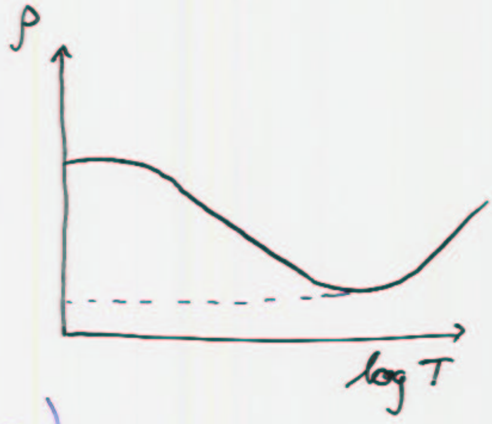
Kondo Model: scattering rate, scaling, phase shifts

$$H = H_0 + H_1$$

$$H_0 = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} \qquad (1)$$

$$H_1 = \sum_{\substack{kk' \\ \sigma\sigma'}} \left(c^\dagger_{k\sigma} \tfrac{1}{2} \vec{\sigma}_{\sigma\sigma'} c_{k'\sigma'} \right) \cdot \vec{S}$$

- Historically, KM was used to explain anomalous resistivity minimum in magnetic alloys (localized spins scatter conduction electrons)



$\boxed{\text{We have to understand scattering problem including spin-flips}}$

KMZ

Scattering states and T-matrix

Consider $\quad H = H_0 + H_1$

Free state: $\quad H_0 |k\sigma\rangle = \varepsilon_k |k\sigma\rangle$

Scattering state: $\quad H |\widetilde{k\sigma}\rangle = \varepsilon_k |\widetilde{k\sigma}\rangle \qquad (2)$

(same eigenvalue as free state)

Ansatz: $$|\widetilde{k\sigma}\rangle = |k\sigma\rangle + \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 |\widetilde{k\sigma}\rangle \qquad (3)$$

Check: $(\varepsilon_k - H_0 + i\eta)|\widetilde{k\sigma}\rangle = (\cancel{\varepsilon_k - H_0} + i\eta)|k\sigma\rangle + H_1 |\widetilde{k\sigma}\rangle$

$i\eta \to 0 \qquad (\varepsilon_k - (H_0 + H_1))|\widetilde{k\sigma}\rangle = 0 \quad \checkmark.$

Iterate (3): $$|\widetilde{k\sigma}\rangle = \left[1 + \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 + \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 + \dots\right] |k\sigma\rangle$$

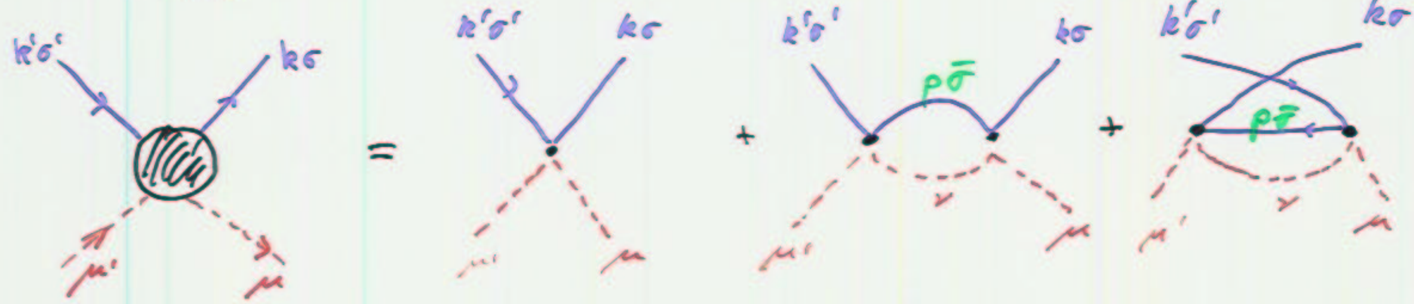
$$= \left[1 + \frac{1}{\varepsilon_k - H_0 + i\eta} T\right] |k\sigma\rangle$$

T-matrix: $$T \equiv H_1 + H_1 \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 + H_1 \frac{1}{(\;)} H_1 \frac{1}{(\;)} H_1 + \dots \qquad (4)$$

Matrix elements of T: $\langle k\sigma| \otimes \langle\mu|\, T\, |k'\sigma'\rangle \otimes |\mu'\rangle$

pert. expansion:

$$T^{\mu\mu'}_{k\sigma,k'\sigma'} = T^{(1)} + T^{(2)} + \dots$$



$$T^{(1)\,\mu\mu'}_{k\sigma,k'\sigma'} = J\ \tfrac{1}{2}\vec{\sigma}_{\sigma\sigma'} \cdot \vec{S}_{\mu\mu'} \qquad (5)$$

$$T^{(2)} \overset{(4)}{=} J^2 \sum_p \frac{\left(\frac{1}{2}\vec{\sigma}_{\sigma\bar{\sigma}} \cdot \vec{S}_{\mu\nu}\right)\left(\frac{1}{2}\vec{\sigma}_{\bar{\sigma}\sigma'} \cdot \vec{S}_{\nu\mu'}\right)}{\varepsilon_k - \varepsilon_p + i\eta}\left[1 - f(\varepsilon_p)\right]$$

$$- J^2 \sum_p \frac{\left(\frac{1}{2}\vec{\sigma}_{\bar{\sigma}\sigma'} \cdot \vec{S}_{\mu\nu}\right)\left(\frac{1}{2}\vec{\sigma}_{\sigma\bar{\sigma}} \cdot \vec{S}_{\nu\mu'}\right)}{\varepsilon_k - (\varepsilon_{k'} + \varepsilon_k - \varepsilon_p) + i\eta}\, f(\varepsilon_p) \qquad (6)$$

relative minus: final state is $c_k^\dagger \overbrace{c_p\, c_p^\dagger}^{1 - f(\varepsilon_p)} c_{k'} |k'\rangle$

versus $\underbrace{c_p^\dagger\, c_{k'}\, c_k^\dagger\, c_p}_{f(\varepsilon_p)} |k'\rangle$

so, $c_k^\dagger$ and $c_{k'}$ act in opposite order

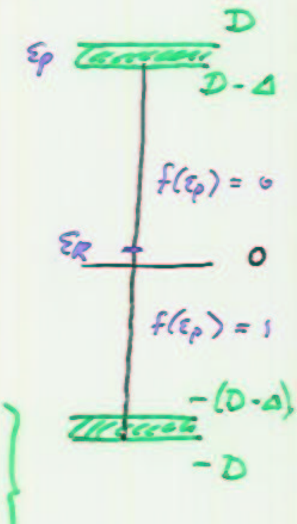
(6): $T^{(2)} = J^2 \sum_{\substack{aa'= \\ x,y,z}} \left(S^a S^{a'}\right)_{\mu\mu'}$ (7a)

$$\times\, \nu \int_{-D}^{D} d\varepsilon_p \;\; \frac{1}{4} \left\{ \left(\sigma^a \sigma^{a'}\right)_{\sigma\sigma'} \frac{f(\varepsilon_p) - 1}{\varepsilon_p - \varepsilon_k - i\eta} - \left(\sigma^{a'} \sigma^{a}\right)_{\sigma\sigma'} \frac{f(\varepsilon_p)}{\varepsilon_p - \varepsilon_k + i\eta} \right\}$$ (7b)

performing entire integral yields divergence! for $T \to 0$

e.g., for $\varepsilon_k = 0$:

$$\frac{1}{4} \left[\sigma^a, \sigma^{a'}\right]_{\sigma\sigma'} \; \nu \underbrace{\int_{-D}^{D} d\varepsilon_p \; \frac{f(\varepsilon_p)}{\varepsilon_p}} \to \simeq \int_{-D}^{T} d\varepsilon_p \; \frac{1}{\varepsilon_p} = \ln T/D \xrightarrow{T \to 0} \infty$$



Anderson (1970): write $T^{(2)}(D) = T^{(2)}_{(D-\Delta)} + \delta T^{(2)}$

where $\delta T^{(2)}$ gives contribution of band edges;

$$\nu \left(\int_{D-\Delta}^{D} d\varepsilon_p + \int_{-D}^{-(D-\Delta)} d\varepsilon_p \right] \frac{1}{\varepsilon_p - \varepsilon_k} \left\{ \begin{matrix} f(\varepsilon_p) - 1 \\ + f(\varepsilon_p) \end{matrix} \right]$$

$$= \nu\Delta \left\{ \begin{matrix} -\frac{1}{D} & + & \frac{0}{D} \\ -\frac{0}{D} & + & -\frac{1}{D} \end{matrix} \right\} = - \frac{\nu\Delta}{D} \left\{ \begin{matrix} 1 \\ +1 \end{matrix} \right\}$$ (8)

- at $D \simeq T$ the two contributions begin to cancel: $\frac{\nu\Delta}{D}\left(-1/2 + 1/2\right)$

so, stop rescaling when $D \simeq T$

Integrated-out strips yield:

$$\delta T^{(2)} = J^2 \left(\frac{-\nu\Delta}{D}\right) \frac{1}{4} \sum_{aa'} \left(S^a S^{a'}\right)_{\mu\mu'} \left[\sigma^a, \sigma^{a'}\right]_{\sigma\sigma'}$$

$$\sum_{aa'} \frac{1}{2}\left(S^a S^{a'} - S^{a'} S^a\right) 2i\varepsilon^{aa'b}\sigma^b$$

$$\underbrace{\sum_{aa'} i\varepsilon^{aa'c} S^c \, i\varepsilon^{aa'b}}_{2\delta^{cb}} \sigma^b = -2\, \vec{S}_{\mu\mu'} \cdot \vec{\sigma}_{\sigma\sigma'}$$

$$\delta T^{(2)} = \underbrace{J^2 \left(\frac{\nu\Delta}{D}\right)}_{\delta J} \frac{1}{2}\, \vec{\sigma}\cdot\vec{S} = T^{(1)}(\delta J) \qquad (9)$$

so, reducing bandwidth $D \to D' = D - \Delta = D + \delta D$

generates a change in $J \to J' = J + \delta J$ (10)

$$\begin{aligned} T(D,J) &= T^{(1)}(J) + T^{(2)}(D,J) \\ &= T^{(1)}(J) + T^{(2)}(D-\Delta, J) + T^{(2)}(J) \\ &= T^{(1)}(J+\delta J) + T^{(2)}(D-\Delta, J+\delta J) + O(J^3) \\ &= T(D', J') \qquad (11) \end{aligned}$$

$\boxed{\text{Repeating this process generates "flowing" coupling constant } J(D)}$

Flowing coupling, Kondo temperature

(9): $$\delta J\nu = J^2 \frac{\nu^2 \Delta}{D} = -J^2 \nu^2 \frac{\delta D}{D} \qquad (12)$$

dimensionless coupling: $g \equiv \nu J$

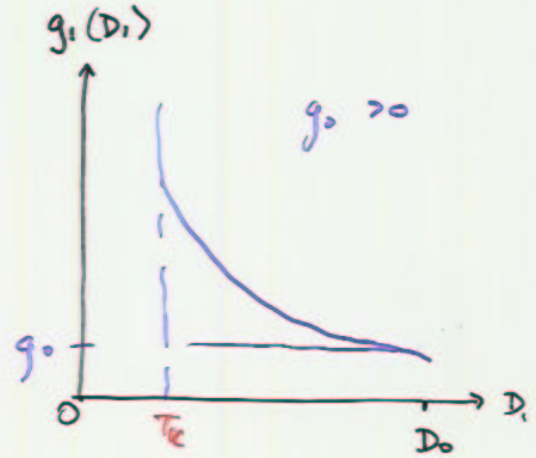
scaling equation: $$-\frac{\delta(g)}{\delta(D/D)} = \boxed{+g^2(D) = -\frac{\partial g(D)}{\partial \ln D}} \qquad (13)$$

integrate:

$$-\int_{g_0}^{g_1} dg \frac{1}{g^2} \overset{(13)}{=} \int_{D_0}^{D_1} \frac{dD}{D}$$

$$\frac{1}{g_1} - \frac{1}{g_0} = \ln D_1/D_0$$

$$\boxed{g_1(D_1) = \frac{1}{\frac{1}{g_0} + \ln D_1/D_0}} \qquad (14)$$



- As D_1/D_0 decreases, $g_1 \begin{cases} \text{increases} & \text{if } g_0 > 0 \\ \text{decreases} & \text{if } g_0 < 0 \end{cases}$
- reduce bandwidth until $D_1 \simeq T$, and use

$$\boxed{g_{eff} \overset{(14)}{=} g_1(D_1 = T) = \frac{g_0}{1 + g_0 \ln T/D}}$$

as effective coupling const. at temp. T

Problem: $g_{eff} \to \infty$ when T approaches the scale T_K:
for $g_0 > 0$

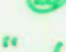
$$\ln T_K/D = -1/g_0 = -\frac{1}{\nu J}$$

$$\boxed{T_K = D e^{-1/g_0} = D e^{-\frac{1}{J\nu}}} \qquad (15)$$

Flow to strong coupling

- As T is lowered, $g_{eff}(T)$ grows
- "KM flows to a strong-coupling regime"

  where $J\vec{s}\cdot\vec{S}$ term dominates everything else
- local spin binds "one" electron from band into a

  singlet: $\uparrow\downarrow$ =  "static scatterer"

  $S_{Tot}=0$

- scattering of other electrons off this object can be described by

  phase shifts: δ_σ, and $\mathcal{S}$-matrix:

  standard relation between $\mathcal{S}$ and T

$$\mathcal{S}_\sigma(\varepsilon_k) = e^{2i\delta_\sigma(\varepsilon_k)} \quad \left[= 1 - i2\pi\nu\, T_\sigma(\varepsilon_k) \right] \tag{16}$$

- Kondo model is invariant under particle-hole symmetry

$$c_{k\sigma} \to \sigma\, c^{+}_{-k-\sigma}$$

$\Rightarrow$ particle (ε_k,σ) scatters same way as hole $(-\varepsilon_k,-\sigma)$

$$\Rightarrow \quad \mathcal{S}_\sigma(\varepsilon) = \mathcal{S}^{+}_{-\sigma}(-\varepsilon)$$

at Fermi level: $\varepsilon=0$ $\Rightarrow$ $\delta_\uparrow(0) = -\delta_\downarrow(0)$ (17)

Friedel sum rule : $\frac{1}{\pi}\delta_\sigma(0) = \Delta n_\sigma$

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

Phase shift $\delta_\sigma(\varepsilon)$ is related to change in DOS. Why?

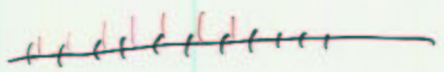
- In a radial box, radius R, momenta of radial waves $j_\ell(kr)$ are quantized :

$$0 = j_\ell(kR) = \frac{\sin(kR - \frac{\pi}{2}\ell)}{kR} \Rightarrow \boxed{k_n = \frac{\pi n}{R}}$$

for $\ell = 0$

- radial momentum sums :

$$\sum_k \simeq R\int_0^\infty \frac{dk}{\pi} = \int_0^\infty d\varepsilon \underbrace{\frac{R}{\pi}\frac{\partial k}{\partial \varepsilon}}_{\nu(\varepsilon)} \Rightarrow \boxed{\nu_\sigma(\varepsilon_k) = \frac{R}{\pi}\frac{\partial k_\sigma}{\partial \varepsilon_k}} \quad (18)$$



$\delta = 0$

$\delta \neq 0$

- a scattering center causes phase shift : $j_\ell(kr - \delta_\sigma(\varepsilon_k))$

$\Rightarrow$ new quantization condition : $$k_n = \frac{\pi n + \delta_\sigma(k)}{R} \quad (19)$$

$\Rightarrow$ DOS changes by

$$\Delta\nu_\sigma(\varepsilon_k) = \frac{R}{\pi}\frac{\partial\, \delta_\sigma(k)/R}{\partial \varepsilon_k} = \frac{1}{\pi}\frac{\partial\, \delta_\sigma(\varepsilon_k)}{\partial \varepsilon_k} \quad (20)$$

$\Rightarrow$ charge of conduction electrons around impurity changes by

$$\Delta n_\sigma = \int_{-D}^{0} d\varepsilon_k\, \Delta\nu_\sigma(\varepsilon_k) = \frac{1}{\pi}\delta_\sigma(0) - \underbrace{\delta_\sigma(-D)}_{=0} \quad (21)$$

Screening of local spin to form singlet:

To screen single localized spin, we need cond. electron spin imbalance of

cond. for perfect screening

$$1 = |\Delta n_\uparrow - \Delta n_\downarrow| \overset{(21)}{=} \frac{1}{\pi}|\delta_\uparrow(0) - \delta_\downarrow(0)| = \frac{2}{\pi}|\delta_\uparrow|$$

$$\Rightarrow \quad \boxed{\delta_\uparrow(0) = -\delta_\downarrow(0) = \pi/2} \qquad (22)$$

phase shifts have maximum possible values! [Nozières, 1974]

Alternative argument: singlet requires

$$\frac{1}{2} = |\Delta n_\sigma| = \frac{1}{\pi}|\delta_\sigma|$$

$$\Rightarrow \quad \boxed{|\delta_\sigma(0)| = \pi/2} \qquad (23)$$

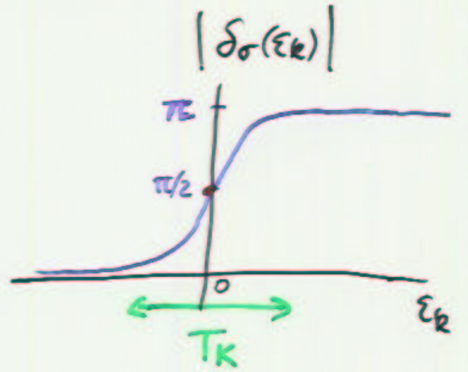
[this is result need in AM-lecture, eq. (27), to explain Kondo plateaux]

Kondo resonance for AM

- $g_1(D_1)$ becomes large only for $D_1 \lesssim T_K$

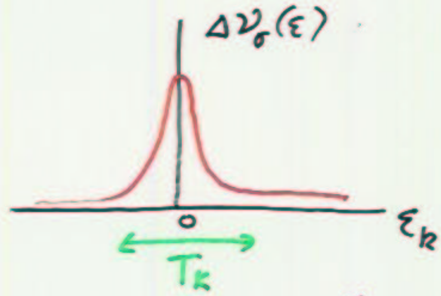
$\Rightarrow$ phase shifts change

on energy scale of T_K

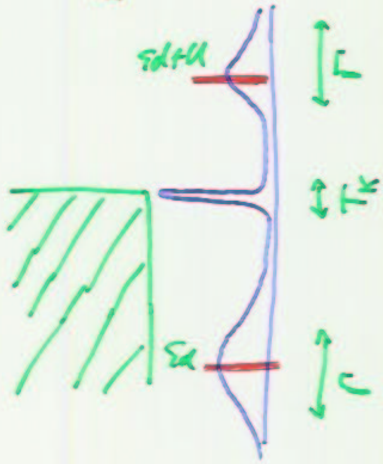


- similarly for DOS:

$$\Delta\nu_\sigma(\varepsilon_k) = \frac{1}{\pi}\frac{\partial\delta_\sigma}{\partial\varepsilon_k}$$



For AM, the local DOS of d-level develops Kondo resonance when $T \lesssim T_K$, which is observed directly in source-drain voltage dependence of $G(V_{SD})$.



Kondo temp. of AM:

$$T_K \overset{(15)}{=} D\,e^{-\frac{1}{\nu J}}, \quad \nu J \overset{(AM11)}{=} \frac{\nu V_{k_F}^2\, U}{|\varepsilon_d|\,|\varepsilon_d+U|}, \quad \underbrace{\nu V_{k_F}^2}_{=\Gamma/\pi}$$

$$= D\exp\left\{-\pi\frac{|\varepsilon_d|\,|\varepsilon_d+U|}{\Gamma U}\right\} \quad (24)$$

[agrees with Bethe Ansatz except for prefactor