Chaire de Physique de la Matière Condensée

Matériaux et dispositifs à fortes corrélations électroniques

I.*2 Blocage de Coulomb vs. Quasiparticules*

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N.B.: Dans cette partie du cours, je vais introduire progressivement le modèle le plus simple permettant de décrire la compétition entre blocage de Coulomb et transport de quasi particules.

Une motivation physique est la physique des points quantiques dans les 2DEG (blocage de Coulomb et sa suppression par l'effet Kondo).

La présentation est introductive et ne fera pas justice aux remarquables développements récents de ce domaine (→ voir les experts Grenoblois ! C.Bauerle,W.Wernsdorfer, N.Roch, S.Florens…)

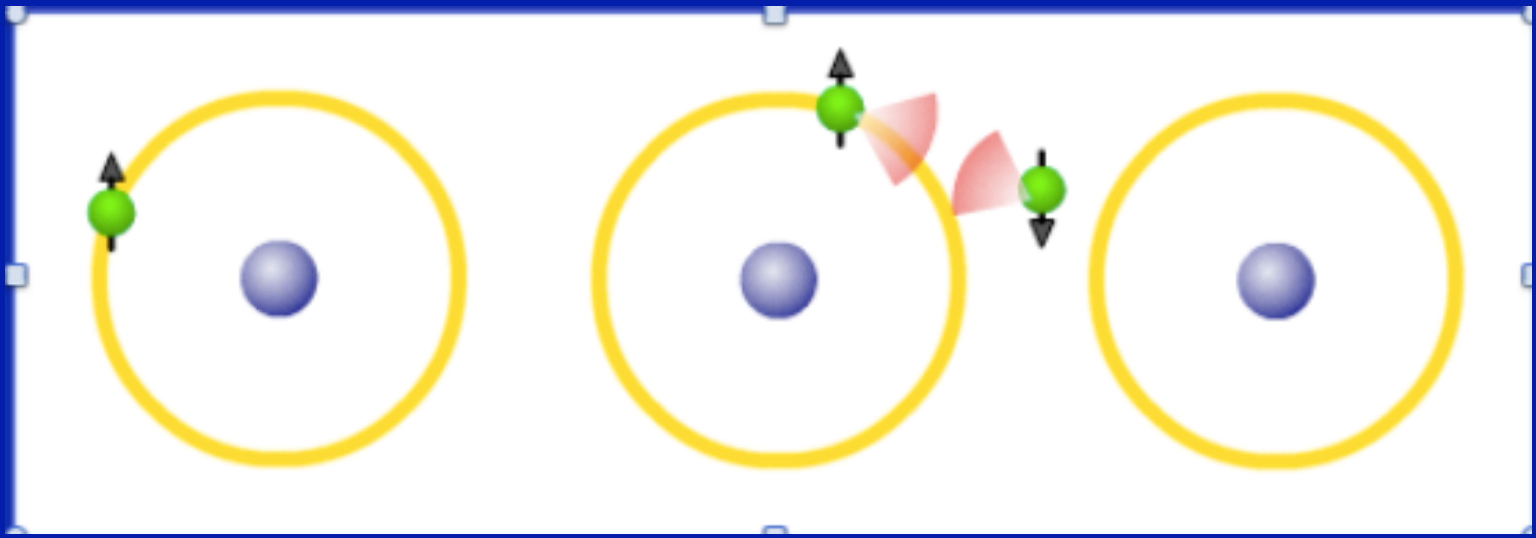
A common thread
through this series of lectures:

Blocking of electronic motion

(and suppression of density fluctuations)

by repulsive interactions

(« Coulomb blockade »)



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:

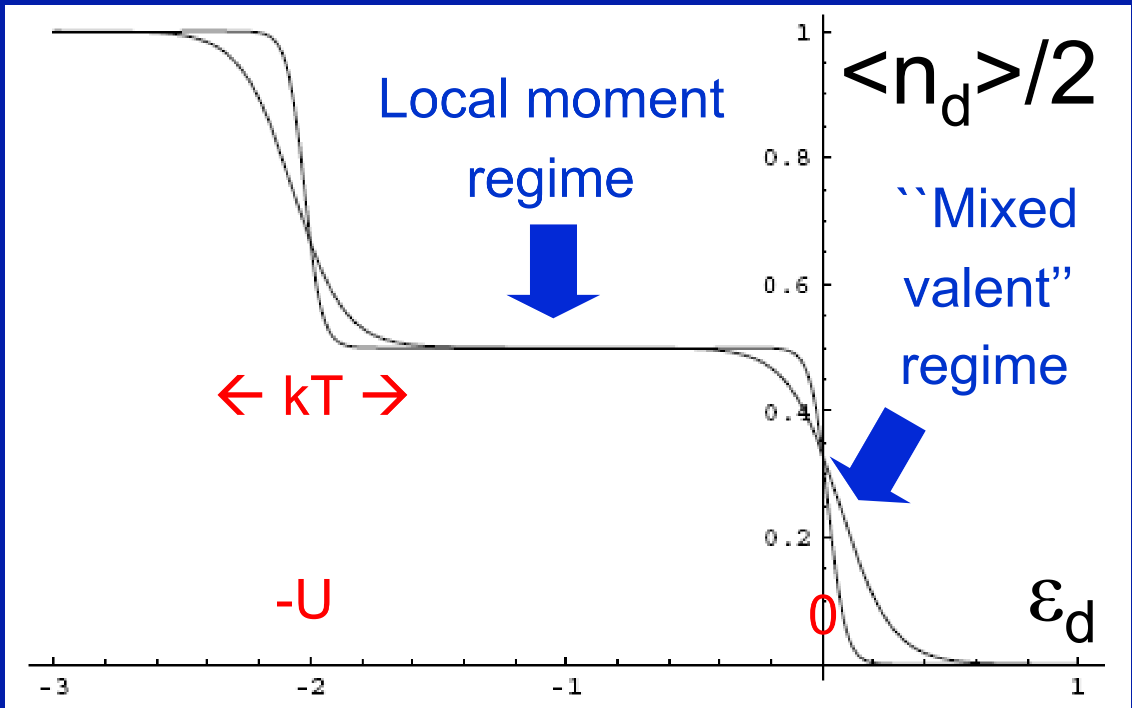
- Between |n=0> and |n=1> at $\varepsilon = 0$

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

Occupancy of the isolated atom :

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

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



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

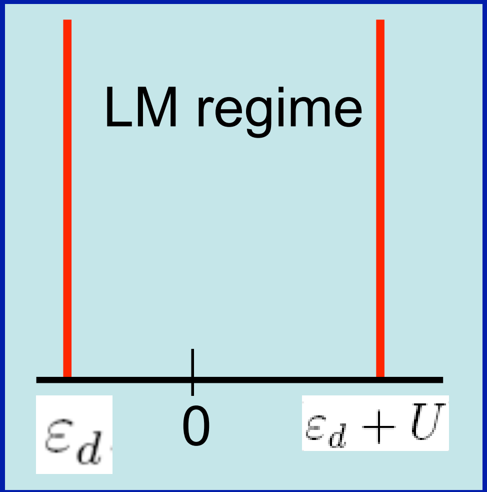
One-particle spectral function, at T=0:

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

and, at finite temperature:

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

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



The (Friedel-, Wolff-) Anderson model

- and other `quantum impurity' models - :

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)

J.Friedel, Can.J.Phys 34, 1190 (1956)
P.W.Anderson, Phys Rev 124, 41 (1961)
P.A.Wolff, Phys. Rev. 124, 1030 (1961)

The model

$$H = H_{\rm c} + H_{\rm at} + H_{\rm hyb}$$

$$H_{\rm c} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

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

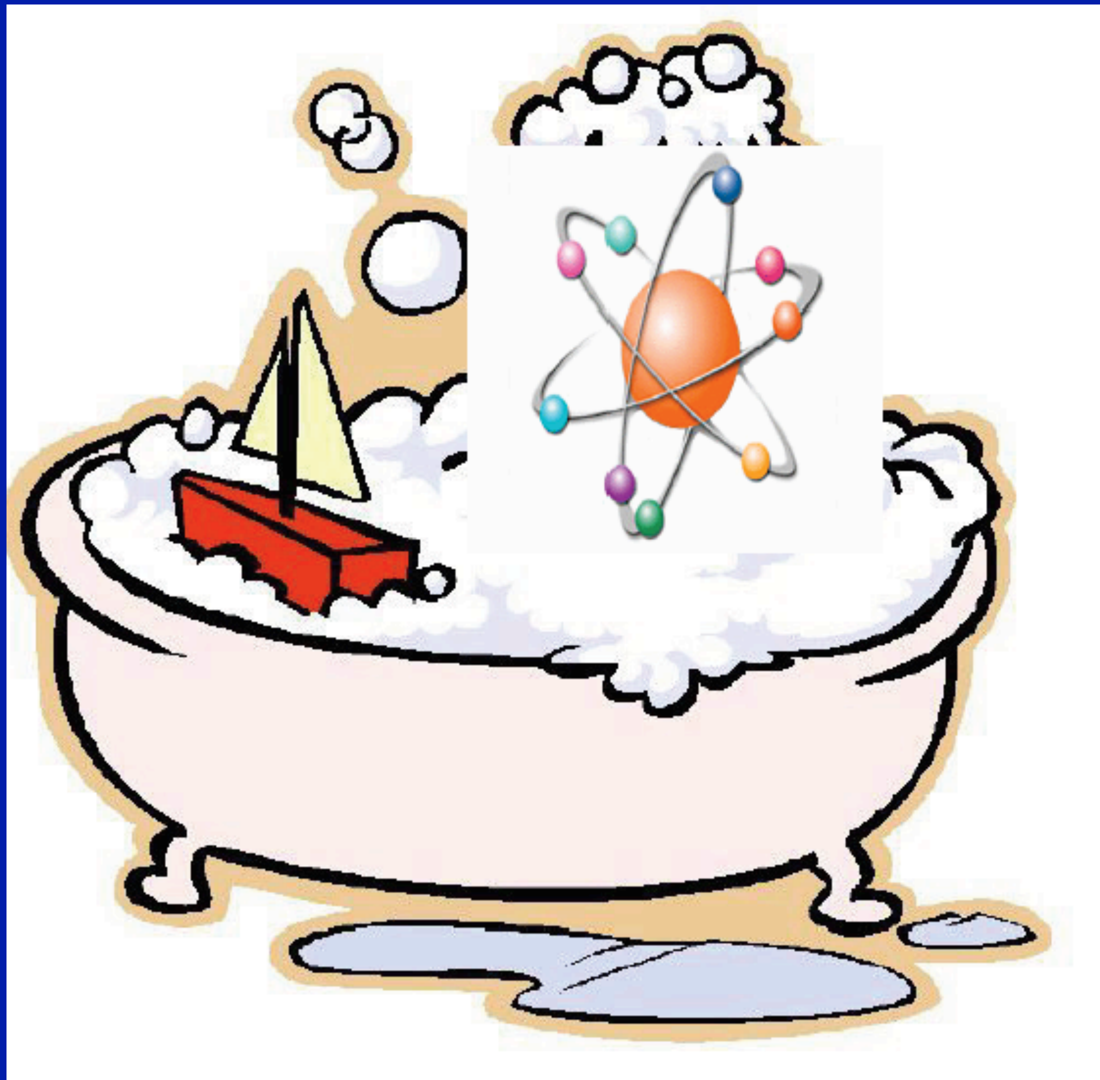
$$H_{\rm at} = \varepsilon_d \sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} + U\, n^d_{\uparrow} n^d_{\downarrow}$$

Single-level ``atom''

$$H_{\rm hyb} = \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} (c^{\dagger}_{\mathbf{k}\sigma} d_{\sigma} + d^{\dagger}_{\sigma} c_{\mathbf{k}\sigma})$$

Transfers electrons between bath and atom – Hybridization, tunneling

``Atom in a bath''



Relevance to physical systems

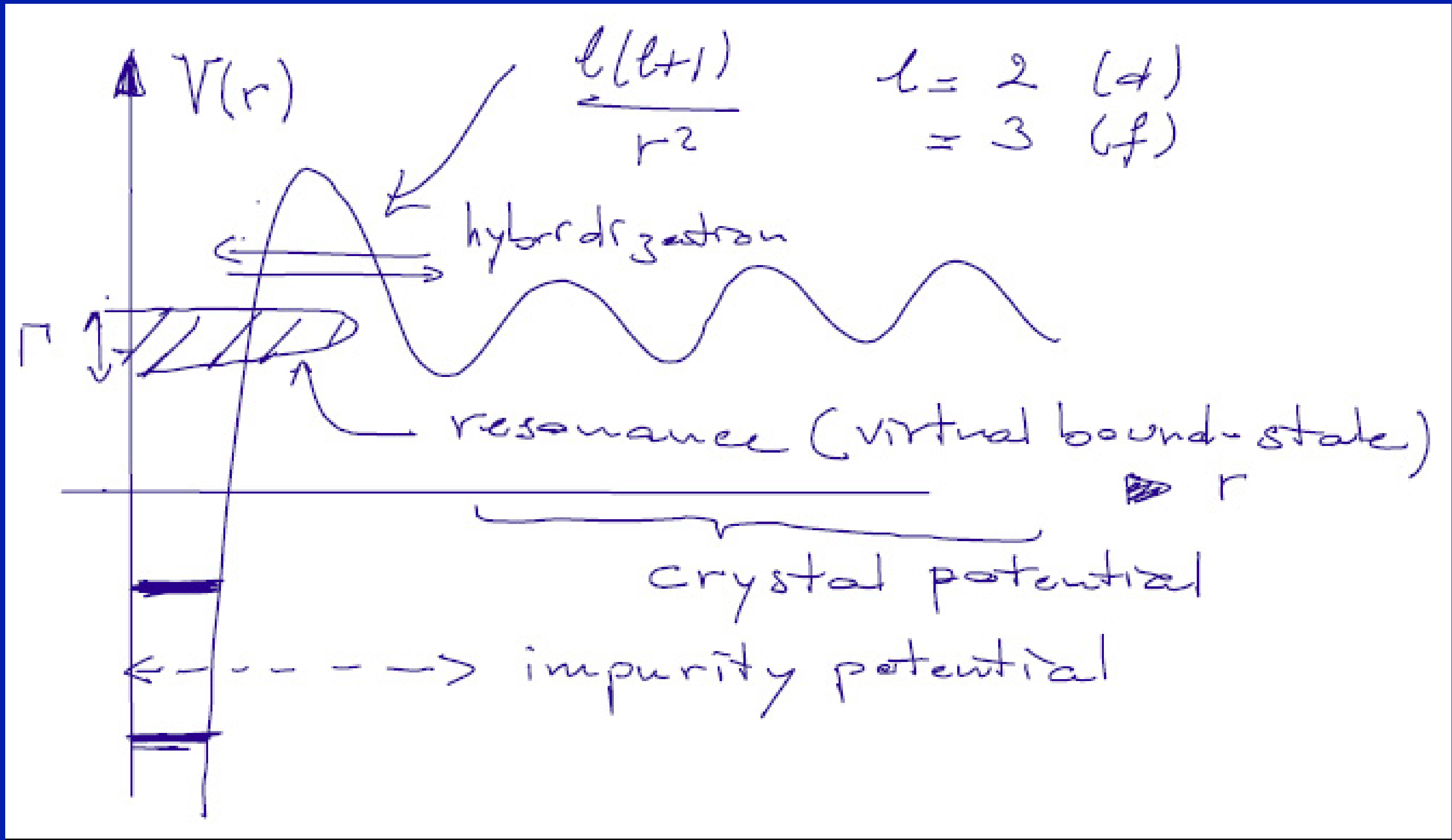
- 1. Magnetic impurities in metals

- 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. $Ce_xLa_{1-x}\,Cu_6$ ($x \ll 1$)

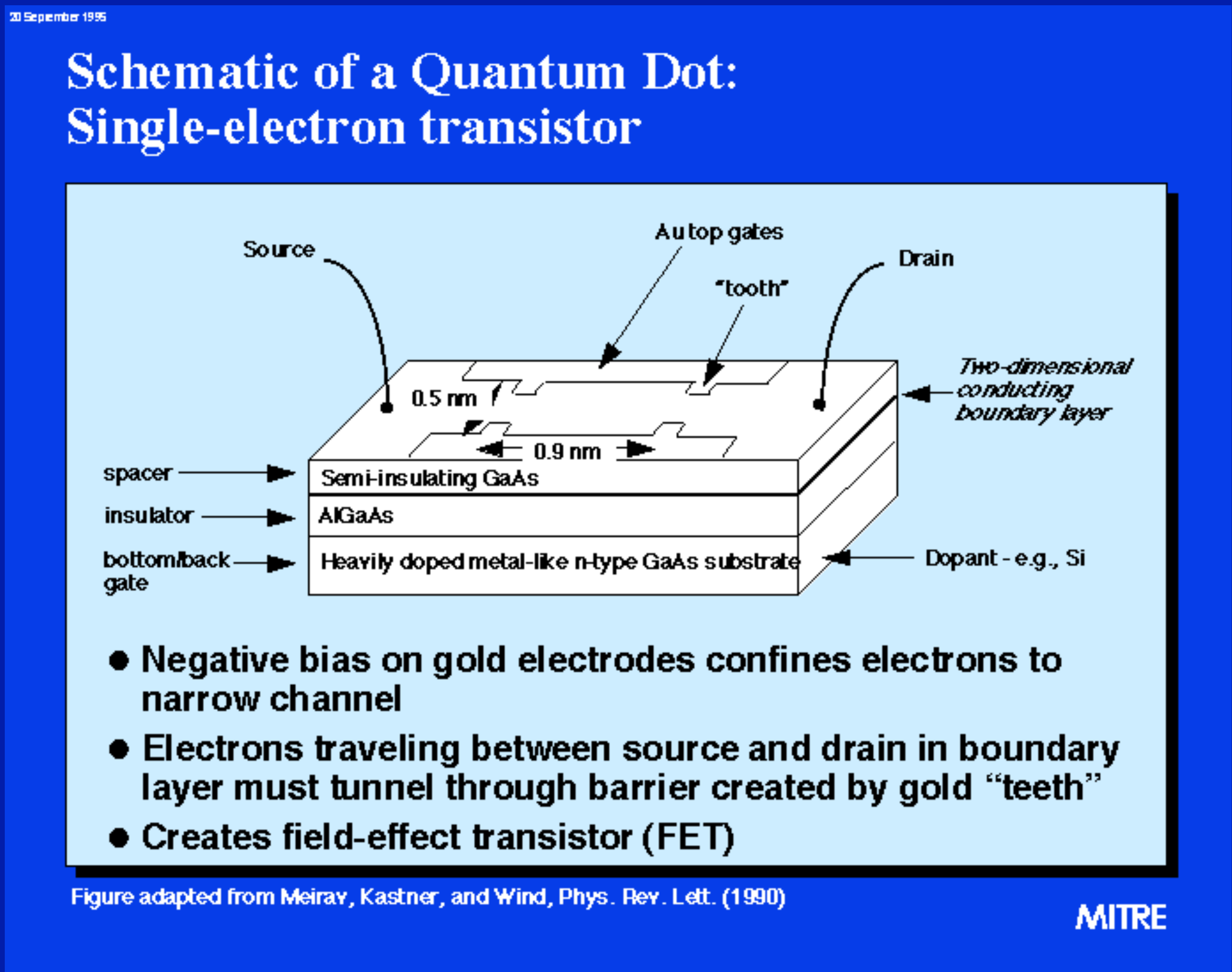
In some cases, all range of solid solution can be studied, from dilute to dense system (Kondo alloy to Heavy-Fermion regime)

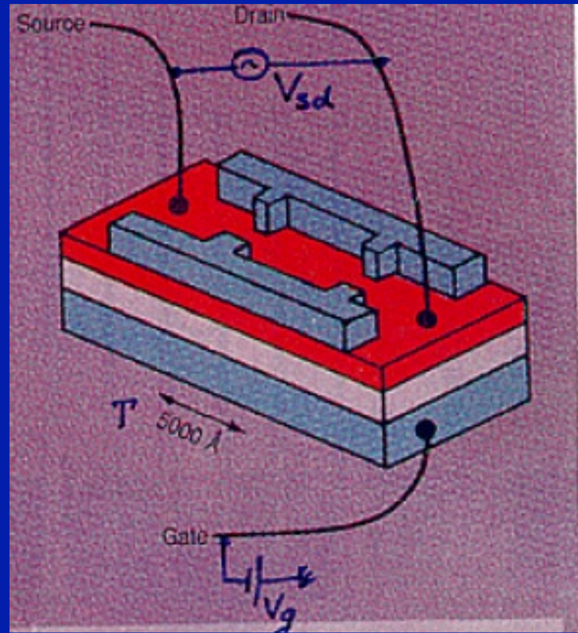
Friedel's virtual bound-state concept



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

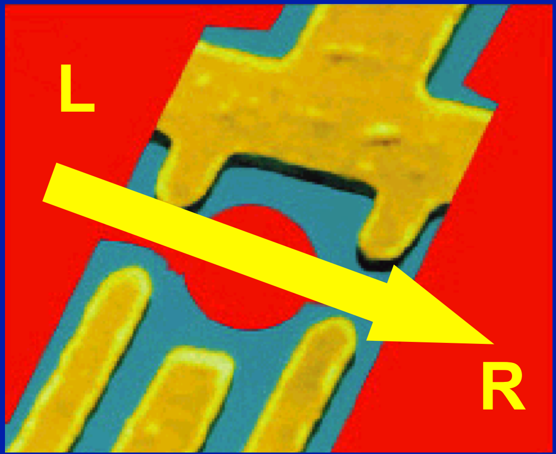
Leads

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

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).

Conductance through dot :



Left junction, Kubo formula:

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

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

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

Adding the 2 junctions in series:

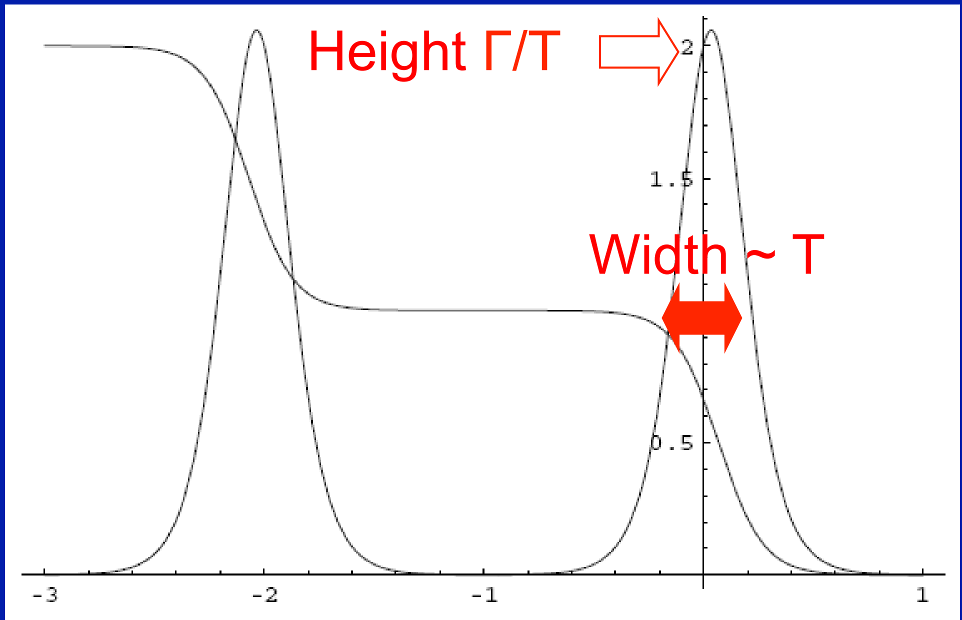
$$\boxed{G = \left[\frac{1}{G_L} + \frac{1}{G_R}\right]^{-1} = \frac{8e^2}{h}\frac{\Gamma_L \Gamma_R}{(\Gamma_L + \Gamma_R)^2}\int_{-\infty}^{+\infty} d\omega \left[-\frac{\partial f}{\partial \omega}\right] \pi \Gamma A_d(\omega, T)}$$

High-temperature regime T>Γ : Coulomb blockade

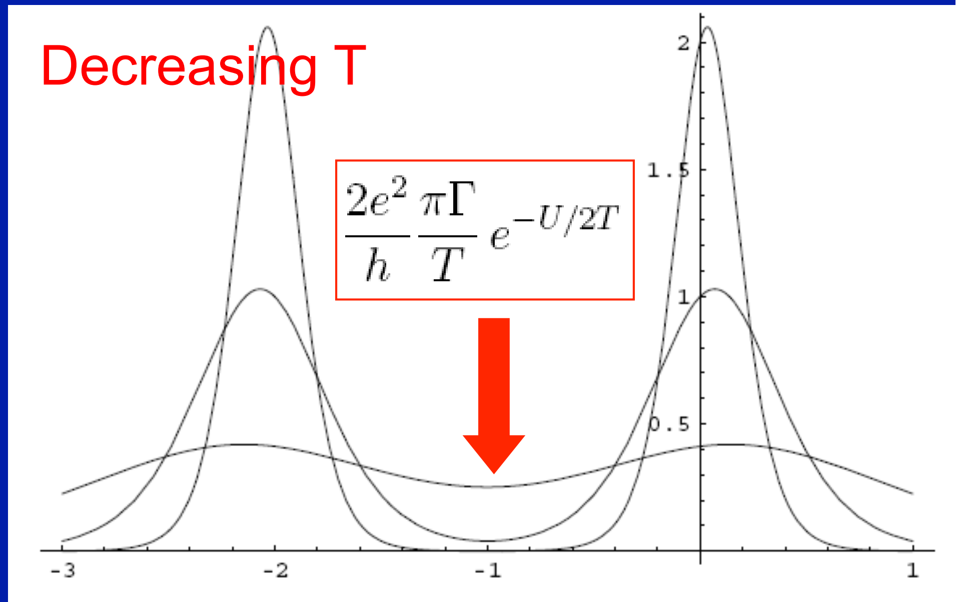
Use isolated atom form of spectral function: $\frac{n_d}{2}\,\delta(\omega-\varepsilon_d-U)+(1-\frac{n_d}{2})\,\delta(\omega-\varepsilon_d)$

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

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



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 $\beta=2,5,10$.

But…
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:

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

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

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

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 $2e^2/h$

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

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

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

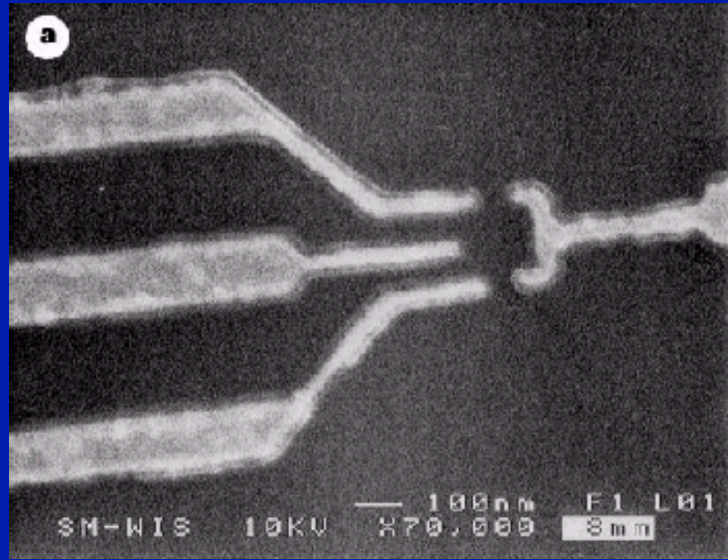
$$|\mathcal{D}\rangle \equiv \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right]$$

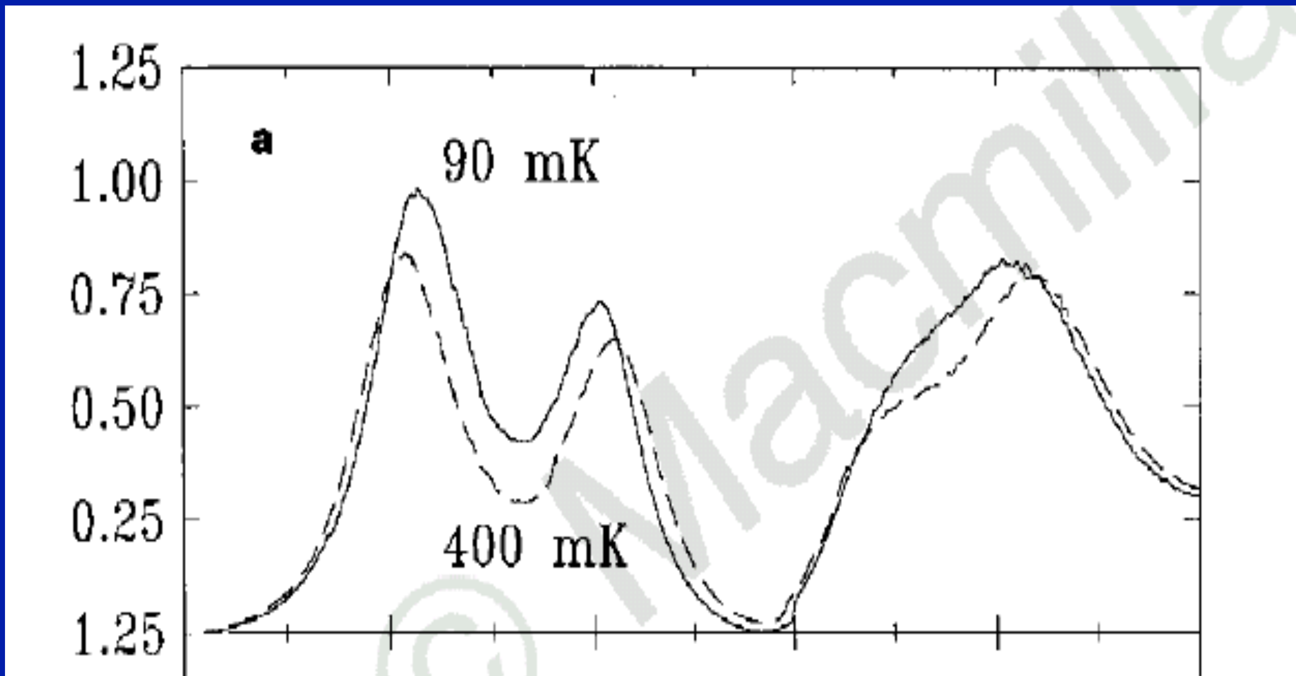
Kondo effect in a single-electron transistor

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





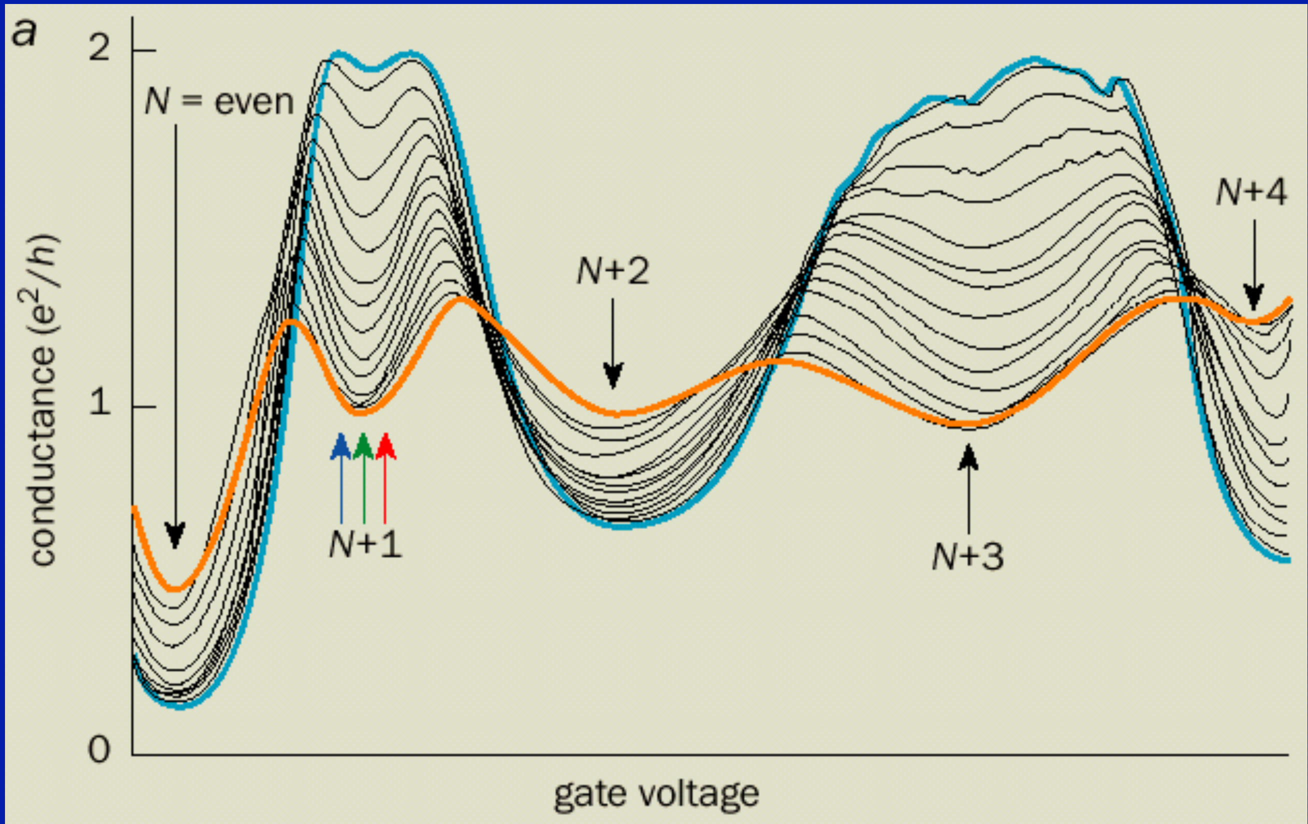
Orders of magnitude:

U ~ 1.9 meV

Γ ~ 0.3 meV

Range of T_K:

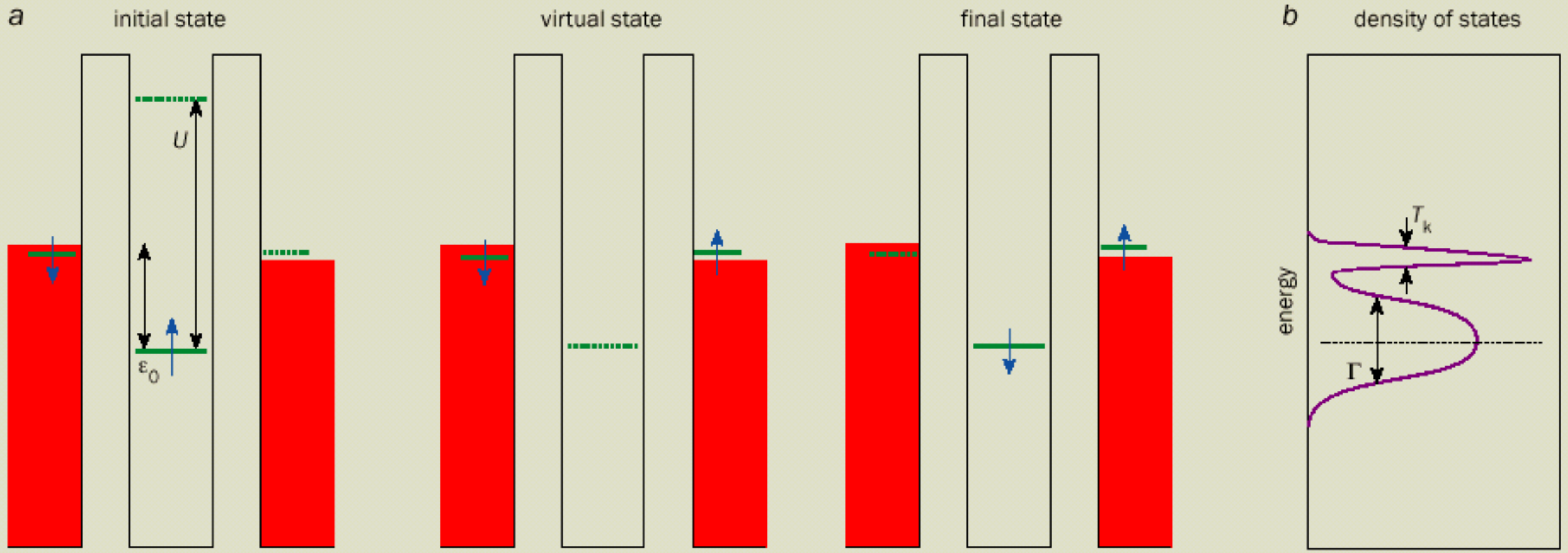
40mK → 2,5 K



(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.

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

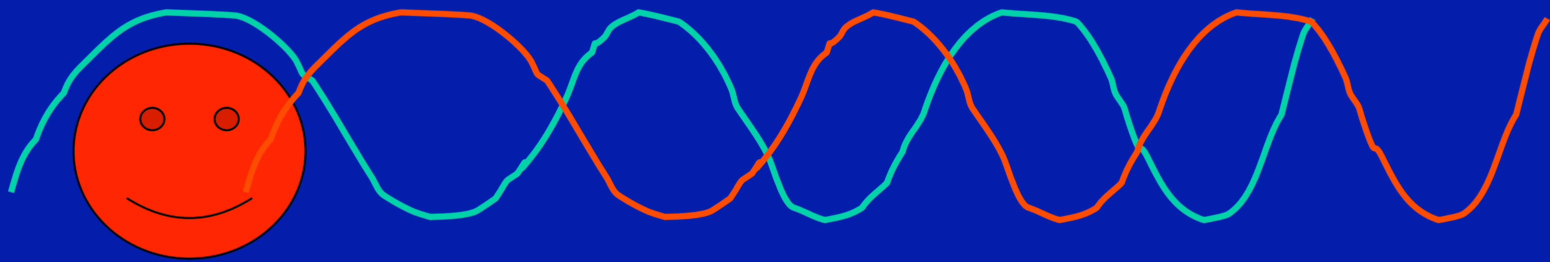
singlet formation and local Fermi liquid

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"**



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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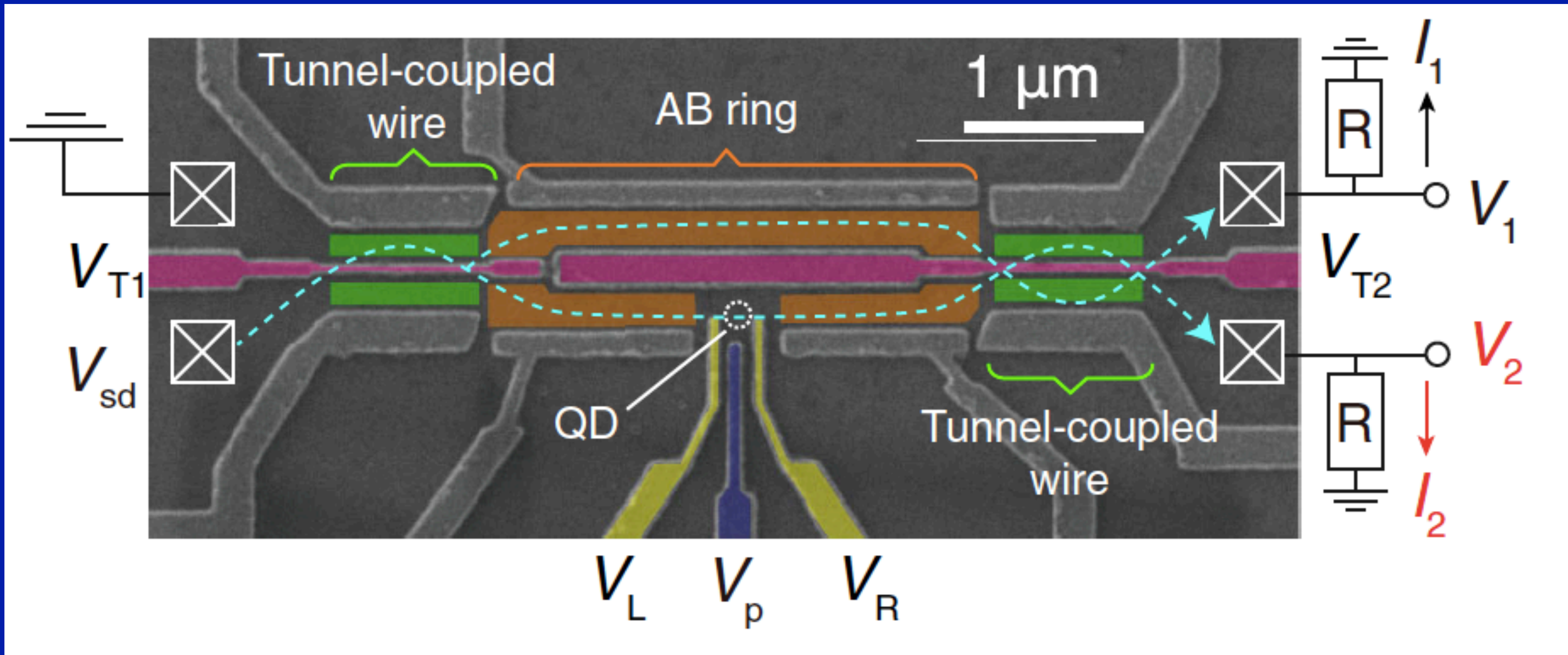
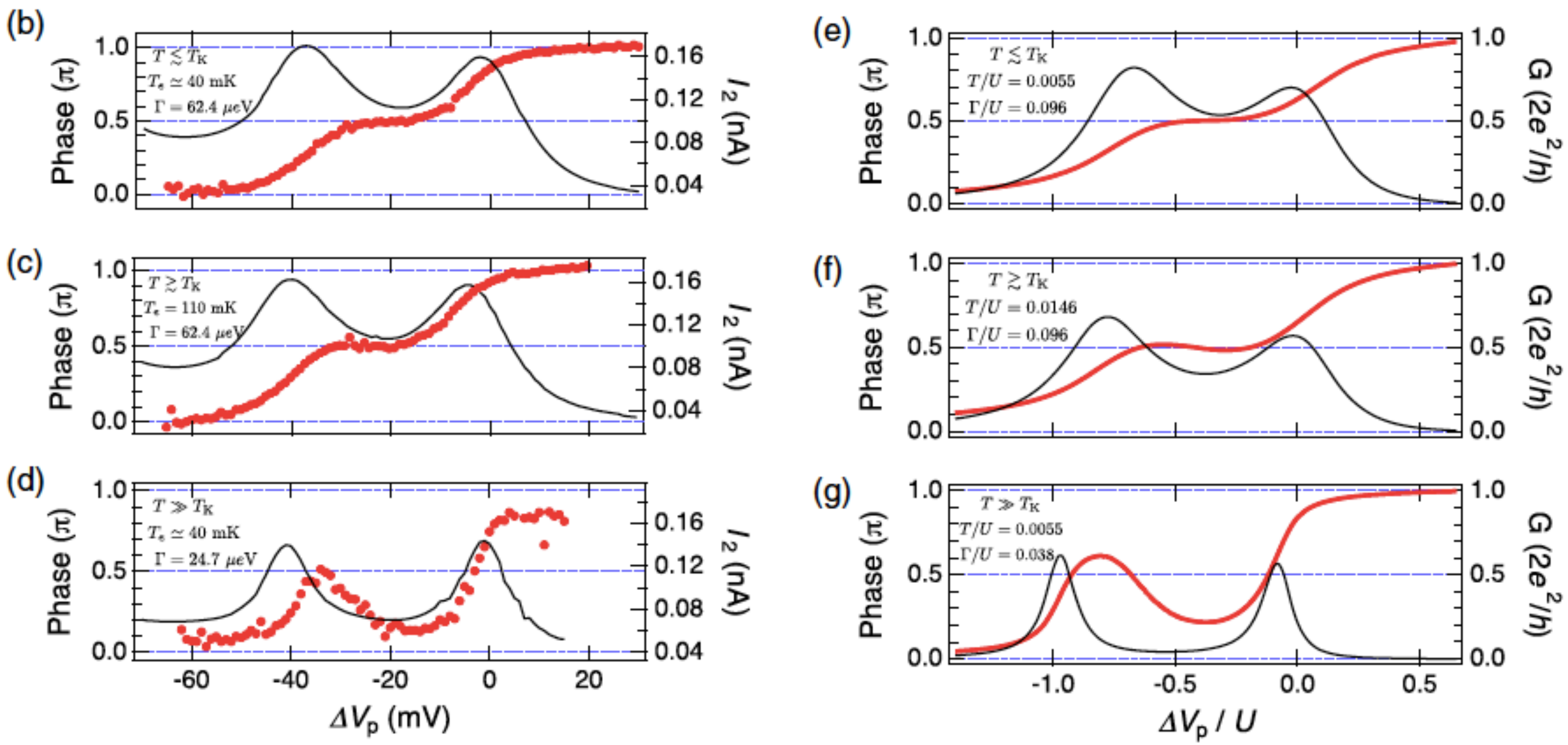




(b)
(c)
(d)
(e)
(f)
(g)
Phase (π)
I_2 (nA)
G ($2e^2/h$)
$T \lesssim T_K$
$T_e \simeq 40$ mK
$\Gamma = 62.4\ \mu$eV
$T \gtrsim T_K$
$T_e = 110$ mK
$\Gamma = 62.4\ \mu$eV
$T \gg T_K$
$T_e \simeq 40$ mK
$\Gamma = 24.7\ \mu$eV
$T \lesssim T_K$
$T/U = 0.0055$
$\Gamma/U = 0.096$
$T \gtrsim T_K$
$T/U = 0.0146$
$\Gamma/U = 0.096$
$T \gg T_K$
$T/U = 0.0055$
$\Gamma/U = 0.038$
ΔV_p (mV)
$\Delta V_p / U$

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: $\boxed{T_{\mathbf{kk'}}(i\omega_n) = V_{\mathbf{k}}^* G_d(i\omega_n) V_{\mathbf{k'}}}$ Scattering T-matrix

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

→ 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: $$\boxed{A_d(0) = \frac{1}{\pi\Gamma}}$$

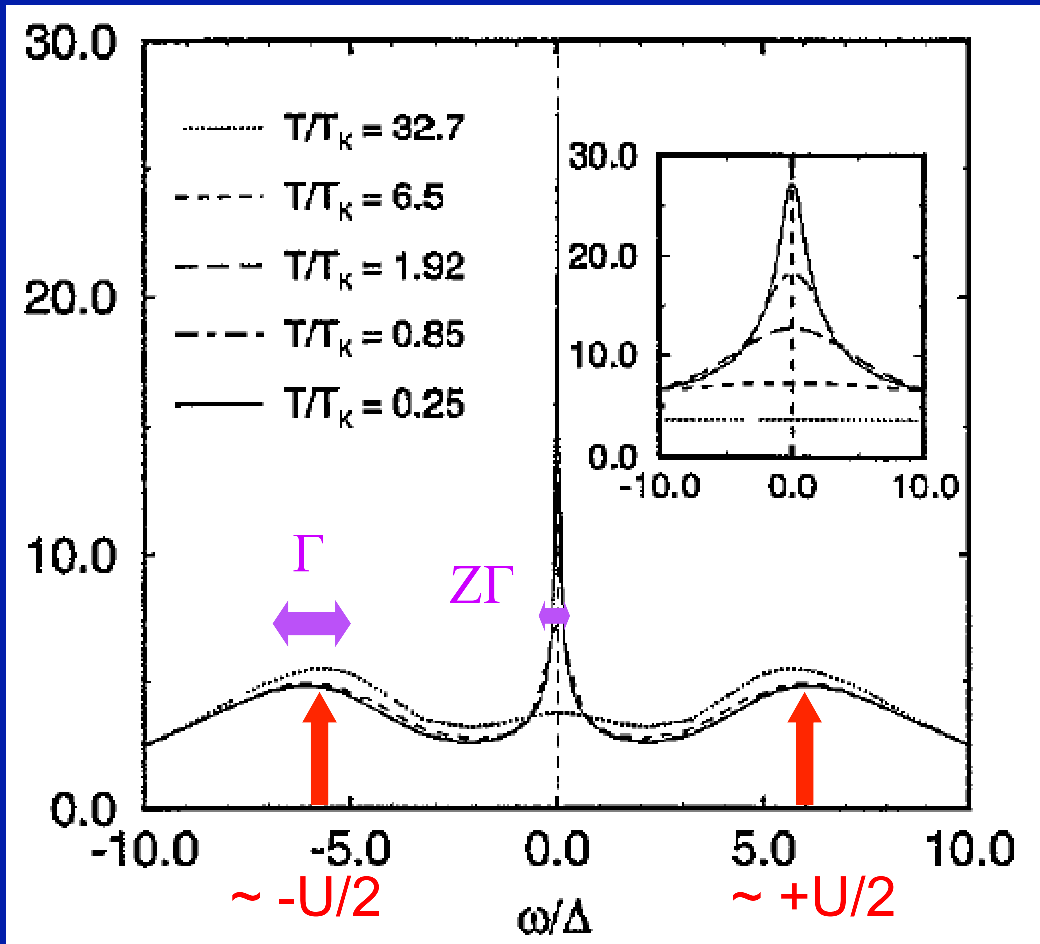
Special case of Friedel's sum rule

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

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:

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

Magnetic impurities in metallic host: 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

Unitary limit resistivity :

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

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

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 :

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

Kubo formula for c-electrons

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

`Optical' theorem

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

Unitary limit resistivity :

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

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

Finite-T, Kondo regime:

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

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

Conductance (cont'd)…

Specialize to L-R symmetric device, for simplicity:

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

Notes:

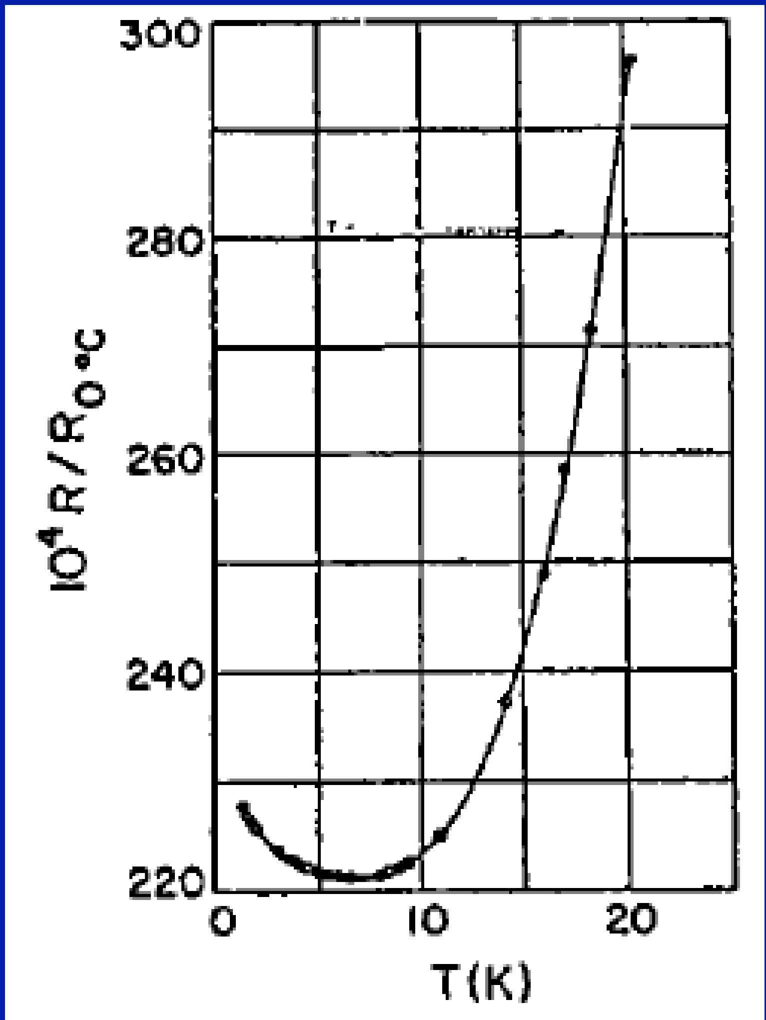
1- Compare to formula for resistivity ! G ~ R quite remarkable !

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

2- → ~ A Landauer formula generalized to tunneling into an interacting system $\Gamma A_d(\omega,T)$ plays the role of transparency of barrier

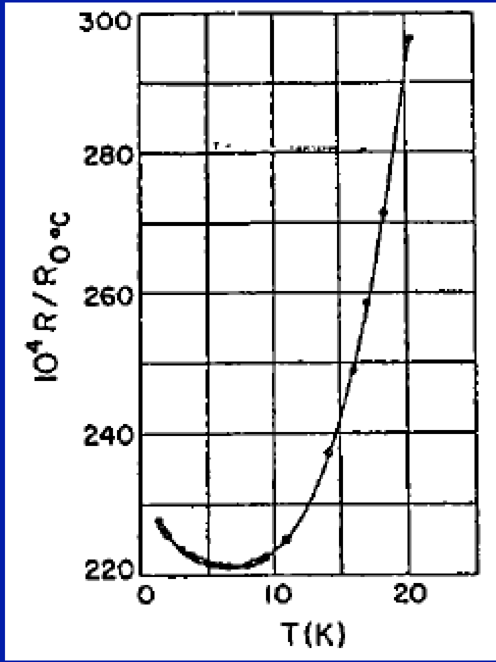
3- Generalization to out of equilibrium, e.g. I(V) for finite voltage Is an outstanding problem. General formula based on Keldysh has been Derived (Meir and Wingreen, PRL 68 (1992) 2512) but concrete calculations Difficult ! Numerous recxent works (Saleur et al., Andrei et al.) – an active field !

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.”

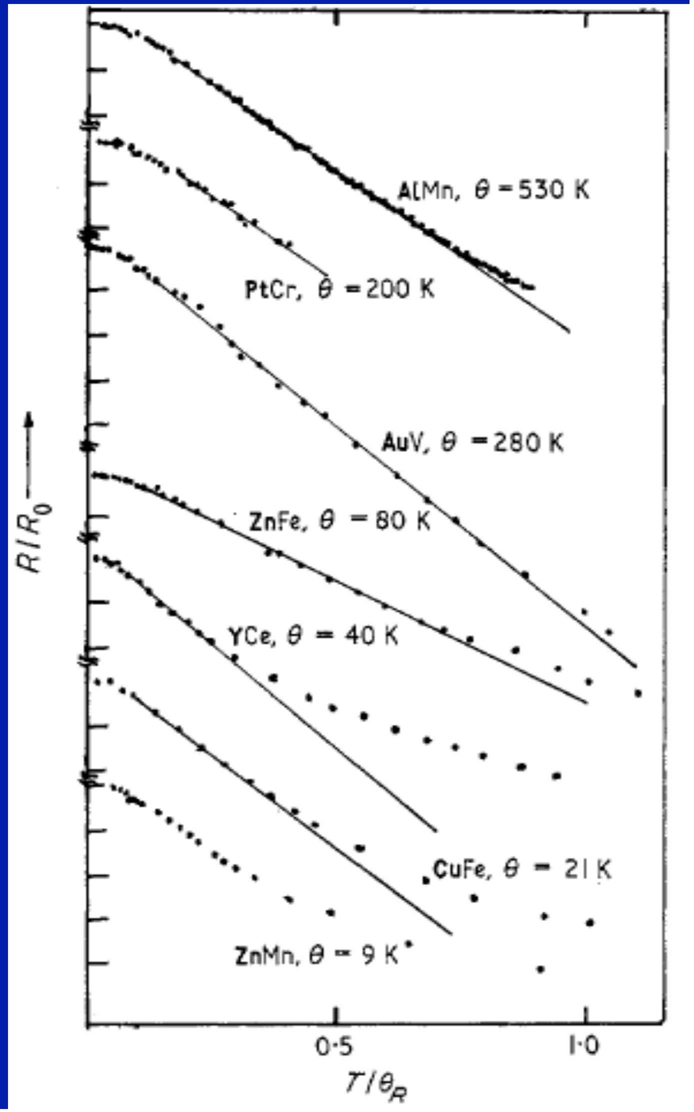


The Kondo effect :

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.

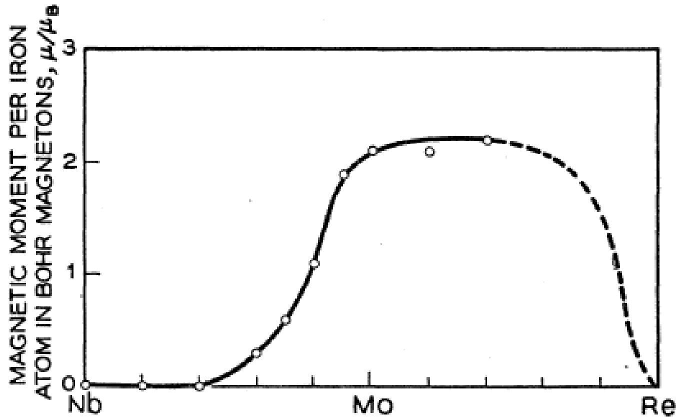


FIG. 1. Magnetic moment of an iron atom dissolved in various Mo-Nb and Mo-Re alloys as a function of alloy composition, according to Clogston *et al.*

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:

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

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

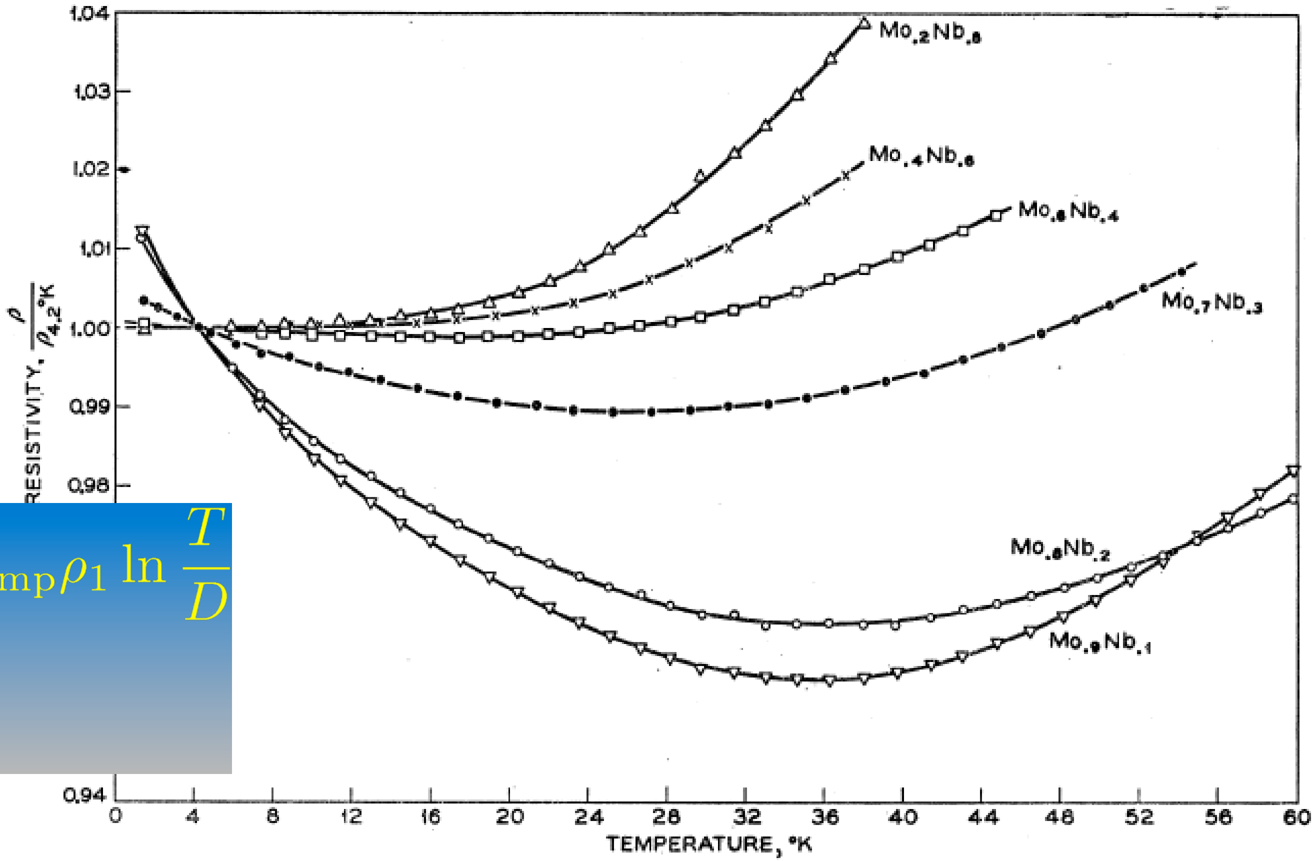


FIG. 3. Resistivity vs temperature for various Mo-Nb alloys containing 1% Fe. Resistivities are normalized at 4.2°K.

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

Effective Hamiltonian at small V: the Kondo model

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

$$H_{\text{eff}} = J_K\, \vec{S}_d \cdot \vec{S}_c \;, \quad J_K = \frac{8V^2}{U}$$

Sd, Sc: spin operators

Can be generalized to a full conduction electron band:

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

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

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

$\rightarrow$ $2V_{\mathbf{k}} V_{\mathbf{k}'} \frac{U}{|\varepsilon_d(\varepsilon_d+U)|}$

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

$\rightarrow$ 0 in symmetric case

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 (when the conduction electron bath is metallic - gapless)

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

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

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

``Kondo temperature''

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

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:

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

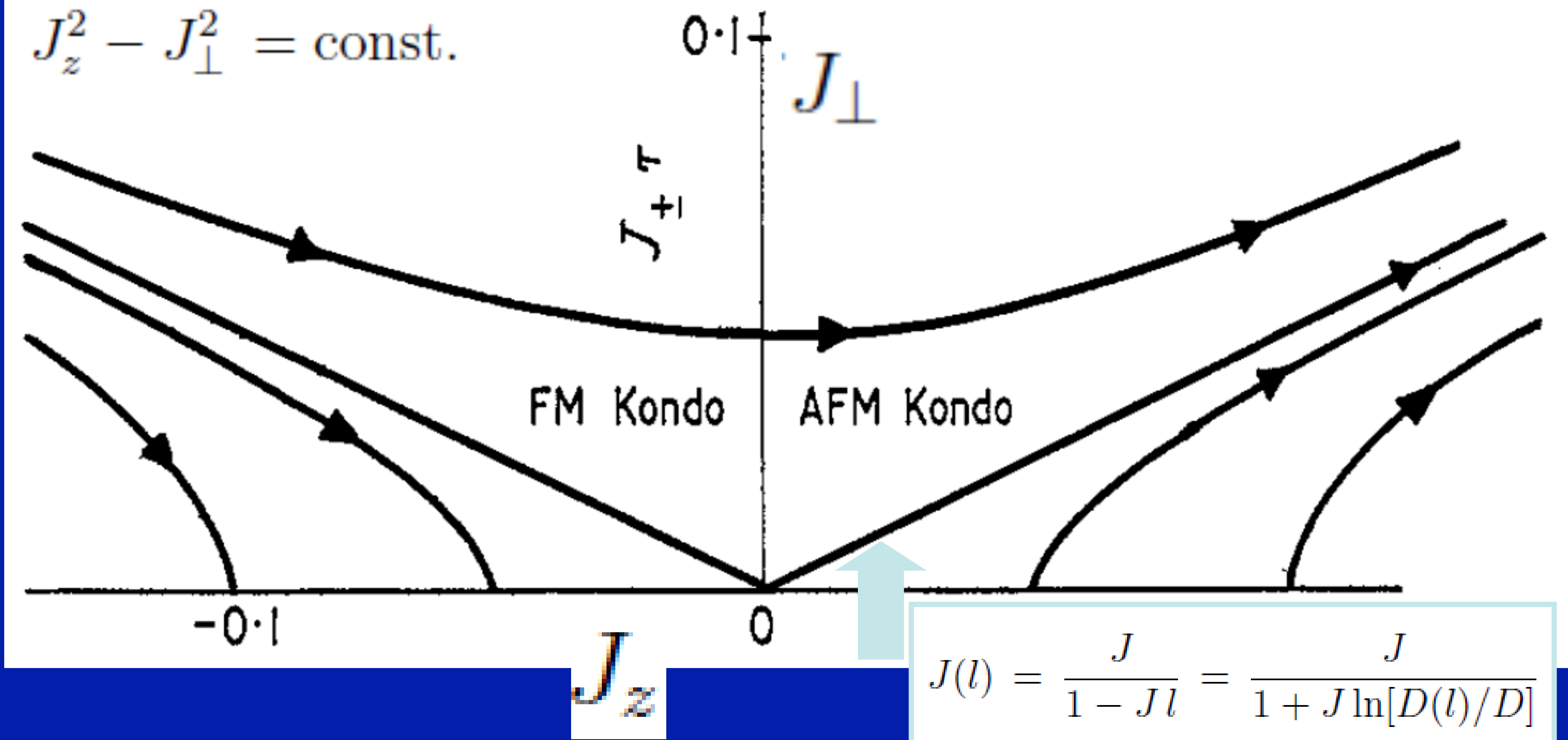
RG flow: AF model flows to strong coupling

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

Coupling becomes large at

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

→ $J_z^2 - J_\perp^2 = \text{const.}$



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

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

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

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

$$\boxed{\chi = \frac{1}{T_K}\tilde{\chi}\left[\frac{T}{T_K}; J(l_K)\right] = \frac{1}{T_K}\tilde{\chi}\left[\frac{T}{T_K}; J^*\right]}$$ + 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:

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

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

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:

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

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

Wilson ratio:

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

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):

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

Scaling of G(T)/G(0) vs. T/T_K

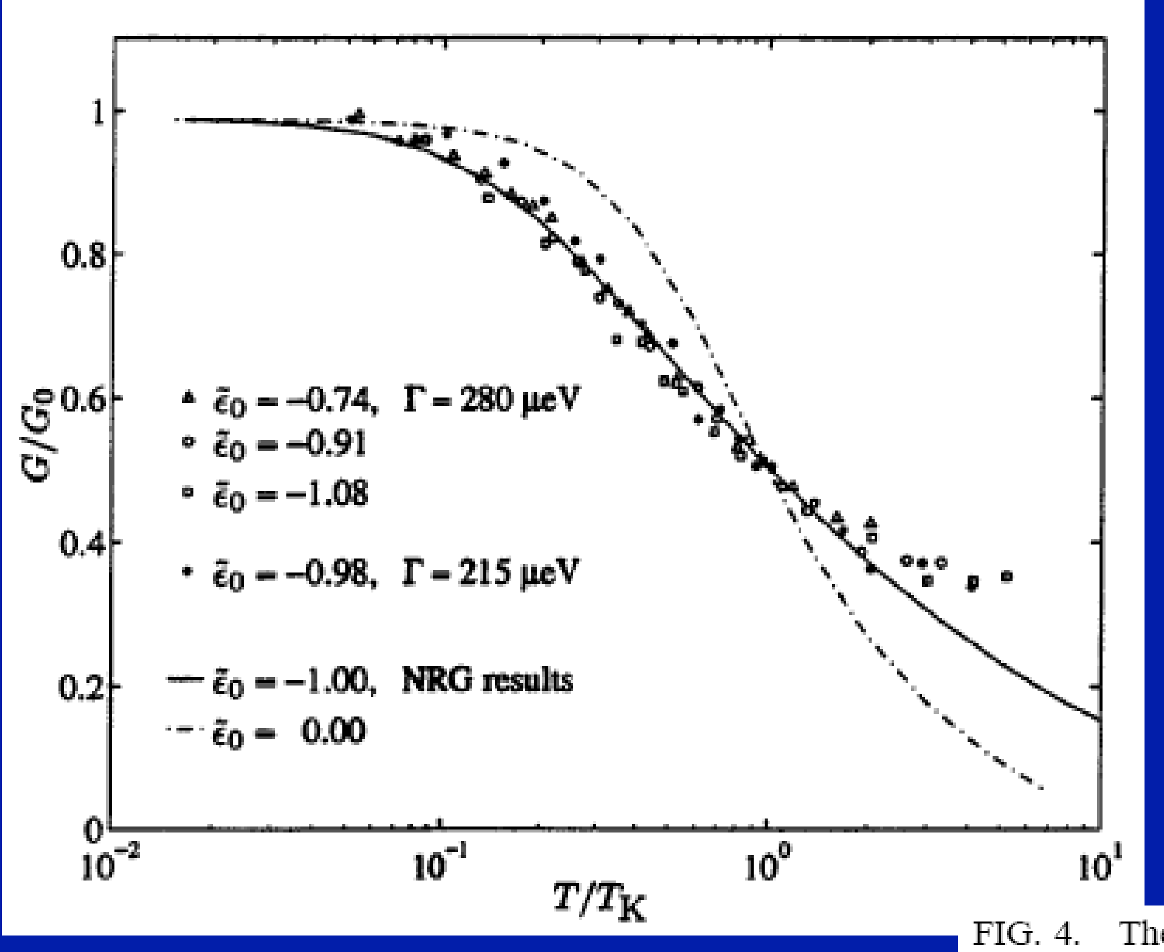
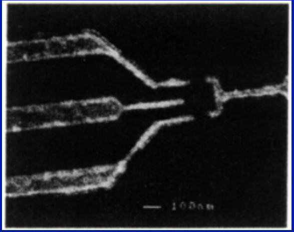


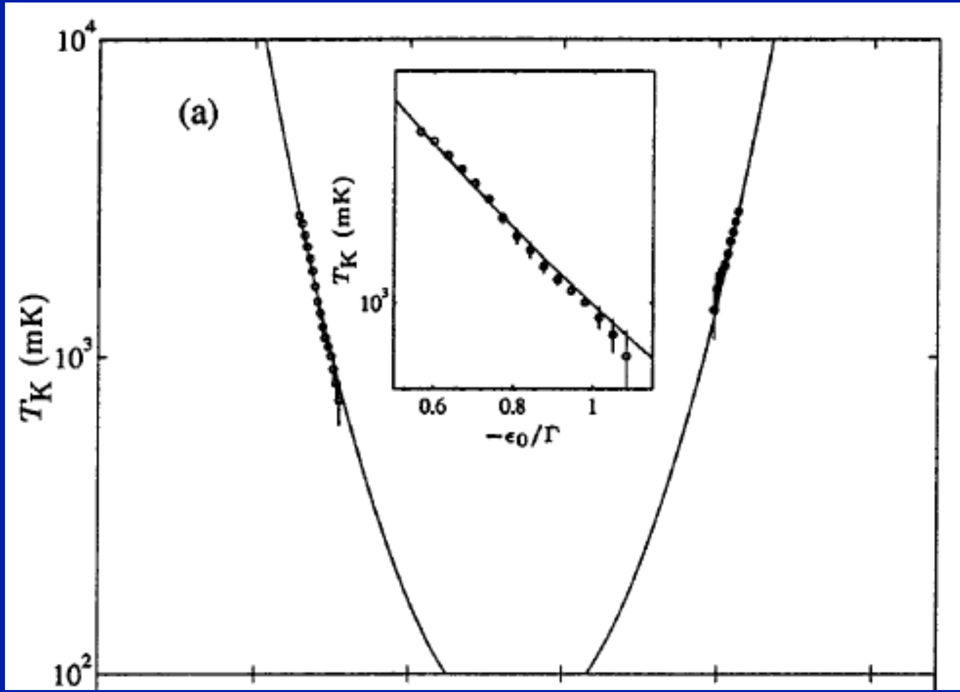
FIG. 4. The normalized conductance $\tilde{G} \equiv G/G_0$ is a universal function of $\tilde{T} \equiv T/T_{\mathrm{K}}$, independent of both $\tilde{\epsilon}_0$ and Γ, in the Kondo regime, but depends on $\tilde{\epsilon}_0$ in the mixed-valence regime. Scaled conductance data for $\tilde{\epsilon}_0 \approx -1$ 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



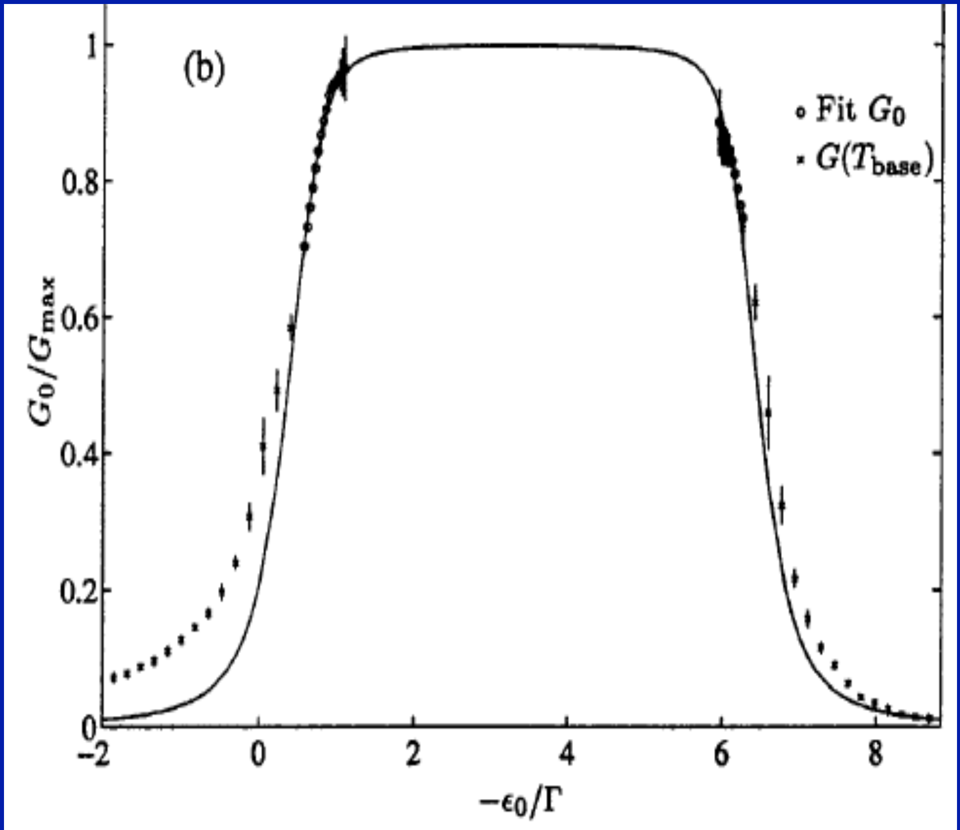


FIG. 5. (a) Fit values of T_K for data such as those in Fig. 3 for a range of values of ϵ_0 [22]. The dependence of T_K on ϵ_0 is well described by Eq. (1) (solid line). Inset: Expanded view of the left side of the figure, showing the quality of the fit. (b) Values of G_0 extracted from data such as 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.

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

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

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

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

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

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

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

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

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

(D→ infinity)

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

\`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

- How does one interpolate from U/Γ=0 limit

(1 broadened atomic level centered at ε_d)

to atomic limit Γ/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:

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

also reads:

$$\begin{aligned}
S &= S_{\text{at}} + S_{\text{hyb}} \\
S_{\text{at}} &= \int_0^\beta d\tau \sum_\sigma d_\sigma^\dagger(\tau) \left(-\frac{\partial}{\partial \tau} + \varepsilon_d \right) d_\sigma(\tau) + U \int_0^\beta d\tau n_\uparrow n_\downarrow \\
S_{\text{hyb}} &= \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma d_\sigma^\dagger(\tau') \Delta(\tau - \tau') d_\sigma(\tau)
\end{aligned}$$

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 <u>self-energy for the d-orbital</u>:

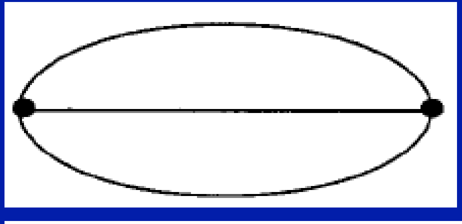
$$G_d(i\omega_n)^{-1} = G_{d0}(i\omega_n)^{-1} - \Sigma(i\omega_n)$$

(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(U^2):



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

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, overall spectral weight Z:

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

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

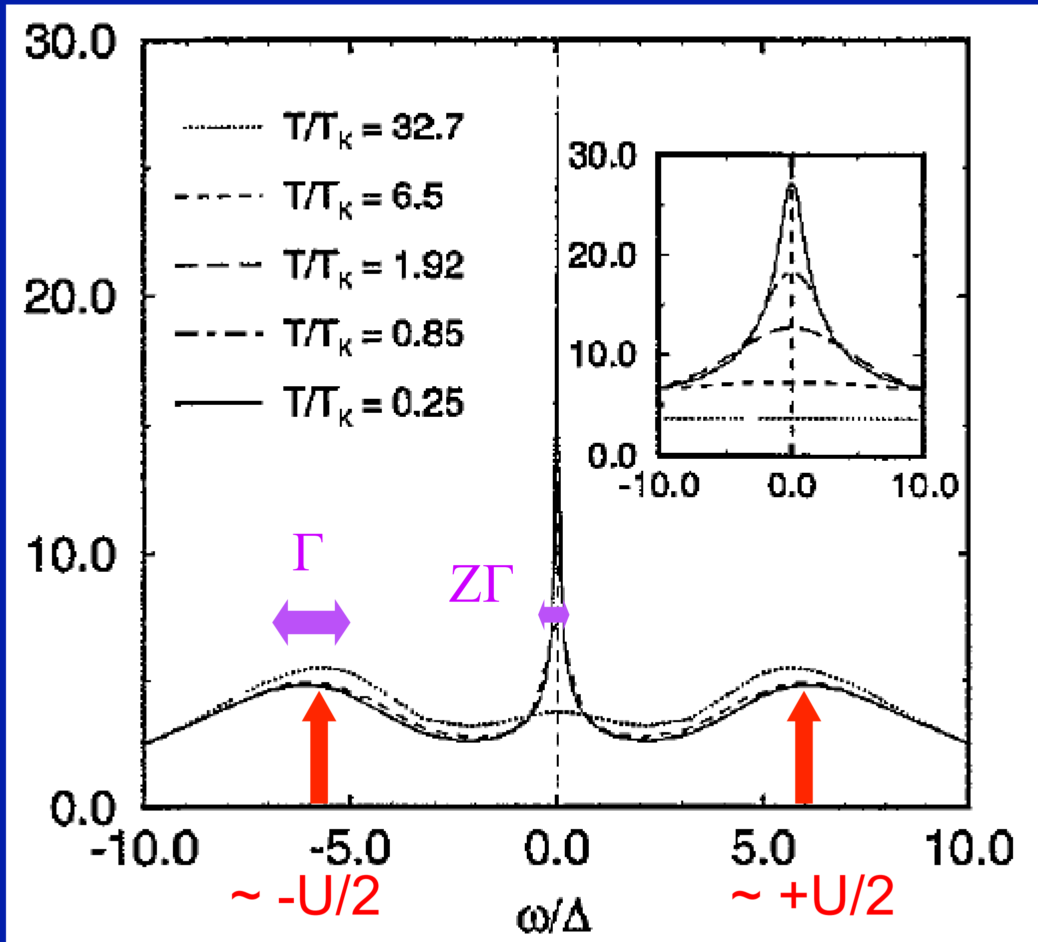
$$A_d(\omega \simeq 0) = \frac{Z}{\pi} \frac{Z\Gamma}{\omega^2 + (Z\Gamma)^2} \qquad A_d(\omega = 0) = \frac{1}{\pi\Gamma}$$

Width, Weight ~ Z

Height unchanged !

Numerical Renormalization Group (NRG) calculation

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



$$Z \sim T_K/\Gamma$$

$$T_K \sim \Lambda\, e^{-1/J_K \rho_c} \sim \Lambda \exp -\frac{\pi U}{8\Gamma}$$

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

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

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

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

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

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.

Bibliography (some)

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- 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…

``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…]