Lecture 2: Kondo effect in quantum dots: Anderson model

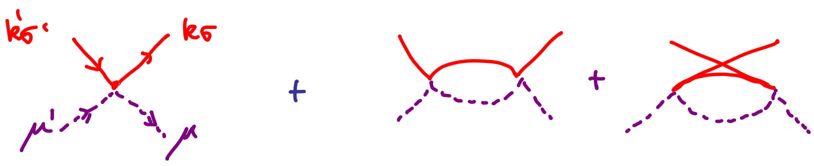
Jan von Delft

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

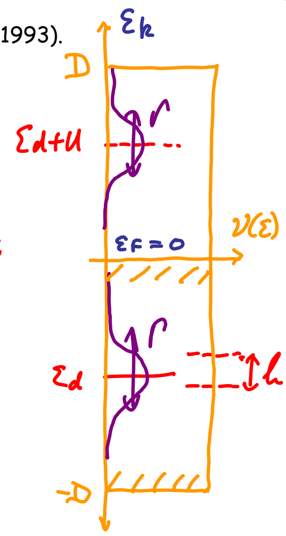
Scattering phase shifts at T = 0: $\delta_\uparrow(0) = -\delta_\downarrow(0) = \pi/2$ (3)

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).



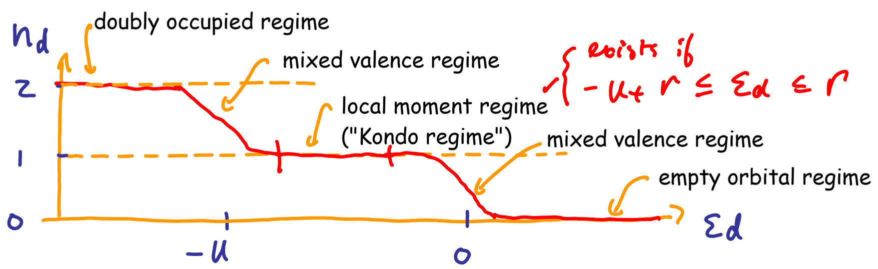
Conduction band: (flat DOS, "wide-band limit": D >> all other scales)
$$H_{band} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} \qquad (1)$$

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

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

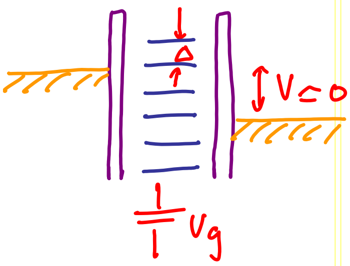
Level width: (from golden rule)
$$\Gamma = \pi \nu v^2 \qquad (4)$$

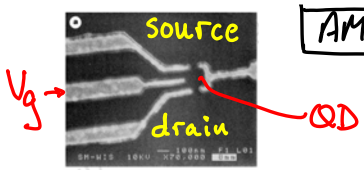
Level occupancy:
$n_d = \langle n_{d\uparrow} + n_{d\downarrow}\rangle$



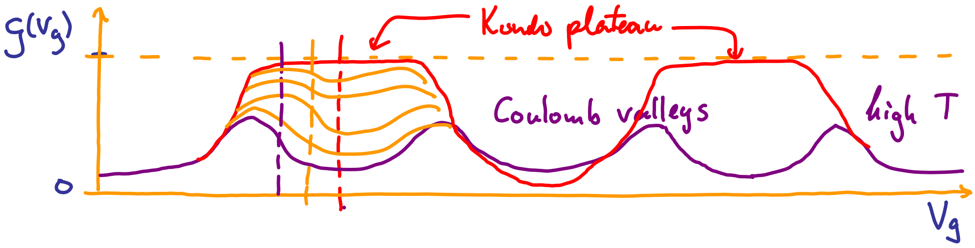
Conductance anomalies for quantum dot in "Kondo regime"

AM3

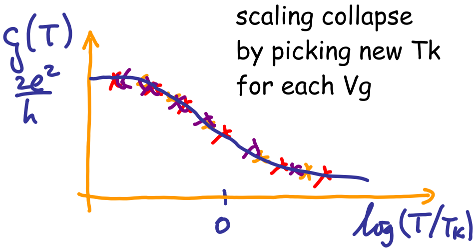




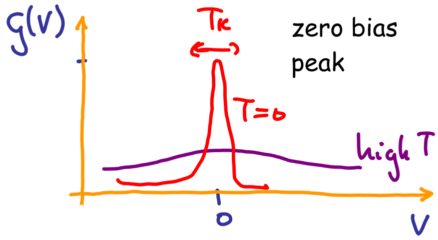
Linear conductance:
Odd Coulomb valleys
become Kondo plateaus



Fixed gate voltage:
Anomalous T- and V-dependence



scaling collapse
by picking new Tk
for each Vg

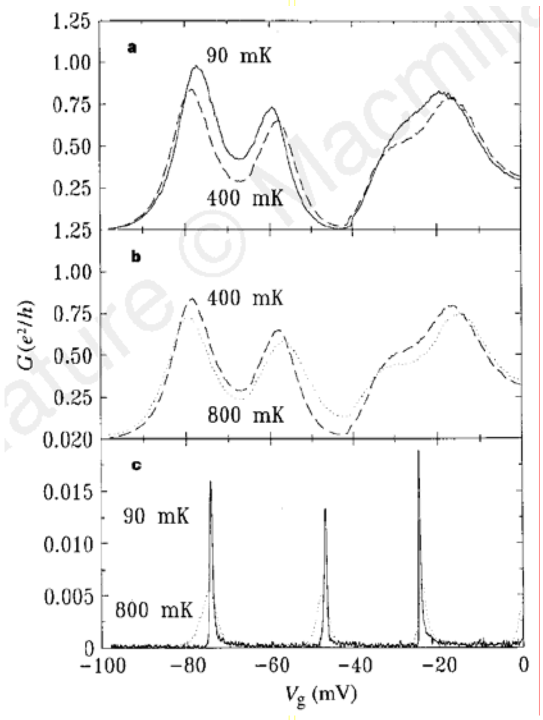


zero bias
peak

Conductance anomalies: real data

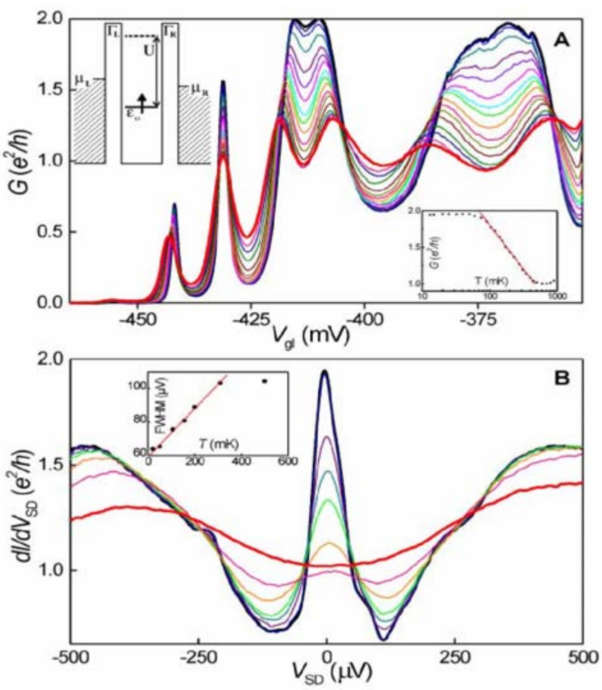
AM4

Weak Kondo effect



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

Strong Kondo effect

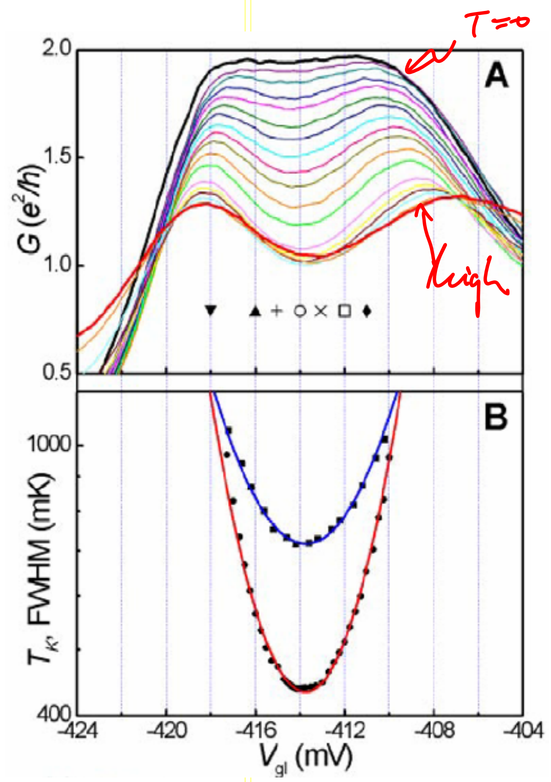


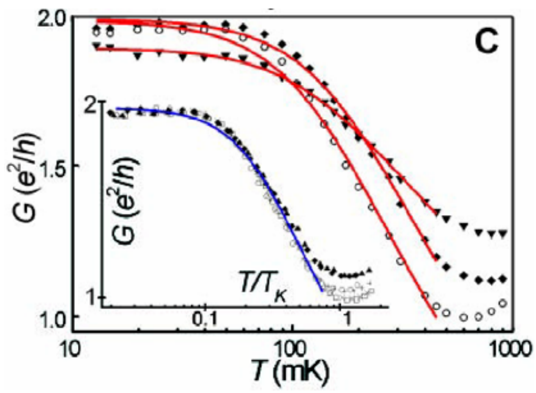
van der Wiel et al., Sience 289, 2105 (2000)

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:

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

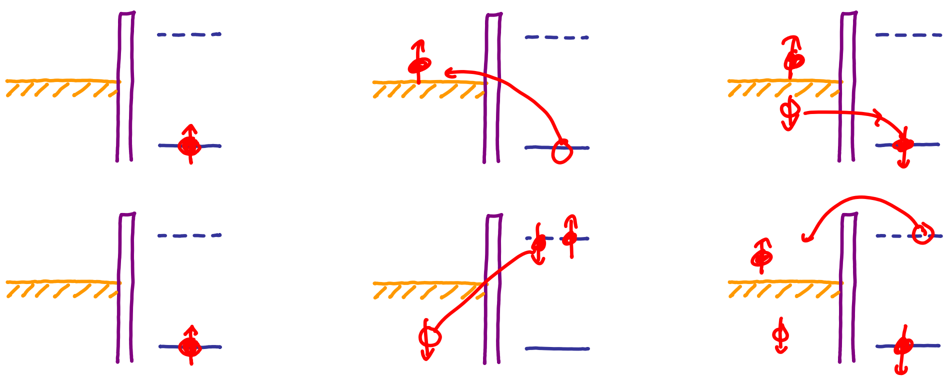
AM6

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)

AM7

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

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

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

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

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

$:= 0$

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

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

AM8

potential scattering

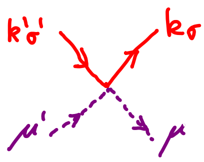
(7.5) yields: $$\tilde{H}\Big|_{n_d=1} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{kk'} \tilde{v}^{(2)}_{kk'} \vec{s}_{kk'} \cdot \vec{S} + (c^\dagger_k c_{k'}\text{-term}) \qquad (1)$$

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

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

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



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

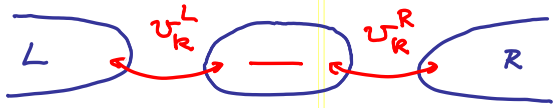
agrees with Bethe Ansatz, except for prefactor

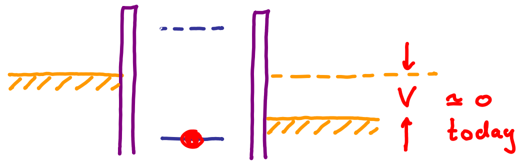
Single-level quantum dot with two leads

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:
$$H = \overbrace{\sum_{k\alpha\sigma} \varepsilon_k c^\dagger_{k\alpha\sigma} c_{k\alpha\sigma}}^{\text{"}H_{2band}\text{"}} + \sum_{k\alpha\sigma} v^\alpha_k c^\dagger_{k\alpha\sigma} d_\sigma + h.c. + H_{loc} \qquad (1)$$

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

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

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

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

$$\sum_{kk'\sigma\sigma'} \left(\psi^\dagger_{k1\sigma}\, \vec\sigma_{\sigma\sigma'}\, \psi_{k'1\sigma'}\right)$$

$$\tilde H^{Kondo}_{scat} \overset{(9.3)}{=} Tr\Big[\underbrace{W^\dagger J W}_{\tilde J}\, \underbrace{W^\dagger \vec s\, W}_{\vec s_1}\Big]\cdot\vec S = J_1\, \vec s_1 \cdot \vec S \qquad (4)$$

J-diagonal Kondo Hamiltonian:
$$H = \sum_{k\gamma\sigma} \varepsilon_k \psi^\dagger_{k\gamma\sigma} \psi_{k\gamma\sigma} + J_1\, \vec s_1 \cdot \vec S \qquad (5)$$

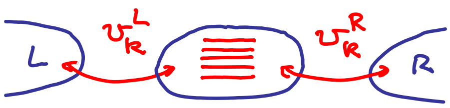
Important conclusion: One mode yields Kondo-Hamiltonian, other mode decouples completely!

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

Then J2 can be nonzero, because $\det J_{\alpha\alpha'} \propto \sum_{jj'} \left(v^L_j v^R_{j'} - v^R_j v^L_{j'} \right)^2 \neq 0$ (6)]

Conductance through (many-level) QD with 2 leads

AM11



lead index: $\alpha = L, R$

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

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

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

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:

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

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

Conductance through 1-level QD with 2 leads

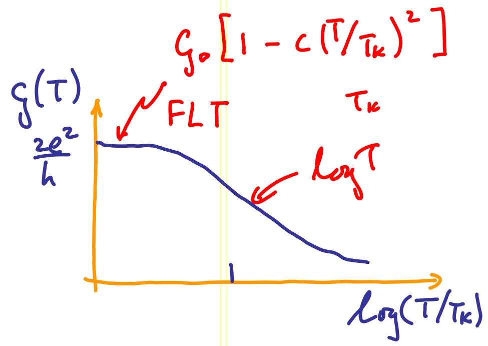
AM12

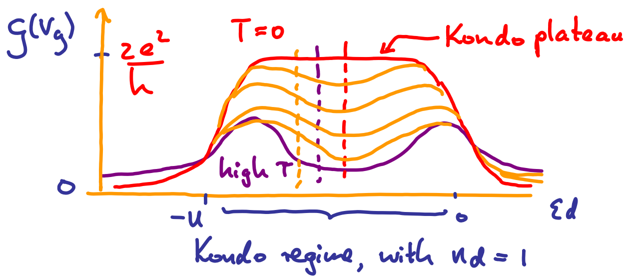
For 1-level AM: $J_2 \overset{(10.2)}{=} 0, \quad \rightarrow \quad \delta_{2\sigma} = 0$ (1)

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

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

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

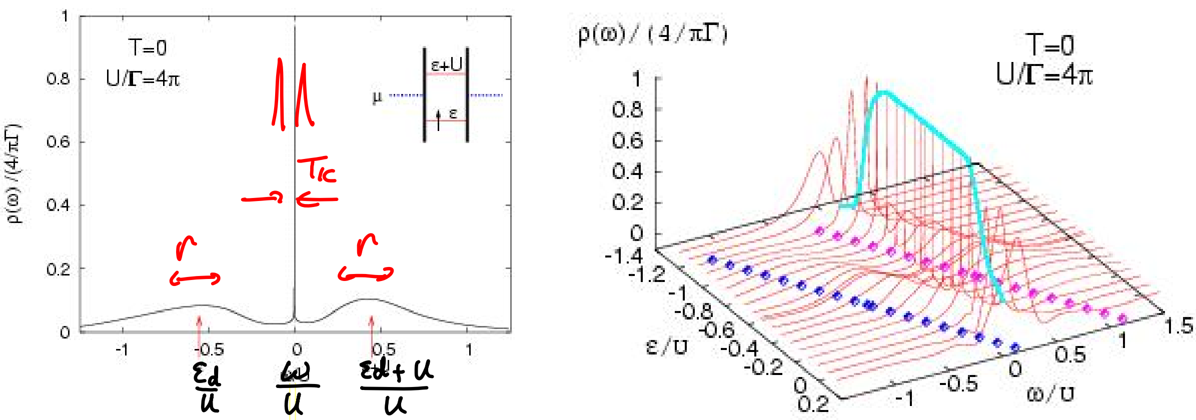




Kondo-Abrikosov-Suhl resonance in local spectral function

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): $A_{d\sigma}(\omega) = -\frac{1}{\pi} \mathrm{Im}\, \mathcal{G}^R_{d\sigma}(\omega) = \nu_{loc}(\omega) = \rho(\omega)$



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