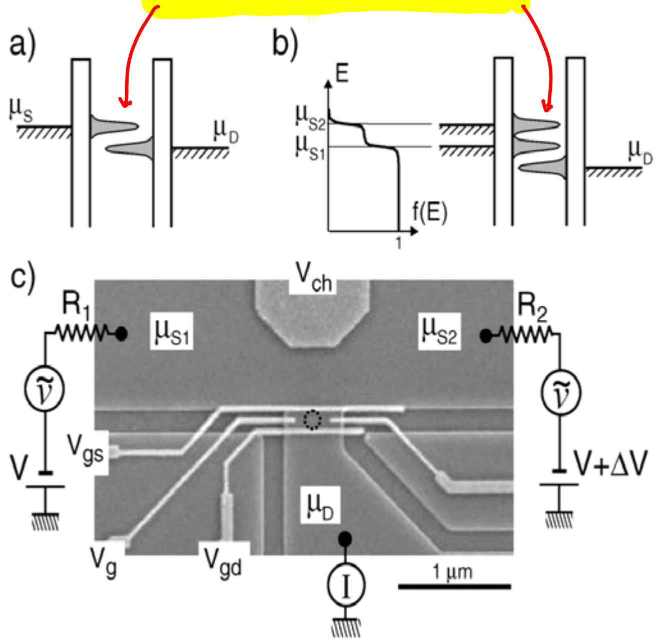
Lecture 3: Flow Equation Renormalization Group

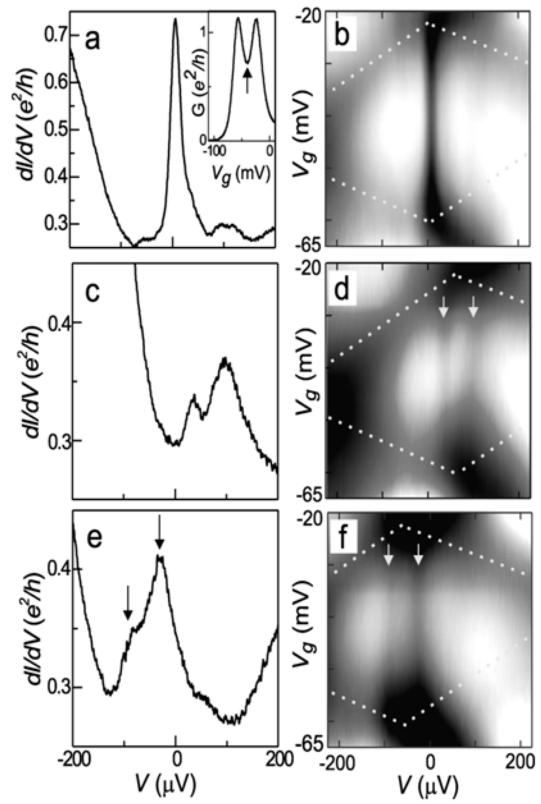
Jan von Delft

FE1

Motivation: Nonequilibrium transport through quantum dots

Kondo resonance splits!

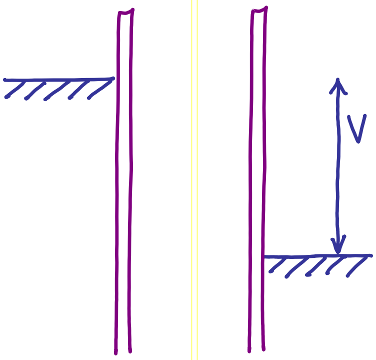




De Franceschi et al., PRL, 89, 156801 (2002)

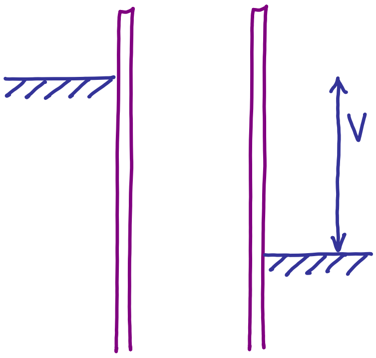
Fundamental limitation of bandwidth reduction scheme

FE2

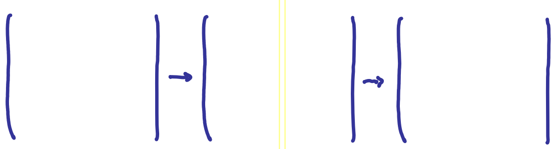


elastic prosseses

possible



$H(0) =$



$H(\lambda) =$

Problem: bandwidth reduction eliminates transport window once

Cure: band-diagonal bandwidth reduction would maintain states in transport window throughout RG-procedure!

Flow Equation Renormalization Group

FE3

Due to: Wegner, Ann. Phys. (Leipzig), 3, 77 (1994), Glazek, Wilson, Phys. Rev. D, 48, 5863 (1993)
Reviewed in: Kehrein, "The Flow Equation Approach to Many-Particle Systems"

Idea: diagonalize H by sequence of infinitesimal unitary transformations:

[RG generalization of Schrieffer-Wolff idea] $H(B) = \mathcal{U}(B)\, H(0)\, \mathcal{U}^\dagger(B)$, $\mathcal{U}^\dagger = \mathcal{U}^{-1}$ (1)

Starting point: $U(0) =$ Goal: $H(\infty) =$

Consider: $\frac{\partial H}{\partial B} = \partial_B H = (\partial_B U) \quad H(0)\, U^{-1} + U\, H(0) \quad \partial_B U^{-1}$ (2)

$\partial_B (U U^{-1})$ (*) where $\eta(B) := (\partial_B U)\, U^{-1} \overset{(*)}{=}$ (3)

"Flow Equation" for Hamiltonian: $\partial_B H(B) \overset{(2)}{=} [\eta(B), H(B)]$ reminiscent of Heisenberg eq. of motion for t-dependence (4)

[solving (4) generates 1-parameter family of unitarily equivalent Hamiltonians H(B)]

Equivalent representation: $U(B) = T_B\, e^{\int_0^B dB' \eta(B')}$, (5)

Canonical choice for η:

FE4

Suppose: $H(B) = H_0(B) + H_{int}(B)$ (1)

Wegner showed that off-diagonal part H1 flows to zero, if we choose

"canonical generator": $\eta(B) := [H_0(B), H_{int}(B)]$ (2)

Theorem: if $Tr[H_0(B)\, H_{int}(B)] = 0$ and $Tr[\partial_B H_0(B)\, H_{int}(B)] = 0$ (3)

(these conditions are satisfied if Ho changes no quantum numbers, and each term in Hint changes at least one)

then off-diagonal terms decrease under flow: $\boxed{Tr[H^2_{int}(B)]}$ (4)

Interpretation of B: Dimensions: $[\eta] \overset{(2)}{=}$ (5)

$[B] \overset{(5)}{=} (\text{energy})^{-2}$ (6)

Limits: $B = \{ \quad \Leftrightarrow \quad \Lambda = \{$ (7)

B acts like $(\text{inverse})^2$ of ultraviolet cutoff (similar, but not identical to D) (8)

Matrix example

$$H(0) = \{h_{ij}\} = \begin{pmatrix} \varepsilon_1 & & H_{int} \\ & \varepsilon_2 & \\ & \ddots & \\ H_{int} & & \varepsilon_n \end{pmatrix} \quad (1)$$

$\boxed{\text{FE5}}$

Diagonal part: $H_0(B)_{ij} = \quad (2)$

Off-diagonal part: $(i \neq j)$ $H_{int}(B)_{ij} = H_{int}(B)_{ji} \quad (3)$

Canonical generator:

$\eta \overset{(4.2)}{=} [H_0, H_{int}]$ $\quad \eta_{ij}(B) = \varepsilon_i h_{ij} - h_{ij}\varepsilon_j = \quad$ (energy difference x off-diag. matrix $\forall\, i \neq j$) $\quad (4)$

Flow eq. (3.4) needs:

$(\partial_B H)_{ij} = [\eta, H]_{ij} \quad (5)$

similar to (4)

$$[\eta, H_0]_{ij} = -(\varepsilon_i - \varepsilon_j)\eta_{ij} \overset{(4)}{=} \quad (6)$$

$$[\eta, H_i]_{ij} = \sum_k [\eta_{ik} h_{kj} - h_{ik}\eta_{kj}] \overset{(4)}{=} \sum_{k \neq i,j} (\qquad) h_{ik} h_{kj} \quad (7)$$

Compare coefficients:

$i = j$: $\quad \partial_B \varepsilon_j(B) = \overset{(6)}{} \qquad \overset{(7)}{} \quad (8a)$

$i \neq j$: $\quad \partial_B h_{ij}(B) = -(\varepsilon_i - \varepsilon_j)^2 h_{ij} + \sum_{k \neq i,j} (\qquad) h_{ik} h_{kj} \quad (8b)$

So far, exact. [Solving (5.8a+b) numerically yiels correct $H(\infty) = H_{diag}$ $\quad\boxed{\text{FE6}}$

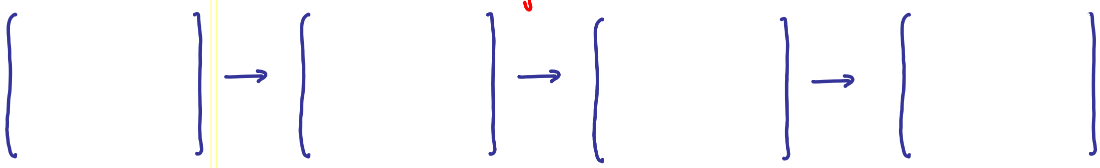
To get feeling for flow, suppose h_{ij} is "small", linearize (5.8) in h_{ij}, i.e. drop last term on RHS:

(5.8b) $$\partial_B h_{ij}(B) = -(\varepsilon_i - \varepsilon_j)^2 h_{ij} + \mathcal{O}(h_{ij}^2) \quad (1)$$

Solution: $$h_{ij}(B) = e^{-B[\varepsilon_i(0) - \varepsilon_j(0)]^2} h_{ij}(0) \quad (2)$$

So, off-diagonal elements $\langle i | H_{int} | j \rangle$ die as

Those with largest energy difference $\varepsilon_i(0) - \varepsilon_j(0)$ die fastest! "Energy scale separation"



(3)

Energy shifts:
(2) into (5.8a) $$\partial_B \varepsilon_j(B) = 2\sum_{k \neq j} [\varepsilon_j(0) - \varepsilon_k(0)]\, h_{jk}^2 + \mathcal{O}(h^3) \quad (4)$$

Integrate: $\int_0^\infty dB$ (4) $$\varepsilon_j(\infty) - \varepsilon_j(0) = \int_0^\infty dB\, \partial_B \varepsilon_j(B) \overset{(4)}{=} \quad (5)$$

2nd. order pert. theory

FERG for 1-lead Kondo Model

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

FE7

S. Kehrein, book, and
PRL. 95, 056602 (2005)

$$H_0 = \sum_{k\sigma} \varepsilon_{k\sigma} :c^\dagger_{k\sigma} c_{k\sigma}: \qquad (2)$$

$$J_{kk'}(0) = \qquad H_1(B) = \sum_{kk'} \Big[\underbrace{\vec{s}_{kk'}}_{\frac{1}{2}\sum_{\sigma\sigma'} :c^\dagger_{k\sigma} \vec{\sigma}_{\sigma\sigma'} c_{k'\sigma'}:} \cdot \vec{S} + \underbrace{\hat{U}_{kk'}}_{:c^\dagger_{k\sigma} c_{k'\sigma}:} \Big] \qquad (3)$$

potential scattering, neglected henceforth,
since it does not scale to strong coupling

Normal ordering: (need to properly include contributions with finite expectation values)

$$:c^\dagger_{k\sigma} c_{k'\sigma'}: = c^\dagger_{k\sigma} c_{k'\sigma'} \qquad f_k = \left[e^{\beta(\varepsilon_k - \mu)} + 1\right]^{-1} \qquad (4)$$

[T- and V-dependence enters <u>here</u>]

$$\begin{aligned} :c^\dagger_{k\sigma} c_{k'\sigma'} c^\dagger_{\bar{k}\bar{\sigma}} c_{\bar{k}'\bar{\sigma}'}: &= :c^\dagger_{k\sigma} c_{k'\sigma'}: \, :c^\dagger_{\bar{k}\bar{\sigma}} c_{\bar{k}'\bar{\sigma}'}: \\ &+ :c^\dagger_{k\sigma} c_{\bar{k}'\bar{\sigma}'}: \, \delta_{k'\bar{k}} \delta_{\sigma'\bar{\sigma}} (1 - f_{k'}) \\ &- :c^\dagger_{\bar{k}\bar{\sigma}} c_{k'\sigma'}: \, \delta_{k\bar{k}'} \delta_{\sigma\bar{\sigma}'} f_k \\ &+ \delta_{k'\bar{k}} \delta_{\sigma'\bar{\sigma}} \, \delta_{k\bar{k}'} \delta_{\sigma\sigma'} (1 - f_{k'}) f_k \end{aligned} \qquad (5)$$

Canonical generator:

$$\eta(B) = [H_0, H_1(B)] \qquad \eta(B) = \sum_{kk'} \quad \vec{s}_{kk'} \cdot \vec{S} + \text{pot. scat.} \qquad (1)$$

FE8

with [compare (5.4)] $\qquad \eta^J_{kk'} = \qquad (2)$

Commutators on RHS of flow eq. $\partial_B H = [\eta, H]$ can be quite complicated, e.g.

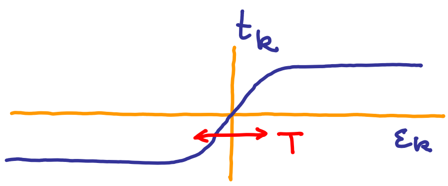
$$[\vec{s}_{kk'} \cdot \vec{S}, \vec{s}_{\bar{k}\bar{k}'} \cdot \vec{S}] = -\tfrac{1}{2} (\vec{s}_{k\bar{k}'} \cdot \vec{S}) \delta_{k'\bar{k}} t_{k'} + \tfrac{1}{2} (\vec{s}_{\bar{k}k'} \cdot \vec{S}) \delta_{k\bar{k}'} t_k \qquad (3a)$$

reminiscent of 2nd order term inpoor man's scaling

$$+ \tfrac{i}{4} :(\vec{s}_{kk'} \times \vec{s}_{\bar{k}\bar{k}'}): \vec{S} + \text{pot. scat.} \qquad (3b)$$

neglect this term for now, it
enters flow eq. only in order $\mathcal{O}(J^3)$

where $\qquad t_k = 1 - 2 f_k = \tanh \frac{\varepsilon_k}{2T} \qquad (4)$



Comparing coeff. of $(\vec{\Delta}_{kk'}\cdot\vec{S})$ and $\hat{v}_{kk'}$ on LHS and RHS of FE (3.4) yields

FE9

$[J_{\varepsilon\varepsilon'} \equiv \quad]$

$$\partial_B J_{\varepsilon\varepsilon'} = -(\varepsilon-\varepsilon')^2 J_{\varepsilon\varepsilon'} - \tfrac{1}{2}\sum_x t_x(\varepsilon+\varepsilon'-2x) J_{\varepsilon x} J_{x\varepsilon'} \qquad (1)$$

+ pot. scat.

Simplify (1) via Ansatz:
[inspired by (6.2)]

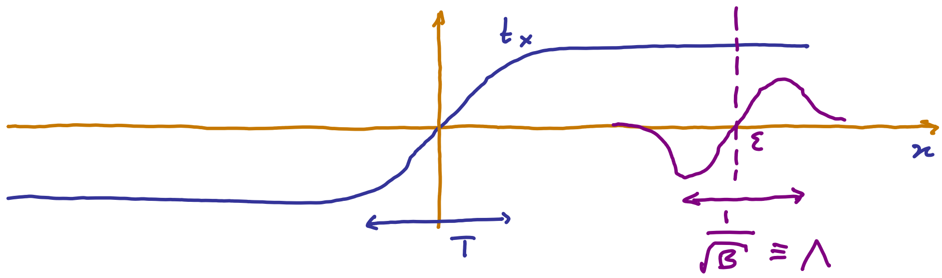
$$J_{\varepsilon\varepsilon'}(B) = \qquad (2)$$

[keeps track of energy dependence of coupling]

[ensures contributions only from energy diff. with: $|\varepsilon-\varepsilon'| \le$]

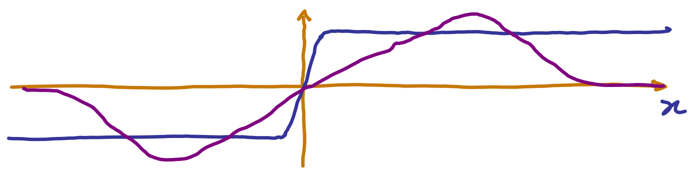
Consider flow eq. for diagonal term:

$$\partial_B \tilde{J}_\varepsilon \overset{(3)\text{ into }(1)}{=} \nu\int_{-\infty}^{\infty} dx \; t_x \left(\tilde{J}_{\frac{\varepsilon+x}{2}}\right)^2 \qquad (3)$$



(i) $|\varepsilon| \ll \Lambda$, $T \ll \Lambda$

FE10



Consider scaling eq. for :

$$\partial_B \tilde{J}_0 \overset{(7.4)}{\simeq} \tilde{J}_0\, 2\nu \int_0^\infty dx \; x\, e^{-2Bx^2} = \qquad (1)$$

dimensionless coupling:

$\nu \tilde{J}_0$:

$$\frac{\partial g_0}{\partial \ln B} \overset{(1)}{=} \frac{g_0^2}{2} \qquad (2)$$

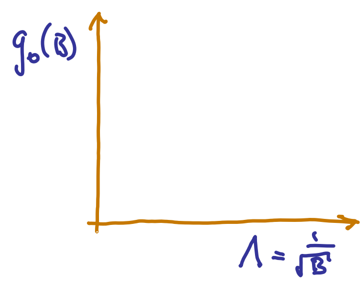
scaling eq. in terms of ultra-violett cutoff:

$$\ln B \overset{(2.8)}{=} \qquad (3)$$

(3) into (1)

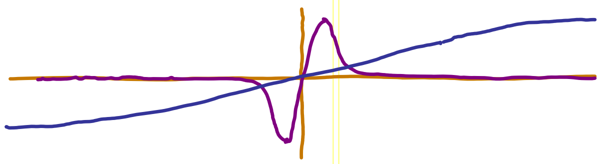
$$\frac{\partial g_0}{\partial \ln \Lambda} =$$

Poor man's scaling recovered!!



$\boxed{FE11}$

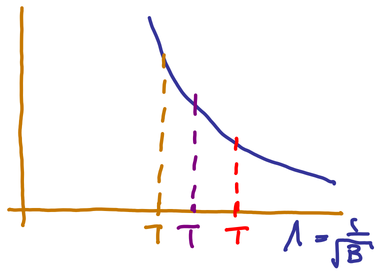
(ii) $|\varepsilon| \ll \Lambda \ll T$



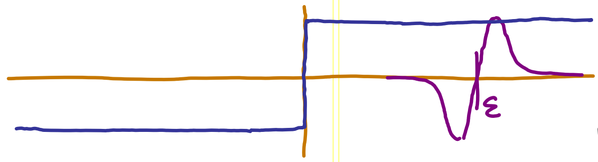
flow stops once decreases below

$\partial_B \tilde{J}_0 \overset{(7.6)}{\simeq}$

[for all relevant x, namely, $|\varepsilon_D| \lesssim \Lambda$ we have: $t_x \simeq$]



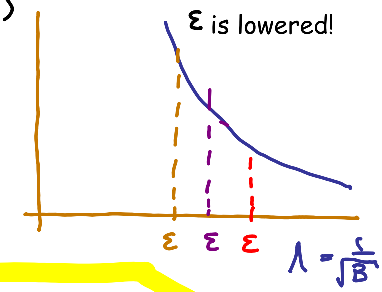
(iii) $T \ll \Lambda \ll |\varepsilon|$



even at T = 0, flow stops once decreases below

$\partial_B \tilde{J}_\varepsilon \overset{(7.6)}{\simeq}$

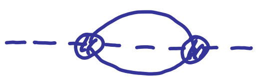
[due to antisymmetry of integrand around ε]



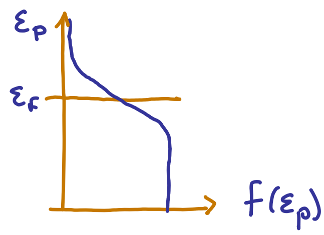
effective coupling: g_{eff}

$\boxed{FE12}$

Spin relaxation rate



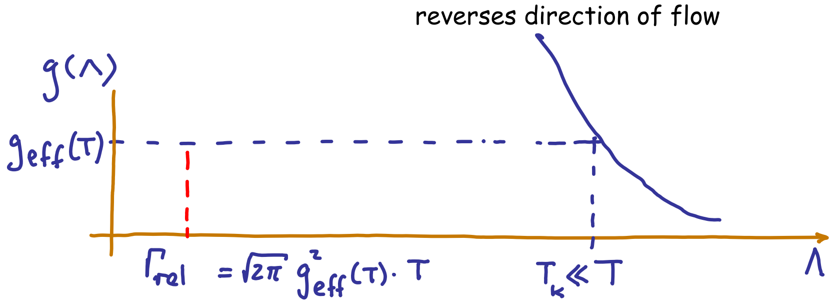
golden rule: $\Gamma_{rel} \propto g^2 \quad T$ (1)



FERG scaling eq. to next-higher order:

$T_K \ll T$: $$\frac{dg_0}{d\Lambda} = \begin{cases} -\frac{g_0^2}{\Lambda} + \frac{1}{2}\frac{g_0^3}{\Lambda} =: \beta(g_0) & \text{for } T \ll \Lambda \quad (2) \\ \frac{\sqrt{2\pi}}{2} g_0^3 \frac{T}{\Lambda^2} & \text{for } \Lambda \ll T \quad (3) \end{cases}$$

dominates at small Λ, reverses direction of flow



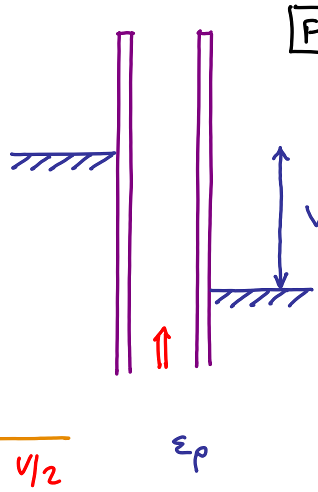
Spin relaxation counteracts logarithmic renormalization of coupling

FERG in nonequilibrium

FE13

Effective Kondo model for coupled channel 1 [compare (AM10.1)]:

$$H = \sum_{k\alpha\sigma} \psi^{+}_{k1\sigma}\psi_{k1\sigma} + J_1 \vec{\sigma}_1 \cdot \vec{S}$$



Effective Fermi function:

$$f_1(\varepsilon_p) = \langle \psi^{+}_{p1\sigma}\psi_{p1\sigma} \rangle$$

$=$

Parametrization of couplings:

$$\nu J_{\varepsilon\varepsilon'} := g_{\frac{\varepsilon+\varepsilon'}{2}}(B)\, e^{-B(\varepsilon-\varepsilon')^2}$$

Coupling at left/right Fermi energy.:

$$g_{l/r}(B) := g_{\varepsilon=\pm V/2}(B)$$

Average coupling in transport window:

$$g_t(B) := \frac{1}{V}\int_{-V/2}^{V/2} d\varepsilon\; g_\varepsilon(B)$$

Flow equations for g_l, g_r, g_t:

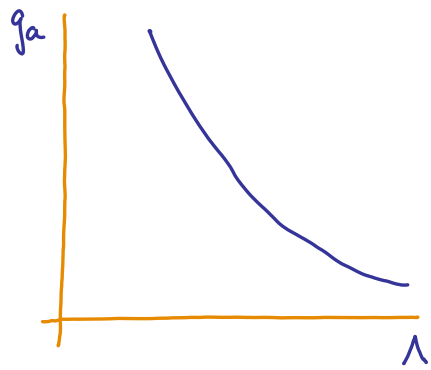
FE14

$V \ll \Lambda$:

$$\frac{dg_l}{d\Lambda} = -\frac{2(g_l^2+g_t^2)}{\Lambda} \quad (1a)$$

$$\frac{dg_r}{d\Lambda} = -\frac{2(g_l^2+g_t^2)}{\Lambda} \quad (1b)$$

$$\frac{dg_t}{d\Lambda} = -\frac{2g_t(g_l+g_r)}{\Lambda} \quad (1c)$$



$\Lambda \ll V$:

$$\frac{dg_l}{d\Lambda} = -\frac{2g_l^2}{\Lambda} + \sqrt{2\pi}\,\frac{V}{\Lambda^2}\, g_l\, g_t^2 \quad (2a)$$

$$\frac{dg_r}{d\Lambda} = -\frac{2g_r^2}{\Lambda} + \sqrt{2\pi}\,\frac{V}{\Lambda^2}\, g_r\, g_t^2 \quad (2b)$$

$$\frac{dg_t}{d\Lambda} = \sqrt{2\pi}\,\frac{V}{\Lambda^2}\, g_t^3 \quad (2c)$$

cut-off of RG flow by finite voltage is generated automatically!

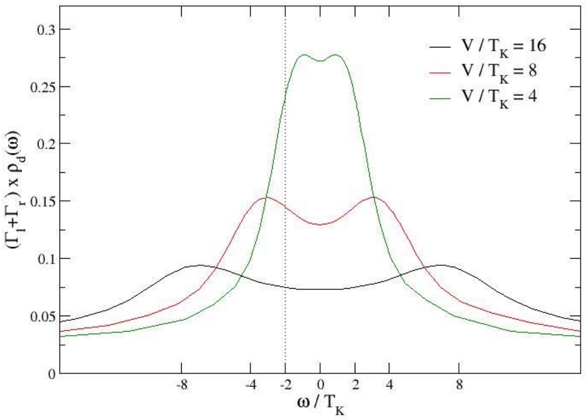
$\Gamma_{rel} \propto$

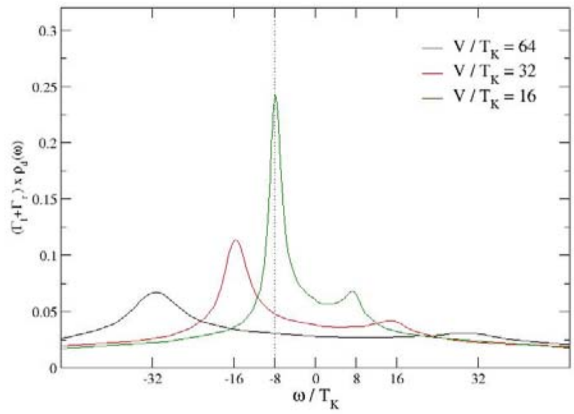
competition between singlet formation and spin relaxation

Finite voltage causes splitting of Kondo resonance

FE 15

S. Kehrein





symmetric couplings

$v_l = v_r$

asymmetric couplings

$v_l \neq v_r$

FERG for Anderson Model ("improve" Schrieffer-Wolff transformation)

FE16

Kehrein, Mielke, Ann. Phys (NY), 252, 1 (1996)

FERG on AM reproduces mapping onto KM for n_d = 1, but with "improved" expressions for J:

Schrieffer-Wolff:

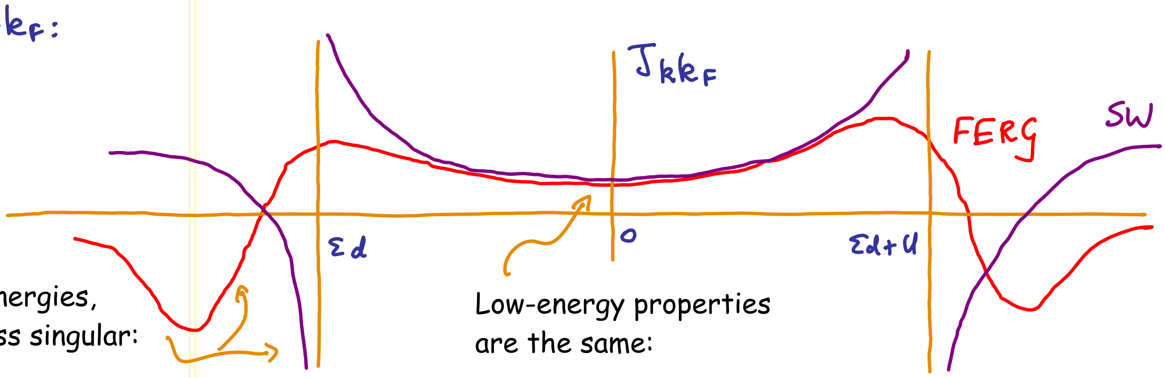
$$J^{SW}_{kk'} = -\frac{1}{2} v_k(0) v_{k'}(0) \left\{ \frac{1}{(\varepsilon_d - \varepsilon_k)(\varepsilon_d + U - \varepsilon_k)} + k \to k' \right\}$$

singular at and at

Flow equations produce les singular result:

$$J^{FERG}_{kk'}(B=\infty) = - v_k(0) v_{k'}(0)\, U \left\{ \frac{(\varepsilon_d - \varepsilon_k)(\varepsilon_d - \varepsilon_k + U) + k \to k'}{(\varepsilon_d - \varepsilon_k)^2 (\varepsilon_d - \varepsilon_k + U)^2 + k \to k'} \right\}$$

For $k' = k_F$:



At large energies, FERG is less singular:

Low-energy properties are the same: