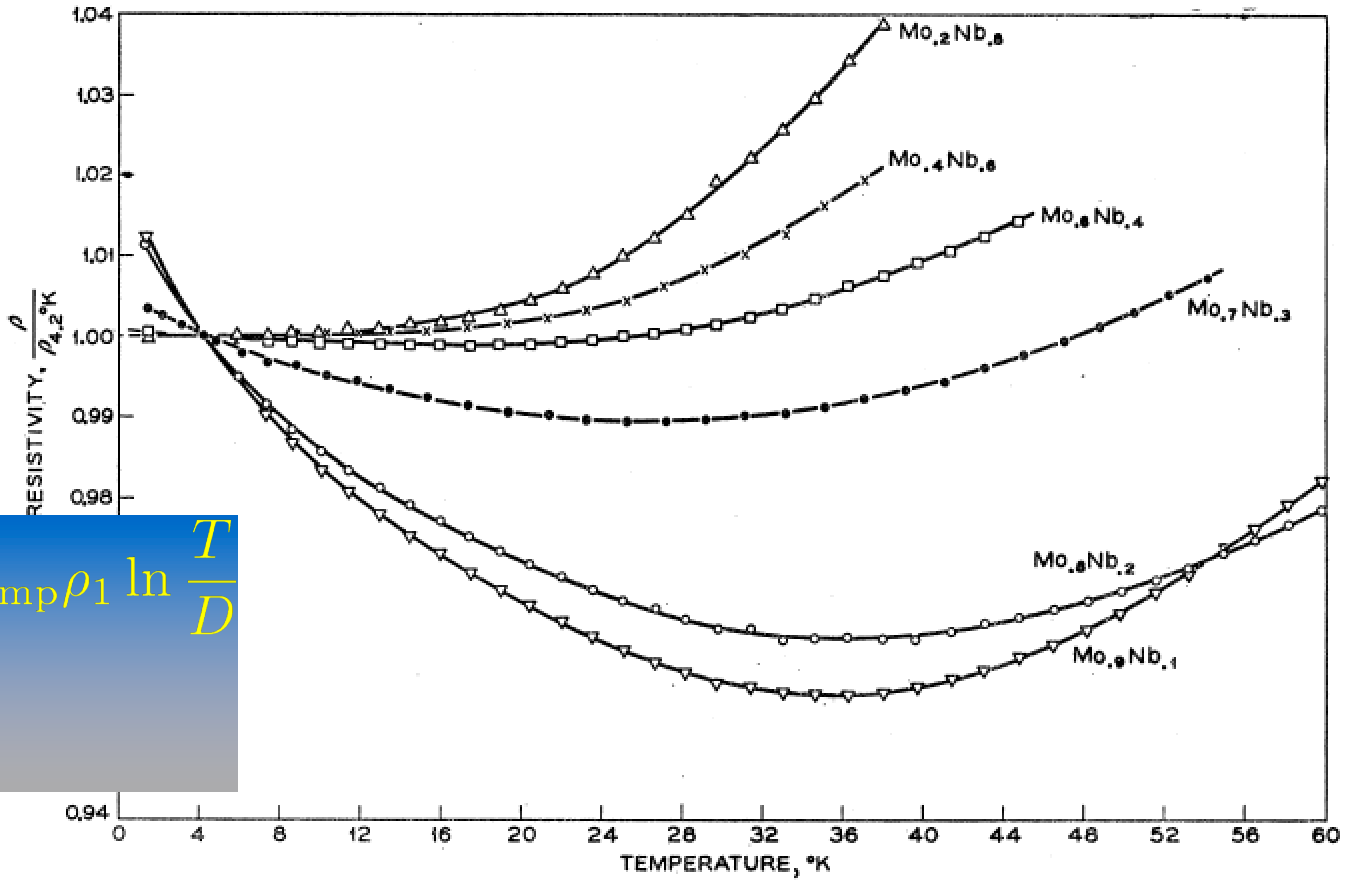


FIG. 3. Resistivity vs temperature for various Mo-Nb alloys containing 1% Fe. Resistivities are normalized at 4.2°K.

Jun Kondo

Expansion in the Kondo coupling (~Γ/U): singularities

Not surprisingly in view of the above, the perturbative expansion in J is plagued w/ singularities
<u>(when the conduction electron bath is metallic - gapless)</u>

The original calculation by Kondo deals w/ the resistivity, in which the log's appear at 3rd order:

$$R_{\mathrm{imp}} \propto (J_K \rho)^2 \left[1 - 2 J_K \rho \ln \frac{T}{D} + \cdots \right]$$

- Hints at an explanation of the `resistance minimum
(R increases as T is lowered)
- Perturbation theory FAILS BELOW a characteristic scale : $T_K \sim D e^{-1/(J_K \rho)}$

``Kondo temperature''

NB: In those RG slides J is dimensionless $J \rightarrow J \rho_0$

Scaling and the Renormalization Group

RG approach: integrate out (recursively) only over high-energy conduction electron states, and reformulate the result as a new Hamiltonian with a scale-dependent coupling.

Integrate only over shell: $\varepsilon_{\mathbf{k}} \in [D - \delta D, D]$

Calculate corresponding change in interactions (2-particle vertex):

$$\delta J_z = J_\perp^2 \frac{\delta D}{D} \; , \; \delta J_\perp = J_z J_\perp \frac{\delta D}{D}$$

Define scale parameter:

$D(l) = De^{-l}$

Flow to Lowest order:

$$\frac{dJ_z}{dl} = J_\perp^2$$
$$\frac{dJ_\perp}{dl} = J_z J_\perp$$

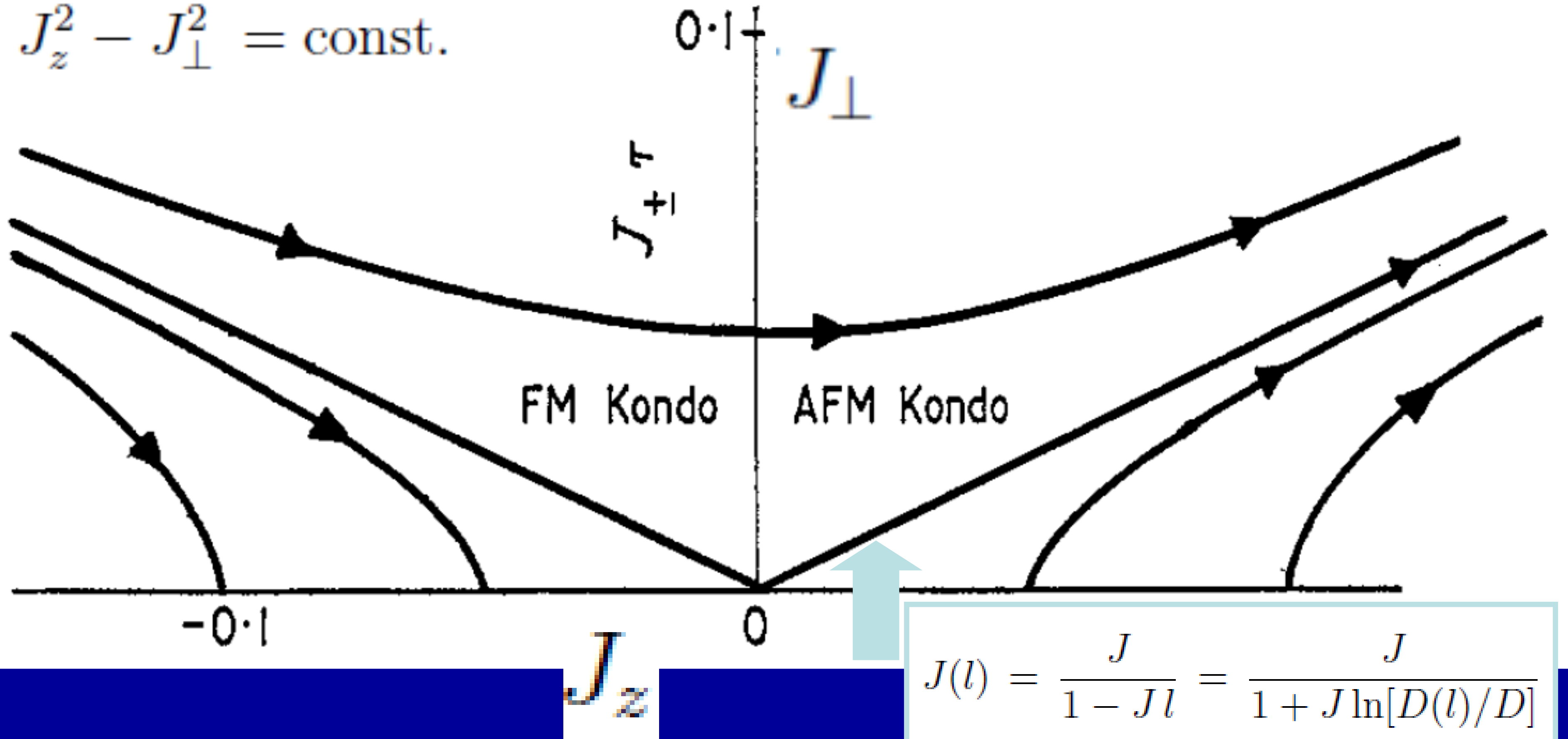
RG flow: AF model flows to strong coupling

$$\frac{dJ_z}{dl} = J_\perp^2$$
$$\frac{dJ_\perp}{dl} = J_z J_\perp$$

Coupling becomes large at

$$D(\ell_K) \sim T_K \sim De^{-1/J_K \rho_0}$$

→ $J_z^2 - J_\perp^2 = \text{const.}$



$$J(l) = \frac{J}{1 - J\,l} = \frac{J}{1 + J\ln[D(l)/D]}$$

Flow of the coupling (all orders): $$\frac{dJ}{dl} = \beta(J)$$ → $$\int_J^{J(l)} \frac{dx}{\beta(x)} = l$$

$$\chi\,[T, D; J] = \chi\,[T, D(l); J(l)] = \frac{1}{D(l)}\,\widetilde{\chi}\left[\frac{T}{D(l)}; J(l)\right]$$

Kondo scale: $$T_K = D(l_K)\ ,\ l_K = \ln\frac{D}{T_K}$$

$$\chi = \frac{1}{T_K}\widetilde{\chi}\left[\frac{T}{T_K}; J(l_K)\right] = \frac{1}{T_K}\widetilde{\chi}\left[\frac{T}{T_K}; J^*\right]$$ + small corrections

Universal scaling function associated with strong-coupling fixed point

Refined estimate to next order: $$T_K = D\sqrt{J}e^{-1/J}$$

Low-T physics: fixed point+leading irrelevant operator = Fermi liquid

This is best described using a one-dimensional description of fermions, associated with s-wave (l=0) channel. Cf. Affleck, arXiv:0809.3474

Kondo Hamiltonian: R- and L-movers on r>0 half-axis

$$H = \frac{v_F}{2\pi} i \int_0^\infty dr \left(\psi_L^\dagger \frac{d}{dr} \psi_L - \psi_R^\dagger \frac{d}{dr} \psi_R \right) + v_F \lambda \psi_L^\dagger(0) \frac{\vec{\sigma}}{2} \psi_L(0) \cdot \vec{S}$$

Folded to full axis, L-movers only, with boundary condition:

$$\psi_R(r) = \psi_L(-r), \quad (r > 0)$$

$$H = \frac{v_F}{2\pi} i \int_{-\infty}^{\infty} dr \psi_L^\dagger \frac{d}{dr} \psi_L + v_F \lambda \psi_L^\dagger(0) \frac{\vec{\sigma}}{2} \psi_L(0) \cdot \vec{S}.$$

Nature of the strong-coupling fixed point and its vicinity:

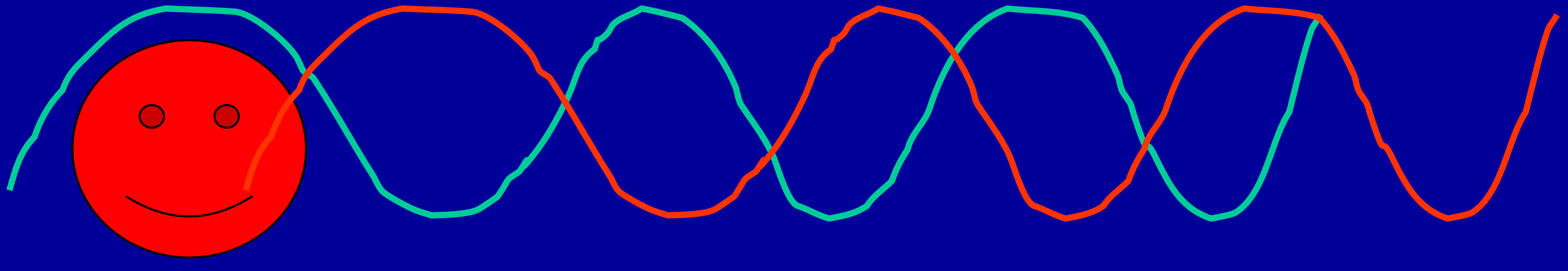
singlet formation and local Fermi liquid

Anderson, Wilson, Nozières, …

- Singlet ground-state formed between impurity spins and conduction electrons (cf. one conduction orbital calculation)

- Seen from the conduction electron viewpoint:

N sites → N-1 sites (impurity site inaccessible) → **$\pi/2$ "phase shift"**



Hamiltonian close to fixed point:

- Impurity degree of freedom is GONE !
- Fermions have undergone a $\pi/2$ phase-shift, i.e a change of b.c
- Operators at fixed point:
- 1) A marginal one $\psi^{\dagger\alpha}(0)\psi_\alpha(0)$ → Potential scattering, forbidden by p-h stry in stric case
- 2) Two leading irrelevant ones of dimension 2, i.e. <O(0)O(t)> ~ $1/t^4$

$J(0)^2$ and $\vec{J}(0)^2$ with: $$J \equiv \psi^{\dagger\alpha}\psi_\alpha, \quad \vec{J} \equiv \psi^{\dagger\alpha}\frac{\vec{\sigma}_\alpha^\beta}{2}\psi_\beta.$$

Only second one has a sizeable coeff (~$1/T_K$, not 1/D)

Effective hamiltonian at s.c. fixed point:

$$H = \frac{v_F}{2\pi} i \int_{-\infty}^{\infty} dr \psi_L^\dagger \frac{d}{dr}\psi_L - \frac{1}{6T_K}\vec{J}_L(0)^2.$$

with modified b.c (phase shift)

$$\psi_R(r) = -\psi_L(-r), \quad (r > 0).$$

Note: coefficient in front of 2nd term specifies a convention for defining T_K

Physical quantities at low-T:

Characteristic behavior of Fermi-liquid

2nd term (LIO) is small and can be treated in perturbation theory, as a weak scattering term:

$$\chi_{\rm imp} = \frac{1}{4T_K}\left[1 - c(\frac{T}{T_K})^2 + \cdots\right]$$

$$S_{imp} \rightarrow \frac{\pi^2 T}{6T_K}.$$

Wilson ratio:

$$R_W \equiv \frac{\chi_{\rm imp}/\chi_{c0}}{\gamma_{\rm imp}/\gamma_{c0}} = \frac{4\pi^2}{3}\frac{\chi_{\rm imp}}{\gamma_{\rm imp}} = 2$$

Resistivity:

$$\rho = \rho_u\left[1 - \frac{\pi^4}{16}\left(\frac{T}{T_K}\right)^2 + \cdots\right]$$

In which ρ_u is the maximal possible resistivity induced by an impurity (unitary limit):

$$\rho_u = \frac{3n_i}{(ev_F\nu)^2}.$$

Friedel's sum-rule

(valid at T=ω=0, wide bandwidth)

Exact relation between

the phase shift and the occupancy of the atomic orbital !

$$\delta = \frac{\pi\, n_d}{2}$$

Why is this remarkable ?

- Phase-shift is a low-energy property (Ad(0))
- Occupancy integrates over all energies (integral of Ad overω<0)

<u>Non-perturbative proof</u> : see later – or see bibliography

(in the context of the AIM: Langreth, Phys Rev 150 (1966) 516

Friedel's sum-rule: non-perturbative proof (sloppy about contours…)

Friedel sum-rule

Wide bandwidth case. Non-perturbative proof, *valid for* $T = 0$.

Note: sloppy about contours and prescription for G.F,

We consider the Green's function $G_d^{-1}(\omega) = \omega - \varepsilon_d + i\Gamma - \Sigma(\omega)$

$$-\frac{\partial}{\partial\omega} \ln G_d(\omega) = \left[1 - \frac{\partial\Sigma}{\partial\omega}\right] G_d(\omega) \tag{1.59}$$

and use:

$$-\frac{1}{\pi}\int_C d\omega G_d(\omega) = \frac{n_d}{2} \tag{1.60}$$

Hence, integrating the above relation:

$$\frac{\pi n_d}{2} = \ln G_d(\omega = 0) - \ln G_d(\omega \to -\infty) + \int_C d\omega \frac{\partial\Sigma}{\partial\omega} G_d(\omega) \tag{1.61}$$

The last term will be shown to vanish, so that we get (remember $\mathrm{Im} G_r < 0$, definition of phase shift, and using a branch-cut of the ln on the negative real axis):

$$\frac{\pi n_d}{2} = (\delta - \pi) - (-\pi) \tag{1.62}$$

so that the occupancy of the d-orbital and the phase-shift are related by

$$n_d = \frac{2}{\pi}\delta \tag{1.63}$$

A manifestation of *Friedel's sum-rule* in this context. This derivation for the AIM is due to Langreth.

To prove that the last term vanishes, we integrate it by part:

$$\int_C d\omega \, \frac{\partial G_d}{\partial \omega} \Sigma(\omega) \tag{1.64}$$

and observe that the self-energy is obtained from the Luttinger-Ward functional as:

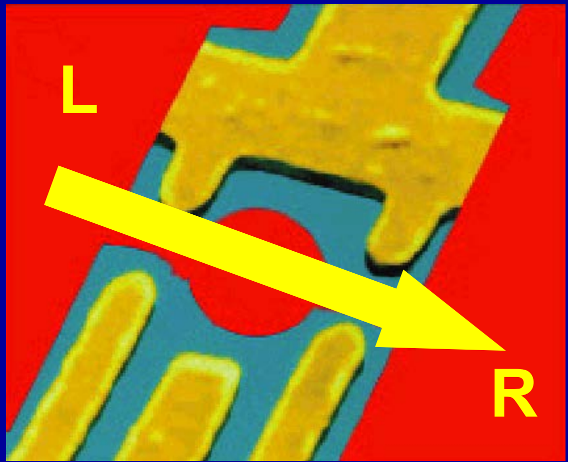
$$\Sigma(\omega) = \frac{\delta \Phi[G]}{\delta G(\omega)} \tag{1.65}$$

so that the above reads:

$$\int_C d\omega \, \frac{\partial G}{\partial \omega} \, \frac{\delta \Phi[G]}{\delta G(\omega)} = \delta \Phi \tag{1.66}$$

This is the change of the LW functional when all frequencies are shifted.

Conductance through dot [Y.Meir, N.Wingreen, 1992] :



Left junction, Kubo formula:

$$G_L \sim \frac{e^2}{h}\frac{1}{\omega}\langle j_{Ld} \cdot j_{Ld}\rangle|_{\omega\to 0}$$

$$j_{Ld} \sim -i\, eV_{\mathbf{k}L}\left(c^\dagger_{\mathbf{k}\sigma L} d_\sigma - d^\dagger_\sigma c_{\mathbf{k}\sigma L}\right)$$

→ $$G_L = \frac{8e^2}{h}\Gamma_L \int_{-\infty}^{+\infty} d\omega \left[-\frac{\partial f}{\partial \omega}\right] \pi A_d(\omega, T)$$

Adding the 2 junctions in series:

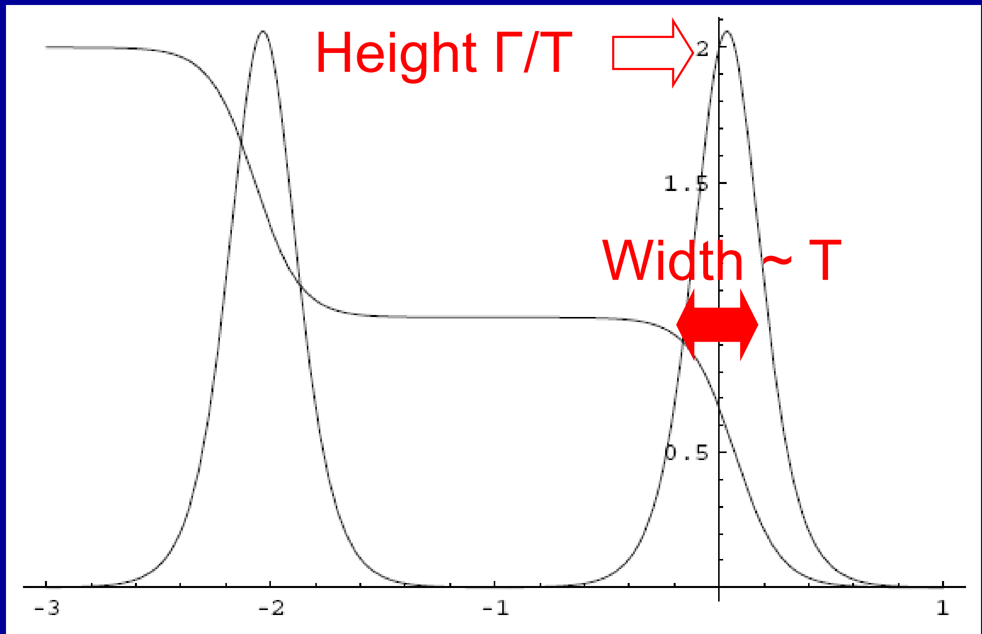
$$G = \left[\frac{1}{G_L} + \frac{1}{G_R}\right]^{-1} = \frac{8e^2}{h}\frac{\Gamma_L\Gamma_R}{(\Gamma_L+\Gamma_R)^2}\int_{-\infty}^{+\infty} d\omega \left[-\frac{\partial f}{\partial \omega}\right] \pi\Gamma A_d(\omega, T)$$

High-temperature regime T>Γ : Coulomb blockade

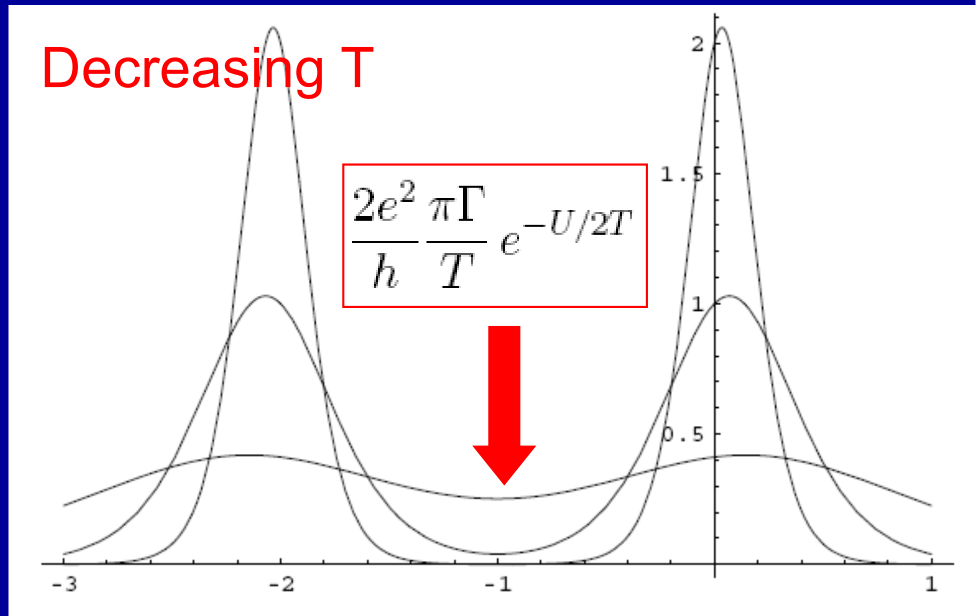
Use isolated atom form of spectral function: $\frac{n_d}{2}\,\delta(\omega-\varepsilon_d-U)+(1-\frac{n_d}{2})\,\delta(\omega-\varepsilon_d)$

$$G(T\gg\Gamma)\simeq\frac{2e^2}{h}\frac{\pi\Gamma}{T}\left[(1-\frac{n_d}{2})\frac{1}{4\cosh^2\frac{\varepsilon_d}{2T}}+\frac{n_d}{2}\frac{1}{4\cosh^2\frac{\varepsilon_d+U}{2T}}\right]$$

$$\frac{n_d}{2}=\frac{1}{Z}\left(1\times e^{-\beta\varepsilon_d}+1\times e^{-\beta(2\varepsilon_d+U)}\right)=n_d(T,\varepsilon_d)$$



Plot of n_d and G vs. ε_d for $U=2$ at $\beta=10$.



Plot of G vs. ε_d for $U=2$ at $\beta=2,5,10$.

Suppression of the Coulomb blockade by the Kondo effect at low-T: Wave-function interpretation (qualitative)

Virtual transitions create admixture of components with
0 or 2 electrons on the dot in the wave-function.

→ Restoration of charge fluctuations

→ Conductance (transmission) takes maximal possible value $2e^2/h$

$$|\Psi_0\rangle = \sqrt{1-\eta^2}\,|\mathcal{S}\rangle + \eta\,|\mathcal{D}\rangle$$

$$|\mathcal{S}\rangle \equiv \frac{1}{\sqrt{2}}\left[|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right]$$

$$|\mathcal{D}\rangle \equiv \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right]$$

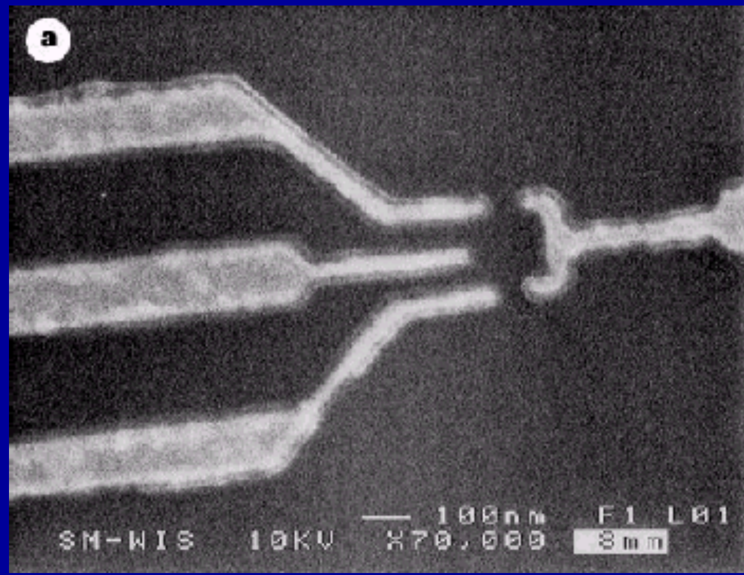
with $\eta \sim \frac{V}{U} \ll 1.$

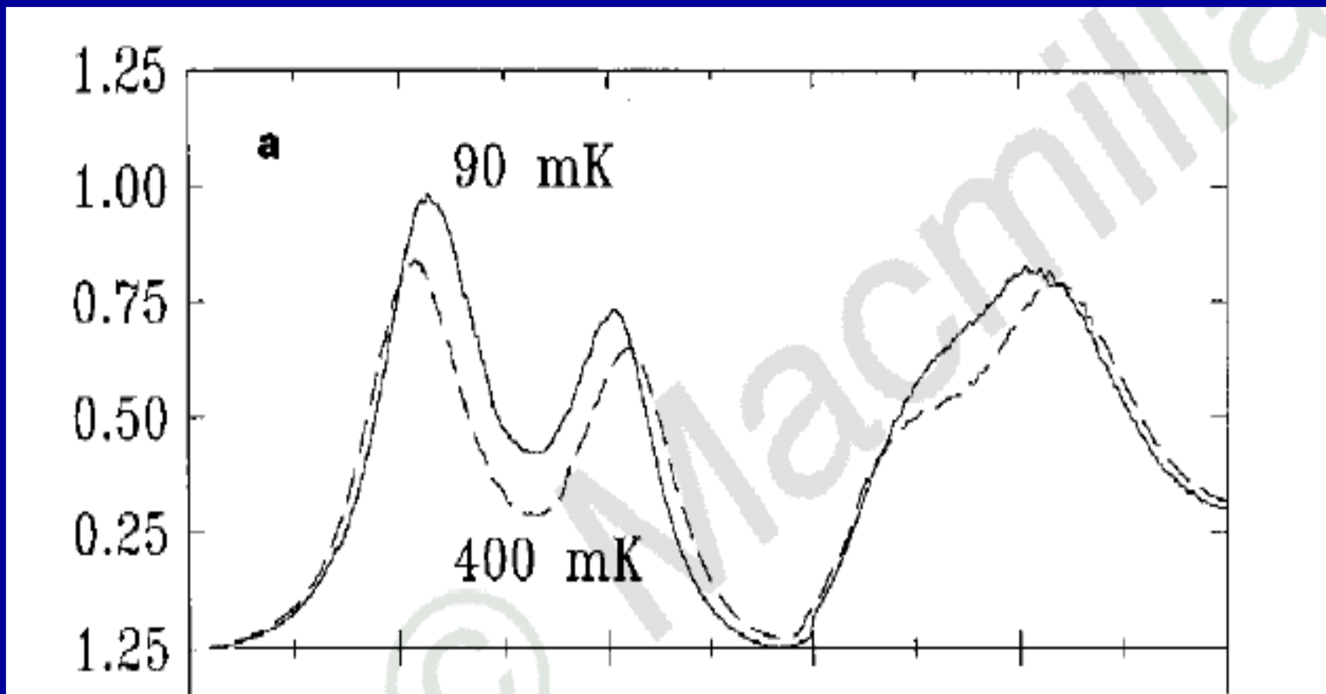
Kondo effect in a single-electron transistor

D. Goldhaber-Gordon*†, Hadas Shtrikman†, D. Mahalu†, David Abusch-Magder*, U. Meirav† & M. A. Kastner*

NATURE | VOL 391 | 8 JANUARY 1998

See also: D. G-G et al. PRL 81 (1998) 5225





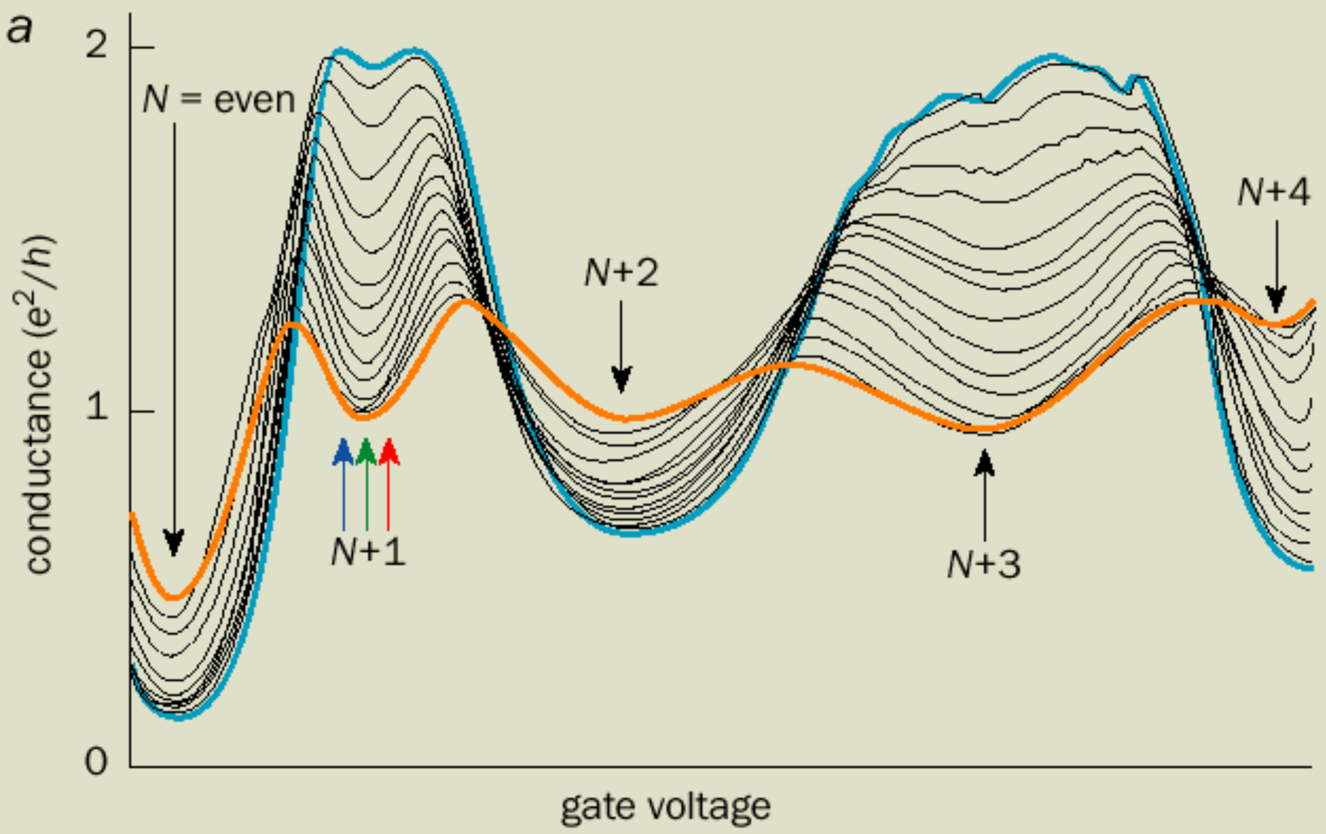
Orders of magnitude:

U ~ 1.9 meV

Γ ~ 0.3 meV

Range of T_K:

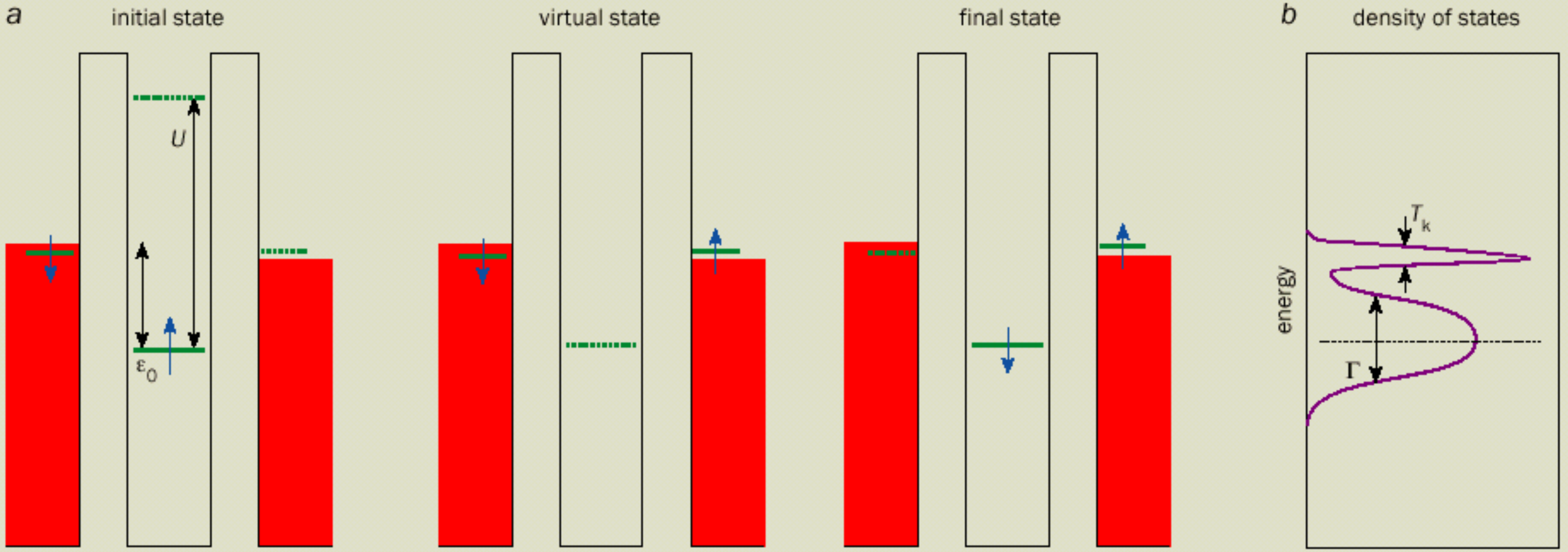
40mK → 2,5 K



(*a*) The conductance (*y*-axis) as a function of the gate voltage, which changes the number of electrons, *N*, confined in a quantum dot. When an even number of electrons is trapped, the conductance decreases as the temperature is lowered from 1 K (orange) to 25 mK (light blue). This behaviour illustrates that there is no Kondo effect when *N* is even. The opposite temperature dependence is observed for an odd number of electrons, i.e. when there is a Kondo effect.

W G van der Wiel *et al*. 2000 The Kondo effect in the unitary limit *Science* **289** 2105–2108

2 Spin flips



(*a*) The Anderson model of a magnetic impurity assumes that it has just one electron level with energy ε_0 below the Fermi energy of the metal (red). This level is occupied by one spin-up electron (blue). Adding another electron is prohibited by the Coulomb energy, *U*, while it would cost at least $|\varepsilon_0|$ to remove the electron. Being a quantum particle, the spin-up electron may tunnel out of the impurity site to briefly occupy a classically forbidden "virtual state" outside the impurity, and then be replaced by an electron from the metal. This can effectively "flip" the spin of the impurity. (*b*) Many such events combine to produce the Kondo effect, which leads to the appearance of an extra resonance at the Fermi energy. Since transport properties, such as conductance, are determined by electrons with energies close to the Fermi level, the extra resonance can dramatically change the conductance.

Conductance (cont'd)…

Specialize to L-R symmetric device, for simplicity:

$$G_{L=R}(T) = \frac{2e^2}{h} \int_{-\infty}^{+\infty} d\omega \left[-\frac{\partial f}{\partial \omega}\right] \pi \Gamma A_d(\omega, T)$$

Notes:

1- Compare to formula for resistivity ! G ~ R quite remarkable !

$$\frac{R_u}{R_{\text{imp}}(T)} = \int_{-\infty}^{+\infty} d\omega \left(-\frac{\partial f}{\partial \omega}\right) \frac{1}{\pi \Gamma A_d(\omega, T)}$$

2- → ~ A Landauer formula generalized to tunneling into an interacting system

$\Gamma A_d(\omega,T)$ plays the role of transparency of barrier

3- Generalization to out of equilibrium, e.g. I(V) for finite voltage
Is an outstanding problem. General formula based on Keldysh has been
Derived (Meir and Wingreen, PRL 68 (1992) 2512) but concrete calculations
Difficult ! Numerous recxent works (Saleur et al., Andrei et al.) – an active field !

Scaling of G(T)/G(0) vs. T/T$_K$

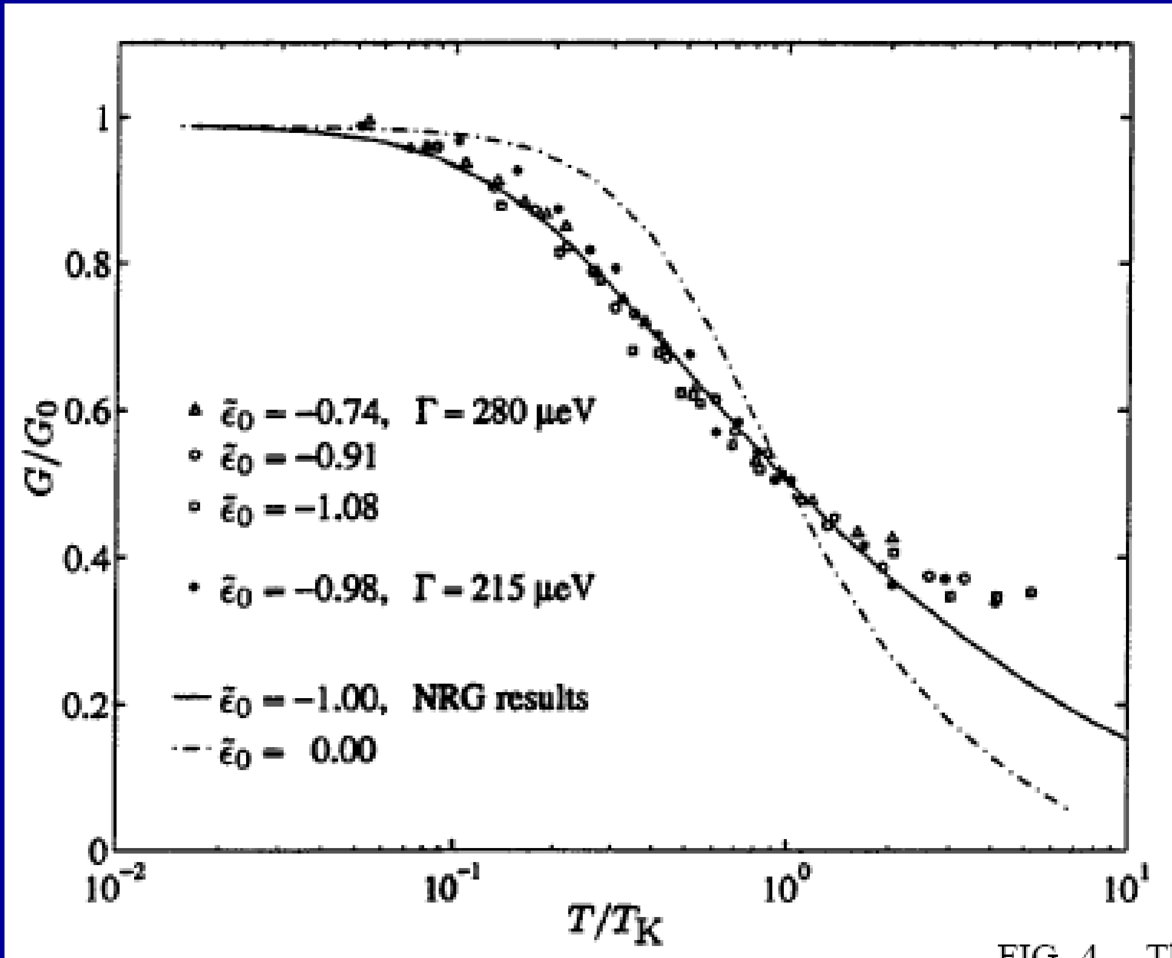
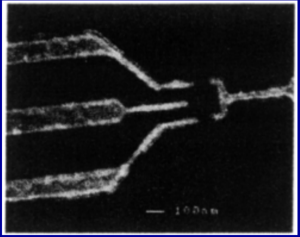


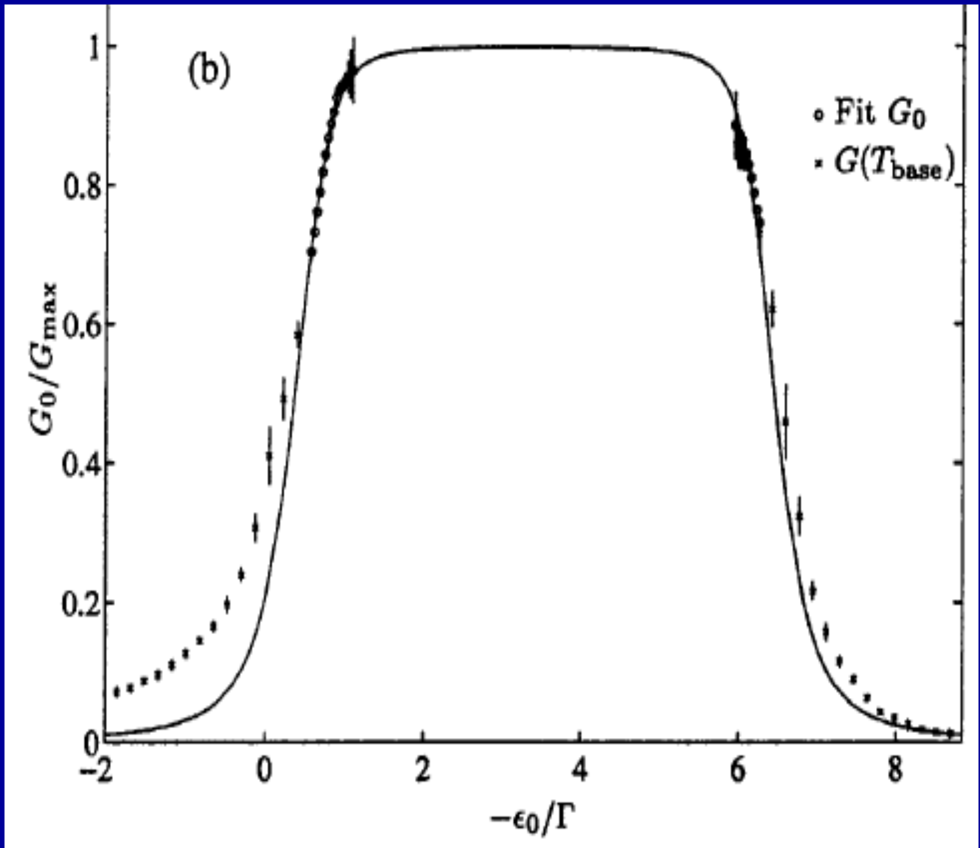
FIG. 4. The normalized conductance $\tilde{G} \equiv G/G_0$ is a universal function of $\tilde{T} \equiv T/T_K$, independent of both $\tilde{\epsilon}_0$ and Γ, in the Kondo regime, but depends on $\tilde{\epsilon}_0$ in the mixed-valence regime. Scaled conductance data for $\tilde{\epsilon}_0 \approx -1$ are compared with NRG calculations [13] for Kondo (solid line) and mixed-valence (dashed line) regimes. The stronger temperature dependence in the mixed-valence regime is qualitatively similar to the behavior for $\tilde{\epsilon}_0 = -0.48$ in Fig. 3(b).



Dependence on gate voltage :

Goldhaber-Gordon et al.

Phys Rev Lett 81 (1998) 5225



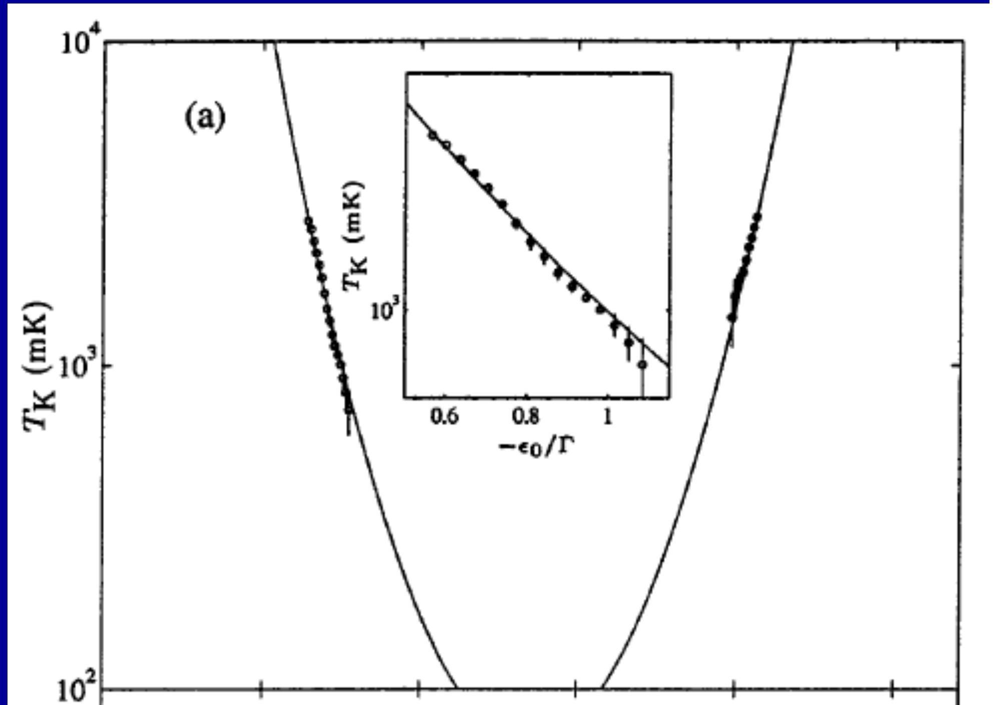


FIG. 5. (a) Fit values of T_K for data such as those in Fig. 3 for a range of values of ϵ_0 [22]. The dependence of T_K on ϵ_0 is well described by Eq. (1) (solid line). Inset: Expanded view of the left side of the figure, showing the quality of the fit. (b) Values of G_0 extracted from data such as those in Fig. 3 at a range of ϵ_0. Solid line: $G_0(\epsilon_0)$ predicted by Wingreen and Meir [4]. $G_{max} = 0.49e^2/h$ for the left peak, and $0.37e^2/h$ for the right peak.

PRL 113, 126601 (2014) PHYSICAL REVIEW LETTERS week ending 19 SEPTEMBER 2014

Transmission Phase in the Kondo Regime Revealed in a Two-Path Interferometer

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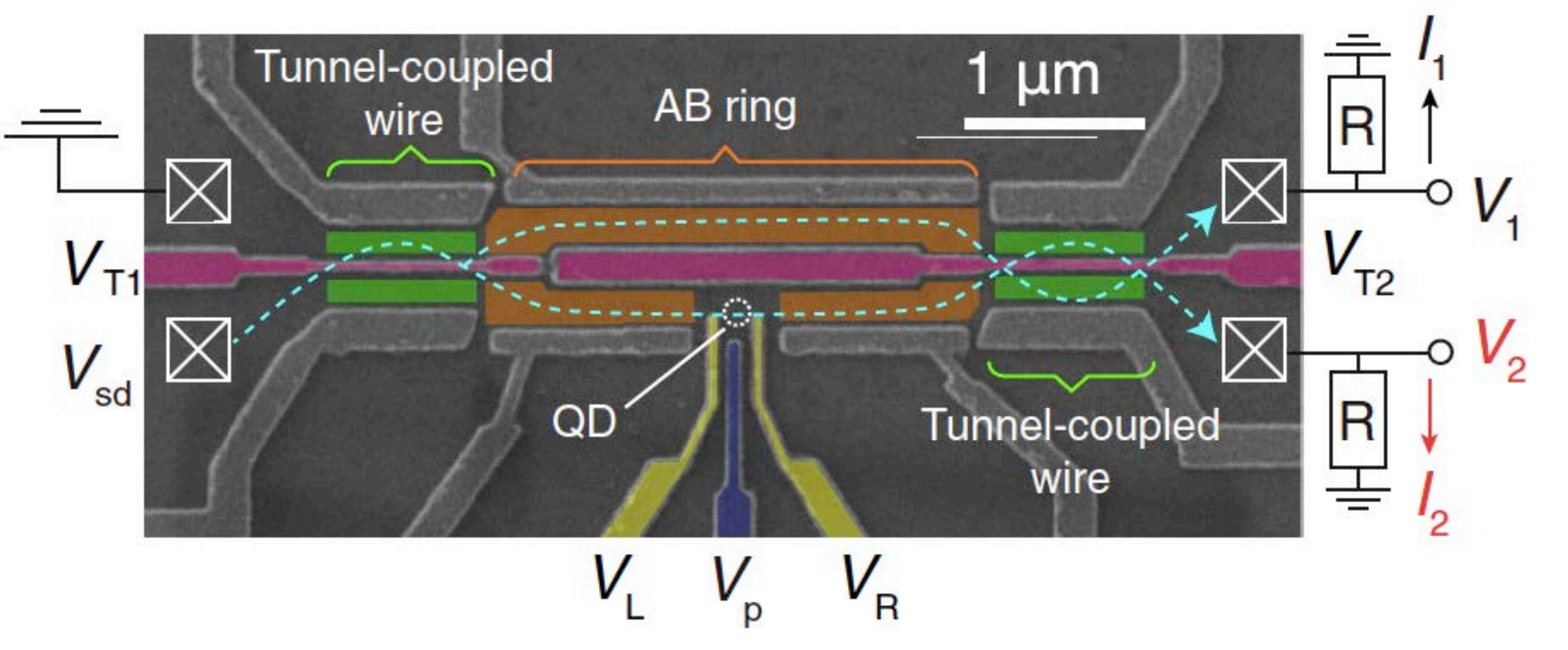
[3]*CNRS, Institut NEEL, F-38042 Grenoble, France*

See also several early papers by Heiblum, Shtrikman et al.



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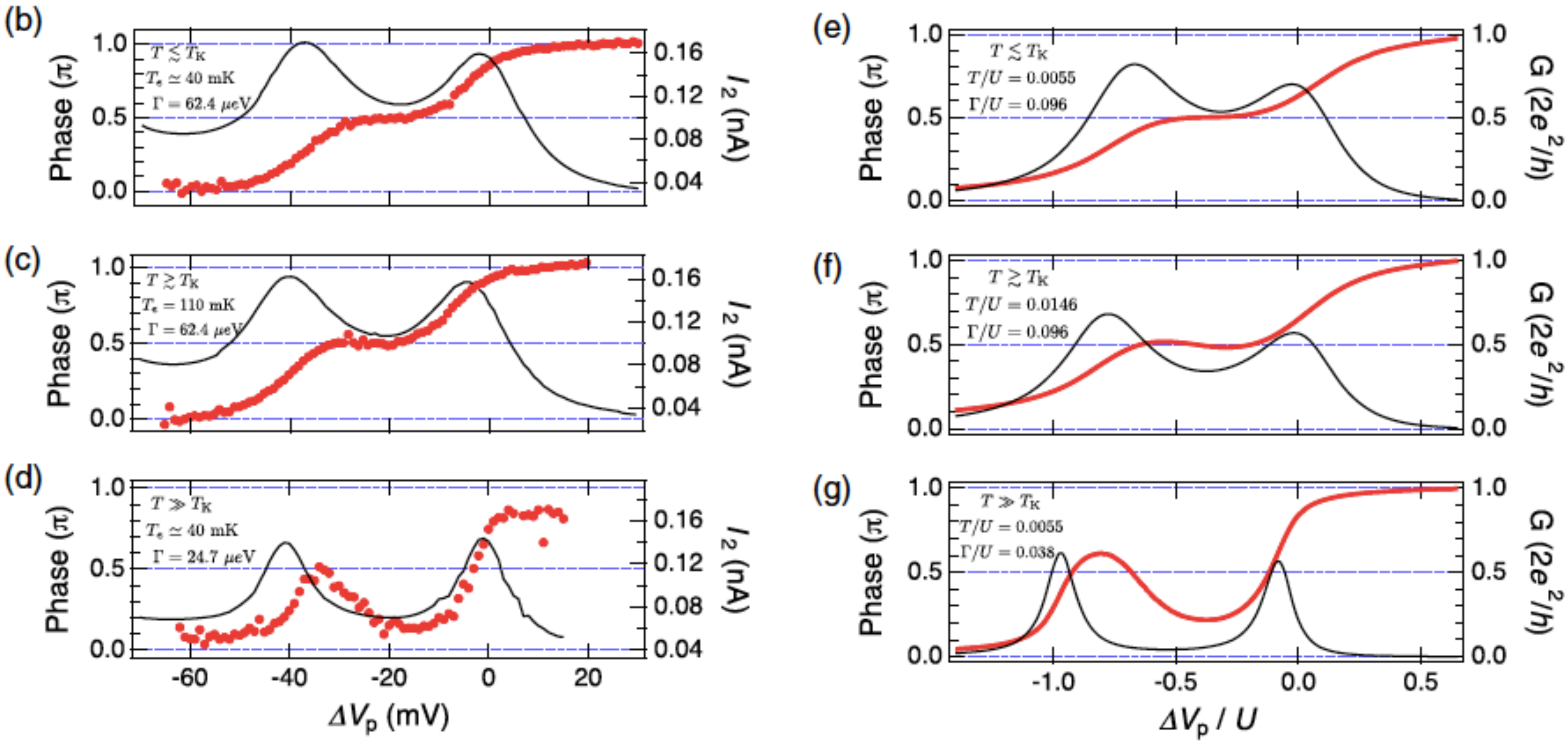

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The conduction electrons viewpoint:

$$G_{\mathbf{kk'}}(i\omega_n) = \frac{1}{i\omega_n - \varepsilon_{\mathbf{k}}}\delta_{\mathbf{kk'}} + \frac{V^*_{\mathbf{k}}}{i\omega_n - \varepsilon_{\mathbf{k}}} G_d(i\omega_n) \frac{V_{\mathbf{k'}}}{i\omega_n - \varepsilon_{\mathbf{k'}}}$$

with:

$$T_{\mathbf{kk'}}(i\omega_n) = V^*_{\mathbf{k}} G_d(i\omega_n) V_{\mathbf{k'}}$$

Scattering T-matrix

Total scattering cross-section ~ Im T ~ $V^2 A_d(\omega)$ - \`optical' theorem

→ Need to understand spectral function of impurity orbital

Conduction electron phase-shift defined by:

$$T_{\mathbf{kk'}}(\omega + i0^+) = -\,|T_{\mathbf{kk'}}|\, e^{i\delta_{\mathbf{kk'}}(\omega)}$$

Note: at particle-hole symmetry: T (and G_d) is purely imaginary → $\delta = \pi/2$

LM case (δ=π/2): Conduction electron density of states vanishes at the impurity site

From the above expression:

$$\sum_{kk'} \mathrm{Im} G_{kk'}(i0^+) = -\pi\rho_0 \left[1 - \pi\Gamma A_d(0)\right]$$

$\Gamma \equiv \pi V^2 \rho_0$ Hence: $$A_d(0) = \frac{1}{\pi\Gamma}$$ Special case of Friedel's sum rule

Thus, the spectral function of the impurity must grow a resonance around zero-energy (Fermi level of the electron gas)
= Abrikosov-Suhl resonance

Formation of the resonance as a tunneling process between spin-up and spin-down states → on board

Magnetic impurities in metallic host: contribution to resistivity :

$$\sigma_{\rm imp}(T) \,=\, \frac{ne^2}{m}\int_{-\infty}^{+\infty} d\omega\, \tau_{\rm tr}(\omega,T)\left(-\frac{\partial f}{\partial\omega}\right)$$

Kubo formula for c-electrons

$$\tau_{\rm tr}^{-1}(\omega,T) \,=\, 2c_{\rm imp}{\rm Im}T^{\rm adv} \,=\, c_{\rm imp}\frac{2}{\rho_c}\Gamma A_d(\omega,T)$$

`Optical' theorem

$$\frac{R_u}{R_{\rm imp}(T)} \,=\, \int_{-\infty}^{+\infty} d\omega\left(-\frac{\partial f}{\partial\omega}\right)\frac{1}{\pi\Gamma A_d(\omega,T)}$$

Unitary limit resistivity :

$$R_u \,=\, c_{\rm imp}\,\frac{2m}{ne^2\pi\rho_c}$$

T→0 limit: maximal (unitary) scattering: $-\frac{\partial f}{\partial\omega}\to\delta(\omega)\ ;\ \pi\Gamma A_d(0)=1$

Contrast to TRANSMISSION: maximal conductance (1/A → A !):

$$G_{L=R}(T) \,=\, \frac{2e^2}{h}\int_{-\infty}^{+\infty} d\omega\left[-\frac{\partial f}{\partial\omega}\right]\pi\Gamma A_d(\omega,T)$$

Impurity contribution to resistivity :

$$\sigma_{\mathrm{imp}}(T) = \frac{ne^2}{m}\int_{-\infty}^{+\infty} d\omega\, \tau_{\mathrm{tr}}(\omega,T)\left(-\frac{\partial f}{\partial \omega}\right)$$

Kubo formula for c-electrons

$$\tau_{\mathrm{tr}}^{-1}(\omega,T) = 2c_{\mathrm{imp}}\mathrm{Im}T^{\mathrm{adv}} = c_{\mathrm{imp}}\frac{2}{\rho_c}\Gamma A_d(\omega,T)$$

`Optical' theorem

$$\frac{R_u}{R_{\mathrm{imp}}(T)} = \int_{-\infty}^{+\infty} d\omega \left(-\frac{\partial f}{\partial \omega}\right)\frac{1}{\pi\Gamma A_d(\omega,T)}$$

Unitary limit resistivity :

$$R_u = c_{\mathrm{imp}}\frac{2m}{ne^2\pi\rho_c}$$

T=0 : $R_{\mathrm{imp}}(T=0) = R_u \sin^2\delta = R_u \sin^2\left(\frac{\pi n_d}{2}\right) = R_u \sin^2\left(\frac{\pi n_d}{2(2l+1)}\right)$

Finite-T, Kondo regime:

$$A_d(\omega,T) \to \frac{1}{\pi\Gamma}\, a\left[\frac{\omega}{T_K},\frac{T}{T_K}\right]$$

$$\frac{R_u}{R_{\mathrm{imp}}(T)} = \int_{-\infty}^{+\infty} dx\, \frac{1}{4\cosh^2\left(\frac{x}{2}\frac{T_K}{T}\right)}\,\frac{1}{a(x,\frac{T}{T_K})}$$