Lecture 2: Kondo effect in quantum dots: Anderson model

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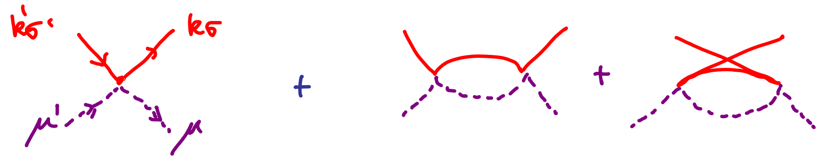
AM1

Main results of lecture 1:

Kondo Model:
$$H = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J \sum_{kk'\sigma\sigma'} \left(c^\dagger_{k\sigma} \tfrac{1}{2}\vec{\sigma}_{\sigma\sigma'} c_{k'\sigma'} \right) \cdot \vec{S} \qquad (1)$$

Spin-flip scattering:



enhanced at low temp:
$T \lesssim T_K = D \exp\left[-\frac{1}{\nu J}\right]$ $\Rightarrow$ ground state = spin singlet $\Downarrow\!\Uparrow$ (2)

Scattering phase shifts at T = 0: $\delta_\uparrow(0) = -\delta_\downarrow(0) = \pi/2$ (3)

How do magnetic moments form in metals?
Answer provided by "Anderson impurity model" (AM) [1961], relevant also to describe transport through quantum dots, which also show Kondo effect [1998].

Single-impurity Anderson model

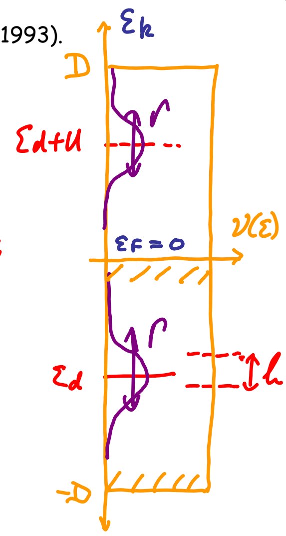
AM2

Anderson, Phys. Rev. 124, 41 (1961); Hewson, "The Kondo Problem to Heavy Fermions", Cambridge (1993).

Conduction band: (flat DOS, "wide-band limit": $D \gg$ all other scales)
$$H_{band} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} \qquad (1)$$

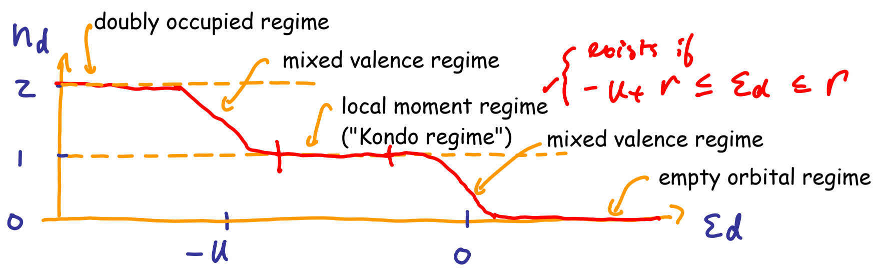
Localized impurity level:
$$H_{loc} = \sum_\sigma (\varepsilon_d + \sigma \underbrace{\cancel{h}}_{=0}) \underbrace{d^\dagger_\sigma d_\sigma}_{\hat{n}_{d\sigma}} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \qquad (2)$$

Hybridization: [Usual convention: $v_k = v =$ real]
$$H_{hyb} = \sum_{k\sigma} v_k \left[c^\dagger_{k\sigma} d_\sigma + h.c. \right] \qquad (3)$$



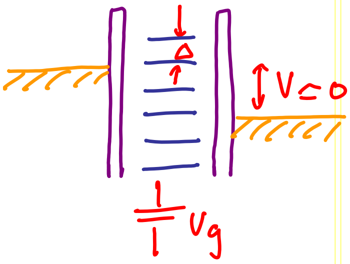
Level width: (from golden rule)
$$\Gamma = \pi \nu v^2 \qquad (4)$$

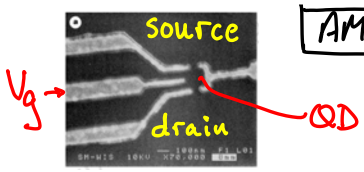
Level occupancy:
$n_d = \langle n_{d\uparrow} + n_{d\downarrow} \rangle$



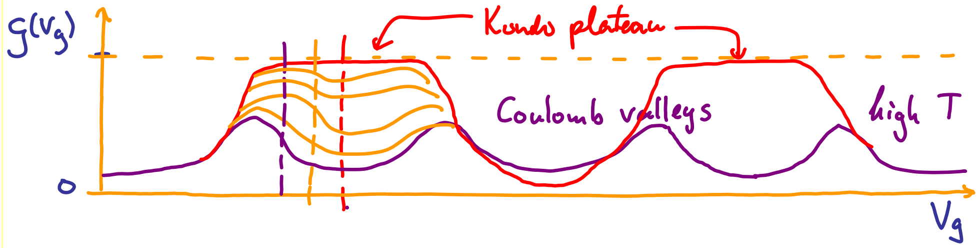
exists if $-U + \Gamma \le \varepsilon_d \le \Gamma$

Conductance anomalies for quantum dot in "Kondo regime"

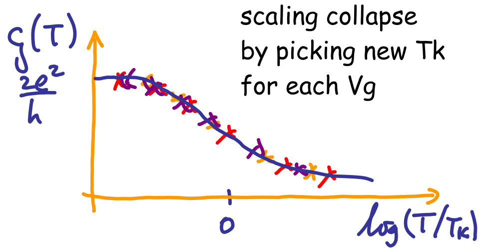


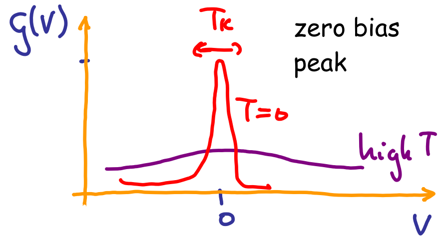


Linear conductance:
Odd Coulomb valleys
become Kondo plateaus



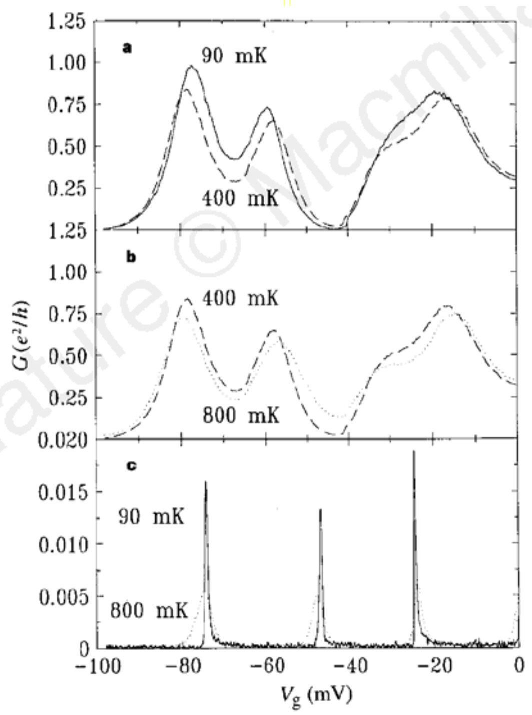
Fixed gate voltage:
Anomalous T- and V-dependence





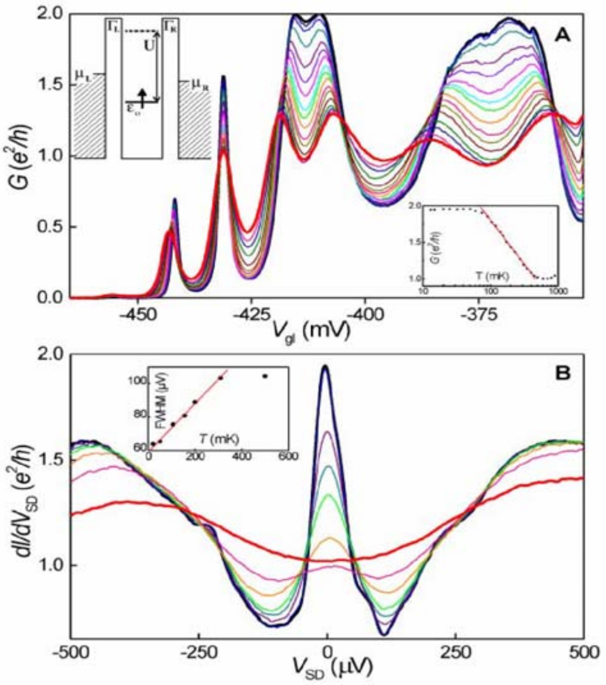
Conductance anomalies: real data

Weak Kondo effect



Goldhaber-Gordon et al., Nature **391**, 156

Strong Kondo effect

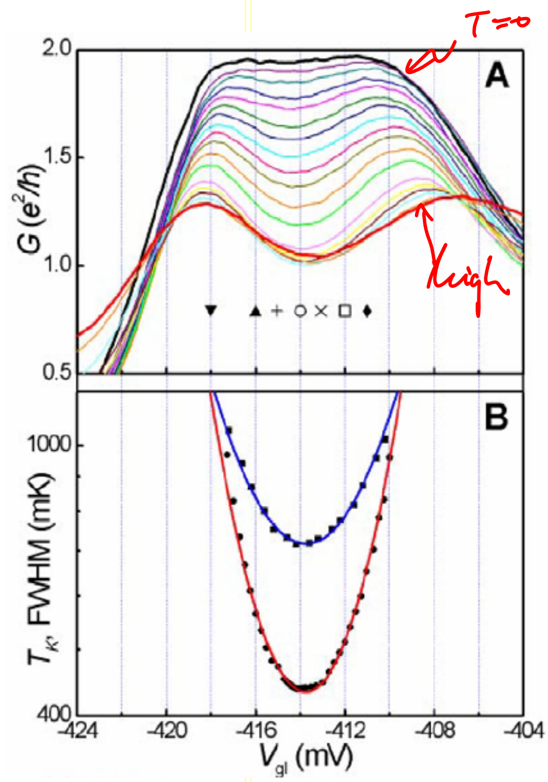


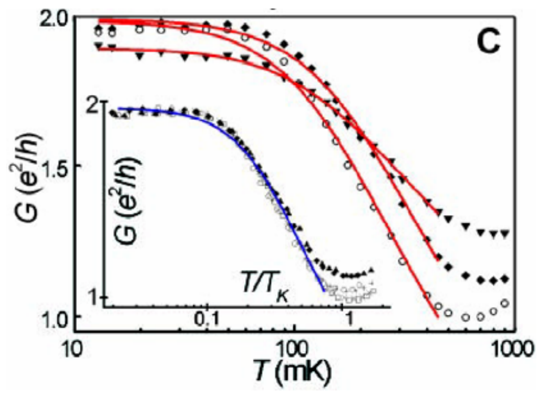
van der Wiel et al., Sience 289, 2105 (2000)

AM5

Ideal Kondo effect

van der Wiel et al., Sience 289, 2105 (2000)





- Beautiful Kondo plateau observed
- T-dependence follows universal form when scaled by Tk
- This allows determination of Tk
- Observed dependence of Tk on εd agrees with theoretical prediction:

$$\log T_K = c_1\, \varepsilon_d(\varepsilon_d + U) + c_2$$

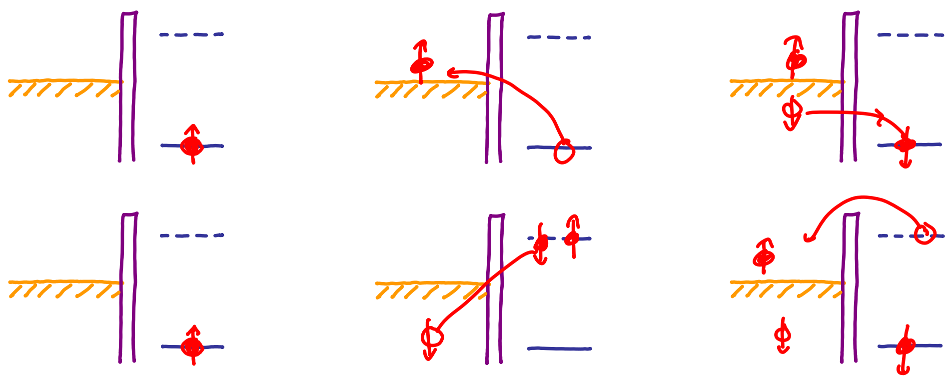
AM6

When does "Kondo plateau" arise?

Occurs for $T \to 0 \quad (T \ll T_K)$

and when $n_d \simeq 1$ (odd) $\Longrightarrow$ localized spin

Loc. spin + cond. band : Kondo model $\Longrightarrow$ Spin-flip scatt. !!



$\Gamma = \pi \nu v^2$

Spin-flip processes occur via virtual intermediate states.

Effective spin-flip rate: $$\nu \frac{v^2}{\varepsilon_d + U} - \frac{v^2}{\varepsilon_d} = - \frac{U\Gamma/\pi}{\varepsilon_d(\varepsilon_d+U)} =: J \quad (>0) \qquad (1)$$

Schrieffer-Wolff transformation

Phys Rev 149, 491 (1966)

$$H_{AM} = \underbrace{H_{band} + H_{loc}}_{H_0} + \underbrace{H_{hyb}}_{H_1 = \mathcal{O}(v)}$$

Idea: seek effective $\tilde{H}$ in subspace of $n_d = 1$

Try unitary transf.: $$\tilde{H} = e^{A} H e^{-A}, \quad \text{with } A^{\dagger} = -A \qquad (1)$$

A has pert. exp. in v : $$A = 0 + \mathcal{O}(v) + \mathcal{O}(v^2) + \dots \qquad (2)$$

Expand $\tilde{H}$: $$\tilde{H} \overset{(2)}{=} (H_0 + H_1) + [A, \underbrace{H_0]}_{:=0} + H_1] + \tfrac{1}{2}[A, \overbrace{[A, H_0}^{(4)\;-H_1} + \cancel{H_1}]] \quad \mathcal{O}(v^3) \qquad (3)$$

Demand: $\tilde{H}$ contains no $\mathcal{O}(v)$: $$H_1 \overset{(3)}{=:} -[A, H_0], \quad (4) \quad \Rightarrow \quad \tilde{H} \overset{(3)}{=} H_0 + \tfrac{1}{2}[A, H_1] + \mathcal{O}(v^3) \qquad (5)$$

check algebra yourself!

(5) is satisfied by: $$A = \sum_{k\sigma} v \left[\frac{1}{\varepsilon_k - \varepsilon_d} c^{\dagger}_{k\sigma} d_{\sigma} + \frac{U}{(\varepsilon_d - \varepsilon_k)(\varepsilon_d + U - \varepsilon_k)} d^{\dagger}_{-\sigma} d_{-\sigma} c^{\dagger}_{k\sigma} d_{\sigma} \right] - h.c. \qquad (6)$$

Effective Hamiltonian for $n_d = 1$ yields Kondo model

(7.5) yields: $$\tilde{H}\Big|_{n_d=1} = \sum_{k\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{kk'} \tilde{v}^{(2)}_{kk'} \vec{s}_{kk'} \cdot \vec{S} + (c^{\dagger}_{k} c_{k'}\text{-term}) \qquad (1)$$

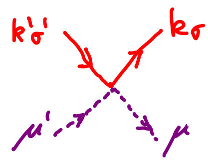
potential scattering

local spin operators: $$S^z = \tfrac{1}{2}\left(d^{\dagger}_{\uparrow} d_{\uparrow} - d^{\dagger}_{\downarrow} d_{\downarrow}\right), \quad S^{+} = d^{\dagger}_{\uparrow} d_{\downarrow}, \quad S^{-} = d^{\dagger}_{\downarrow} d_{\uparrow} \qquad (2)$$
$$:= \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad := \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

conduction band spin operators: $$\vec{s}_{kk'} = \tfrac{1}{2} \sum_{\sigma\sigma'} c^{\dagger}_{k\sigma} \vec{\sigma}_{\sigma\sigma'} c_{k'\sigma'} \qquad (3)$$

coupling: $$\tilde{v}^{(2)}_{kk'} = \frac{-\tfrac{1}{2} v_k v_{k'} U}{(\varepsilon_d - \varepsilon_k)(\varepsilon_d + U - \varepsilon_k)} + k \to k' \quad \xrightarrow[\ll\, |\varepsilon_d|,\ |\varepsilon_d + U|]{|\varepsilon_k|,\ |\varepsilon_{k'}|} \quad \simeq \frac{v_{k_F}^2 U}{|\varepsilon_d||\varepsilon_d + U|} =: J \qquad (4)$$

Low-en. properties of AM for nd = 1 described by KM: $$H_{Kondo} = H_{band} + J \sum_{\substack{kk' \\ \mu\mu'}} \underbrace{\vec{s}_{kk'} \cdot \vec{S}_{\mu\mu'}}_{SU(2)\text{ symmetric!}} \qquad (6)$$



Eff. Kondo temp:
(observed: see AM 5!)

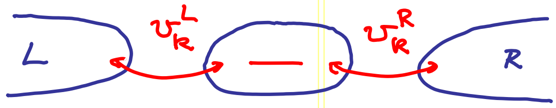
$$T_K \overset{(K6.5)}{=} D e^{-\frac{1}{\nu J}} \overset{(4)}{=} D \exp\left[- \frac{\pi |\varepsilon_d||\varepsilon_d + U|}{\Gamma U} \right] \qquad (7)$$

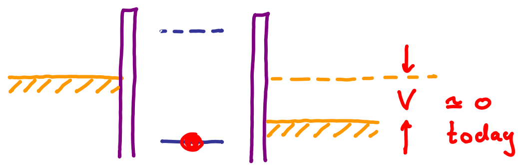
agrees with Bethe Ansatz, except for prefactor

Single-level quantum dot with two leads

Pustilnik, Glazman, PRL 87, 216601 (2001) **AM9**

Recent review: "Nanophysics: Coherence and Transport," eds. H. Bouchiat et al., pp. 427-478 (Elsevier, 2005).





lead index: $\alpha = L, R$

Two-lead Hamiltonian:
$$H = \overbrace{\sum_{k\alpha\sigma} \varepsilon_k c^\dagger_{k\alpha\sigma} c_{k\alpha\sigma}}^{\text{"}H_{2\,band}\text{"}} + \sum_{k\alpha\sigma} v_k^\alpha c^\dagger_{k\alpha\sigma} d_\sigma + h.c. + H_{loc} \qquad (1)$$

Schrieffer-Wolff as before, with:
$$\sum_k v_k \longrightarrow \sum_{k\alpha} v_k^\alpha \left(\ldots \right)^\alpha \qquad (2)$$

Effective Hamiltonian for nd = 1:
$$H^{Kondo}_{scat.} = \sum_{\alpha\alpha'} \underbrace{\left(- \frac{v^\alpha_{k_F} v^{\alpha'}_{k_F} U}{\varepsilon_d(\varepsilon_d + U)} \right)}_{:= J_{\alpha\alpha'}} \underbrace{\left(\sum_{kk'\sigma\sigma'} c^\dagger_{k\alpha\sigma} \vec{\sigma}_{\sigma\sigma'} c_{k'\alpha'\sigma'} \right) \cdot \vec{S}}_{\vec{s}_{\alpha\alpha'} \cdot \vec{S}} = \overbrace{\sum_{\alpha\alpha'} J_{\alpha\alpha'} \vec{s}_{\alpha'\alpha}}^{Tr(J\vec{s})} \cdot \vec{S} \qquad (3)$$

Coupling matrix:
$$J_{\alpha\alpha'} = \tilde{c} \begin{bmatrix} v_L^2 & v_L v_R \\ v_R v_L & v_R^2 \end{bmatrix}, \quad \text{with} \quad v_\alpha = v^\alpha_{k_F}, \quad \tilde{c} = \frac{-U}{\varepsilon_d(\varepsilon_d + U)} \qquad (4)$$

Determinant:
$$\det J_{\alpha\alpha'} = \tilde{c}^2 \left[v_L^2 v_R^2 - (v_L v_R)^2 \right] = 0 \qquad (5)$$
one eigenvalue = 0

Diagonalization of coupling matrix J

AM10

J is diagonalized by:
$$W = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}, \quad \tan\theta = -v_R/v_L \qquad (1)$$

diagonal form:
$$\tilde{J} = W J W^\dagger = \begin{bmatrix} J_1 & 0 \\ 0 & J_2 \end{bmatrix} = \begin{bmatrix} \tilde{c}(v_L^2 + v_R^2) & 0 \\ 0 & 0 \end{bmatrix} \qquad (2)$$

Rotate basis:
$$\psi_{k\gamma\sigma} = \sum_\alpha c_{k\alpha\sigma} W_{\alpha\gamma} \qquad (3)$$

$$\sum_{kk'\sigma\sigma'} (\psi^\dagger_{k1\sigma} \vec{\sigma}_{\sigma\sigma'} \psi_{k'1\sigma'})$$

$$\tilde{H}^{Kondo}_{scat} \overset{(9.3)}{=} Tr\Big[\underbrace{W^\dagger J W}_{\tilde{J}} \underbrace{W^\dagger \vec{s} W}_{\vec{s}_1} \Big] \cdot \vec{S} = J_1 \vec{s}_1 \cdot \vec{S} \qquad (4)$$

J-diagonal Kondo Hamiltonian:
$$H = \sum_{k\gamma\sigma} \varepsilon_k \psi^\dagger_{k\gamma\sigma} \psi_{k\gamma\sigma} + J_1 \vec{s}_1 \cdot \vec{S} \qquad (5)$$

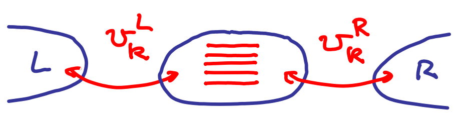
Important conclusion: One mode yields Kondo-Hamiltonian, other mode decouples completely!

[Comment: for multilevel AM, coupling matrix is more complicated: $v_k^{\alpha j} c^\dagger_{k\alpha\sigma} d_{j\sigma}$

Then J2 can be nonzero, because $\det J_{\alpha\alpha'} \propto \sum_{jj'} \left(v_j^L v_{j'}^R - v_j^R v_{j'}^L \right)^2 \neq 0$ (6)]

Conductance through (many-level) QD with 2 leads

AM11



Consider $T=0$, $B \neq 0$ but $\to 0$
which ensures non-degenerate ground state

lead index: $\alpha = L, R$

Then incident electrons experience only potential scattering, described by 2x2 S-matrix:

$$S_{\sigma,\alpha\alpha'}(0) = W^\dagger D_\sigma W , \qquad D_\sigma = \begin{bmatrix} e^{2i\delta_{1\sigma}} & 0 \\ 0 & e^{i2\delta_{2\sigma}} \end{bmatrix} \qquad (1)$$

same as in (10.1)

Phase shifts: $\delta_{\gamma\sigma}$, with $\gamma = 1,2$, $\sigma = \uparrow, \downarrow$

Landauer formula for conductance:

$$G(T=0) = \frac{e^2}{h}\sum_\sigma \left| S^\gamma_{\sigma,RL}(0)\right|^2 = G_0 \, \frac{1}{2}\sum_\sigma \sin^2(\delta_{1\sigma} - \delta_{2\sigma}) \qquad (2)$$

Prefactor:

$$G_0 = \frac{2e^2}{h}\sin^2 2\theta \overset{(10.1)}{=} \frac{2e^2}{h}\,\frac{4(v_L v_R)^2}{(v_L^2+v_R^2)^2} = \frac{2e^2}{h} \text{ if } v_L = v_R \qquad (3)$$

Important conclusion: T = 0 conductance is determined purely by phase shifts!

Conductance through 1-level QD with 2 leads

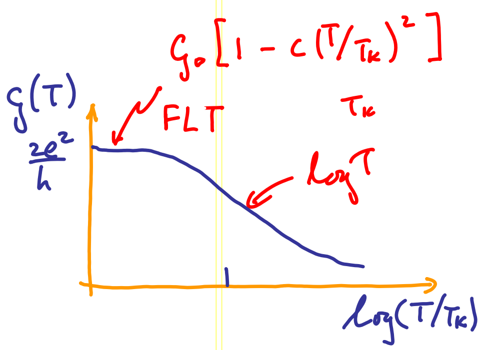
AM12

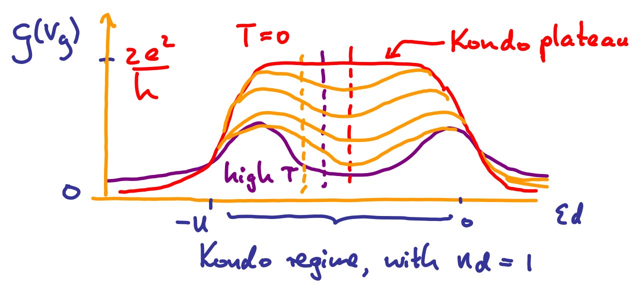
For 1-level AM: $J_2 \overset{(10.2)}{=} 0 , \quad \to \quad \delta_{2\sigma} = 0$ (1)

From lecture 1, (K9.4): at $T=0$, $\delta_{1\uparrow} = -\delta_{1\downarrow} = \pi/2$ (2)

Conductance at T = 0: $G(T=0) \overset{(11.2)}{=} G_0 \, \frac{1}{2}\sum_\sigma \sin^2(\overset{=\pi/2}{\delta_{1\sigma}} - \overset{=0}{\cancel{\delta_{2\sigma}}}) = G_0$ (3)

for symmetric couplings $(v_L = v_R)$ $= \frac{2e^2}{h}$ = "unitarity limit", maximal possible value, as though channel were completely open! (4)



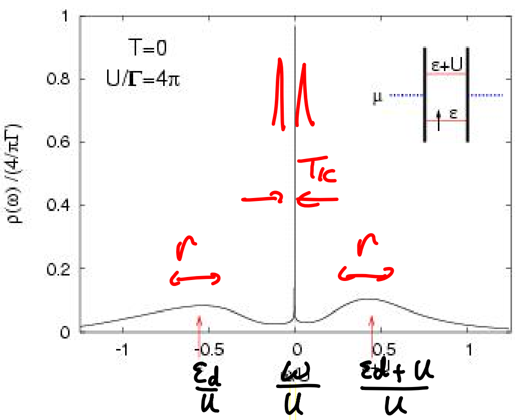


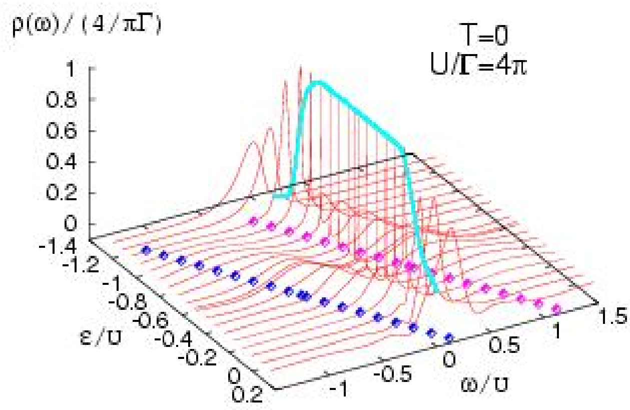
Kondo-Abrikosov-Suhl resonance in local spectral function

AM13

Local Green's function: $\mathcal{G}^R_{d\sigma}(\omega) = \int_0^\infty dt\, e^{-i\omega t} (-i) \langle \{ d_\sigma(t), d_\sigma(0) \} \rangle$

Spectral function = local density of states (LDOS): $A_{d\sigma}(\omega) = -\frac{1}{\pi} \operatorname{Im} \mathcal{G}^R_{d\sigma}(\omega) = \nu_{loc}(\omega) = \rho(\omega)$





For T < Tk, LDOS develops Kondo resonance...

which is observed directly in V-dep. of G (see AM4)

Numerical Renormalization Group calculations by Michael Sindel, 2004