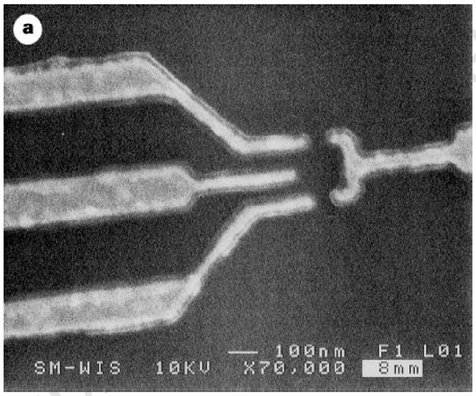
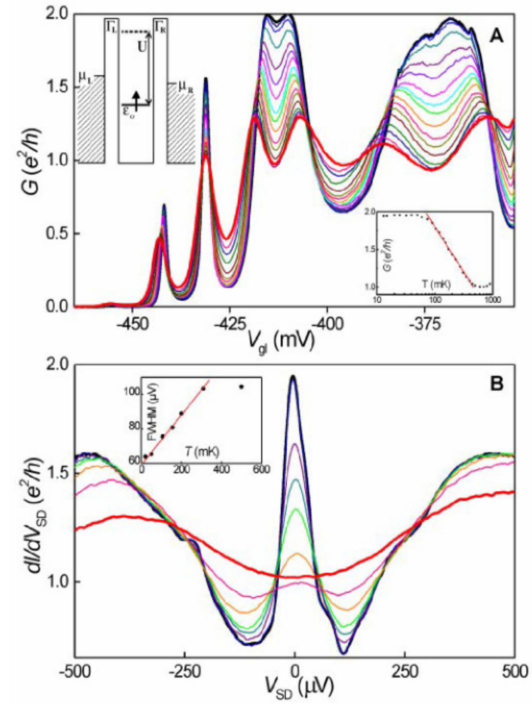
Kondo Effect in Metals and Quantum Dots

(i)



Goldhaber-Gordon et al., Nature **391**, 156 (1998)
Cronenwett et al., Science **281**, 540 (1998)
Simmel et al., PRL **83**, 804 (1999)
van der Wiel et al., Sience 289, 2105 (2000)

... very many subsequent groups ...



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

(ii)

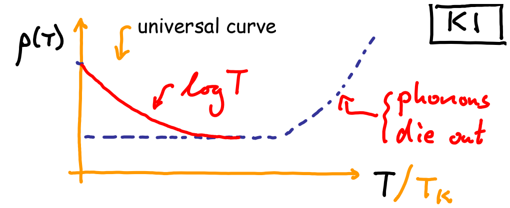
Lecture 1: Kondo effect in metals: Kondo model
- T-matrix in perturbation theory, log(T/D) divergencies
- Anderson's "poor man's scaling", Kondo temperature
- Strong coupling regime, Fermi liquid theory, Friedel sum rule
- Kondo resonance

Lecture 2: Kondo effect in quantum dots: Anderson model
- Experimental Results
- Mapping of Anderson to Kondo model by Schrieffer-Wolff transformation
- Anderson model with two leads

Lecture 3: Numerical Renormalization Group
- General idea: map model to linear chain and diagonalize numerically
- Wilson's iterative RG scheme
- Matrix product states
- Relation to DMRG
- Finite temperature

<u>Lecture 1: Kondo model</u> [Kondo, Phys Rev 1964]

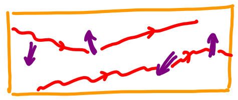
K1



anomalous resistivity minimum in dilute magnetic alloys
(localized spins scatter conduction electrons)

Kondo Model:

$$H_{Kondo} = H_{band} + H_{scat}$$



$$H_{band} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} \qquad (1)$$

$$H_{scat} = J \sum_{kk'\sigma\sigma'\mu\mu'} \underbrace{\left(c^\dagger_{k\sigma} \tfrac{1}{2}\vec{\sigma}_{\sigma\sigma'} c_{k'\sigma'}\right)}_{=:\vec{s}} \cdot \vec{S}_{\mu\mu'} \qquad (2)$$

conduction electron spin

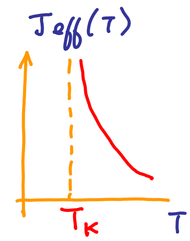
magnetic impurity

Spin-flip scattering:

final state: initial state:

turns out to be enhanced at low temperatures:

$$T \lesssim T_K = D\, e^{-\frac{1}{\nu J}} \qquad (3)$$



T = 0: Fermi liquid theory

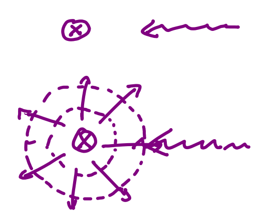
ground state = spin singlet

$$\frac{e^{i(kr-\delta_\sigma)}}{r} \longleftarrow \frac{e^{-ikr}}{r}$$

<u>Scattering states and T-matrix</u>

K2

$$H = H_0 + H_1 \qquad (1)$$



Free state: $H_0 |k\sigma\rangle = \varepsilon_k |k\sigma\rangle$ (2)

Scattering state: $H |\widetilde{k\sigma}\rangle = \varepsilon_k |\widetilde{k\sigma}\rangle$ (3)

Ansatz:

$$|\widetilde{k\sigma}\rangle = |k\sigma\rangle + \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 |\widetilde{k\sigma}\rangle \qquad (4)$$

Check:

$$(\varepsilon_k - H_0 + \cancel{i\eta}^{\,0})|\widetilde{k\sigma}\rangle = \underbrace{(\varepsilon_k - H_0 + \cancel{i\eta}^{\,0})|k\sigma\rangle}_{(2)} + H_1|\widetilde{k\sigma}\rangle \qquad (5)$$

$$(\varepsilon_k - H_0 - H_1)|\widetilde{k\sigma}\rangle \overset{(3)}{=} 0 \quad \checkmark$$

Iterate (4):

$$|\widetilde{k\sigma}\rangle = \left[1 + \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 + \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 + \dots\right]$$

$$= \left[1 + \frac{1}{\varepsilon_k - H_0 + i\eta} \mathcal{T}\right] |k\sigma\rangle \qquad (6)$$

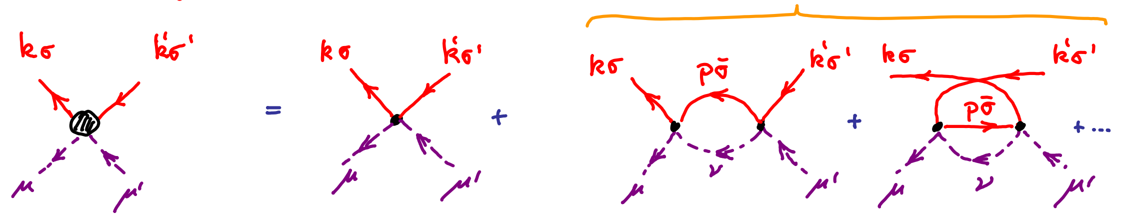
T-matrix:

$$\mathcal{T} = H_1 + H_1 \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 + H_1 \frac{1}{(\ )} H_1 \frac{1}{(\ )} H_1 + \dots \qquad (7)$$

Matrix elements of T

$\langle k\sigma| \otimes \langle \mu| \; \mathcal{T} \; |k'\sigma'\rangle \otimes |\mu'\rangle$ **K3**

pert. exp:
$$\mathcal{T}^{\mu\mu'}_{k\sigma,k'\sigma'} = \mathcal{T}^{(1)} + \underbrace{\mathcal{T}^{(2)}}_{} + \dots \qquad (1)$$



(2)

$$\mathcal{T}^{(1)\,\mu\mu'}_{k\sigma,k'\sigma'} = \tfrac{1}{2} J \, \vec{\sigma}_{\sigma\sigma'} \cdot \vec{S}_{\mu\mu'} \qquad (3)$$

$$\mathcal{T}^{(2)\,\mu\mu'}_{k\sigma,k'\sigma'} = J^2 \sum_{p\bar{\sigma},\nu} \frac{(\tfrac{1}{2}\vec{\sigma}_{\sigma\bar{\sigma}} \cdot \vec{S}_{\mu\nu}) \cdot (\tfrac{1}{2}\vec{\sigma}_{\bar{\sigma}\sigma'} \cdot \vec{S}_{\nu\mu'})}{\varepsilon_k - \varepsilon_p + i\eta} [1 - f(\varepsilon_p)] \qquad (4a)$$

relative minus: final state is $\overbrace{c_k c^\dagger_p}^{1-f(\varepsilon_p)} c_p c^\dagger_{k'} |k\sigma\rangle$

versus $\underbrace{c^\dagger_p c_{k'}}_{f(\varepsilon_p)} c^\dagger_k c_p |k\sigma\rangle$

$c^\dagger_k, \; c_{k'}$ act in opposite order

$$\leftarrow \ominus J^2 \sum_{p\bar{\sigma},\nu} \frac{(\tfrac{1}{2}\vec{\sigma}_{\bar{\sigma}\sigma'} \cdot \vec{S}_{\mu\nu}) \cdot (\tfrac{1}{2}\vec{\sigma}_{\sigma\bar{\sigma}} \cdot \vec{S}_{\nu\mu'})}{\cancel{\varepsilon_k} - (\cancel{\varepsilon_k} + \varepsilon_{k'} - \varepsilon_p) + i\eta} f(\varepsilon_p) \qquad (4b)$$

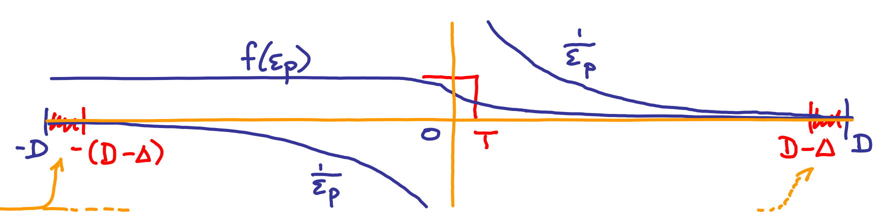
K4

$$\mathcal{T}^{(2)} \overset{(3.6)}{=} J^2 \sum_{\substack{aa'=\\xyz}} (S^a S^{a'})_{\mu\mu'} \left[\nu \int_{-D}^{D} d\varepsilon_p \frac{1}{4} \left\{ (\sigma^a \sigma^{a'})_{\sigma\sigma'} \frac{f(\varepsilon_p) - 1}{\varepsilon_p - \varepsilon_k - i\eta} - (\sigma^{a'}\sigma^a)_{\sigma\sigma'} \frac{f(\varepsilon_p)}{\varepsilon_p - \varepsilon_{k'} + i\eta} \right\} \right] \qquad (1)$$

Consider $\varepsilon_k \simeq \varepsilon_{k'} \simeq \varepsilon_F$: $\quad \frac{1}{4}[\sigma^a, \sigma^{a'}]_{\sigma\sigma'} \, \nu \int_{-D}^{D} d\varepsilon_p \frac{f(\varepsilon_p)}{\varepsilon_p} \propto \int_{-D}^{T} d\varepsilon_p \frac{1}{\varepsilon_p} = \ln\frac{T}{D} \xrightarrow{T\to 0} \infty \qquad (2)$

performing entire integral yields log. divergence

Anderson "poor man's scaling" idea: split off contribution from strips near band edges:



$$\mathcal{T}^{(2)}(D) = \mathcal{T}^{(2)}(D-\Delta) + \delta \mathcal{T}^{(2)} \qquad (3)$$

$$\delta \mathcal{T}^{(2)} = J^2 \sum_{aa'} (S^a S^{a'})_{\mu\mu'} \, \underbrace{\tfrac{1}{4}[\overbrace{\sigma^a, \sigma^{a'}}^{\frac{1}{2} i \varepsilon_{aa'b} \sigma^b}]_{\sigma\sigma'}} \, \nu \underbrace{\left[\int_{D-\Delta}^{D} d\varepsilon_p + \int_{-D}^{-(D-\Delta)} d\varepsilon_p \right] \frac{f(\varepsilon_p)}{\varepsilon_p}} \qquad (4)$$

check algebra yourself! $\boxed{\Sigma}$

$$= J^2 \left(-\tfrac{1}{2} \vec{S}_{\mu\mu'} \cdot \vec{\sigma}_{\sigma\sigma'}\right) \nu\Delta \begin{cases} \frac{0}{D} + \frac{1}{-D} & \text{for } T \ll D \quad (5a) \\ \frac{1/2}{D} + \frac{1/2}{-D} \simeq 0 & \text{for } D \ll T \quad (5b) \end{cases}$$

K5

Integrated-out strips yield term of same form as bare vertex:

$\mathcal{T}^{(1)} \overset{(3.3)}{=} \frac{1}{2} J \, \vec{\sigma}\cdot\vec{S}$

$$\delta\mathcal{T}^{(2)}(J) \overset{(4.5a)}{=} \underbrace{J^2 \frac{\nu\Delta}{D}}_{\delta J} \frac{1}{2}\vec{\sigma}\cdot\vec{S} = \mathcal{T}^{(1)}(\delta J) \quad (1)$$

Scaling of T-matrix under band-width reduction:

$$\mathcal{T}(D,J) \overset{(3.2)}{=} \mathcal{T}^{(1)}(J) + \mathcal{T}^{(2)}(D,J) + \cancel{\mathcal{O}(J^3)} \quad (2)$$

$$\overset{(4.4)}{=} \mathcal{T}^{(1)}(J) + \mathcal{T}^{(2)}(D-\Delta,J) + \delta\mathcal{T}^{(2)}(J) \overset{(1)}{=} \mathcal{T}^{(1)}(\delta J) \quad (3)$$

$$\overset{(1)}{=} \mathcal{T}^{(1)}(J+\delta J) + \mathcal{T}^{(2)}(D+\delta D, J+\delta J) + \cancel{\mathcal{O}(J^3)} \quad (4)$$

$$= \mathcal{T}(D', J') \quad (5)$$

So, reducing bandwidth $D \to D' = D + \delta D$, $\delta D = -\Delta$ (6)

generates increase in coupling constant: $J \to J' = J + \delta J$, $\underbrace{\delta J \nu}_{\delta g} \overset{(1)}{=} -\underbrace{J^2\nu^2}_{g^2} \frac{\delta D}{D}$ (7)

Scaling eq. for dimensionless coupling: $g(D) := \nu J$ $\boxed{\frac{dg}{d(\ln D)} = -g^2}$ (8)

K6

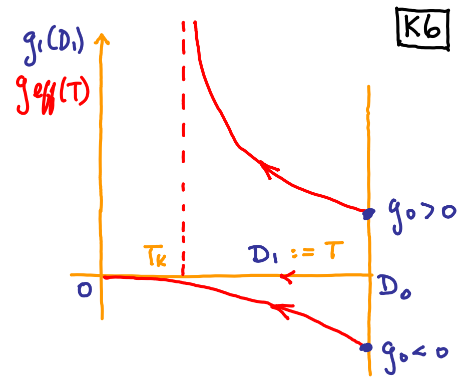
Flow to strong coupling; Kondo temperature

Scaling equation:

$$-\int_{g_0}^{g_1} \frac{dg}{g^2} \overset{(5.8)}{=} \int_{D_0}^{D_1} d(\ln D) \quad (1)$$

$$\frac{1}{g_1} - \frac{1}{g_0} = \ln D_1/D_0 \quad (2)$$

$$g_1(D_1) = \frac{1}{\frac{1}{g_0} - \underbrace{\ln(D_0/D_1)}_{>0,\ \text{grows as } D_1 \to 0}} \quad (3)$$



Reduce bandwidth until $D_1 = T$, [because by (4.5b), renormalization of coupling stops for $D_1 \ll T$]

and use as effective coupling constant at temperature T:

$$g_{eff}(T) = g_1(D_1 = T) = \frac{1}{\frac{1}{g_0} - \ln(D/T)} \overset{(5)}{=} \frac{1}{\ln(T/T_K)} \quad \text{for } T > T_K \quad (4)$$

For $g_0 > 0$, scaling approach eventually breaks down: eff. coupling diverges at a scale T_K:

$$\ln D/T_K := \frac{1}{g_0} \Rightarrow \boxed{T_K = D e^{-\frac{1}{g_0}}} \quad (5)$$

Strong coupling fixed point: Fermi liquid theory

P. Nozières, J. Low Temp. Phys. 17, 31 (1974)

K7

* Scaling approach breaks down for $T \lesssim T_K$. Nevertheless, it allows qualitative conclusion:

$$J \vec{s} \cdot \vec{S} \quad (1)$$

* For T-> 0, "KM flows to strong-coupling fixed point", dominated by

* Local spin binds "one" electron from band into a singlet: (conduction band "screens" local spin to form a singlet)

* Other electrons form ~~Fermi liquid~~, for which singlet acts a (static) potential scatterer, causing only phase shifts:

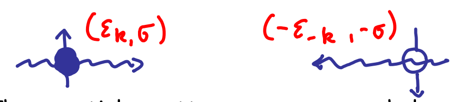
$$\frac{e^{i(kr-\delta_\sigma)}}{r} \longleftarrow \frac{e^{-ikr}}{r} \quad (2)$$

standard relation between S and T

S- [or T-] matrix: $$e^{2i\delta_\sigma(\varepsilon_k)} = S_\sigma(\varepsilon_k) \quad \left[=: 1 - i2\pi\nu\, T_\sigma(\varepsilon_k) \right] \quad (3)$$

Choose: $|\delta_\sigma| \le \pi/2$

KM is invariant under particle-hole symmetry: $$c_{k\sigma} \to \sigma c^\dagger_{-k-\sigma} \quad (4)$$



Thus, particle scatteres same way as hole

This relates phase shifts for spin up and down: $$e^{i2\delta_\sigma(\varepsilon_k)} = S_\sigma(\varepsilon_k) \overset{(4)}{=} S^\dagger_{-\sigma}(-\varepsilon_{-k}) = e^{-i2\delta_{-\sigma}(-\varepsilon_{-k})} \quad (5)$$

At Fermi level: $\varepsilon_k = 0$ $$\boxed{\delta_\uparrow(0) = -\delta_\downarrow(0)} = ? \quad (6)$$

Friedel sum rule:

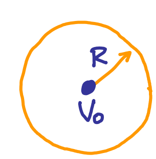
Friedel, Can. J. Phys. 34, 1190 (1956)

K8

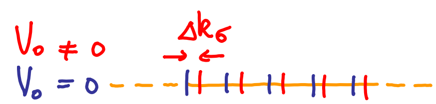
$$\boxed{\frac{1}{\pi}\delta_\sigma(0) = \Delta n_\sigma} = \text{charge displaced by local potential scatterer} \quad (1)$$

Derivation:

Use radial box, radius R, radial wavefunctions $j_\ell(kr)$: $$0 = j_{\ell=0}\left(kR - \delta_\sigma(\varepsilon_k)\right) = \frac{\sin(kR - \delta_\sigma(\varepsilon_k))}{kR} \quad (2)$$



to quantize momenta of radial waves: $$k_n = \frac{\pi n}{R} + \underbrace{\frac{\delta_\sigma(\varepsilon_k)}{R}}_{=:\Delta k_\sigma} \quad (3)$$



Radial momentum sums: $\xi_k = \frac{k^2}{2m} = \varepsilon_F + \varepsilon_k$

$$\sum_k \simeq R\int\frac{dk}{\pi} = \int d\varepsilon_k \underbrace{\frac{R}{\pi}\frac{\partial}{\partial\varepsilon_k}}_{\nu(\varepsilon_k)}\left(k + \Delta k_\sigma\right) \quad (4)$$
$$\nu(\varepsilon_k) + \Delta\nu_\sigma(\varepsilon_k)$$

Potential scatterer $\delta_\sigma(\varepsilon_k)$, $$\Delta k_\sigma \overset{(3)}{=} \frac{\delta_\sigma(\varepsilon_k)}{R}, \qquad \Delta\nu_\sigma(\varepsilon_k) \overset{(4)}{=} \frac{1}{\pi}\frac{\partial\delta_\sigma(\varepsilon_k)}{\partial\varepsilon_k} \quad (5)$$

Change in charge of cond. electrons around impurity ("screening charge"): $$\Delta n_\sigma \overset{(T=0)}{=} \int_{-D}^{0} d\varepsilon_k\, \Delta\nu_\sigma(\varepsilon_k) \overset{(5)}{=} \frac{1}{\pi}\left[\delta_\sigma(0) - \delta_\sigma(-D)\right] = (1) \quad (6)$$

$= 0$ if $|D| \gg V_0$

for Kondo problem, scattering near band edge is weak, $\simeq 0$ see (6.3)

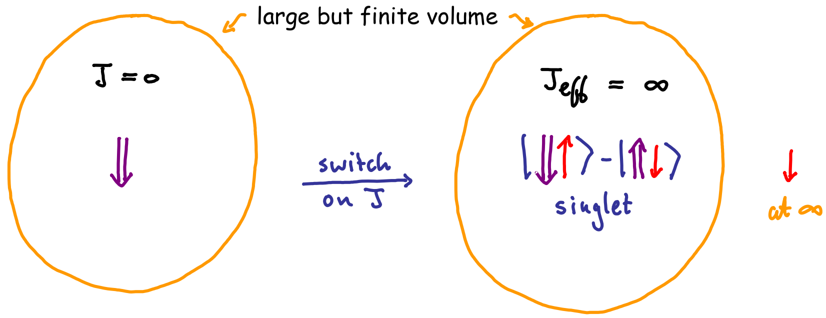
□

Screening of local spin to form singlet:

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

K9

Consider how charge inside a large but finite volume changes when J is switched on:



total spin inside volume: $S_{z,tot} = -\frac{1}{2}$ $\qquad$ $S_{z,tot} = 0$ (1)

conduction band is initially unpolarized: $n_\uparrow - n_\downarrow = 0$ $\qquad$ change in cond. band charge inside volume to achieve screening: $\Delta n_\uparrow - \Delta n_\downarrow = 1$ (2)

$$\downarrow (8.6)$$

$$\frac{1}{\pi}\left[\delta_\uparrow(0) - \delta_\downarrow(0)\right] = 1 \quad (3)$$

Phase shifts at Fermi energy:

$$\boxed{\delta_\uparrow(0) \overset{(7.6)}{=} -\delta_\downarrow(0) \overset{(3)}{=} \frac{\pi}{2}}$$

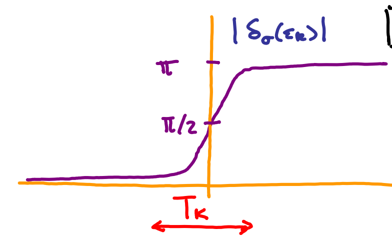
maximal possible value (4)

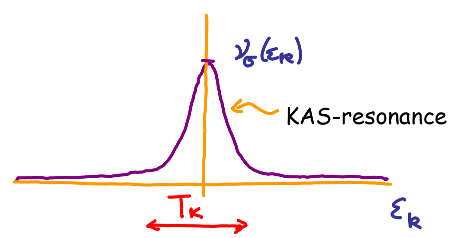
Kondo-Abrikosov-Suhl resonance in density of states

K10

* $g_{eff}(D')$ becomes large only for $D' \lesssim T_K$

* phase shifts change on scale of T_K





* similarly for DOS: $\Delta\nu_\sigma(\varepsilon) \overset{(8.5)}{=} \frac{1}{\pi}\frac{\partial\delta_\sigma(\varepsilon_k)}{\partial\varepsilon_k}$

This resonance also arises in:

- T-matrix
- electron scattering rate (causing resistivity anomaly)
- in dynamical correlation function of composite operator F:

Costi, Phys. Rev. Lett. 85, 1504 (2000)

$$F_\sigma := \sum_{k\sigma'} \vec{S}\cdot\vec{\sigma}_{\sigma\sigma'}\, c_{k\sigma} \quad (1)$$

$$-\frac{\mathrm{Im}\,T(\omega)}{\pi\ \sigma\sigma} = A_{\sigma\sigma}(\omega) := \mathrm{Im}\int_0^\infty \frac{dt}{\pi} e^{-i\omega t}(-i)\langle\{F_\sigma(t), F_\sigma^\dagger(0)\}\rangle \quad (2)$$