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Nonequilibrium functional RG for the Anderson impurity model

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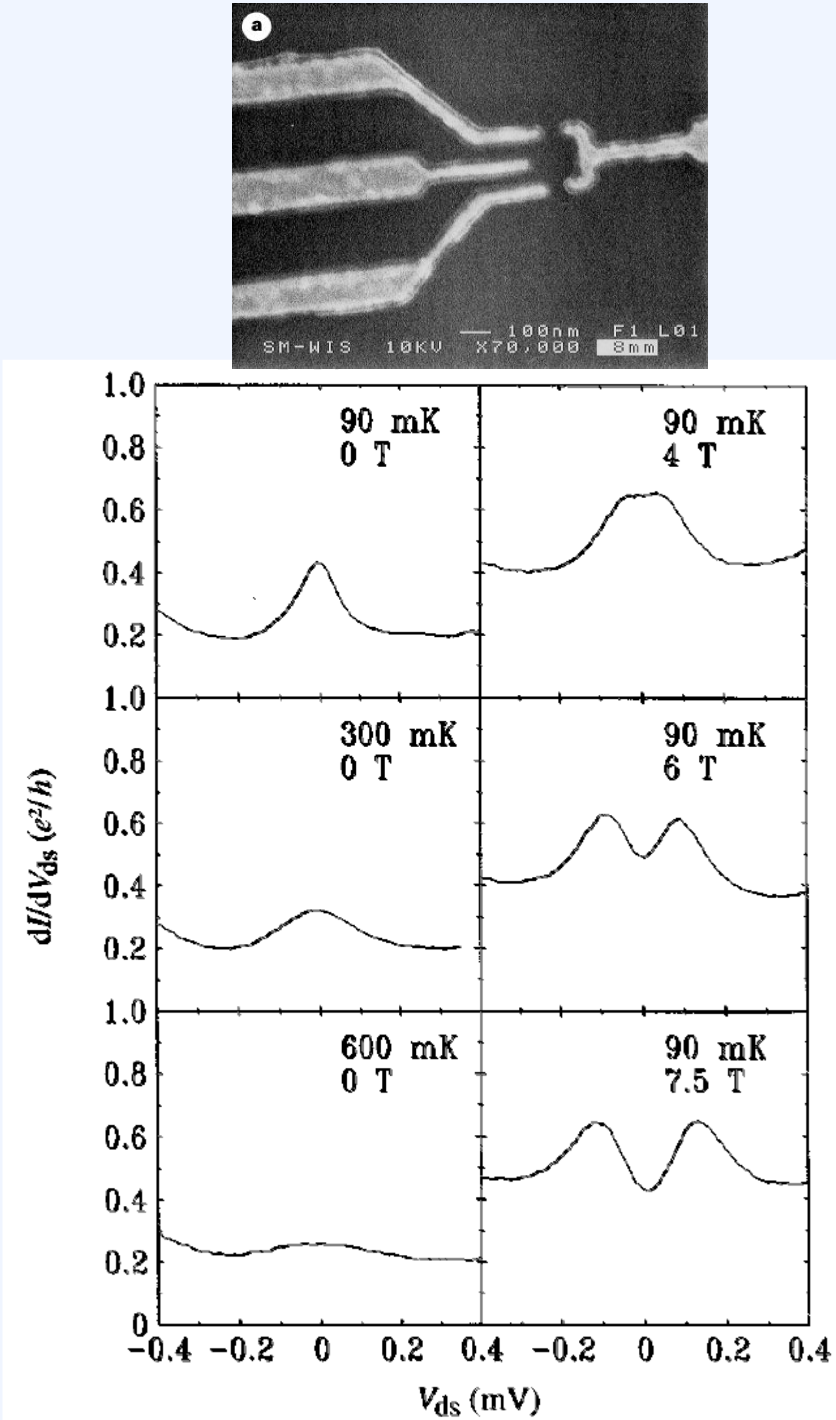
Jakobs, Pletyukhov, Schoeller – PRB **81**, 195109 (2010)
Jakobs, Pletyukhov, Schoeller – J Phys A: Math Theor **43**, 103001 (2010)
Eckel, Heidrich-Meisner, Jakobs et al – NJP **12**, 043042 (2010)

Outline

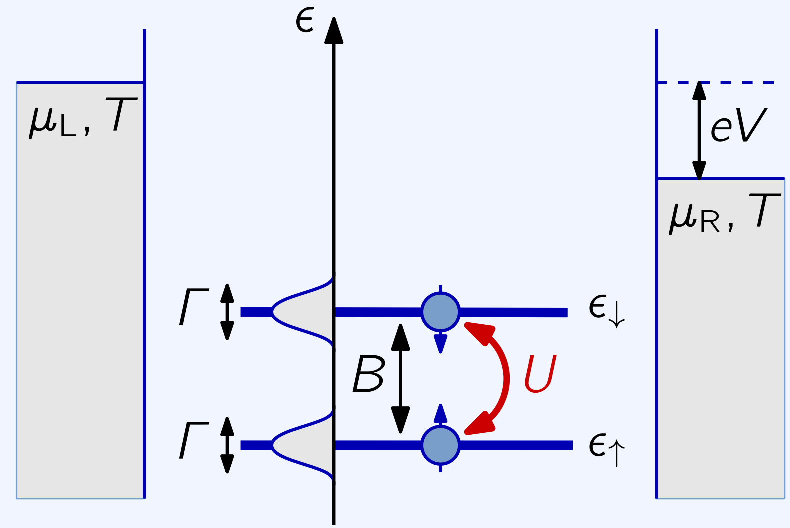
1. Model: Anderson impurity in nonequilibrium
2. Method: fRG within Keldysh formalism
3. Discussion of results
4. Conclusion

A model for transport through quantum dots

Goldhaber-Gordon et al, Nature (1998)



- Noneq. transport through QDot has been studied experimentally
- Challenge for theory: strong correlations, current-carrying state
- Model: Anderson impurity with contacts

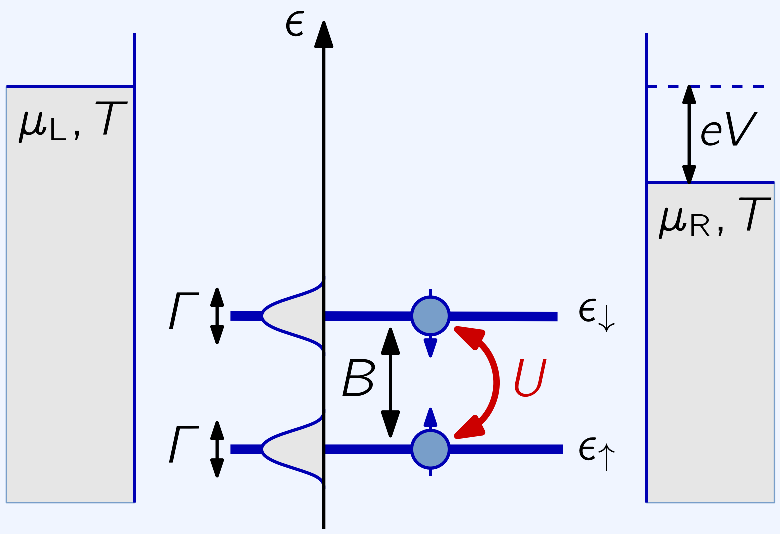


- Describes charge *and* spin fluctuations.

  (Reson. level model → charge fluct.

  Kondo model → spin fluct.)

Anderson impurity in nonequilibrium



$$H_{imp} = \sum_\sigma (eV_{gate} - \sigma B - \tfrac{U}{2}) n_\sigma + U n_\uparrow n_\downarrow$$

$$H_{leads} = \sum_{r=R,L} \sum_\sigma \int dk\, \epsilon_k n_{rk\sigma}$$

$$H_{coup} = \sum_{r=L,R} \sum_\sigma \int dk\, V_{rk} d_\sigma^\dagger c_{rk\sigma} + \text{h.c.}$$

$$\Gamma_r = 2\pi \frac{|V_r|^2}{v_r}, \quad \Gamma = \Gamma_L + \Gamma_R = 2\Delta$$

Properties of the Anderson model

- Perturbation theory in U is regular.
- Large U, low energies $\rightarrow$ $T_K \sim \exp\left(-\frac{\pi}{4}\frac{U}{\Gamma}\right)$ $\rightarrow$ RG-treatment
- Equilibrium: good description by NRG, Bethe Ansatz.

Equilibrium-fRG studies of the model

- Based on expansion in U [Hedden et al '04, Karrasch et al '06, '08]
- Based on Hubbard-Stratonovich fields [Bartosch et al '09, '10]

$\rightarrow$ our guideline for noneq. fRG

High interest in noneq. properties of Anderson model

Recent investigations of nonequilibrium Anderson model

- Perturbation theory ($V_g = 0, B = 0$) [Hershfield et al '91, '92; Fujii, Ueda '03]
- Real time RG (mixed valence, empty orbital) [Schoeller, König '00]
- Imag. voltage QMC (difficult analyt. cont.) [Han, Heary '07, Dirks et al '10]
- Nonequilibrium fRG (lowest order truncation) [Gezzi et al '07]
- Scattering states NRG (data still noisy) [Anders '08]
- ISPI (moderate U, no small T) [Weiss et al '08]
- Real time QMC ($V_g = 0, B = 0$) [Werner et al '09, '10]
- GW approach (Coulomb blockade regime) [Spataru et al '09]
- tDMRG (from the transient regime) [Heidrich-Meisner et al '09]
- Scattering Bethe Ansatz (phenomenological distr. funct.) [Chao, Palacios '10]

Role of noneq. fRG

- flexible tool for $U \lesssim 3\Gamma$ allowing for finite B, T, V_g, V
- based on single-particle-states $\rightarrow$ good scaling with system size
  $\rightarrow$ applicable to larger systems (eg q-wires)

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Keldysh formalism describes time evolved density matrix

- formulated for real times/frequencies
  → no analytic continuation
- can describe nonequilibrium

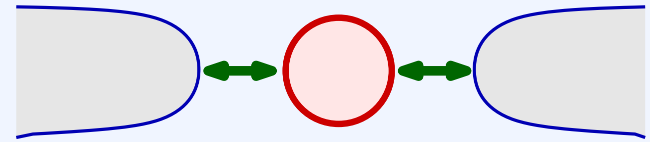
$t = -\infty$

$$\rho_0 = \rho_L \otimes \rho_{imp} \otimes \rho_R$$

switch on interaction
and coupling

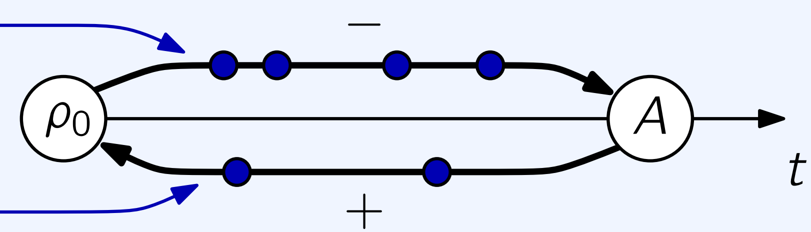
time evolution

finite t



$$\rho(t) \equiv \rho \text{ (stat. state)}$$

$$\langle A(t) \rangle = \mathrm{Tr}\, \rho_0\, U_I(-\infty, t)\, A_I(t)\, U_I(t, -\infty)$$



$$G^{Ret} = \frac{1}{\omega - \epsilon - \Sigma^{Ret}}$$ → quasi-part. energies, lifetimes

$$G^K = G^{Ret} \Sigma^K G^{Av}$$ → particle distribution: $g^K = [1 - 2f_{eff}(\omega)][g^{Ret} - g^{Av}]$

Flow parameters for the Keldysh fRG

Exact relations that approximation should satisfy:

- Causality, eg $G^{\mathrm{Ret}}(t) \sim \Theta(t)$
- KMS conditions in equilibrium, eg $G^{\mathrm{K}} = [1 - 2f(\omega)][G^{\mathrm{Ret}} - G^{\mathrm{Av}}]$

If g_Λ respects relations, **then** result of truncated flow respects them. [Jakobs et al '10]

Real frequency cut-off [Jakobs '03; Gezzi et al '07]

$$g_\Lambda(\omega) = \Theta(|\omega| - \Lambda)g(\omega)$$

+ fast

− causality violated → KMS violated

Momentum cut-off

$$g_{k,\Lambda} = \Theta(|\epsilon_k| - \Lambda)g_k$$

+ causality *and* KMS conserved

− not applicable to dot system

Imaginary frequency cut-off [Jakobs et al '07]

$$f_\Lambda(\omega) = T \sum_{\omega_n} \frac{\Theta(|\omega_n| - \Lambda)\, \mathrm{e}^{\mathrm{i}\,\omega_n 0^+}}{\mathrm{i}\,\omega_n - \omega}$$

+ causality conserved

− KMS violated

Hybridization flow [Jakobs et al '10]

$$\Gamma_\Lambda = \Gamma + \Lambda$$

+ causality *and* KMS conserved

− slow

↓

used here

fRG with hybridization as flow parameter

Hybridization Γ as flow parameter:

$$\Gamma \longrightarrow \Gamma_\Lambda = \Gamma + \Lambda$$

$$\Gamma^{L/R} \longrightarrow \Gamma_\Lambda^{L/R} = \Gamma^{L/R} + \frac{\Gamma^{L/R}}{\Gamma}\Lambda$$

with Λ flowing $\infty \longrightarrow 0$.

Reservoir dressed propagator depends on Λ:

$$g_\Lambda^{\mathrm{Ret}} = \frac{1}{\omega - \epsilon + \frac{i}{2}\Gamma_\Lambda}$$

$$g_\Lambda^{K} = \left[1 - 2 f_{\mathrm{eff}}(\omega)\right]\left[g_\Lambda^{\mathrm{Ret}} - g_\Lambda^{\mathrm{Av}}\right]$$

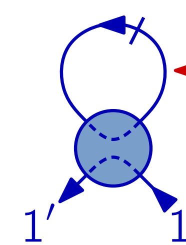
- Irreduc. vertex functions γ_n depend on Λ:

$$\gamma_n^{\Lambda=\infty} = \bar{v}_n \quad \rightarrow \quad \gamma_n^{\Lambda=0} = \gamma_n$$

- Hierarchy of flow equations
- Approximate by truncation, effective parametrization

Wetterich (1993), Morris (1994)

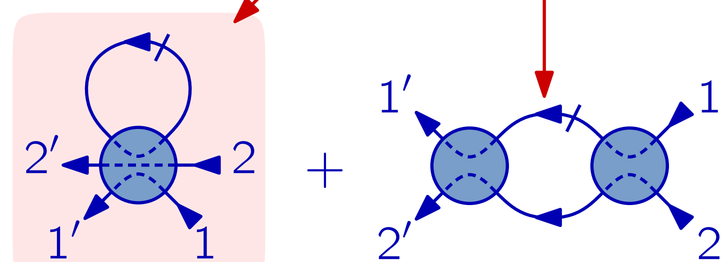
$$\frac{d}{d\Lambda}\Sigma(1'|1) =$$



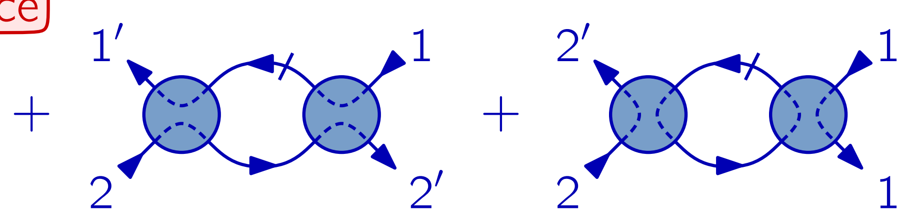
feed back only static Σ

neglect

$$\frac{d}{d\Lambda}\gamma(1'2'|12) =$$

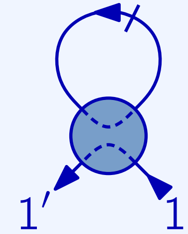


make Ansatz for freq.-dependence

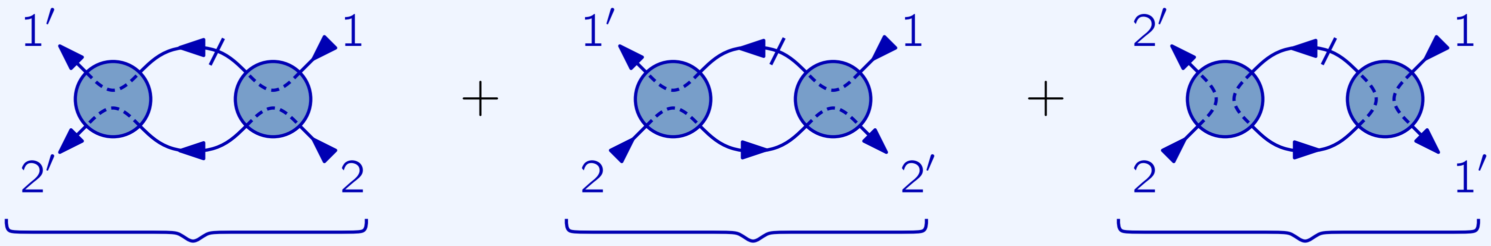


Flow equation couples three channels

$$\frac{\mathrm{d}}{\mathrm{d}\Lambda}\Sigma(1'|1) \;=$$



$$\frac{\mathrm{d}}{\mathrm{d}\Lambda}\gamma(1'2'|12) \;=$$



pp-channel: $\Pi = \omega_1 + \omega_2 = \omega_1' + \omega_2'$

xph-channel: $X = \omega_2' - \omega_1 = \omega_2 - \omega_1'$

dph-channel: $\Delta = \omega_1' - \omega_1 = \omega_2 - \omega_2'$

Approximation for frequency-dependence

$$\gamma(\Pi, X, \Delta) \;=\; \bar{v} + \varphi_{\mathrm{p}}(\Pi) + \varphi_{\mathrm{x}}(X) + \varphi_{\mathrm{d}}(\Delta)$$

- Each channel feeds back into own flow exactly
- Each channel feeds into flow of other channels as constant (renormalizing the interaction)
- Only static part of self-energy fed back into flow

[cf Karrasch et al, J Phys: Cond Mat **20**, 345205 (2008)]

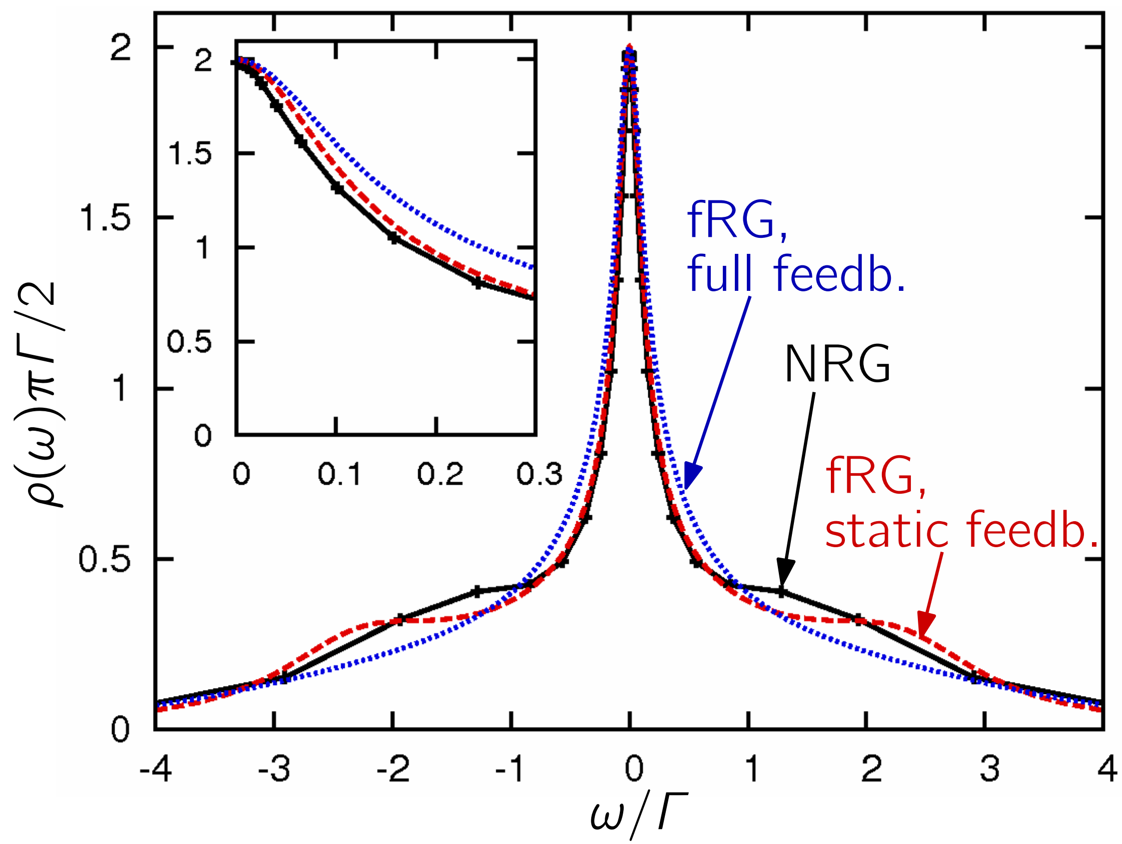
Range of applicability

- Approximations valid only for moderate U/Γ
- Some aspects of Kondo for large U/Γ captured
- For $U/\Gamma \to 0$: second order PT is asymptot. approached

Outline

Full Σ-feedback vs. static Σ-feedback

Spectral function for $U = 3\Gamma, V = 0, V_g = 0, B = 0, T = 0$



Full Σ-feedback into flow $\rightarrow$ features too smooth

Reason:

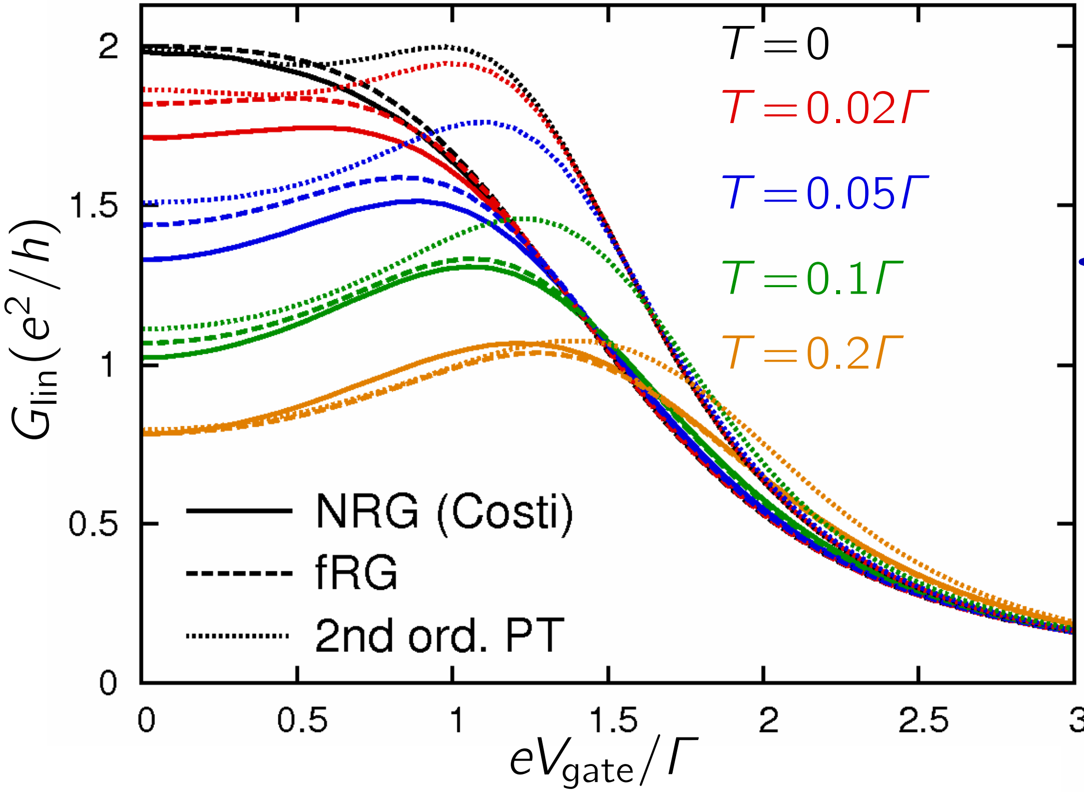
Flow of γ_3 neglected $\rightarrow$ $\frac{\partial}{\partial\Lambda}\gamma_2^\Lambda(\Pi=0, X=0, \Delta=0) = 0$

instead of $\gamma_2(\Pi=0, X=0, \Delta=0) \overset{U\to\infty}{\sim} \exp\left(\frac{\pi}{4}\frac{U}{\Gamma}\right)$

[Yamada, Yosida '75]

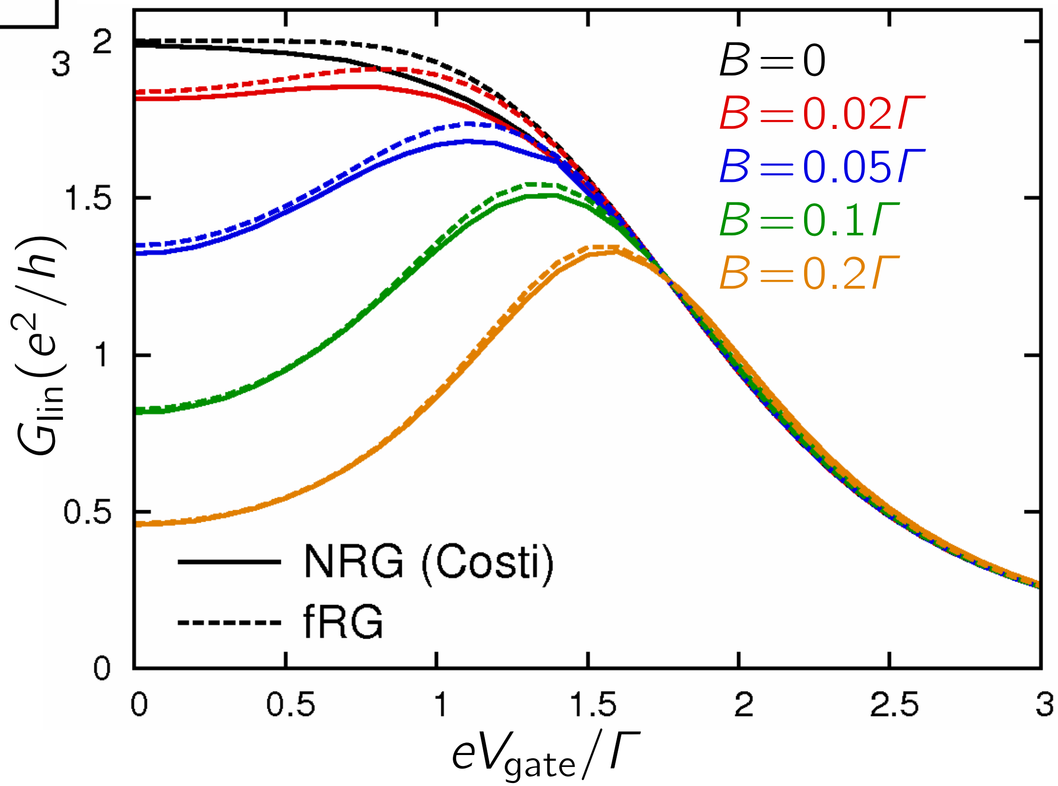
Choose static Σ-feedback.

Good description of $G_{\text{lin}}(V_{\text{gate}}; B, T)$

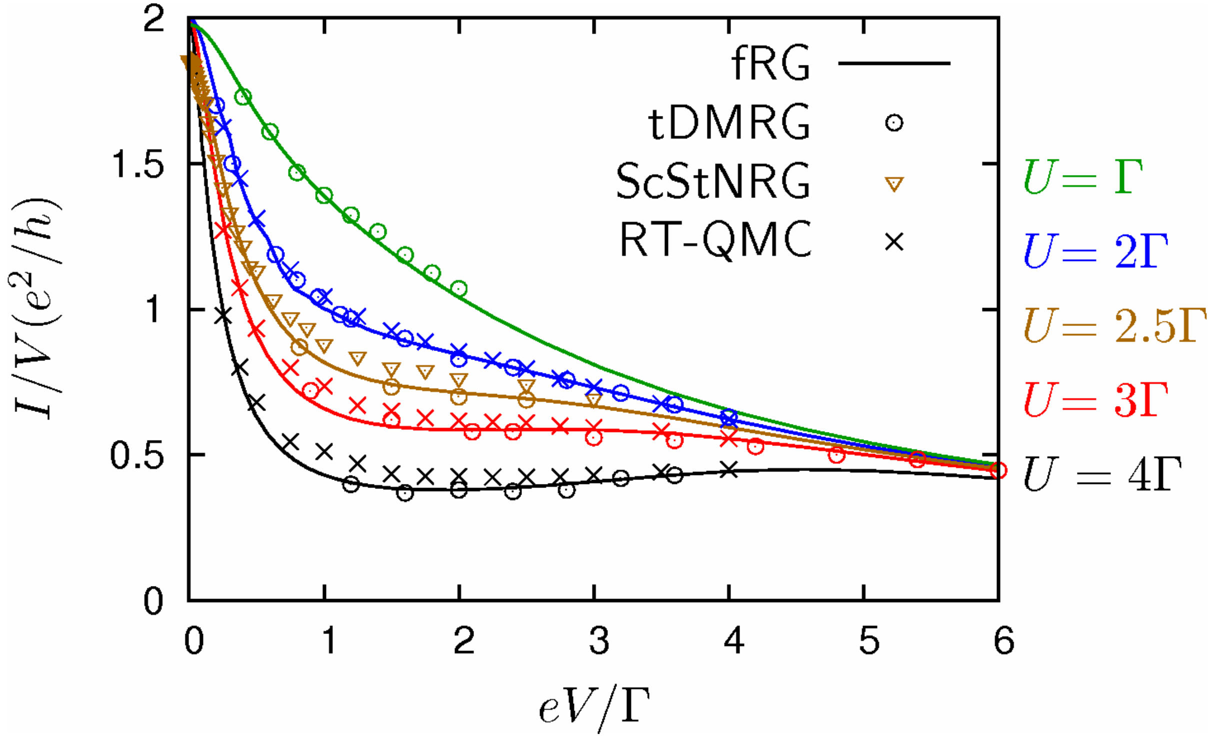


$U = 3\Gamma (= 6\Delta)$,
$B = 0, V = 0$
good agreement with NRG,
inaccessible to static fRG

$U = 4\Gamma (= 8\Delta)$,
$T = 0, V = 0$
very good agreement with NRG,
comparable to static fRG
[cf Karrasch et al '06]



Nonequilibrium – good agreement with ISPI and tDMRG



Heidrich-Meisner et al, PRB 2009

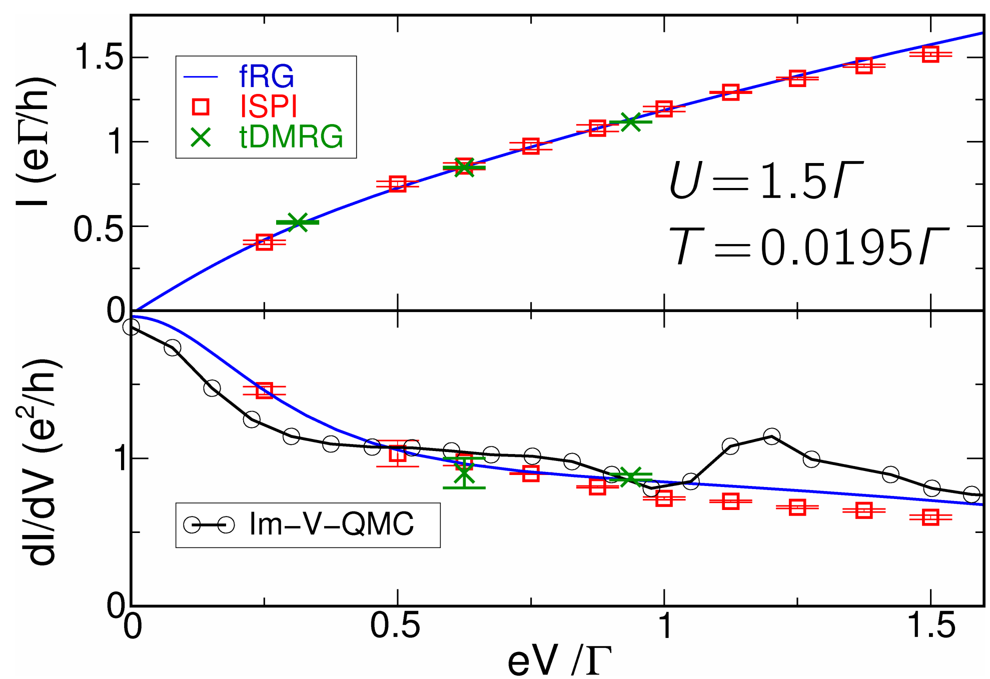
Anders, PRL 2008

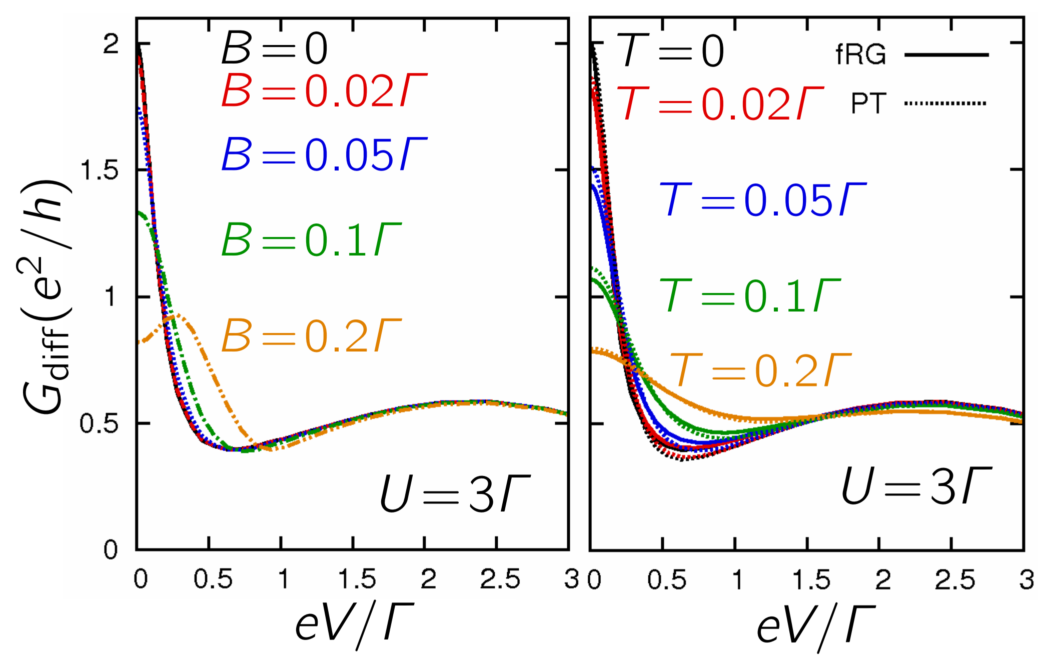
Werner et al, PRB 2009

Weiss et al, PRB 2008

Han, Heary, PRL 2007

see Eckel et al, NJP 2010



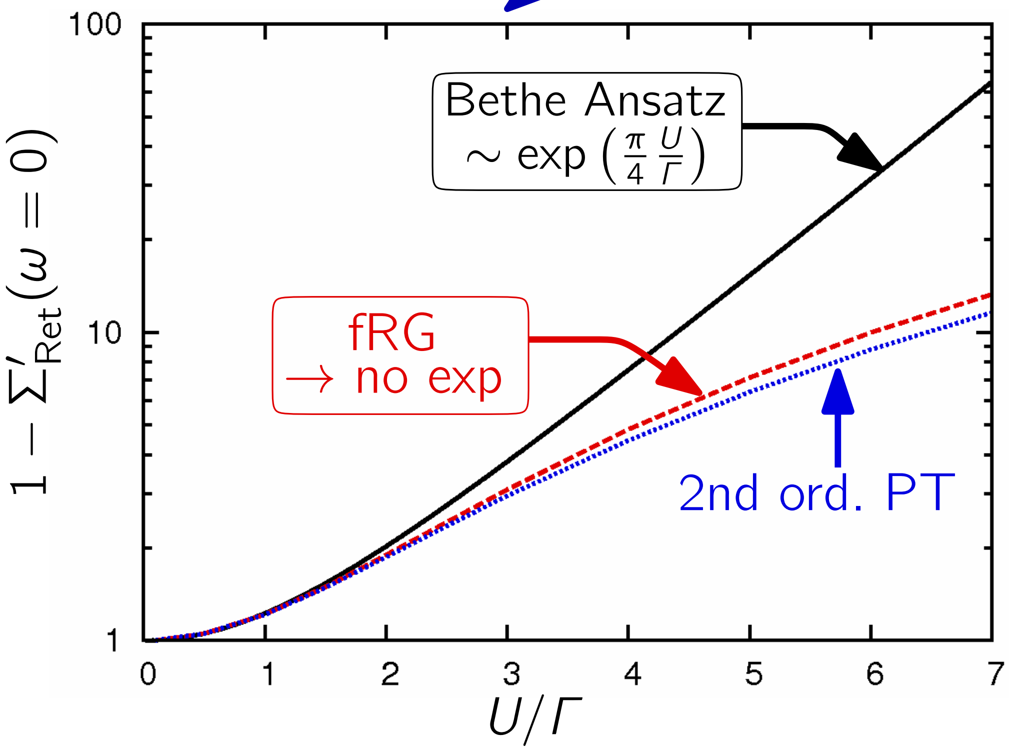


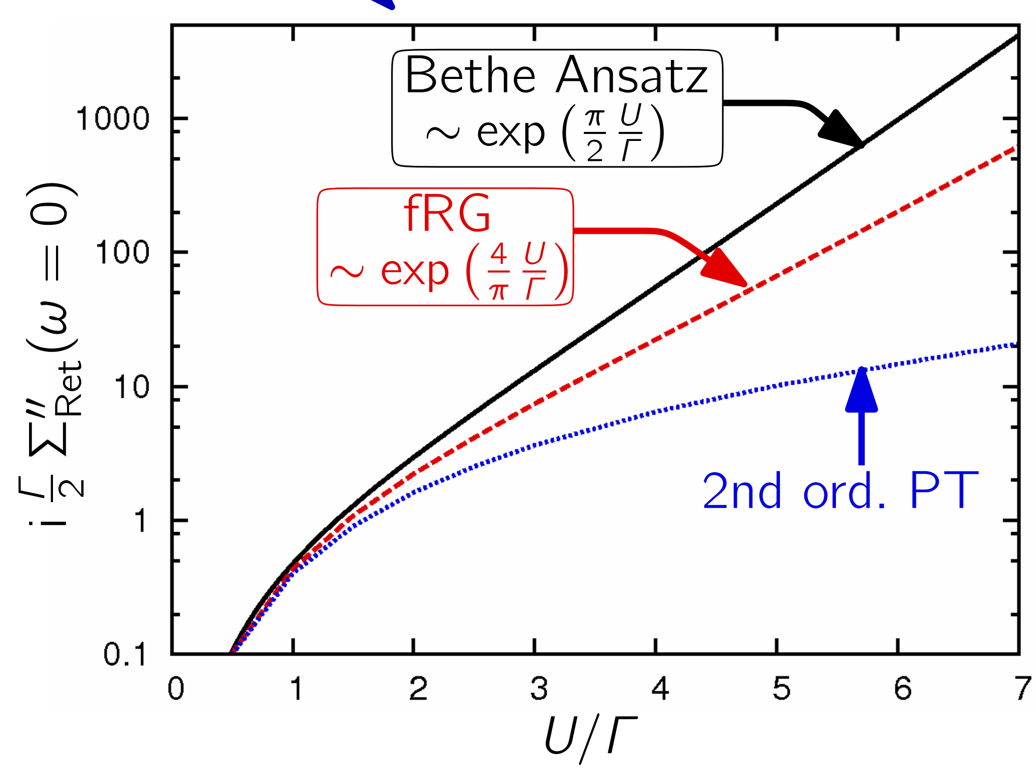
Kondo scale in Fermi liquid coefficient

In particle-hole symmetric case [Oguri '01]

$$\Sigma_{\mathrm{Ret}} \simeq \frac{U}{2} + \Big(1 - \underbrace{\frac{\tilde{\chi}_{\mathrm{s}} + \tilde{\chi}_{\mathrm{c}}}{2}}_{= m^* = Z^{-1}}\Big)\omega - \mathrm{i}\,\frac{(\tilde{\chi}_{\mathrm{s}} - \tilde{\chi}_{\mathrm{c}})^2}{4\Gamma}\Big[\omega^2 + (\pi T)^2 + \frac{3}{4}(eV)^2\Big]$$

fRG: prefactors correct





Wilson Ratio: $R = \dfrac{2\tilde{\chi}_{\mathrm{s}}}{\tilde{\chi}_{\mathrm{s}} + \tilde{\chi}_{\mathrm{c}}} < 2,$ $\quad R \xrightarrow{U\to\infty} 2.$ $\quad$ fRG: $R > 2$ for $U > 4\Gamma$.

Conclusion

Topic: Steady state transport through Anderson impurity

Method: Functional RG
- in Keldysh formalism
- with hybridization as flow parameter
- with frequency dependent 2-particle vertex

Findings:
- for $U \lesssim 3\Gamma (= 6\Delta)$: flexible tool
  - $\rightarrow$ good agreement with other nonequilibrium methods
  - $\rightarrow$ finite V, T, B, V_g accessible
- larger U: Kondo scale in Fermi liquid coefficient (but not in effective mass)

Jakobs, Pletyukhov, Schoeller – PRB **81**, 195109 (2010)

Jakobs, Pletyukhov, Schoeller – J Phys A: Math Theor **43**, 103001 (2010)

Eckel, Heidrich-Meisner, Jakobs et al – NJP **12**, 043042 (2010)

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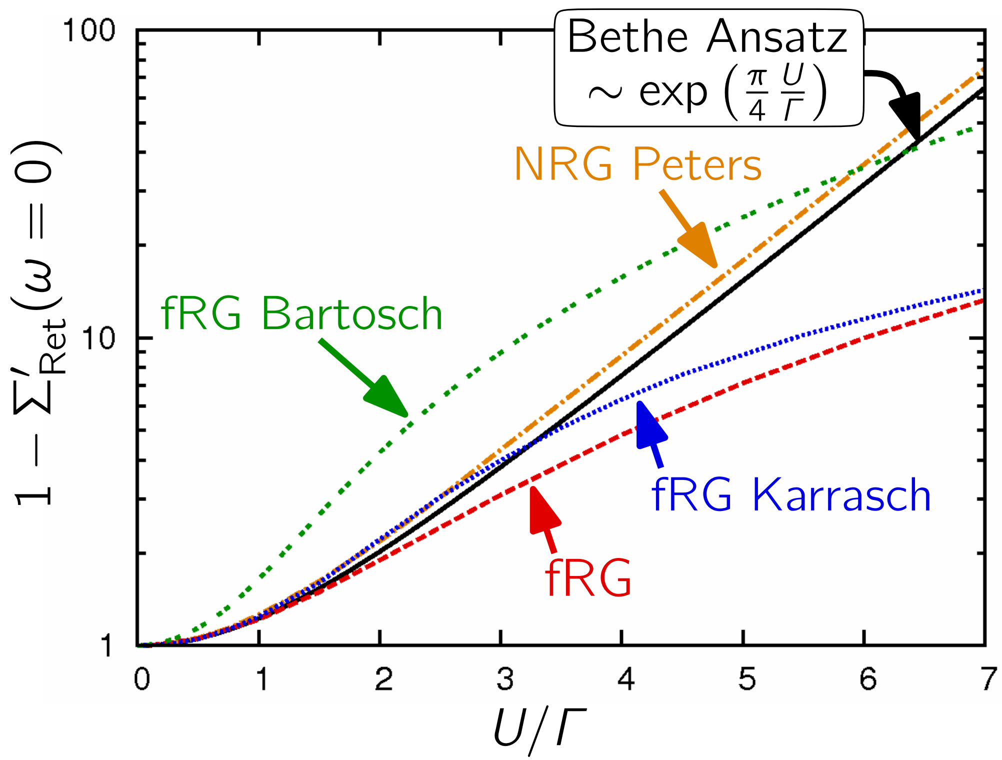
Extra 1: Comparison of fRG-methods



Zlatić, Horvatić, PRB **28**, 6904 (1983)

Karrasch et al, J Phys: Cond Mat **20**, 345205 (2008)

Bartosch et al, J Phys: Cond Mat **21**, 305602 (2009)