KITP Program on Dynamics in Closed Thermally Isolated Systems, S. Barbara October 2012

Non-Equilibrium Dynamics across Impurity Quantum Critical Points

Marco Schiro'

Princeton Center For Theoretical Science

M. Schiro', Phys. Rev. B **86** 161101(R) (2012)

Outline

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☑ Motivations (Theory): Local Quenches in Impurity Models

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- ☑ Motivations (Experiment): Kondo Effect in the Optical Spectrum of Quantum Dots

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- ☑ Basic Questions, Quick Answers and Few Examples

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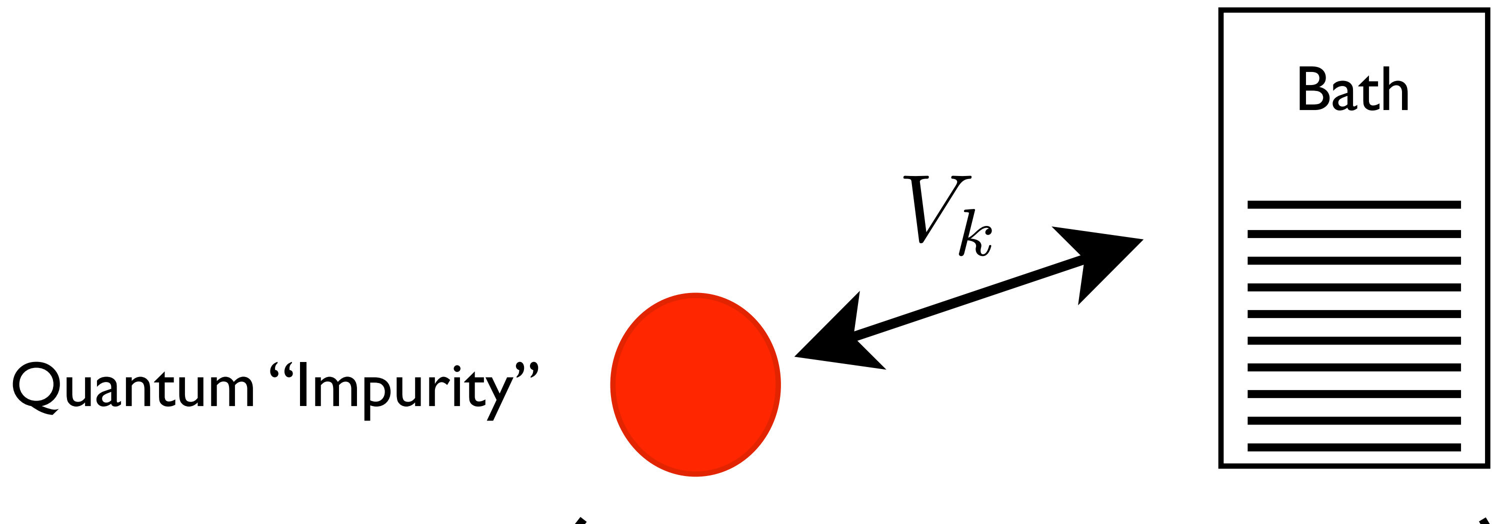
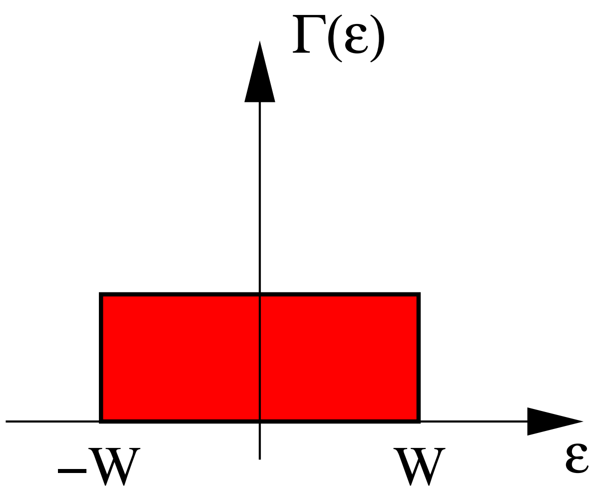
- ☑ Motivations (Theory): Local Quenches in Impurity Models
- ☑ Motivations (Experiment): Kondo Effect in the Optical Spectrum of Quantum Dots
- ☑ Basic Questions, Quick Answers and Few Examples
- ☑ A Less Trivial (?) Example -- The Role of Kondo Effect

Small quantum systems coupled to a "*bath*"





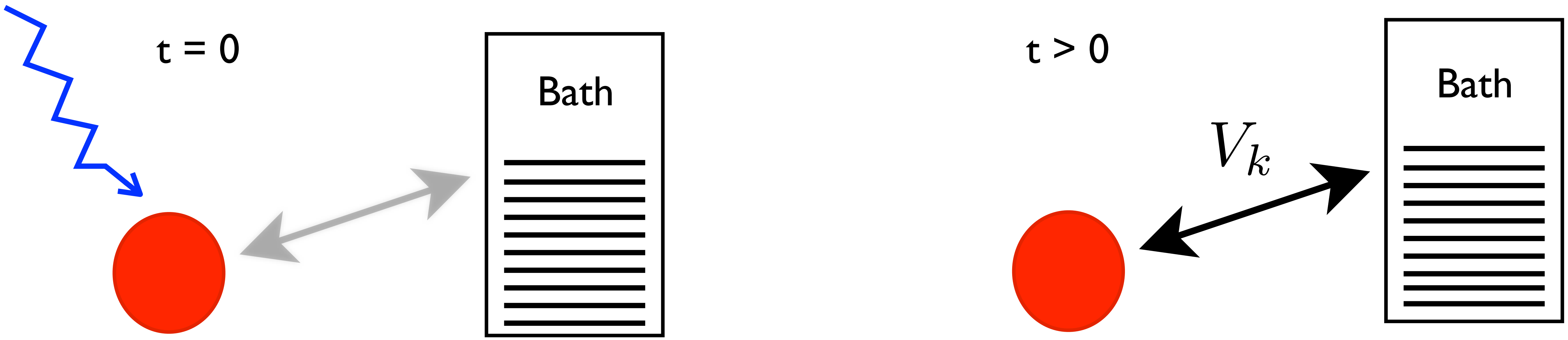
Few interacting quantum degrees of freedom

<u>Continuum</u> of Excitations

Example: Anderson Impurity Model

$$H = \frac{U}{2}(n-1)^2 + \sum_{k\sigma} \epsilon_k \, f^\dagger_{k\sigma} f_{k\sigma} + \sum_{k\sigma} V_k \, \left(c^\dagger_\sigma f_{k\sigma} + h.c.\right)$$

Dynamics after Local Quenches



☑ Long time dynamics after a local perturbation: does the system thermalize?

$$\langle O \rangle_t = Tr[\rho_0 \, e^{iHt} \, O \, e^{-iHt}] \qquad t \to \infty \qquad \langle O \rangle_t = \langle O \rangle_{eq} \; ???$$

☑ Non trivial (universal) off equilibrium dynamics?

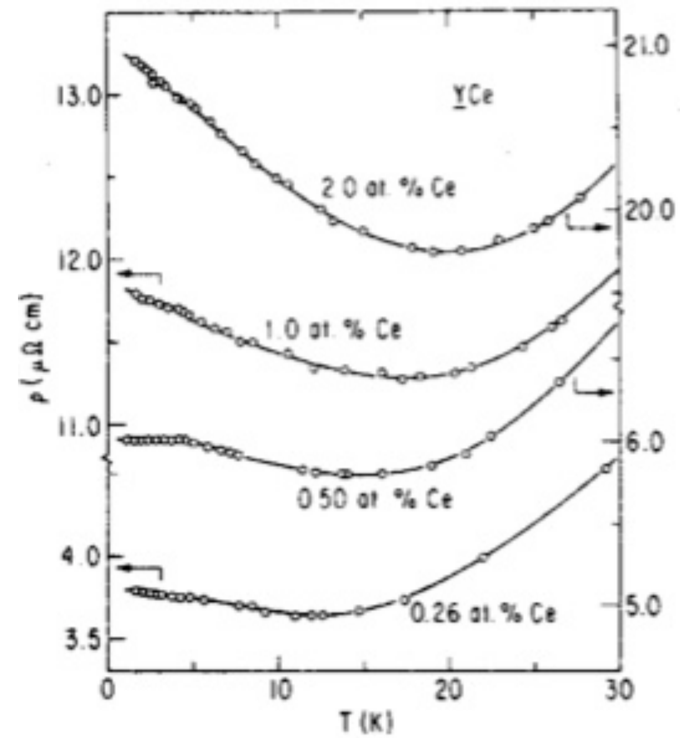
☑ Also relevant for closed systems through DMFT mapping

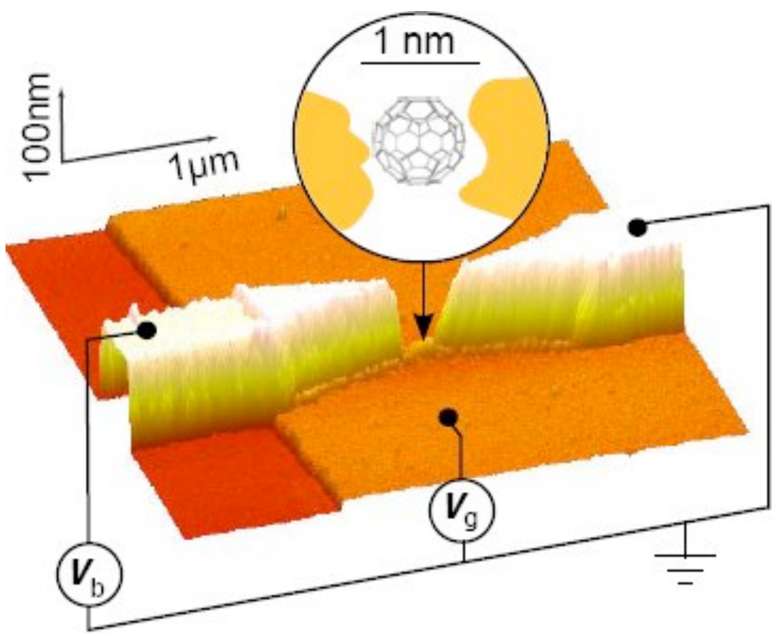
See recent works:

Ratiani & Mitra, PRB **81** 125110(2010), Vinkler, Schiller & Andrei PRB **85** 035411 (2012), ...

Experimental Motivations

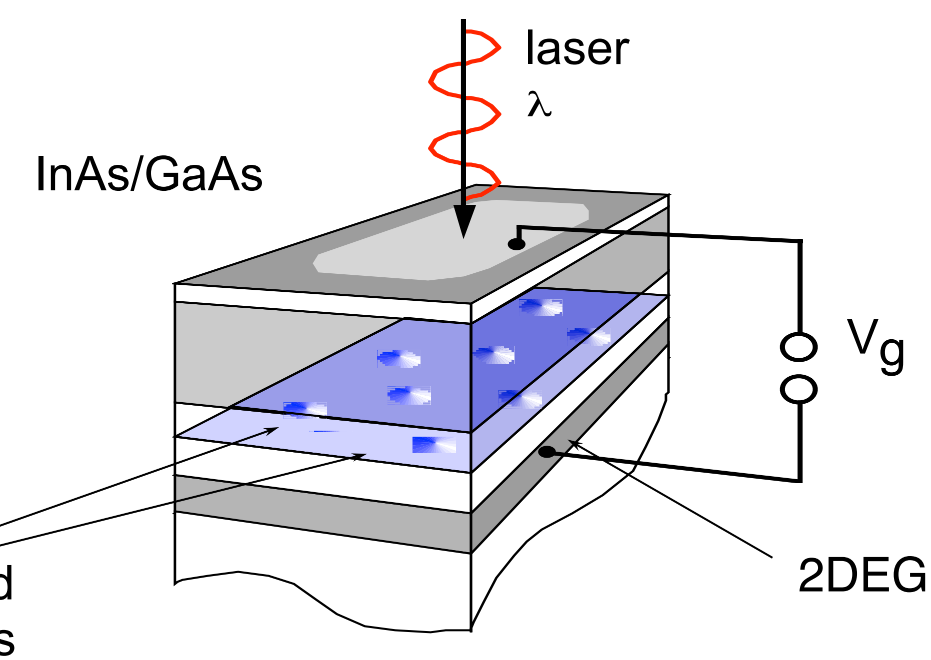
Diluted Magnetic Impurities in Metals ~ 1960





Quantum Dots and Single Molecule Devices ~1998

Optically controlled Self-Assembled Quantum Dots ~ 2005



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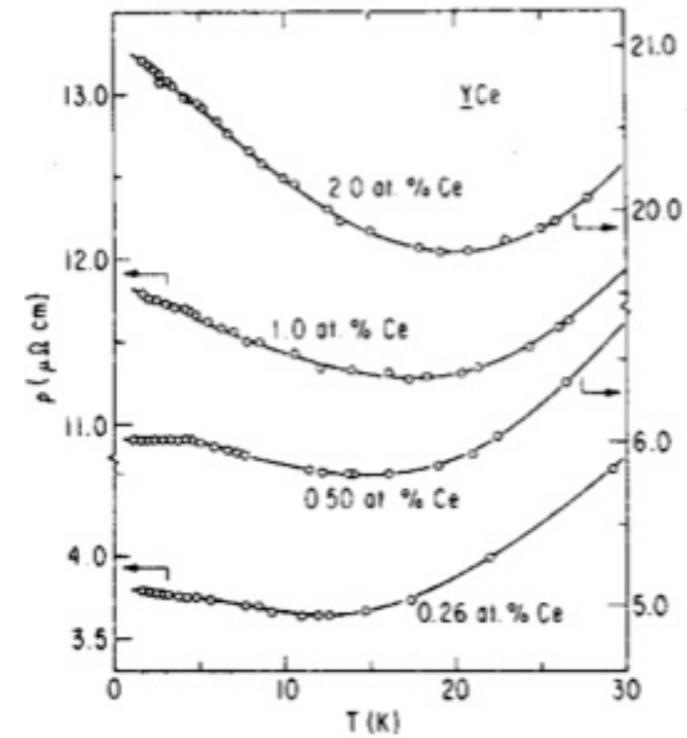

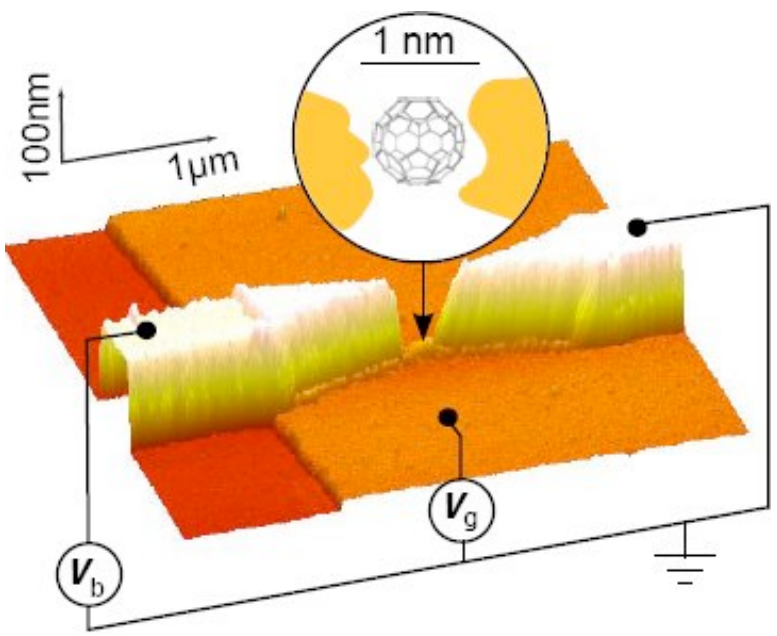

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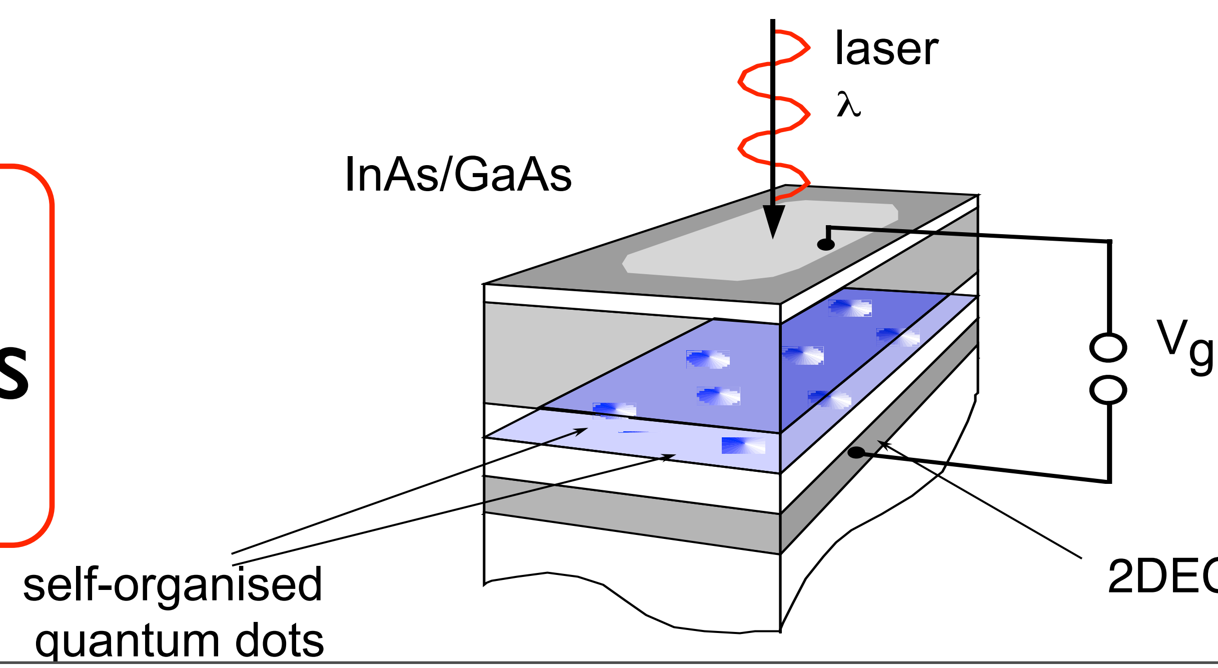
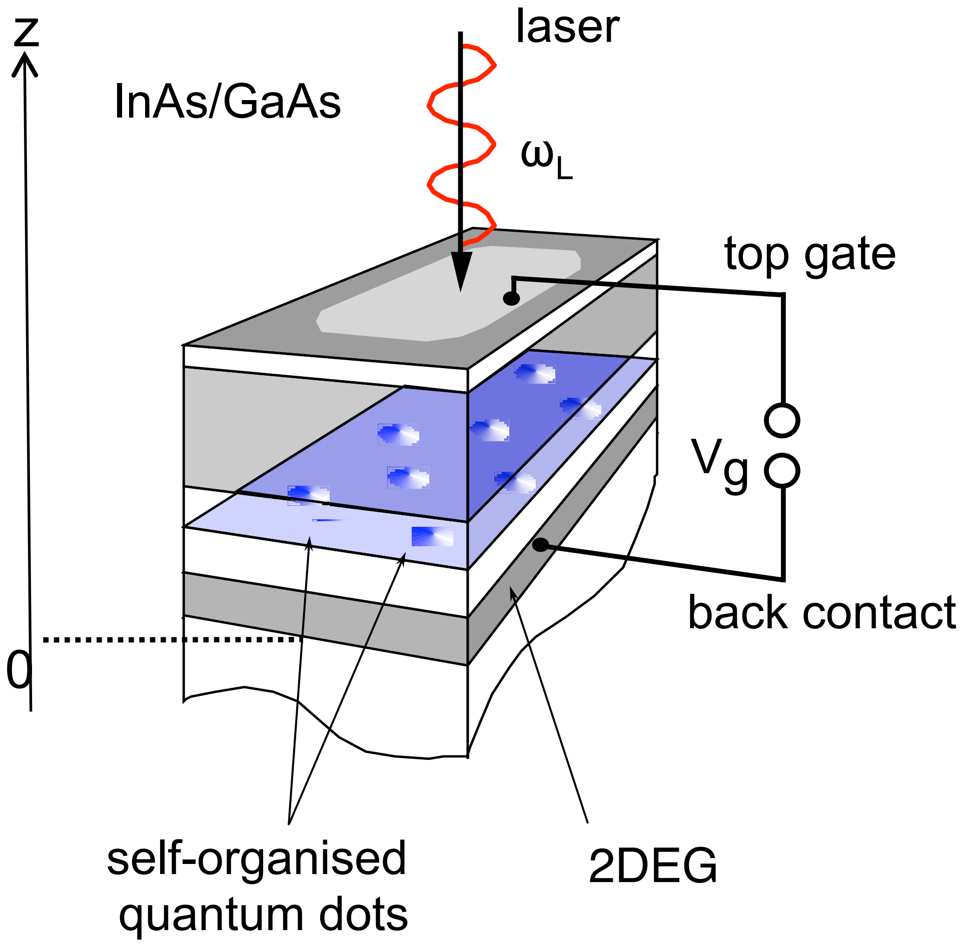
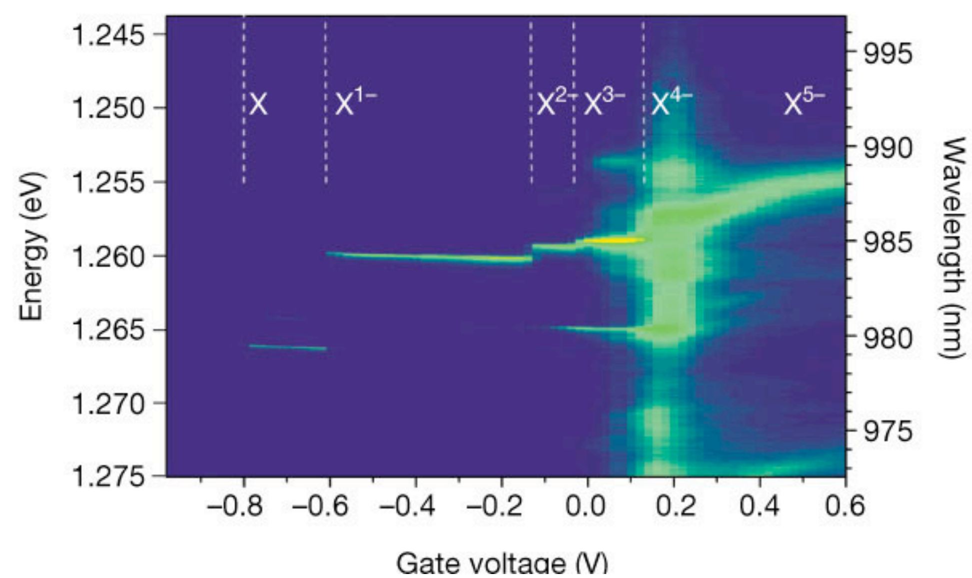


New All Optical Set-up: Self Assembled QuantumDots



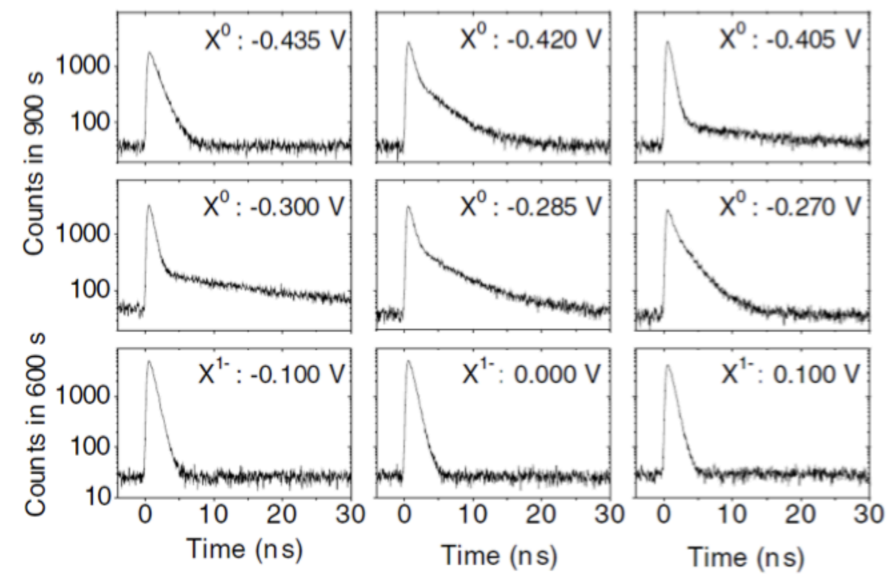
Absorption/Emission spectrum of a single Quantum Dot!

Warburton et *al.*, Nature **405**, 926 (2000)



Evidence of Strong Hybridization to the Fermi Sea

Karrai et al, Nature (2004),
Dalgarno et al, PRL (2008)

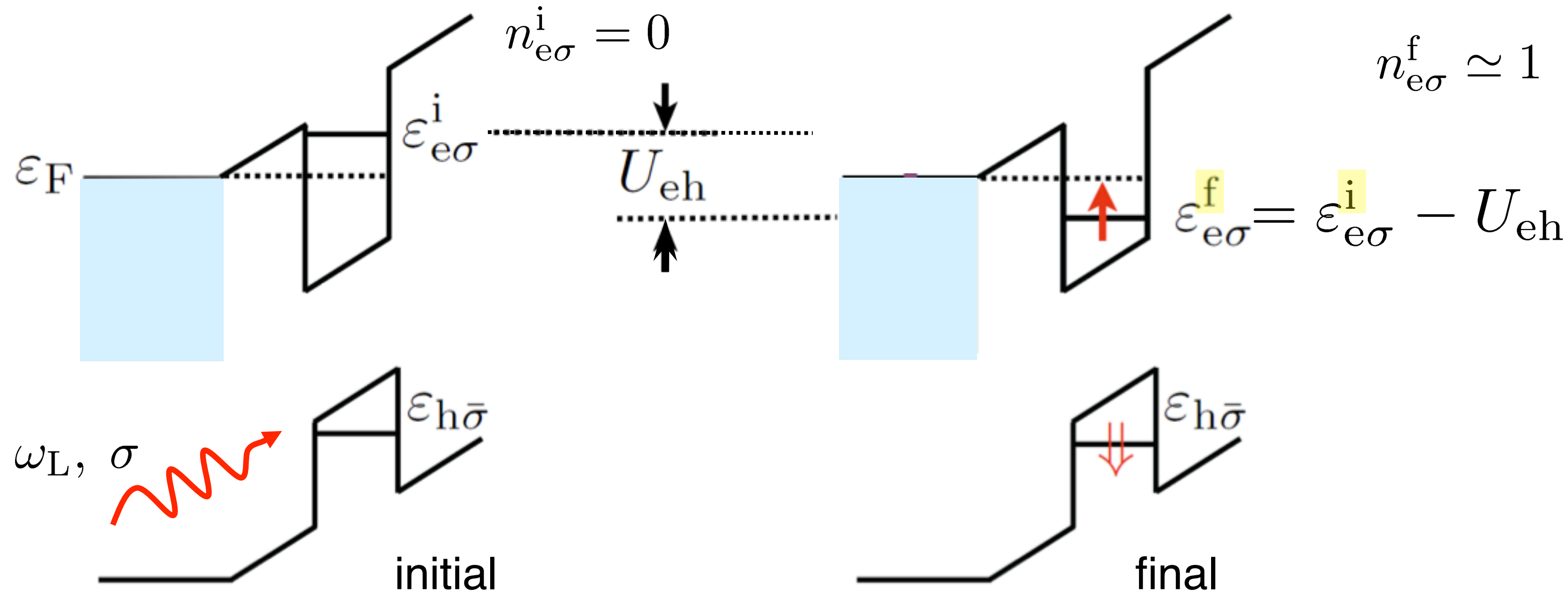


Light-Induced Local “Quantum Quench”

Helmes et al, PRB **72** 125301 (2005)
Tureci et al, PRL **106** 107402 (2011)
Munder et al, PRB **85** 235104 (2012)

$$H_{dot} = \sum_{\sigma} (\varepsilon_{e\sigma}\, n_{e\sigma} + \varepsilon_{h\sigma}\, n_{h\sigma}) +$$
$$+U\, n_{e\uparrow}\, n_{e\downarrow} - \sum_{\sigma\sigma'} U_{eh} n_{e\sigma}\, n_{h\sigma'}$$

$$H_L \sim e^{\dagger}_{\sigma}\, h^{\dagger}_{\bar\sigma}\, e^{-i\omega_L\, t} + h.c.$$



Optical Absorption Spectrum

$$A_\sigma(\omega_L) = 2\pi \sum_{nm} \rho^i_m\, |\langle\, n; f\,|\, e^{\dagger}_{\sigma}\,|\, m; i\rangle|^2\, \delta(\omega_L - E^f_n + E^i_m)$$

Work Statistics!

Silva, PRL **101** 120603 (2008)
Heyl&Kehrein, PRL **108** 190601 (2012)

Pump-Probe Dynamics (soon??)

Connection with Work Statistics

Heyl&Kehrein, PRL **108** 190601 (2012)

☑ Sudden Local Quench:

$$H_i \to H_f \qquad \delta H \sim U_{eh} \sum_\sigma n_{e\sigma}$$
$$H_i \leftarrow H_f$$

☑ Non-equilibrium Correlators

Absorption!

$$P_F(W) = \int \frac{dt}{2\pi}\, e^{iWt} \langle e^{iH_i t} e^{-iH_f t} \rangle_i \sim A(\nu = W)$$

$$P_B(W) = \int \frac{dt}{2\pi}\, e^{iWt} \langle e^{iH_f t} e^{-iH_i t} \rangle_f \sim E(\nu = W)$$

Emission!

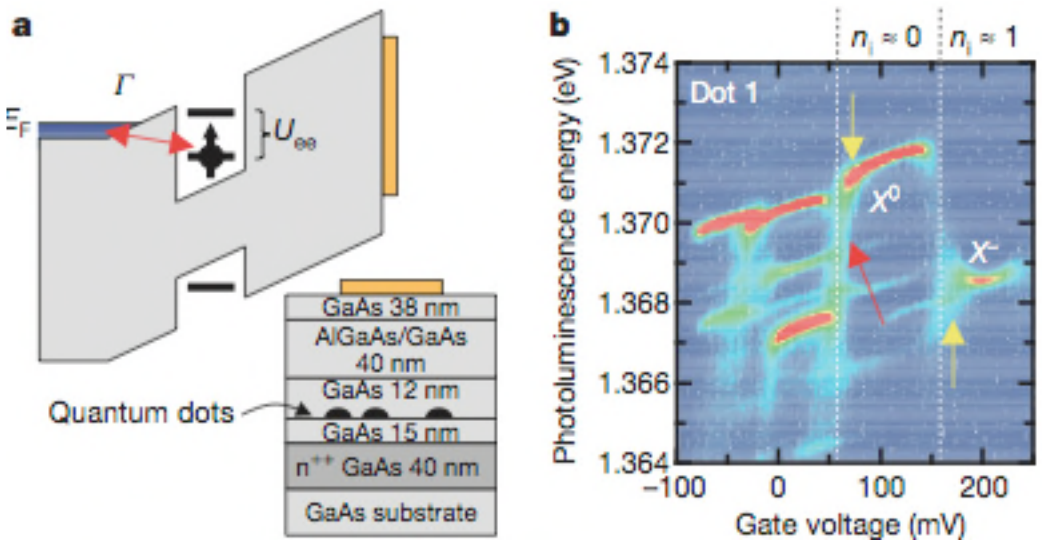
☑ Crooks Relation

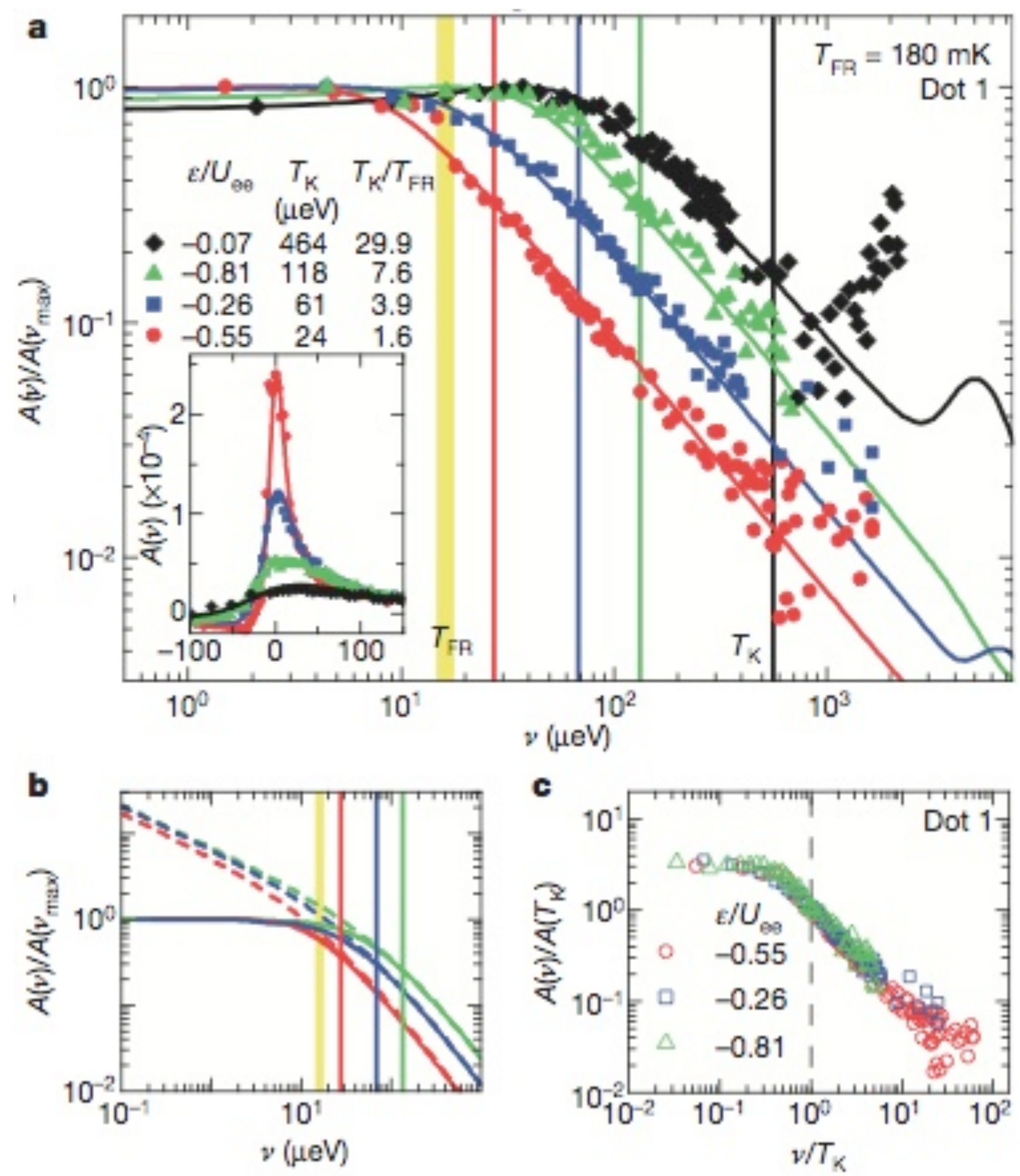
$$\frac{A(\nu)}{E(\nu)} \sim e^{\beta\,(\nu - \Delta F)}$$

NB: Also in a single shot, for weak perturbation

Kondo Effect in the Optical Absorption Spectrum

C. Latta et *al.*, Nature **474**, 627 (2011)





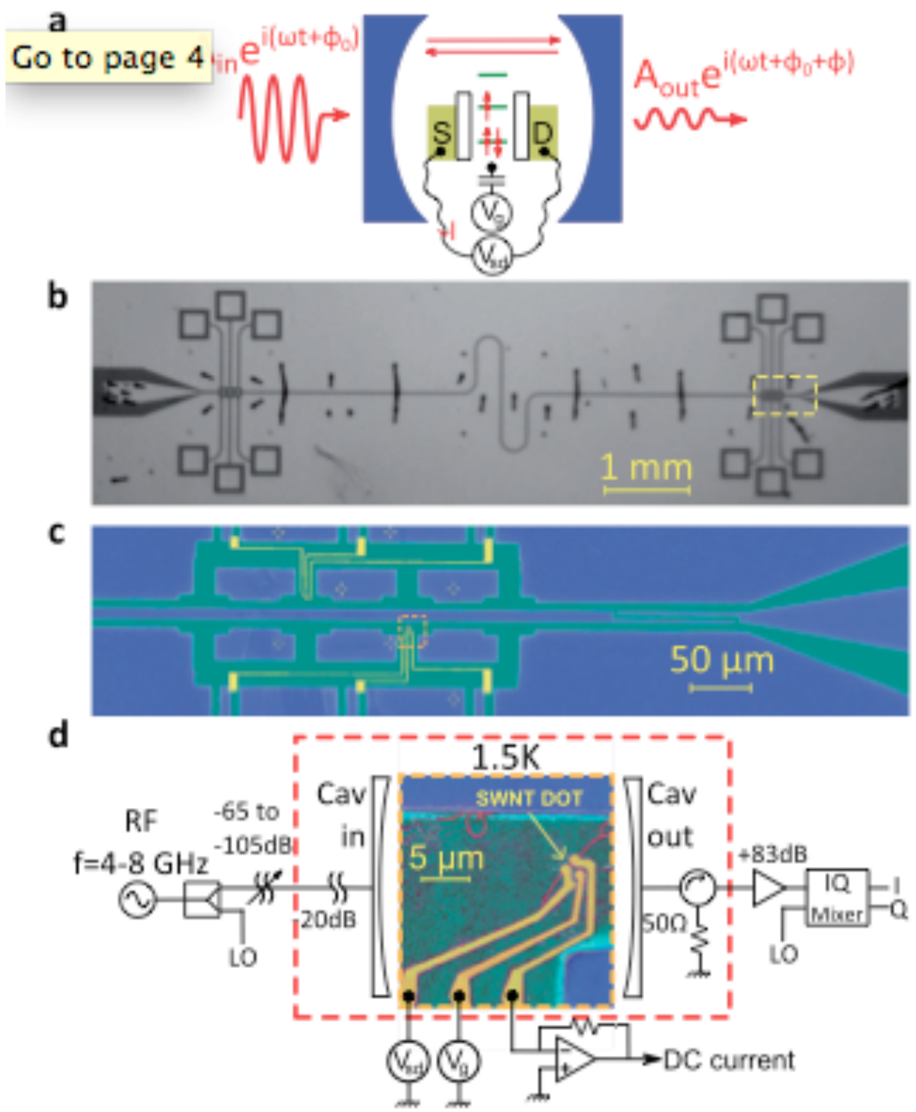
☑ Edge Singularity in the Optical Absorption Spectrum!

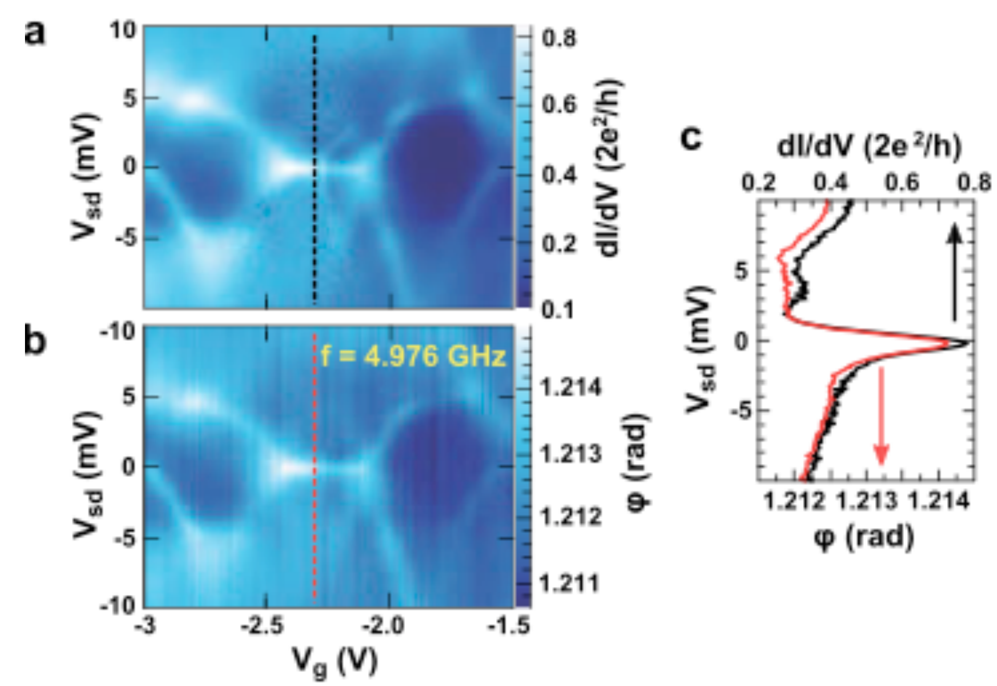
$$A(\nu) \sim \nu^{-\eta}$$

☑ Exponent tunable by magnetic field/gate voltage

Toward Hybrid Light-Matter Quantum Impurity Systems

Delbecq et al , PRL (2011) ENS-LPA (Kontos Lab)

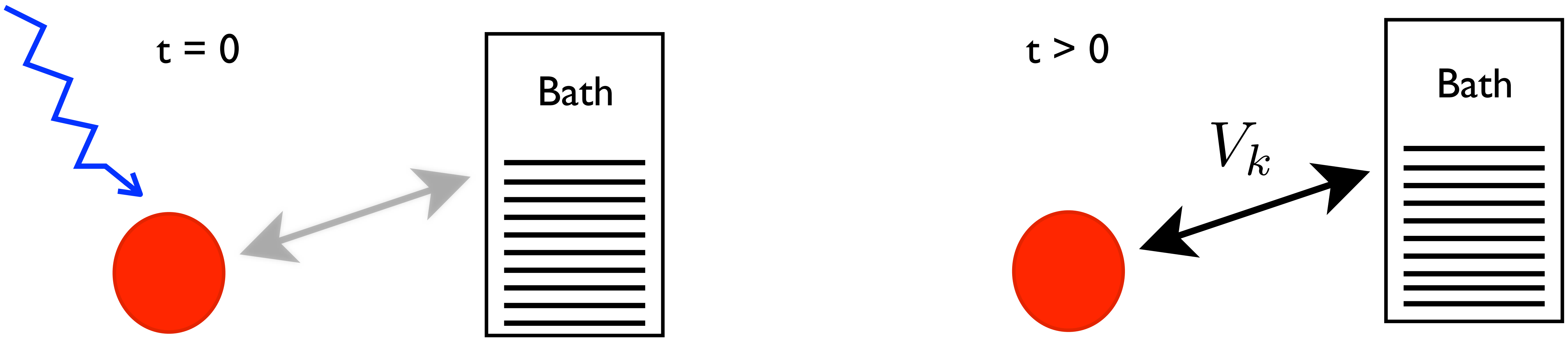




☑ Coupling Electrons with quantum light (Photons)

☑ Response of Kondo State to microwave signals

Theoretical Question & Quick Answers



☑ Long time dynamics after a local perturbation: does the system thermalize? How?

$$\langle O \rangle_t = Tr[\rho_0\, e^{iHt}\, O\, e^{-iHt}] \qquad t \to \infty \qquad \langle O \rangle_t = \langle O \rangle_{eq}\ ???$$

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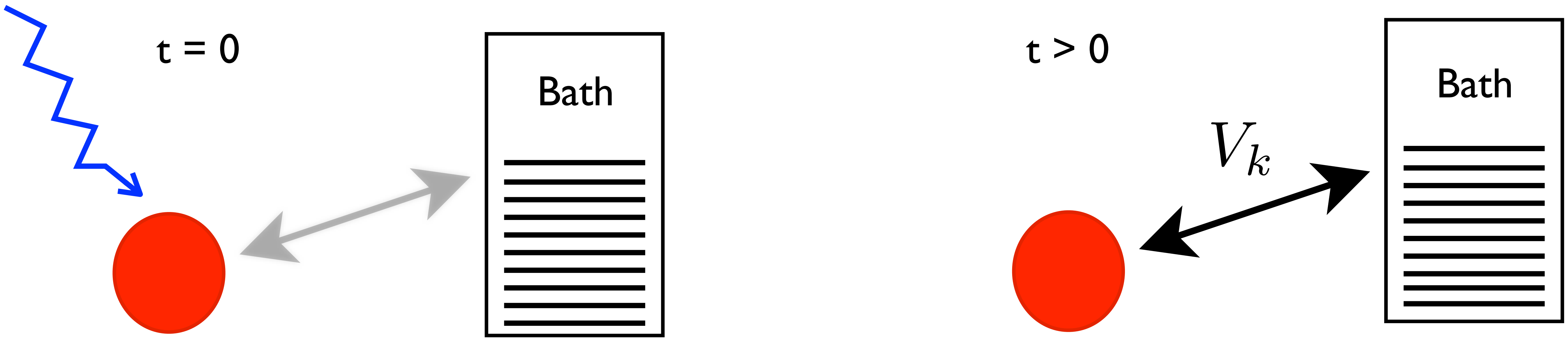

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☑ YES!

- Conserved quantities (energy, particle number, spin,..) flow across the system due to V_k
- Reservoir is infinite and gapless (and if proper order of limit is taken)

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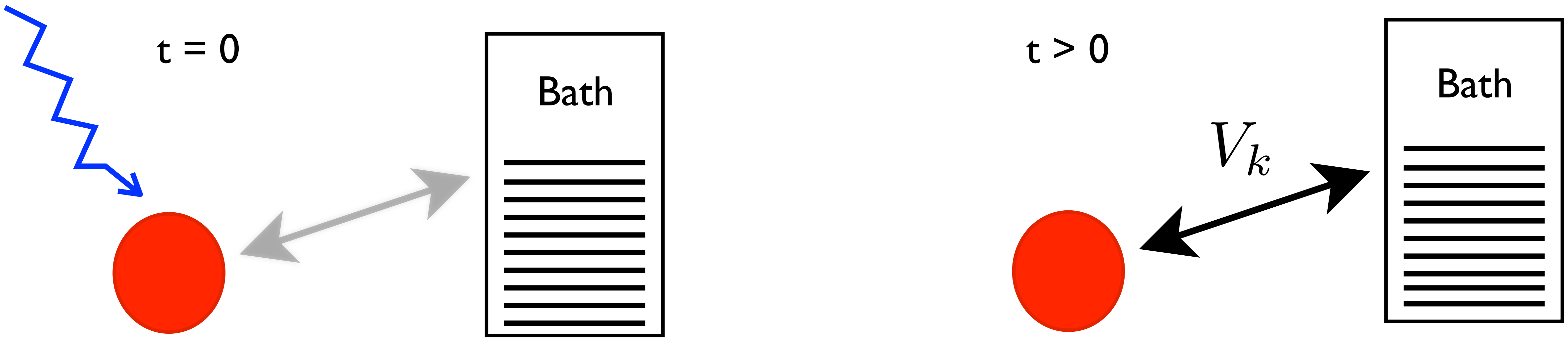

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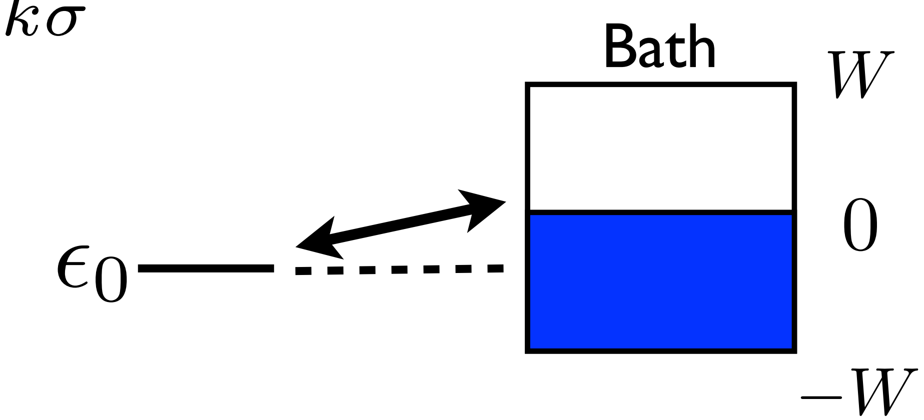
NO!

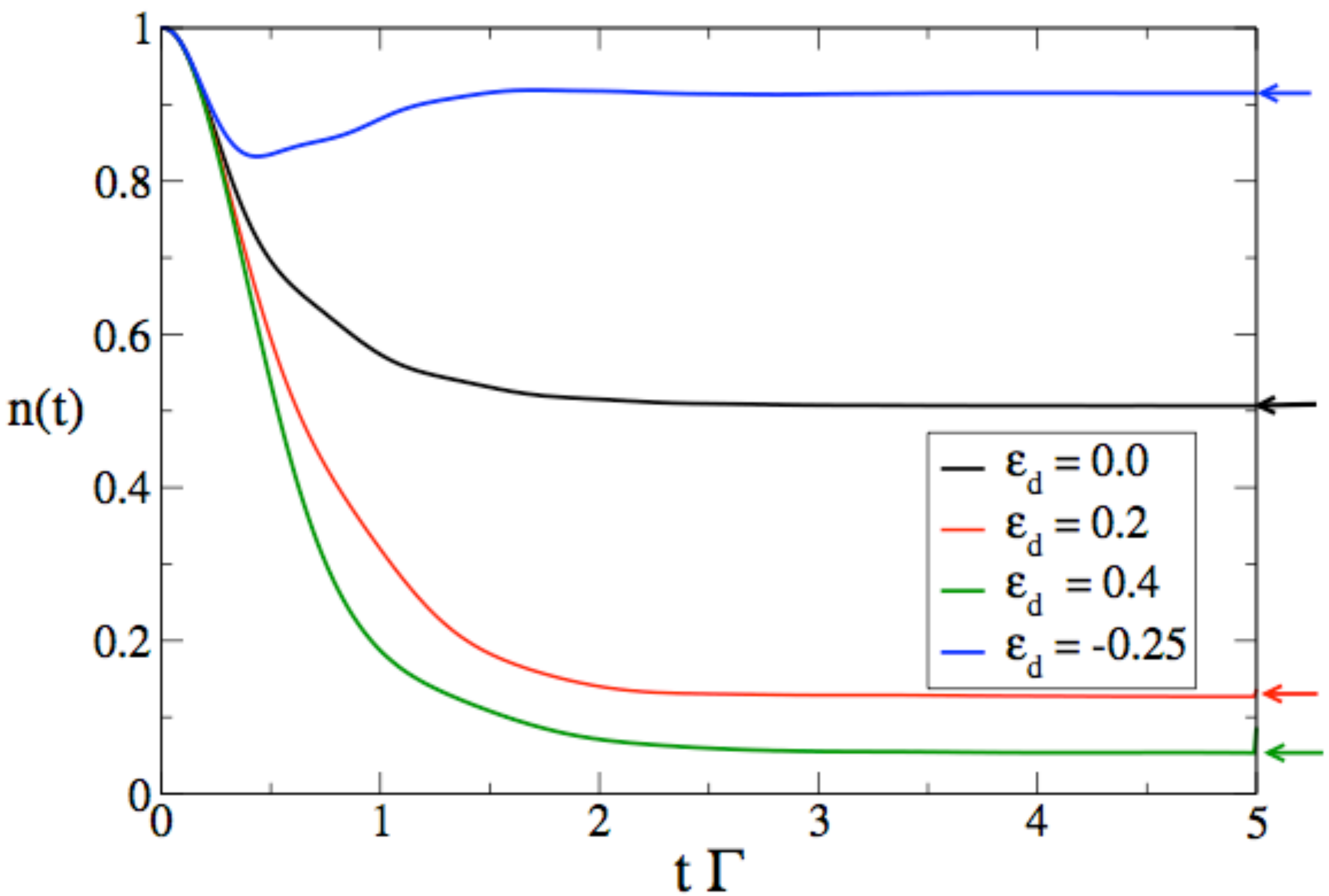
- Anderson Impurity Model (or similar) is integrable -- Bethe Ansatz Solvable

Example (simple): Electrons coupled to a Fermi Sea

$$H = \epsilon_0 \sum_{\sigma} c^\dagger_\sigma c_\sigma + \sum_{k\sigma} \epsilon_k f^\dagger_{k\sigma} f_{k\sigma} + \sum_{k\sigma} V_k \left(c^\dagger_\sigma f_{k\sigma} + h.c. \right)$$



Model is quadratic, solution easy!



$$\Gamma = \pi \sum_k V_k^2 \, \delta(\epsilon_k)$$

Long time dynamics: relaxation to the ground state $t \gg 1/\Gamma$

End of the story??

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Not Yet ..!!

End of the story??

Not Yet ..!!

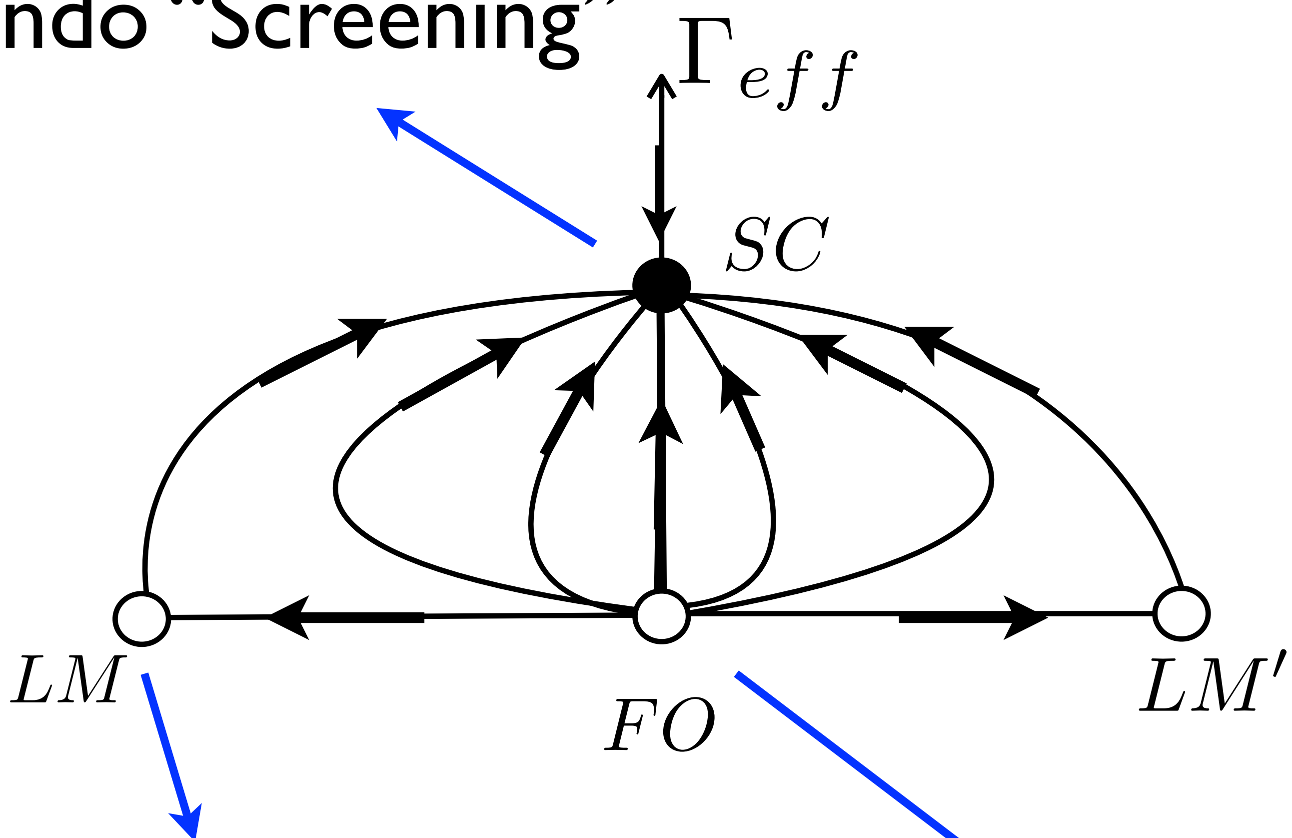
- We are assuming system+bath always 'effectively' coupled
- Local Many Body Interactions can change this picture?

Anderson impurity model...

$$H = \boxed{\frac{U}{2}(n-1)^2} + \sum_{k\sigma} \epsilon_k \, f^\dagger_{k\sigma} \, f_{k\sigma} + \sum_{k\sigma} V_k \, \left(c^\dagger_\sigma \, f_{k\sigma} + h.c.\right)$$

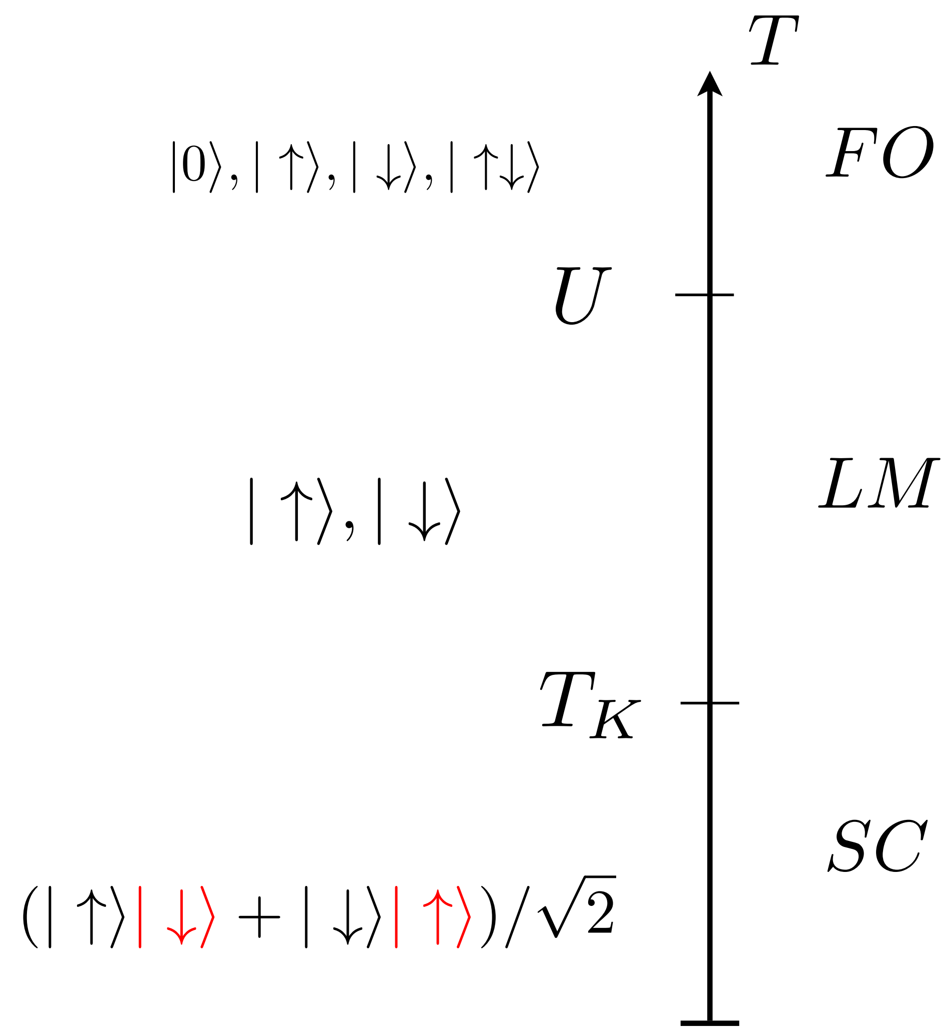
Anderson, Kondo, Haldane, Nozieres, Wilson,...
(~1960-1975)

Strong Couplig FP:
Kondo “Screening”



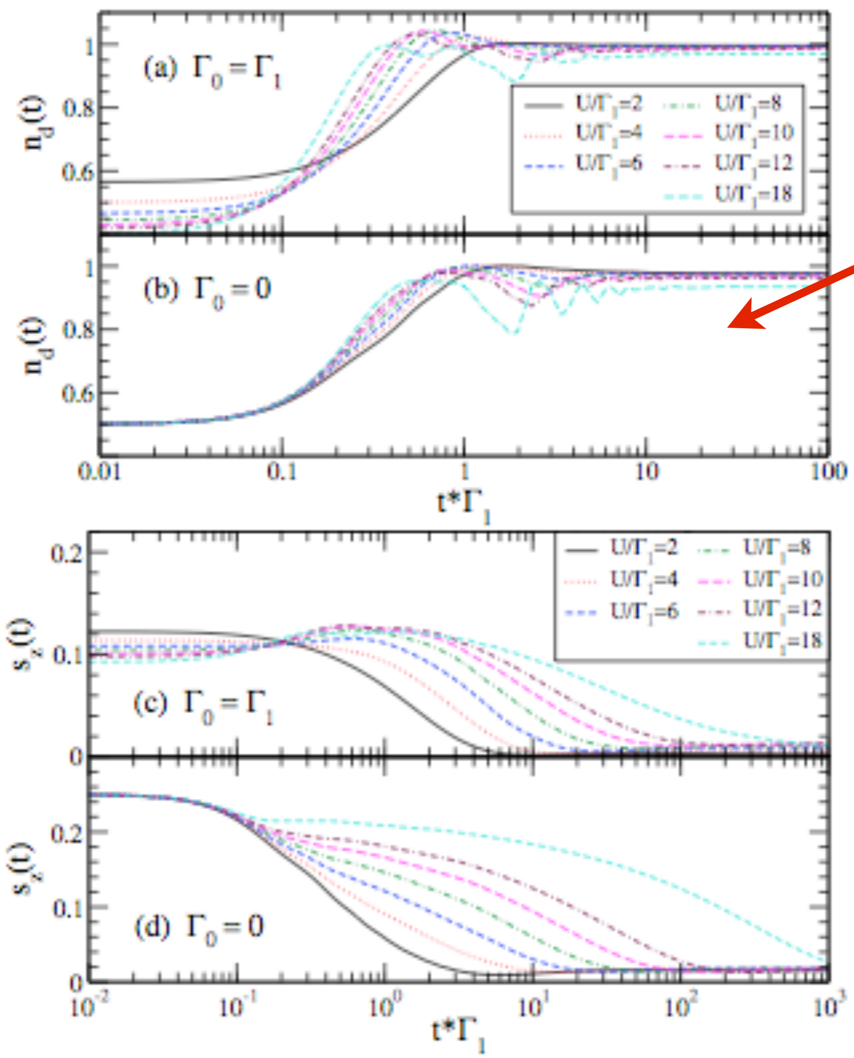
Local Moment FP:
Spin Fluctuations

Free Orbital FP:
Charge Fluctuations

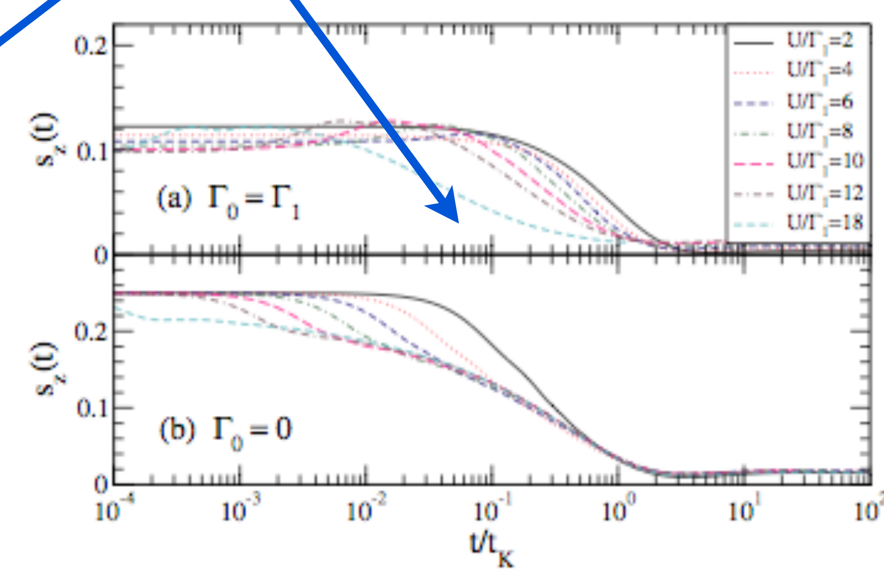


... and its out of equilibrium dynamics

TD-NRG: Anders&Schiller PRL(2005)



- Charge relaxation time $t_{charge} \sim 1/\Gamma$
- Spin relaxation time $t_{spin} \sim 1/T_K$



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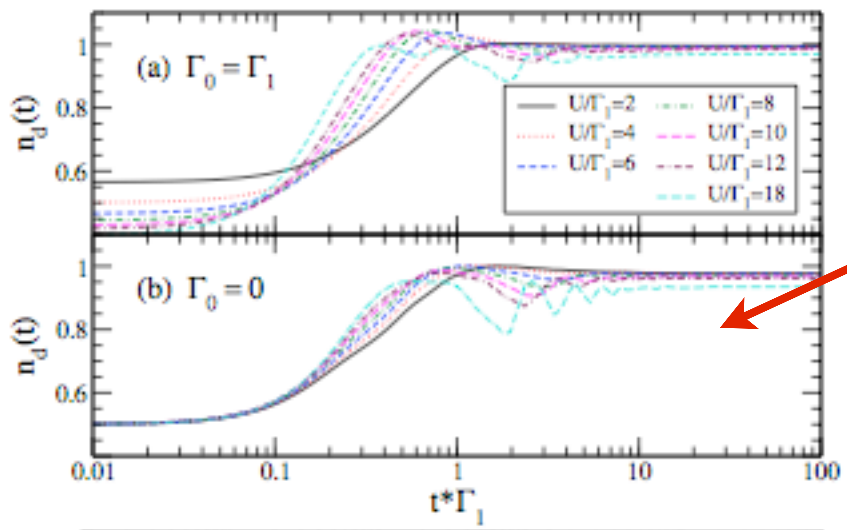

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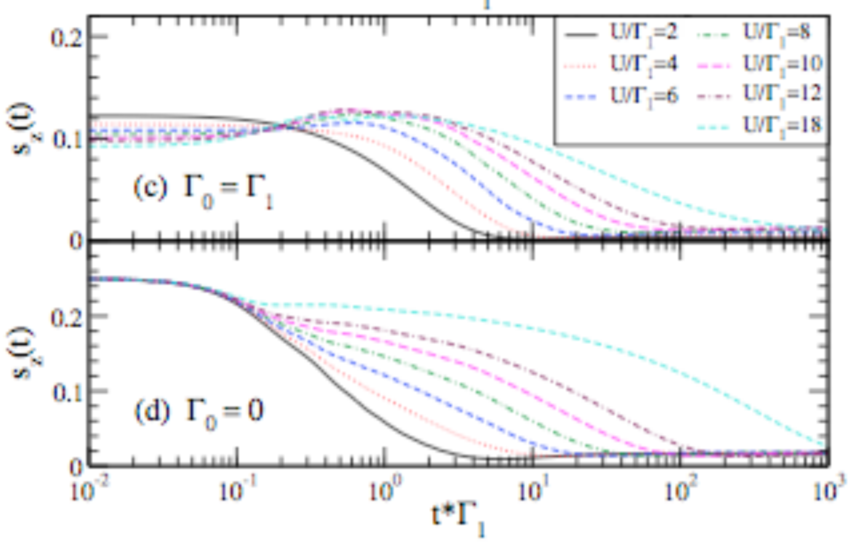
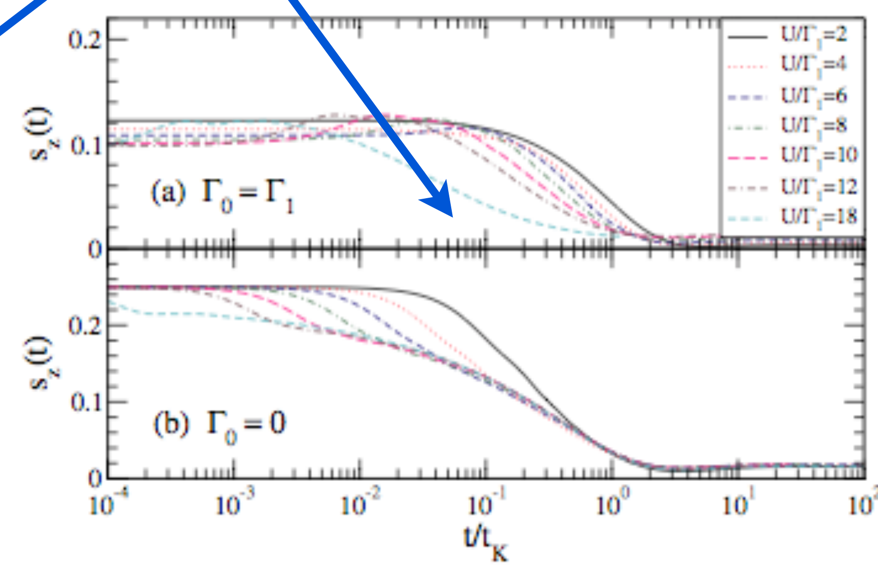
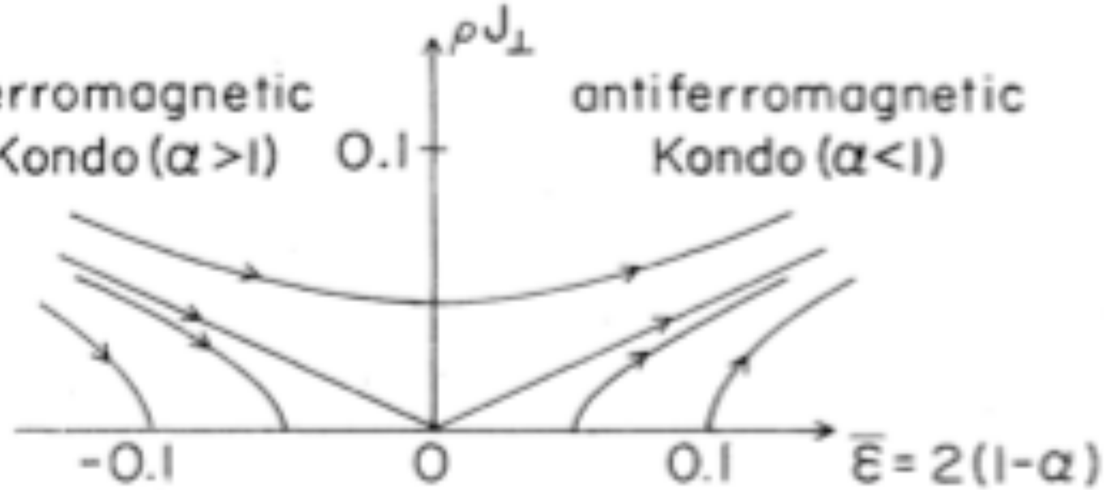




Take-home message:

Kondo Effect, always thermal, but RG flow matters!

Ferromagnetic Kondo Model

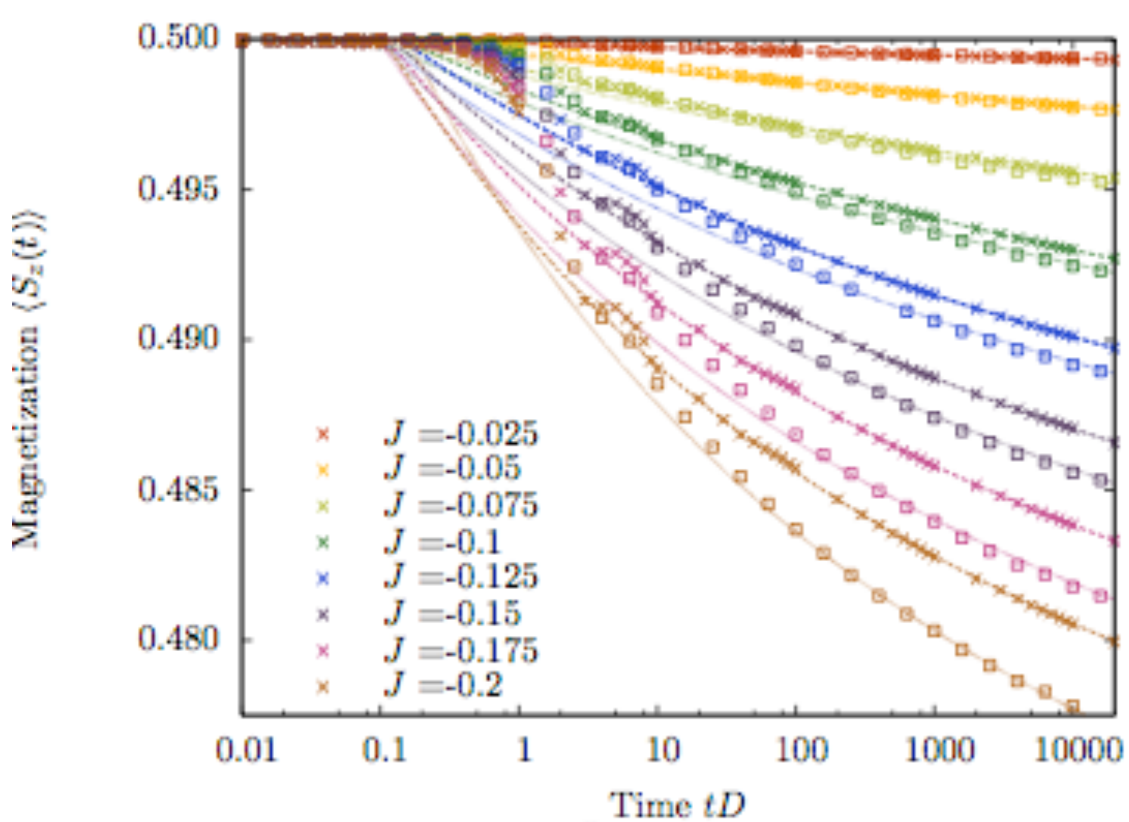


$$J_\perp \to 0$$

$$J_\perp(\Lambda) = J/(1 + \rho_F \, J \, log(\Lambda/D))$$

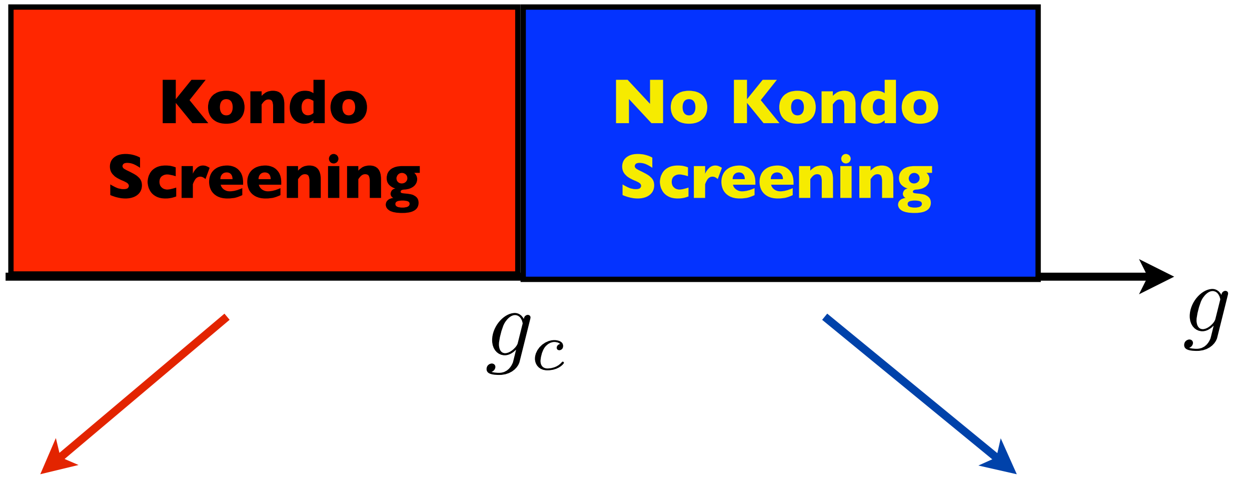
Quench Dynamics from a decoupled initial state

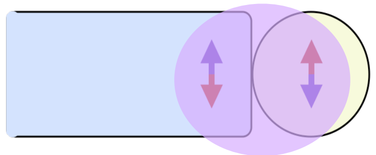
Hackl et al, PRL **102** 196101 (2009)
Flow-Equation, tdNRG



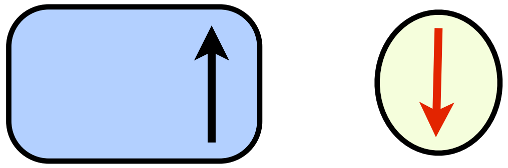
☑ Relaxation, yet very slow
☑ Memory of Initial Condition

To Screen or Not to Screen...





Flow to Strong Coupling FP
Thermalization at long times

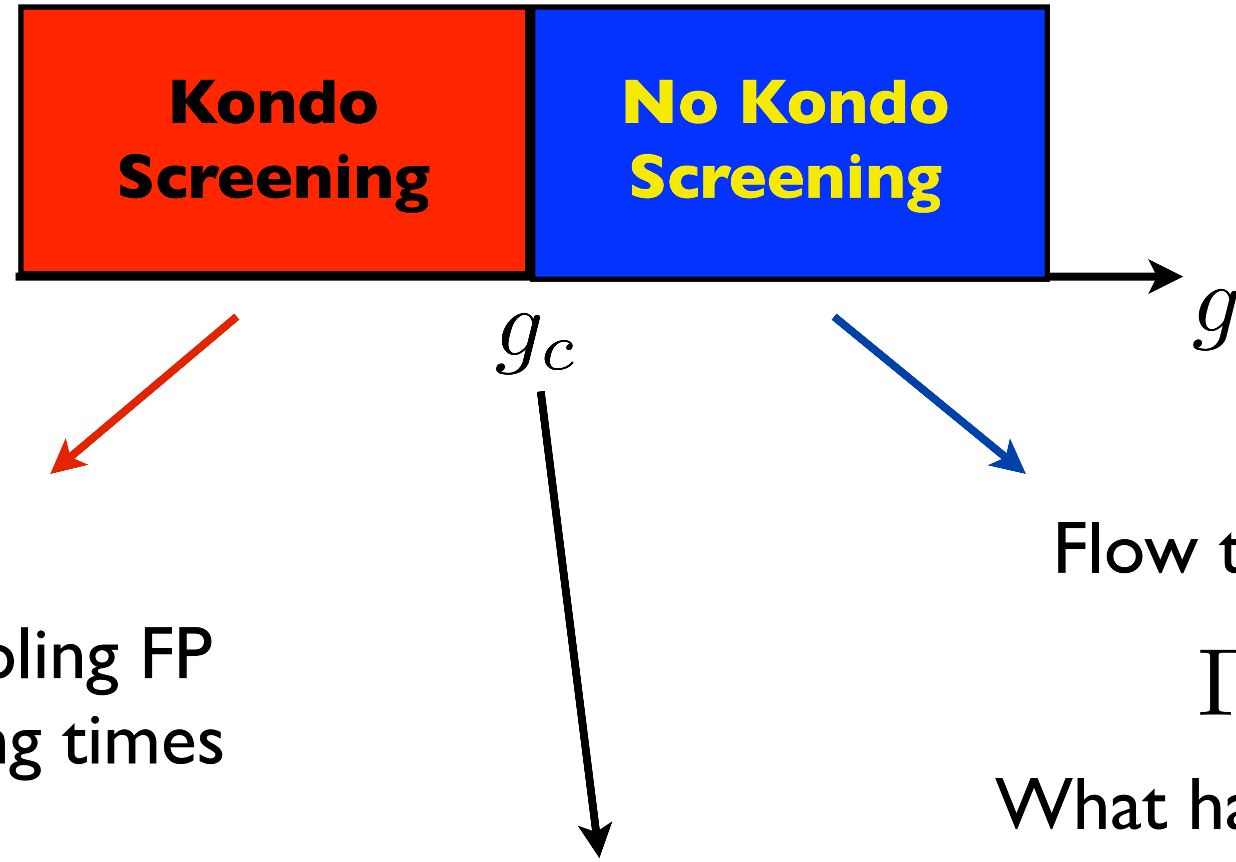


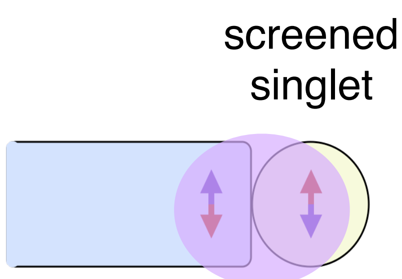
Flow to Local Moment FP

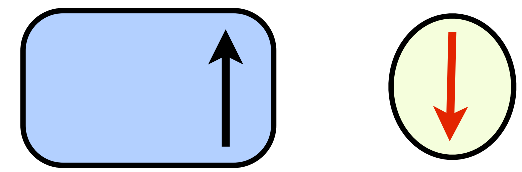
$$\Gamma_{eff}(t) \rightarrow 0$$

What happens at long times??

To Screen or Not to Screen...







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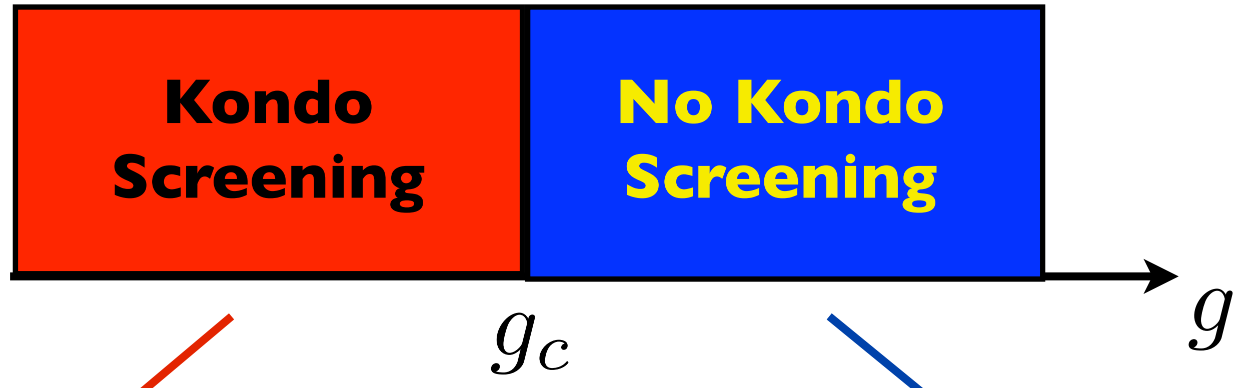

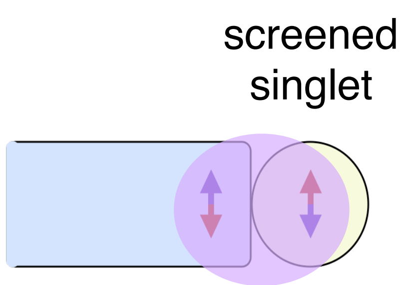

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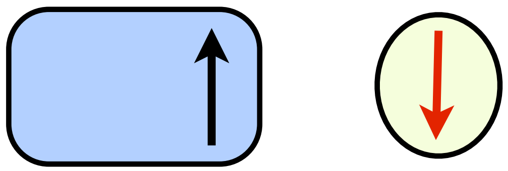

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How these dynamical regimes are connected?

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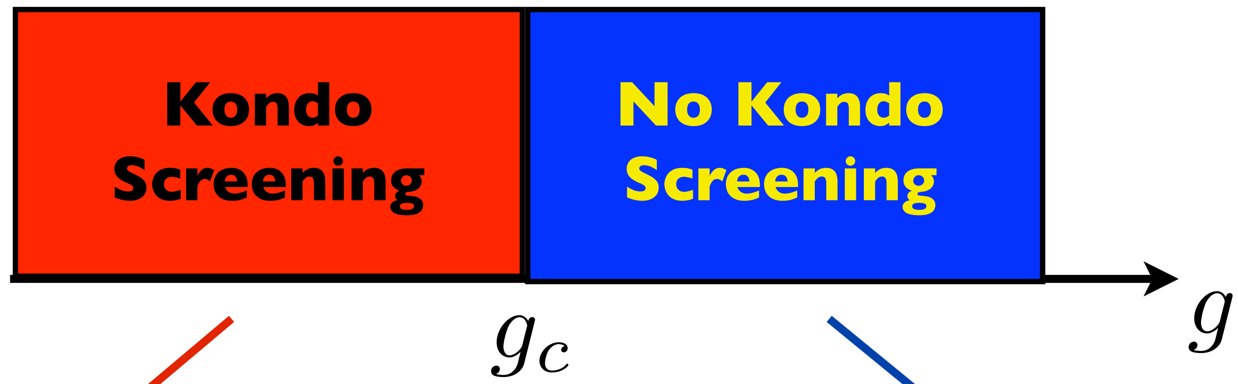

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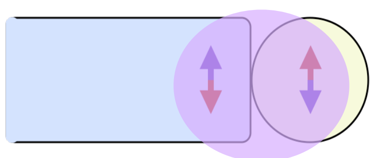

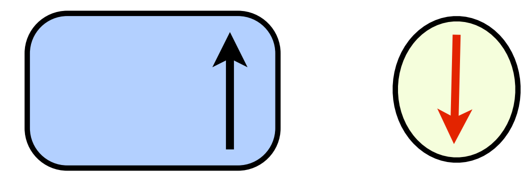

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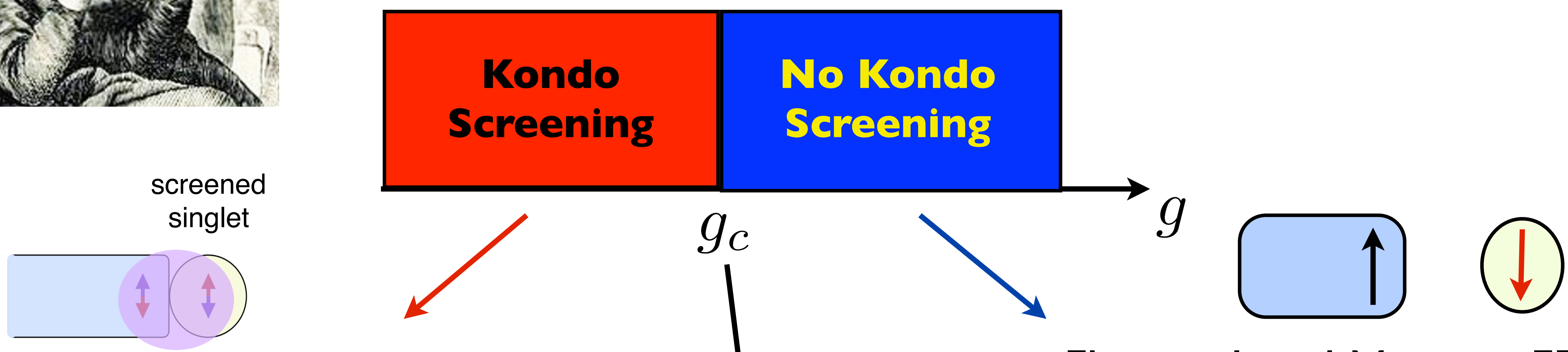

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- ☑ Pseudo-Gap Anderson Model

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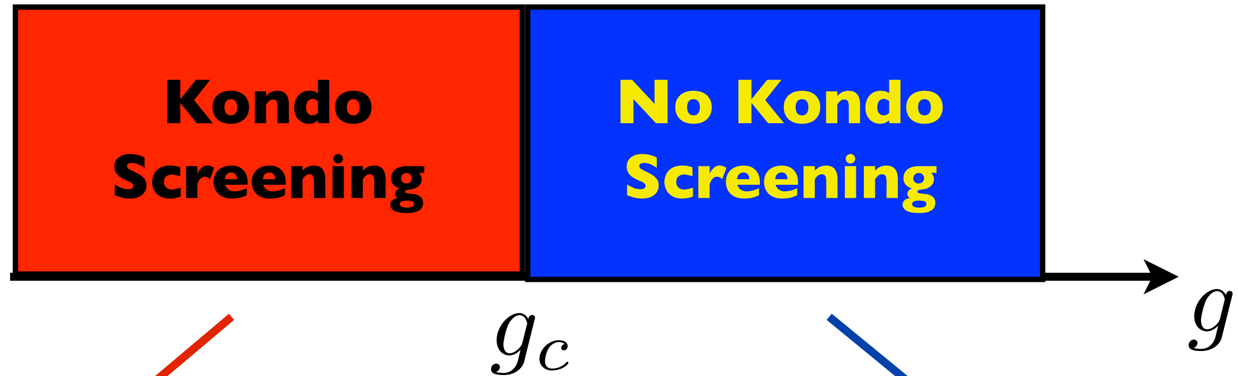

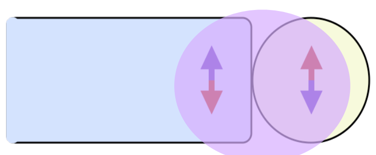

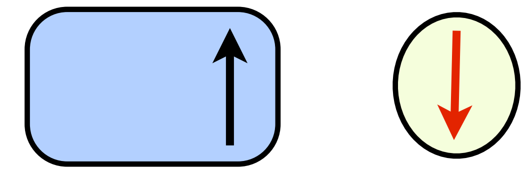

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Fradkin, Ingersent, Vojta, ...

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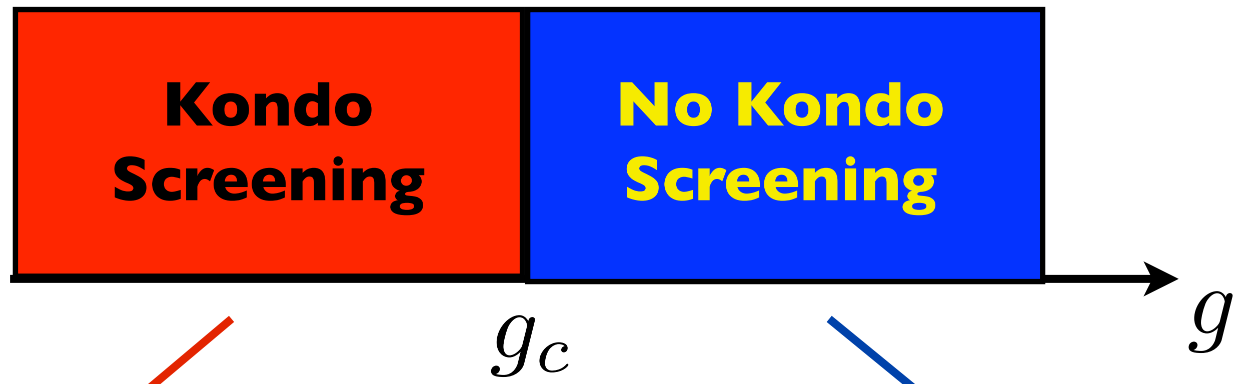

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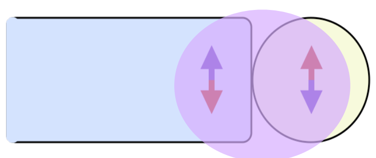

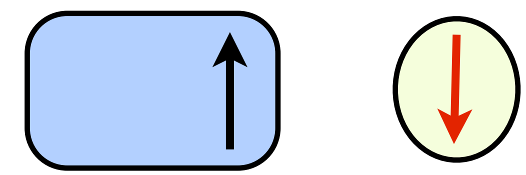

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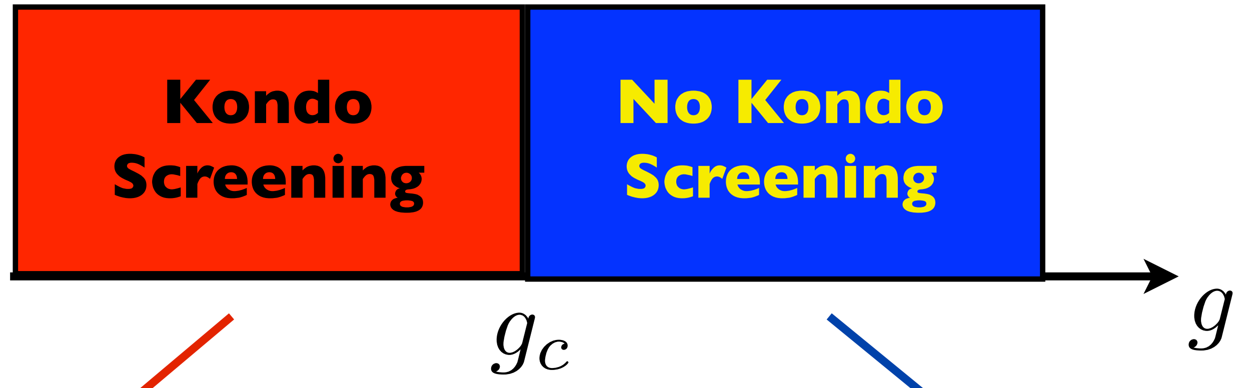
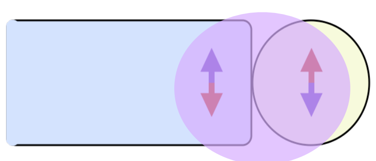
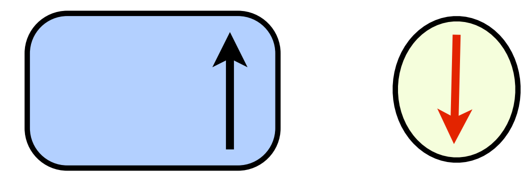
- ☑ Two Impurity Kondo Model — Jones&Varma, Jones,Millis&Kotliar, Affleck,Ludwing&Jones,..
- ☑ Pseudo-Gap Anderson Model — Fradkin, Ingersent,Vojta, ...

To Screen or Not to Screen...



screened singlet





Flow to Local Moment FP

$$\Gamma_{eff}(t) \to 0$$

What happens at long times??

Flow to Strong Coupling FP
Thermalization at long times

How these dynamical regimes are connected?

Relevant Examples:

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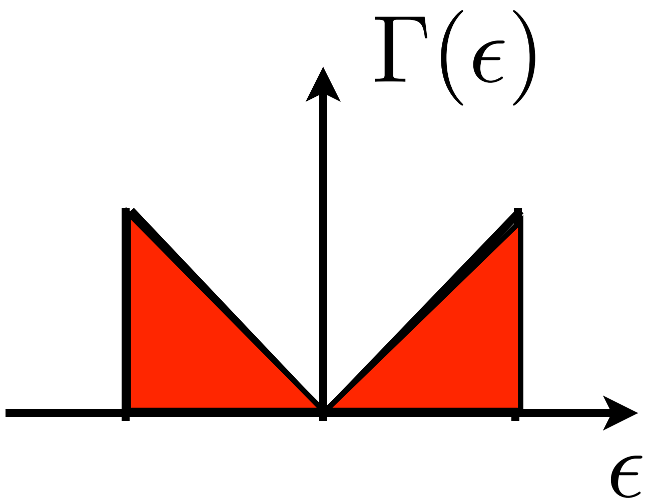
Anderson Impurity in a power-law bath

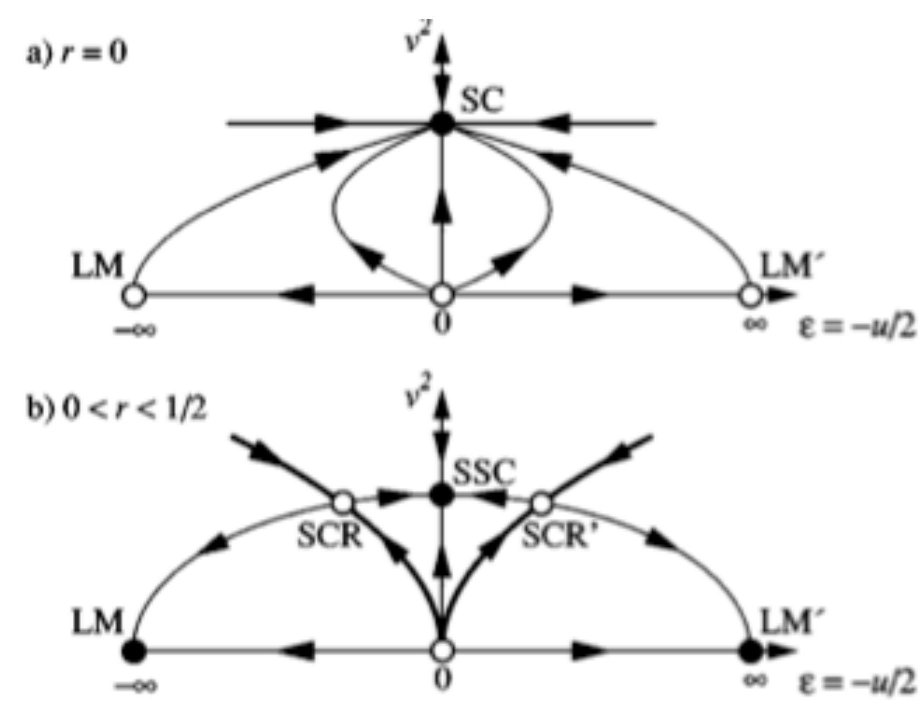
$$H = \frac{U}{2}(n-1)^2 + \sum_{k\sigma} \epsilon_k\, f^\dagger_{k\sigma} f_{k\sigma} + \sum_{k\sigma} V_k\, (c^\dagger_\sigma f_{k\sigma} + h.c.)$$

AIM in a pseudo-gap

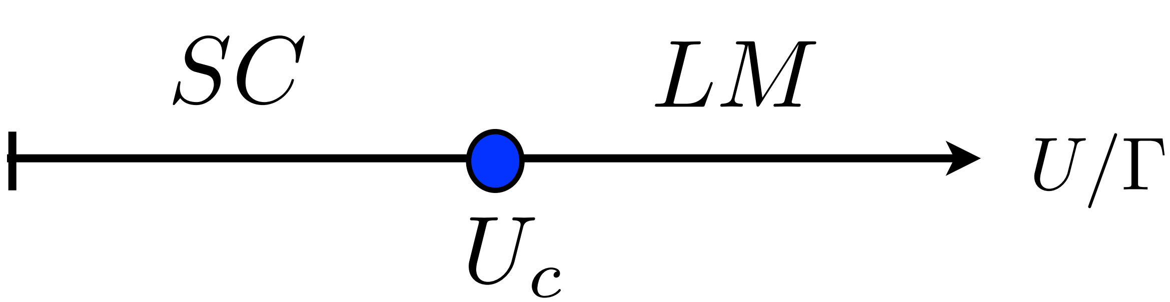
Fradkin, Ingersent, Vojta, Polkovnikov,..



$$\Gamma(\epsilon) \sim |\epsilon|^r$$



$r < 1/2$ Quantum Critical Point!



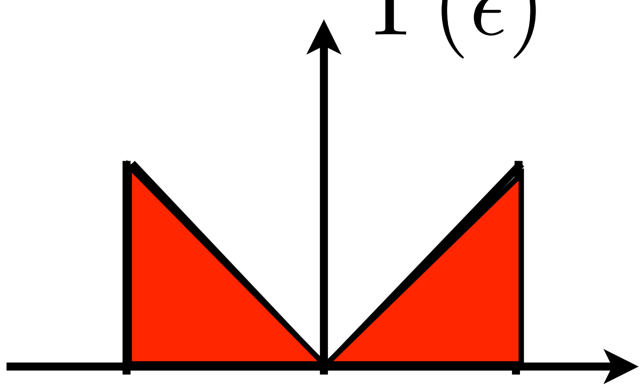
No QCP for $r > 1/2$

Out of Equilibrium Dynamics

$$H = \frac{U}{2}(n-1)^2 + \sum_{k\sigma} \epsilon_k \, f^\dagger_{k\sigma} f_{k\sigma} + \sum_{k\sigma} V_k \, (c^\dagger_\sigma f_{k\sigma} + h.c.)$$

Initial Condition

- ✦ No Coupling with Bath $V_k = 0$
- ✦ No Local Interaction $U = 0$



$\Gamma(\epsilon) \sim |\epsilon|^r$

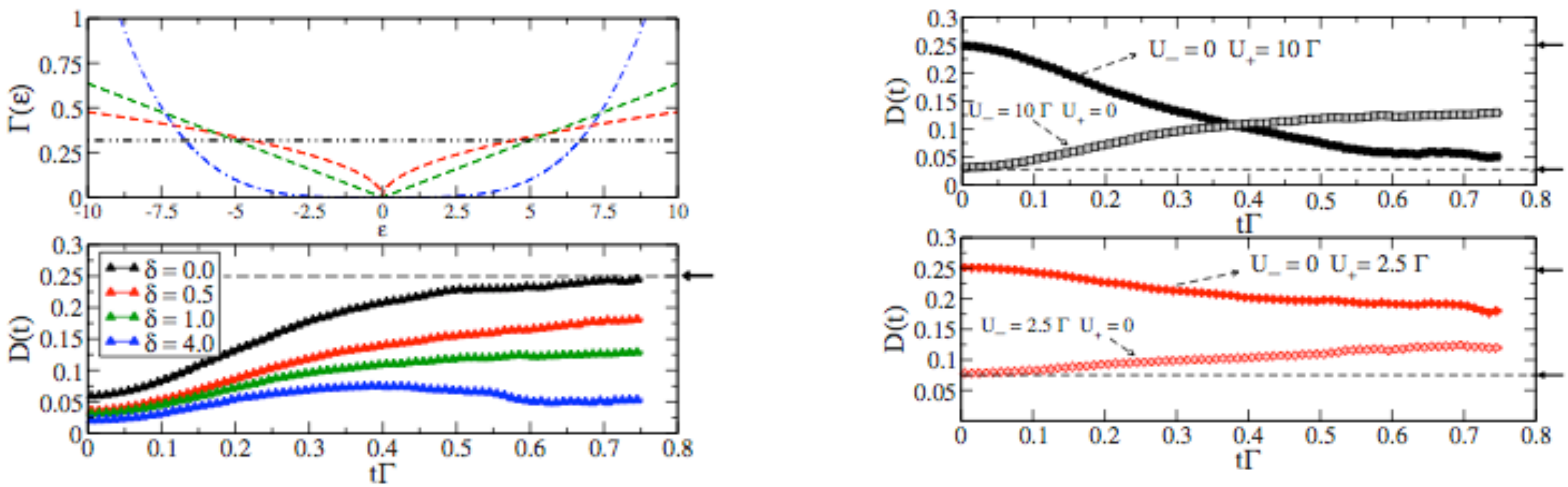
Real-Time Dynamics: how to solve?

- ☐ time-dep NRG → Finite Size Effects due to Wilson Chain
  cfr A. Rosch, Eur. Phys. J. B **85** 6 (2012)
- ☑ diagrammatic MC
- ☑ time-dep variational method

$$\frac{dN}{d\mu} \sim N \qquad \frac{dE}{dT} \sim \frac{1}{log\Lambda}$$

Dynamics with Real-Time QMC

MS, PRB **81**, 103232 (2010)



- Seemingly slow dynamics for large $r > 1/2$ but...
- Short time dynamics <u>only</u>, due to "sign" problem
- Finite Temperature in the bath, no QCP!

A Time Dependent Variational Approach

$$\delta \int dt \, \langle \Psi(t) | \, i\partial_t - \mathcal{H} | \Psi(t) \rangle = 0$$

Ansatz on the time dep
Many Body Wave Function

$$|\Psi(t)\rangle = e^{iHt} |\Psi(0)\rangle \simeq P(t) \, |\Phi(t)\rangle$$

Variational parameters:

$$P(t) = \sum_{a=|0\rangle,..,|\uparrow\downarrow\rangle} \lambda_a(t) \, e^{i\phi_a(t)} \, | \, a \rangle\langle \, a |$$

Gutzwiller WF:
change weight of atomic configurations

$$i\partial_t |\Phi(t)\rangle = \mathcal{H}_\star(t) |\Phi(t)\rangle$$

Non interacting model with $V_k(t)$

$$\mathcal{H}_\star(t) = \sum_{k\sigma} \epsilon_k \, f^\dagger_{k\sigma} \, f_{k\sigma} + \sqrt{Z(t)} \sum_{k\sigma} V_k \, \left(c^\dagger_\sigma \, f_{k\sigma} + h.c. \right)$$

A Time Dependent Variational Approach

Dynamics of Variational Parameters

$D(t), \phi(t)$

$$\dot{D} = 4\,\mathcal{E}_{hyb}(t)\,\sqrt{D\,(1/2 - D)}\,sin\phi$$

$$\dot{\phi} = U + \mathcal{E}_{hyb}(t)\,\frac{1-4D}{\sqrt{D\,(1/2-D)}}\,cos\phi$$

$$\mathcal{E}_{hyb}(t) = \sum_{k\sigma} V_k\,\langle\Phi(t)|\,\left(f^{\dagger}_{k\sigma}\,c_\sigma + h.c.\right)|\Phi(t)\rangle$$

Dynamics of non-equilibrium bath

$$i\partial_t|\Phi(t)\rangle = \mathcal{H}_\star(t)|\Phi(t)\rangle$$

$$\mathcal{H}_\star(t) = \sum_{k\sigma}\epsilon_k\,f^{\dagger}_{k\sigma}\,f_{k\sigma} + \sqrt{Z(t)}\sum_{k\sigma}V_k\,\left(c^{\dagger}_\sigma\,f_{k\sigma} + h.c.\right)$$

Variational Ground State

$$|\Psi\rangle = \left(\sum_{a=|0\rangle,\dots,|\uparrow\downarrow\rangle} \lambda_a \, |a\rangle\langle a| \right) |\Phi\rangle$$

Ground-State of $\mathcal{H}_\star$

$$\mathcal{H}_\star = \sum_{k\sigma} \epsilon_k \, f^\dagger_{k\sigma} \, f_{k\sigma} + \sqrt{Z} \sum_{k\sigma} V_k \, \left(c^\dagger_\sigma \, f_{k\sigma} + h.c. \right)$$

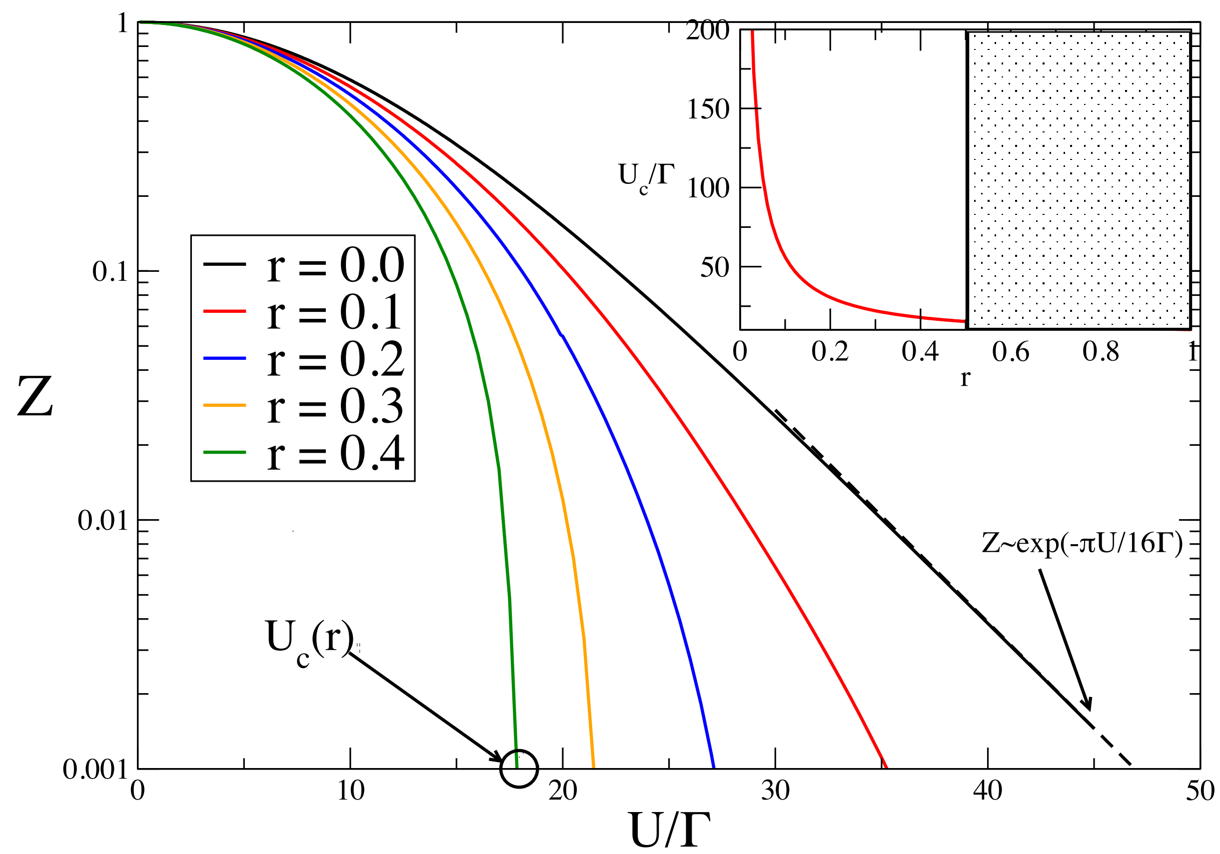
Variational Energy

$$E[\lambda_a, \sqrt{Z}] = \langle \Psi | \mathcal{H} | \Psi \rangle$$

A QCP between Kondo and Local moment regime

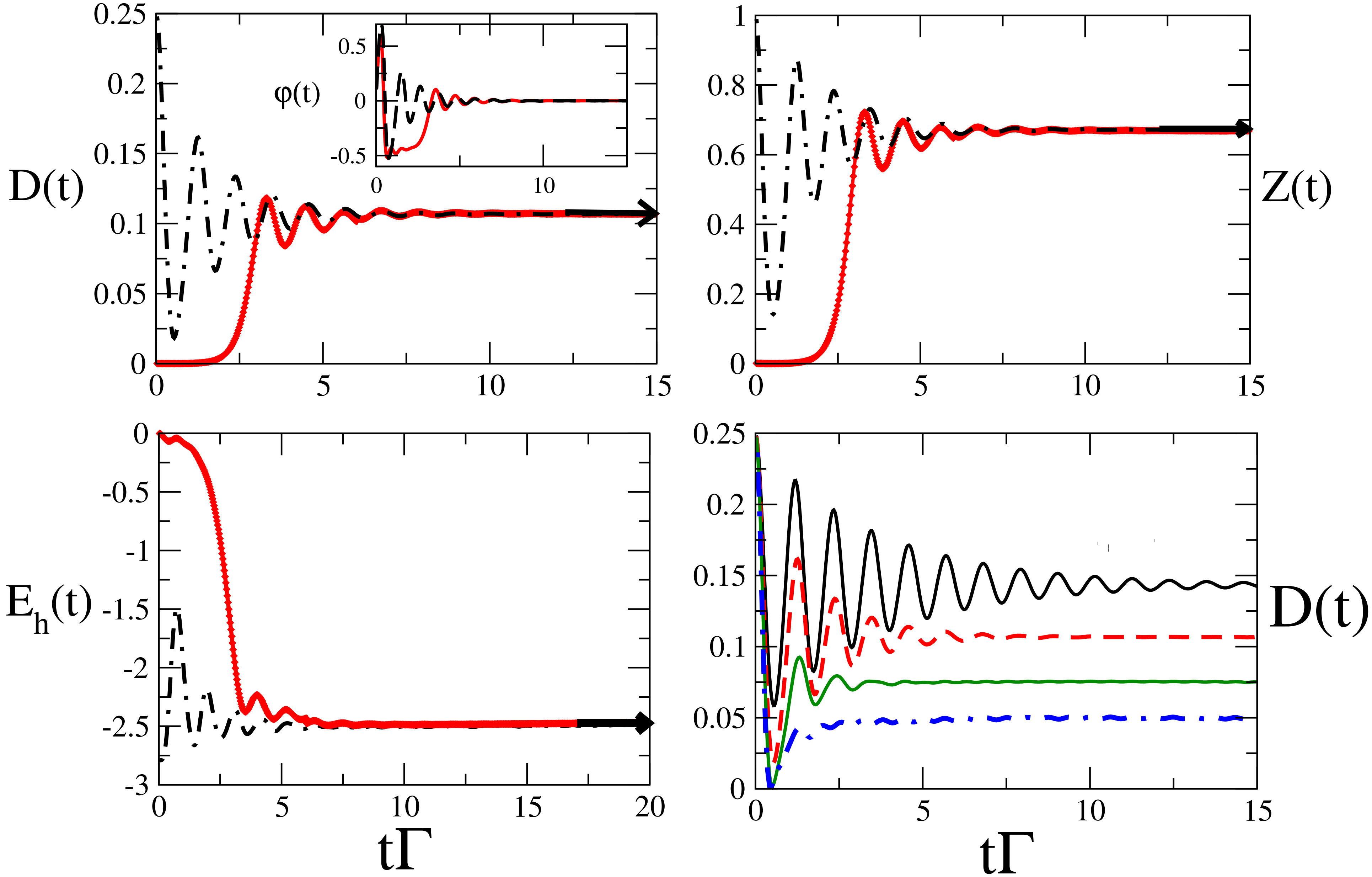
$$U_c/\Gamma = \frac{16(1+r)}{\pi \, r}$$

NB: $U_c \to \infty$ for $r \to 0$



Dynamics in the Kondo Screened Phase

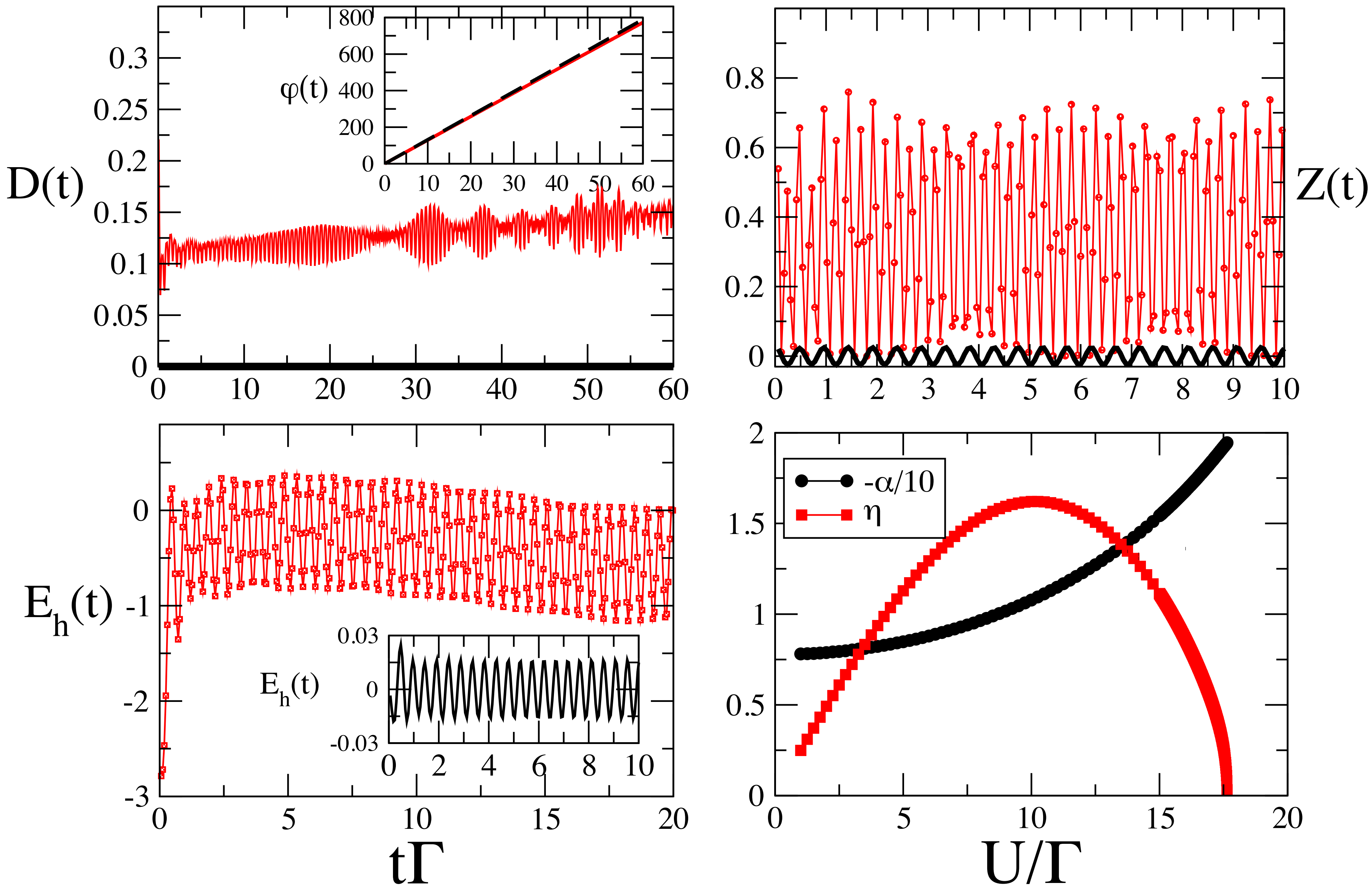
$r = 0.4 \quad U < U_c(r)$



☑ Relaxation to the thermal steady state

Dynamics in the Local Moment Phase

$U > U_c(r)$



☑ No Damping, No Relaxation, No Steady State

How these regimes are connected?

- ☑ In the Kondo Phase, linearize dynamics around steady state

$$\delta \ddot{O} = \alpha \delta O + \eta \delta E_{hyb}$$

$$\delta O = O(t) - O_\star$$

Equilibrium Properties:

$$\eta \sim E^\star_{hyb} \qquad \alpha \sim -E^{\star 2}_{hyb}/Z_\star \qquad E^\star_{hyb} \sim \sqrt{Z_\star}$$

- ☑ Relaxation time diverges at the quantum critical point!

$$\tau_{rel} \sim 1/\sqrt{Z_\star} \sim |U - U_c(r)|^{-1/2}$$

- ☑ Dynamical transition between thermal and non thermal regime

Conclusions

- Thermalization in Quantum Impurity Models after local perturbations

- Long-Time physics is sensitive to Low-Energy features, i.e. RG Fixed Points, Kondo Effect

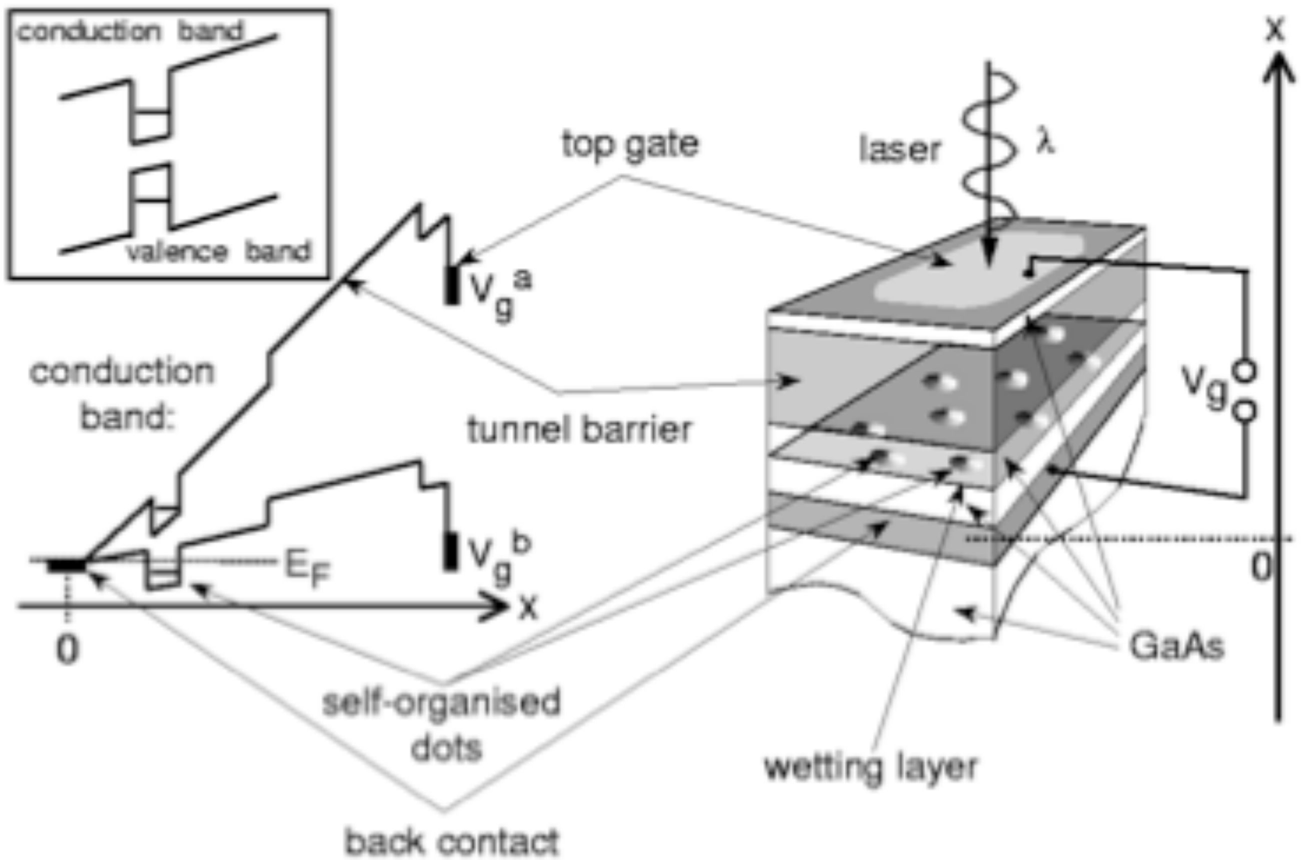
- Non trivial Dynamics across a Kondo-to-Local Moment QCP

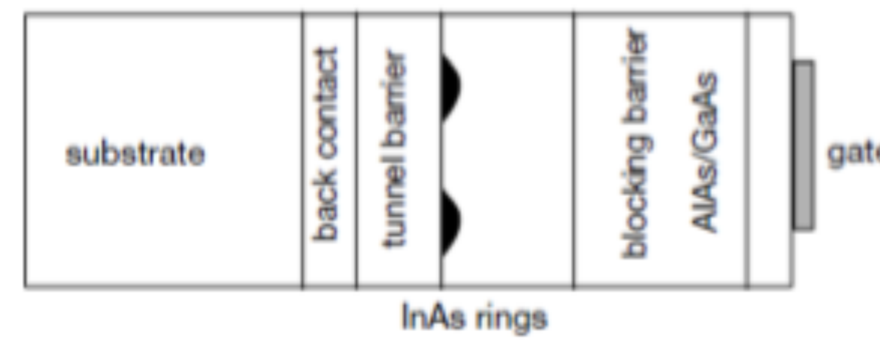
Open Questions:

- ☑ Role of Quantum Fluctuations: damping in the LM?
- ☑ Correlation Functions (Aging?), Statistics of Work
- ☑ Other Models: 2IKM (Bosonization?),...

Thanks!

Experimental Setup



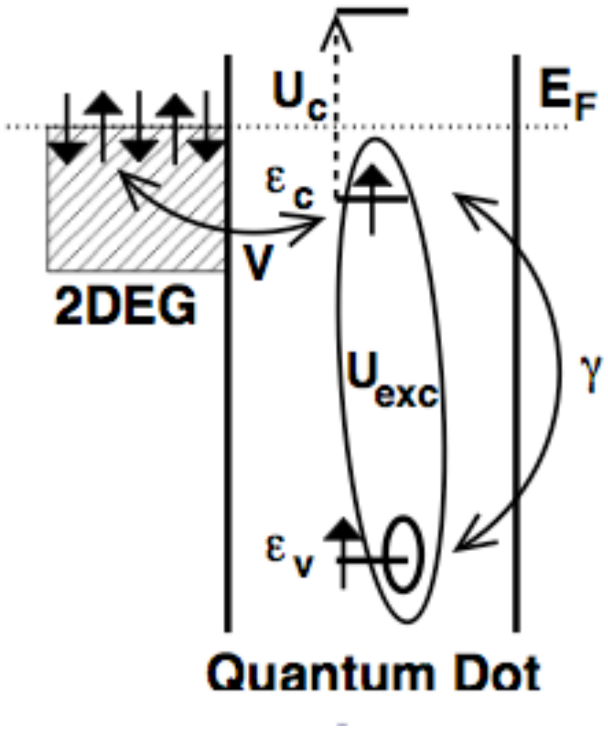


Helmes et al, PRB **72** 125301 (2005)
Latta et al, Nature **474** 627 (2011)

- ☑ InAs/GaAs Tunnel Barriers result into dips in conduction/valence band gap: quantum dots!
- ☑ Light excites e-h pairs that recombine emitting photons
- ☑ Number of electrons tunable by Vg

Excitonic Anderson Model

Helmes et al, PRB **72** 125301 (2005)



$$H = H_{QD} + H_{bath} + H_{hyb}$$

$$H_{QD} = \sum_{\sigma} \varepsilon_c n_{c\sigma} + U_c n_{c\uparrow} n_{c\downarrow} +$$

$$+ \sum_{\sigma} \varepsilon_v n_{v\sigma} + U_v (1 - n_{v\uparrow})(1 - n_{v\downarrow})$$

Exciton Binding Energy:
e-h attraction

$$- \sum_{\sigma\sigma'} U_{exc} n_{c\sigma} (1 - n_{v\sigma'})$$

☑ Light-Matter Interaction: absorption vs emission

$$H_{LM} = \sum_{k\sigma} (\gamma_k a_k e^{-i\omega_k t} c_\sigma^\dagger v_\sigma + hc)$$