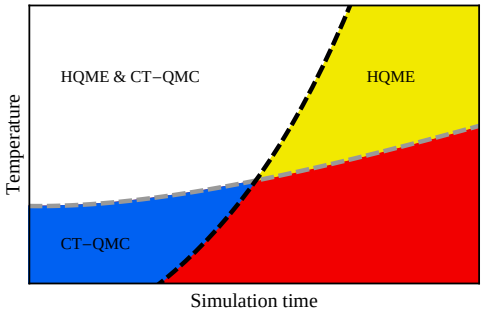
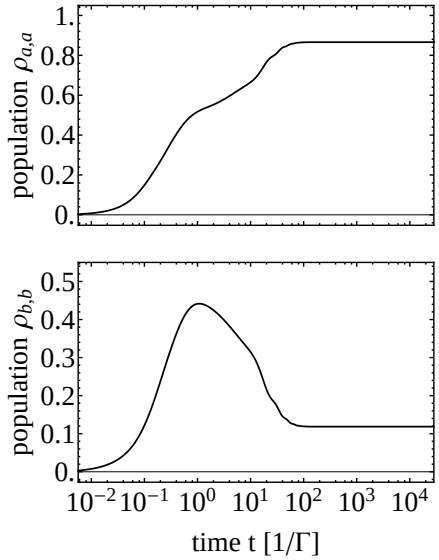
Hierarchical quantum master equations and driven long-term impurity dynamics

Rainer Härtle

Institut für theoretische Physik,
Universität Göttingen





PRB **92**, 085430 (2015)

PRB **90**, 245426 (2014)

A. J. Millis,
G. Cohen, D. R. Reichman
S. Kehrein, T. Pruschke

DFG
HA 7380/1-1

Unterstützt von / Supported by
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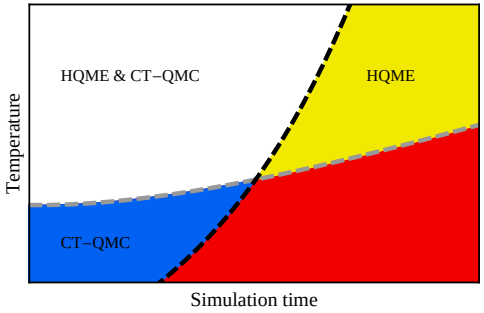
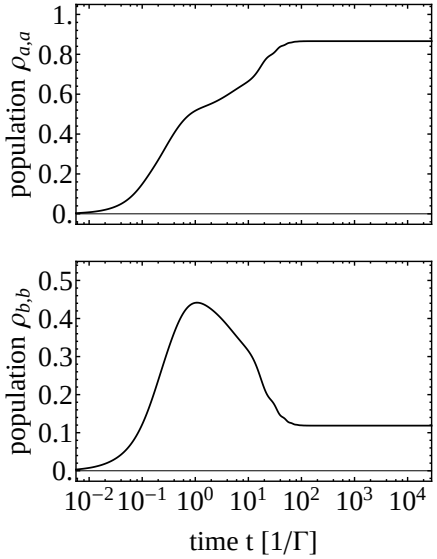
Stiftung/Foundation

Outline

- Motivation
- Hierarchical Master Equation Method (HQME)
- Usability of HQME vs quantum Monte Carlo (CT-HYB)
- Magnetization dynamics ($t \sim 100/\Gamma$)
- Slow buildup of coherence



PRB **92**, 085430 (2015)

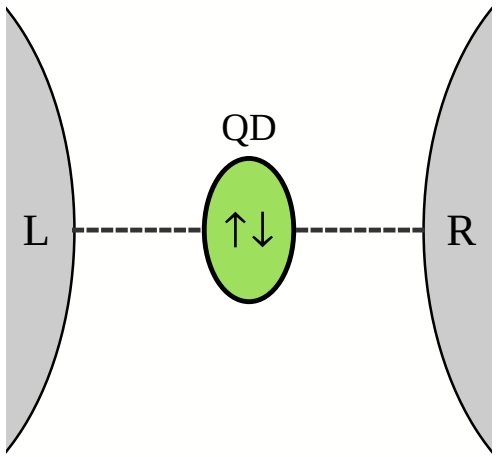


PRB **90**, 245426 (2014)

Motivation

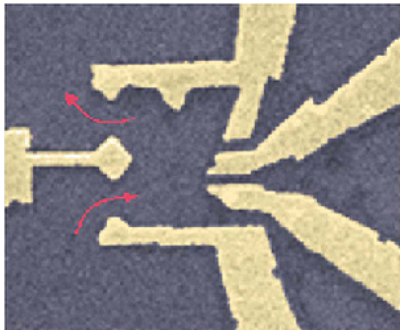
Impurity problems

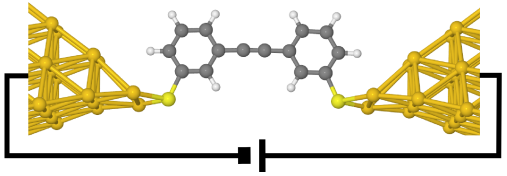
$$H_{\text{imp}} = \sum_m \epsilon_m d_m^\dagger d_m + \sum_{m>n} U_{mn} d_m^\dagger d_m d_n^\dagger d_n,$$
$$H_{\text{env}} = \sum_k \epsilon_k c_k^\dagger c_k,$$
$$H_{\text{tun}} = \sum_{k;m} (V_{kn} c_k^\dagger d_m + \text{h.c.}).$$

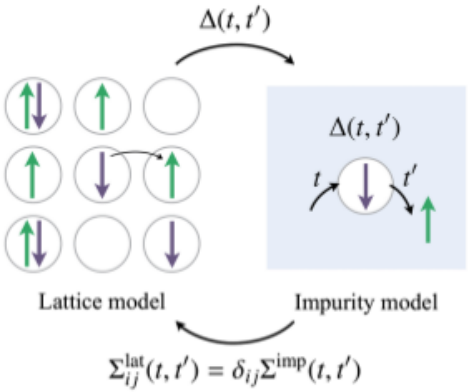


Ubiquitous in

Quantum transport —— Strongly Correlated Materials



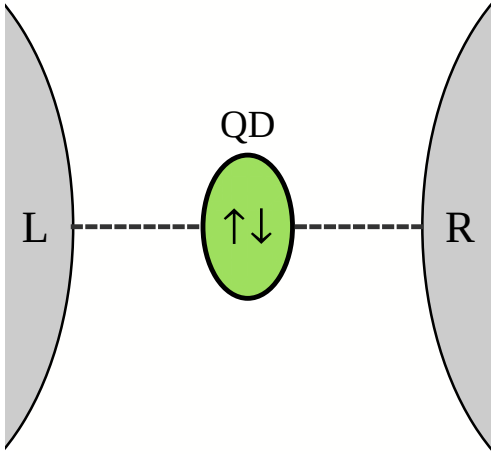




from www.int.washington.edu

from RMP 86, 779 (2014).

Motivation



Given an impurity problem
with ϵ_m, U_{mn}, Γ, T, B, Φ, ..

.. involving long-term dynamics, e.g.
due to Kondo or other correlations,

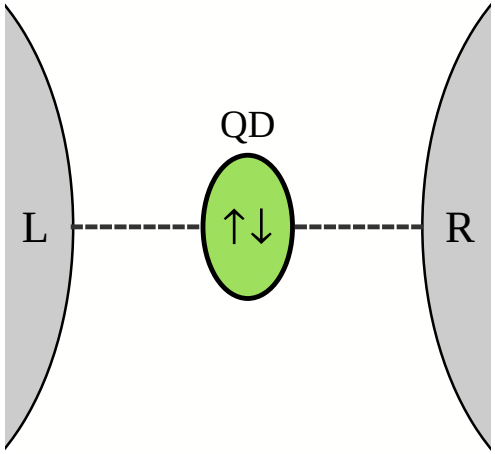
Which solution scheme to use?

$\rightarrow$ Approximate schemes (can be ok, but ...)

$\rightarrow$ Numerically exact schemes (exact, but numerics!)

- Quantum Monte Carlo
- Density-matrix renormalization group
- Numerical Renormalization Group
- Multi-Configurational Time-Dependent Hartree
- Quantum Master Equation

Motivation



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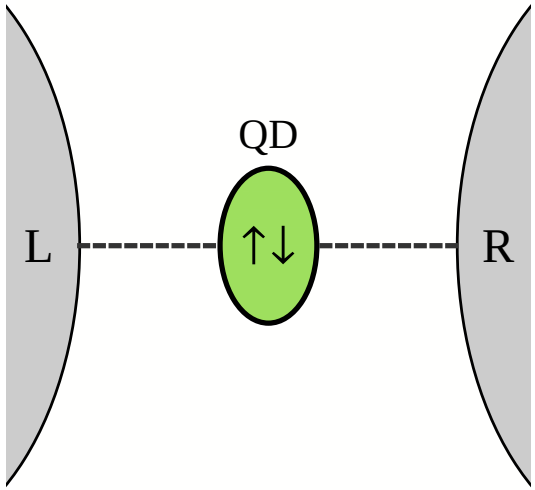
- Cont.-REAL-time Quantum Monte Carlo (CT-HYB)
- Density-matrix renormalization group
- Numerical Renormalization Group
- MultiConfigurational Time-Dependent Hartree
- Hierarchical Quantum Master Equation (HQME)

Hierarchical Master Equations (HQME)

EOM for impurity density matrix ρ
(H_{env}-interaction picture)

$$\partial_t \rho(t) = -i\left[H_{\text{imp}}, \rho(t)\right] - i\tilde{\rho}(t)$$

with $\tilde{\rho}(t) = \text{Tr}_{\text{env}}\left\{[H_{\text{tun}}(t), \varrho(t)]\right\}$



Step I of HQME

$$\tilde{\rho}(t) = \sum_{K\in\{\text{env}\},mn,s\in\{+,-\}} \int_0^t \mathrm{d}\tau\, C^s_{K,mn}(t-\tau)\times \Big(\Big[d^{\bar{s}}_m, \text{Tr}_{\text{env}}\left\{U(t,\tau)d^s_n U(\tau,0)\varrho(0)U^\dagger(t,0)\right\}\Big] - \Big[d^{\bar{s}}_m, \text{Tr}_{\text{env}}\left\{U(t,0)\varrho(0)U^\dagger(\tau,0)d^s_n U^\dagger(t,\tau)\right\}\Big]\Big)$$

with $C^s_{K,mn}(t-\tau) = \sum_{k\in K} V^{\bar{s}}_{mk} V^s_{nk} \text{Tr}_K\left\{\rho_K c^s_k(t) c^{\bar{s}}_k(\tau)\right\}$,
$\varrho(0) = \rho_{\text{env}}\rho$, $s = \{+,-\}$, ..

Jin *et al.*, JCP **128**, 234703 (2008)

Hierarchical Master Equations (HQME)

EOM for impurity density matrix ρ
(H_{env}-interaction picture)

$$\partial_t \rho(t) = -i\left[H_{\text{imp}}, \rho(t)\right] - i\tilde{\rho}(t)$$

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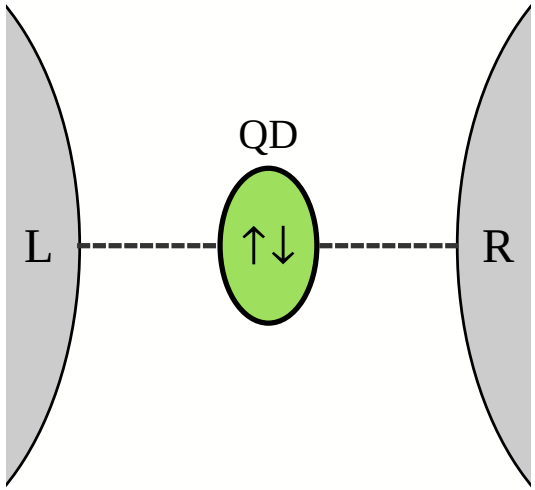


Step II of HQME

$$\tilde{\rho}(t) = \sum_{K,mn,s,p} \int_0^t \mathrm{d}\tau\, \eta^s_{R_r,mn,p} \mathrm{e}^{-\omega^s_{R_r,p}(t-\tau)} \times \Big(\Big[d^{\bar{s}}_m, \text{Tr}_{\text{env}}\left\{U(t,\tau) d^s_n U(\tau,0)\varrho(0) U^\dagger(t,0)\right\}\Big] - \Big[d^{\bar{s}}_m, \text{Tr}_{\text{env}}\left\{U(t,0)\varrho(0)U^\dagger(\tau,0) d^s_n U^\dagger(t,\tau)\right\}\Big]\Big)$$

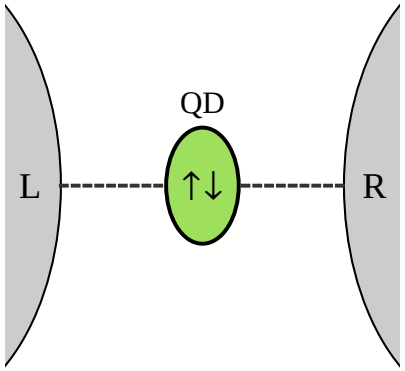
with $C^s_{K,mn}(t-\tau) = \sum_{k\in K} V^{\bar{s}}_{mk} V^s_{nk} \text{Tr}_K\left\{\rho_K c^s_k(t) c^{\bar{s}}_k(\tau)\right\}$,
$\varrho(0) = \rho_{\text{env}}\rho$, $s = \{+,-\}$, ..

Jin *et al.*, JCP **128**, 234703 (2008)

Hierarchical Master Equations (HQME)

Using superoperators

$$\rho^{(1)}_{j_1}(t) \equiv B_j \rho(t) \equiv \rho_{K,mn,s,p}(t),$$
$$\rho^{(\alpha)}_{j_1..j_\alpha}(t) \equiv B_{j_\alpha}..B_{j_1}\rho(t),$$



ρ can be determined by the hierarchy of time-local EOMs

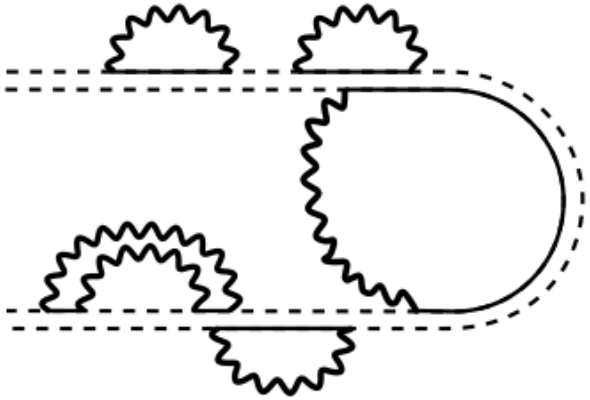
$$\partial_t \rho^{(\alpha)}_{j_1..j_\alpha}(t) = -i\left[H_{\text{imp}}, \rho^{(\alpha)}_{j_1..j_\alpha}(t)\right] - \sum_{\beta\in\{1..\alpha\}} \omega_{j_\beta} \rho^{(\alpha)}_{j_1..j_\alpha}(t)$$
$$+ \sum_\beta (-1)^{\alpha-\beta} \eta_{j_\beta} d^{s_\beta}_{\sigma_\beta} \rho^{(\alpha-1)}_{j_1..j_\alpha/j_\beta}(t) + (-)^\beta \eta^*_{\overline{j_\beta}} \rho^{(\alpha-1)}_{j_1..j_\alpha/j_\beta}(t) d^{s_\beta}_{\sigma_\beta}$$
$$- \sum_{j_{\alpha+1},\sigma_{\alpha+1}} d^{\bar{s}_{\alpha+1}}_{\sigma_{\alpha+1}} \rho^{(\alpha+1)}_{j_1..j_\alpha j_{\alpha+1}}(t) - (-1)^\alpha \rho^{(\alpha+1)}_{j_1..j_\alpha j_{\alpha+1}}(t) d^{\bar{s}_{\alpha+1}}_{\sigma_{\alpha+1}}.$$

Systematic truncation: Härtle *et al.*, PRB **88**, 235426 (2013).
$\longrightarrow$ hybridization expansion w.r.t. temperature scale.

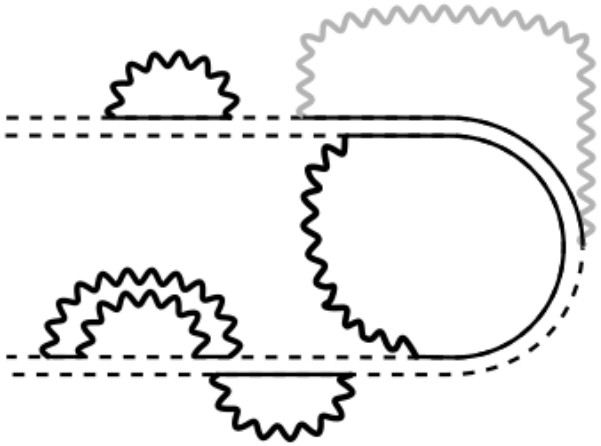
Cont.-real-time Quantum Monte Carlo

Stochastic sum of diagrams on the Keldysh contour:

bare propagation



measuring observables, GF, ..

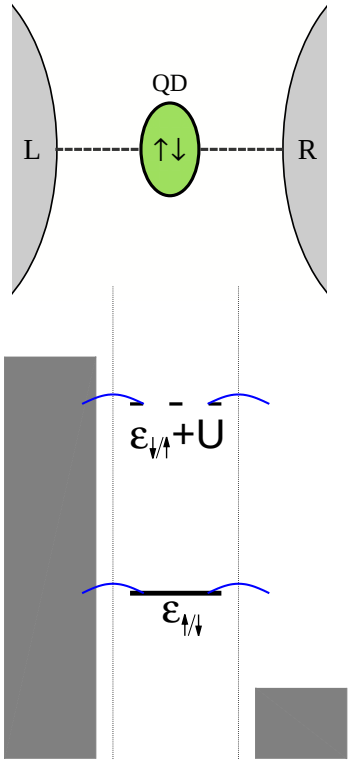


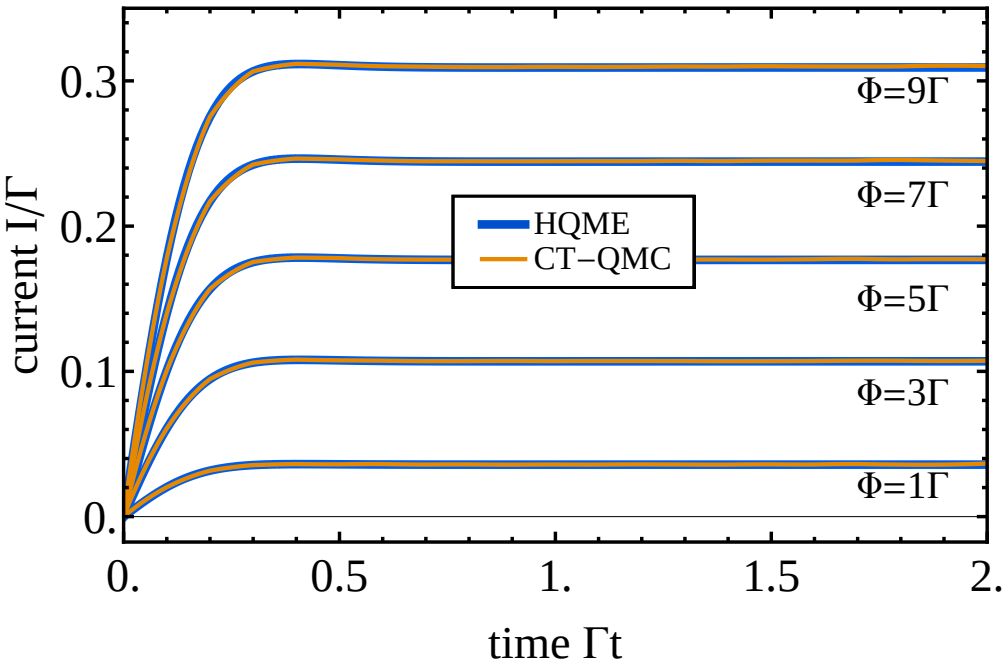
Again, **hybridization expansion**.

Number of relevant diagrams increases with simulation time
$\rightarrow$ statistical error grows polynomially
until one hits an 'exponential wall'.

Gull *et al.*, RMP **83**, 349 (2011)

Current through Anderson impurity





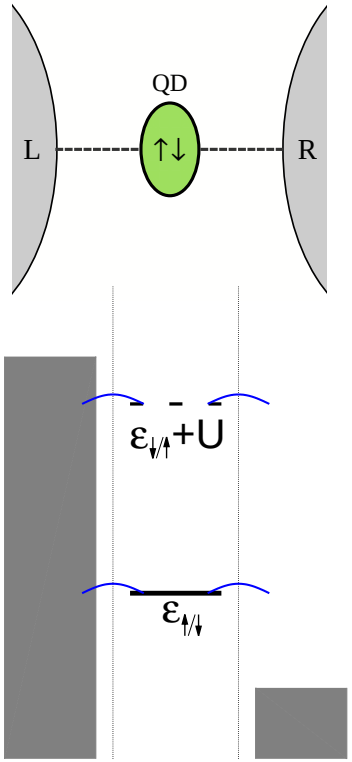
High temperature, *i.e.* $\beta = 0.2/\Gamma$ ($\beta_{\text{Kondo}} \approx 15/\Gamma$)

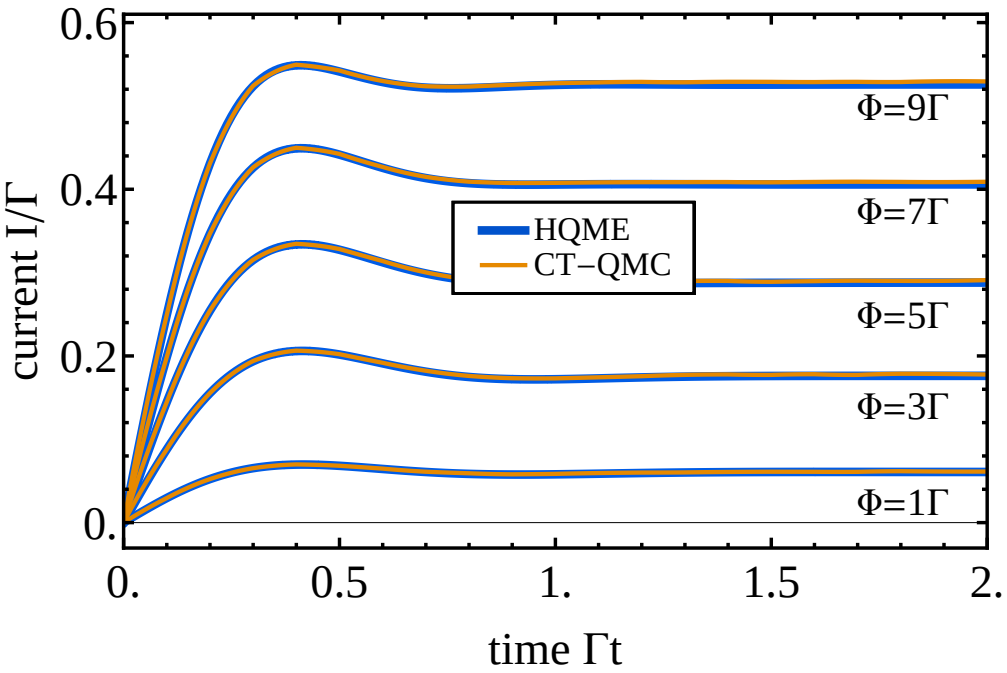
$\epsilon_{\uparrow/\downarrow} = -4\Gamma$, $U = 8\Gamma$, $\Gamma_{\text{L/R}}(\epsilon) = \Gamma \cdot \frac{D^2}{\epsilon^2 + D^2}$, $D = 10\Gamma$,

starting from product initial state with empty impurity.

RH, Cohen, Reichman, Millis, PRB **92**, 085430 (2015)

Current through Anderson impurity





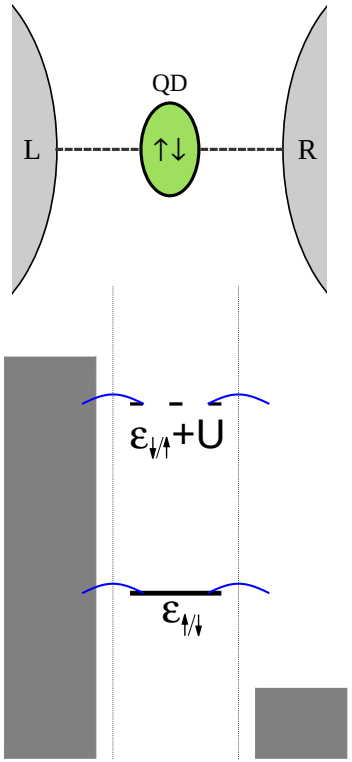
Intermediate temperature, *i.e.* $\beta = 1/\Gamma$ ($\beta_{\text{Kondo}} \approx 15/\Gamma$)

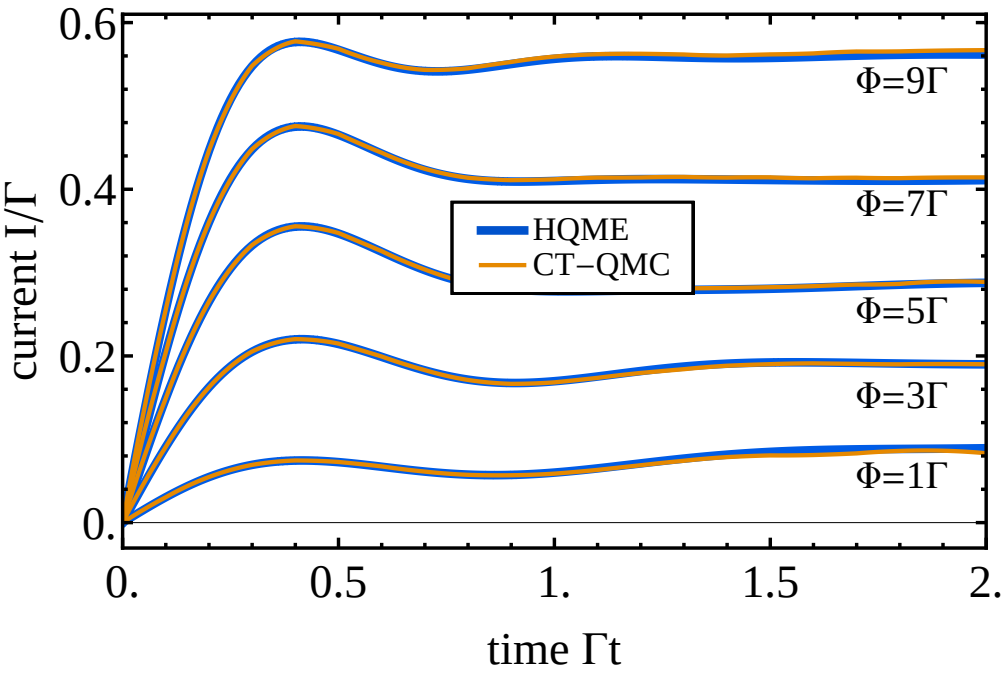
$\epsilon_{\uparrow/\downarrow} = -4\Gamma$, $U = 8\Gamma$, $\Gamma_{\text{L/R}}(\epsilon) = \Gamma \cdot \frac{D^2}{\epsilon^2 + D^2}$, $D = 10\Gamma$,

starting from product initial state with empty impurity.

RH, Cohen, Reichman, Millis, PRB **92**, 085430 (2015)

Current through Anderson impurity





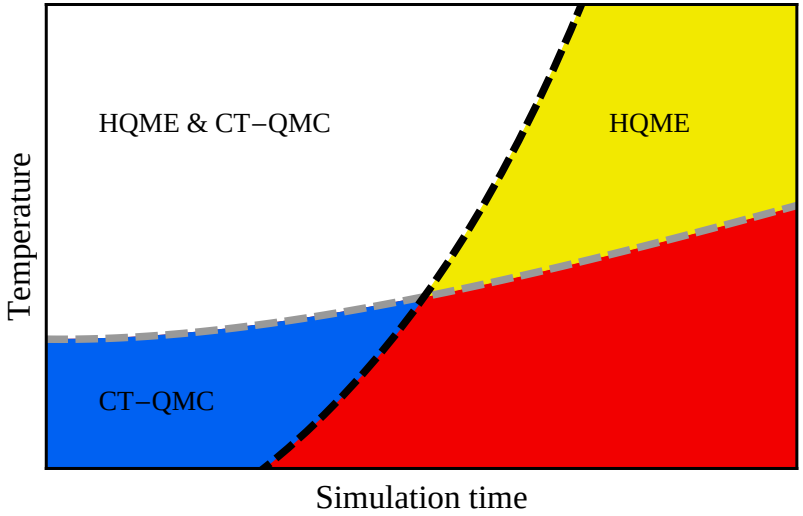
Low temperature, *i.e.* $\beta = 5/\Gamma$ ($\beta_{\text{Kondo}} \approx 15/\Gamma$)

$\epsilon_{\uparrow/\downarrow} = -4\Gamma$, $U = 8\Gamma$, $\Gamma_{\text{L/R}}(\epsilon) = \Gamma \cdot \frac{D^2}{\epsilon^2 + D^2}$, $D = 10\Gamma$,

starting from product initial state with empty impurity.

RH, Cohen, Reichman, Millis, PRB **92**, 085430 (2015)

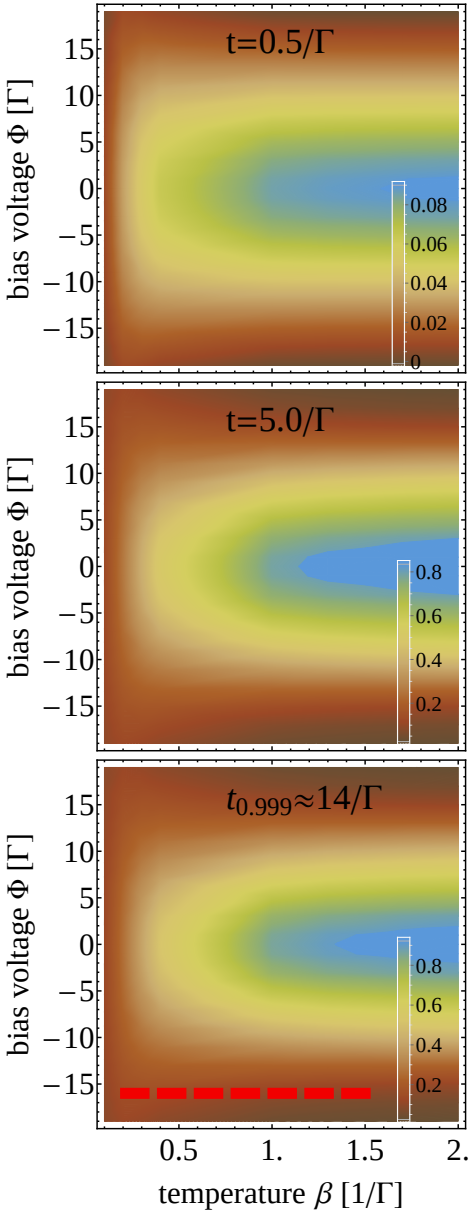
HQME vs CT-HYB



For an Anderson impurity	HQME	CT-HYB
Hybridization exp. of	$U(t)$	time evolution
Numerics	$\sim t$ = linear	$t^{\alpha} - a^{t}$
Temperature	$T > T_{\mathrm{K}}$	all T
Time scales	all	$t \lesssim 10/\Gamma$

RH, Cohen, Reichman, Millis, PRB **92**, 085430 (2015)

Magnetization dynamics for $\epsilon_\uparrow - \epsilon_\downarrow = 2\Gamma$



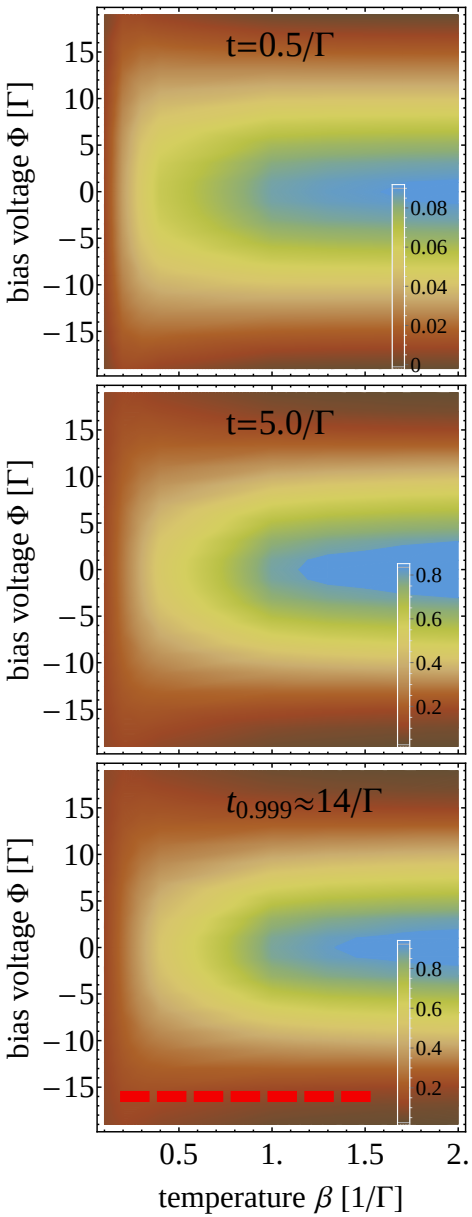
Left figure:

$$\Gamma_L = \Gamma_R = \Gamma$$

$$\beta = \Gamma$$

PRB **92**, 085430 (2015)

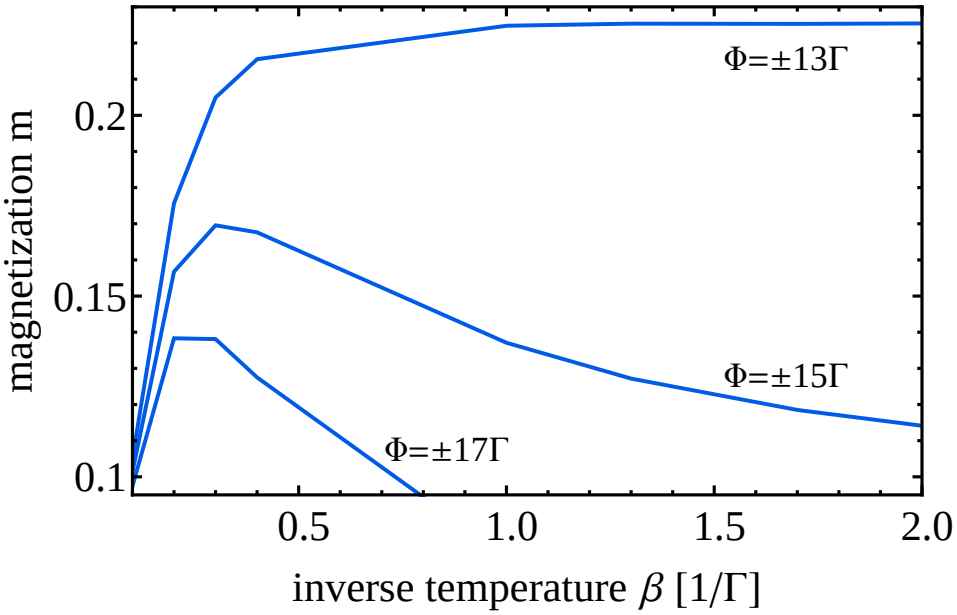
Magnetization dynamics for $\epsilon_\uparrow - \epsilon_\downarrow = 2\Gamma$



Left figure:

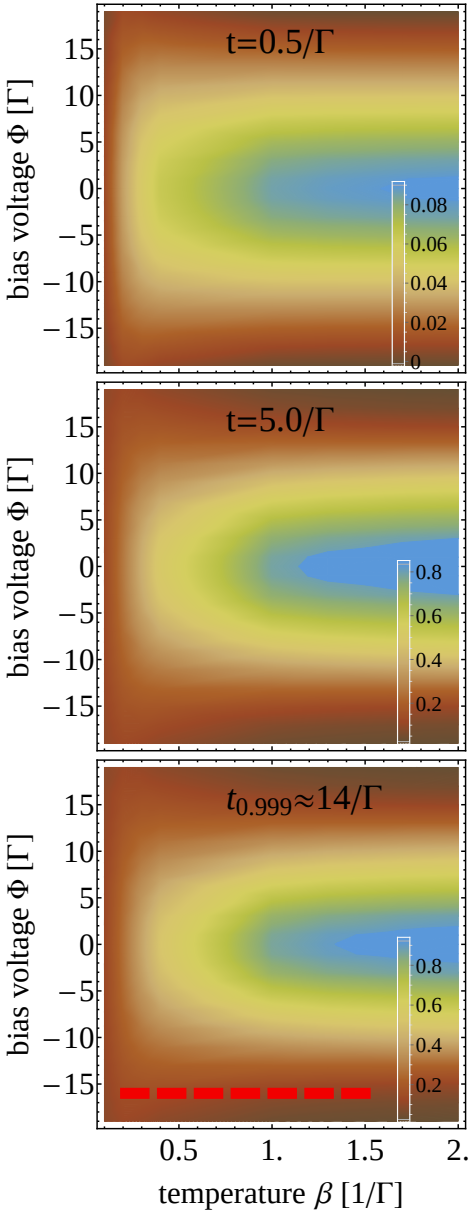
$\Gamma_L = \Gamma_R = \Gamma$

$\beta = \Gamma$



PRB **92**, 085430 (2015)

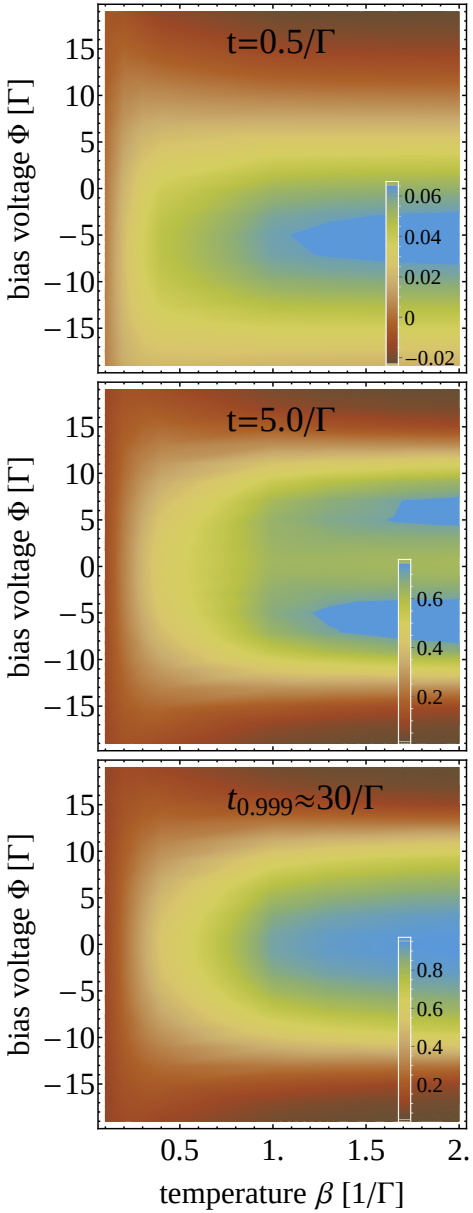
Magnetization dynamics for $\epsilon_\uparrow - \epsilon_\downarrow = 2\Gamma$



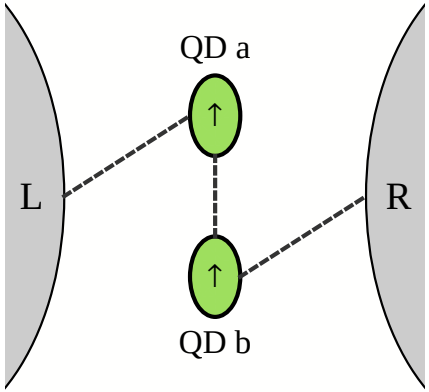
Left figure:
$\Gamma_L = \Gamma_R = \Gamma$
$\beta = \Gamma$

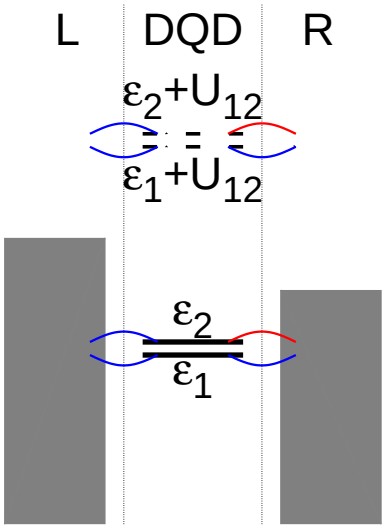
Right figure:
$\Gamma_L = 4\Gamma_R = \Gamma$
$\beta = \Gamma$

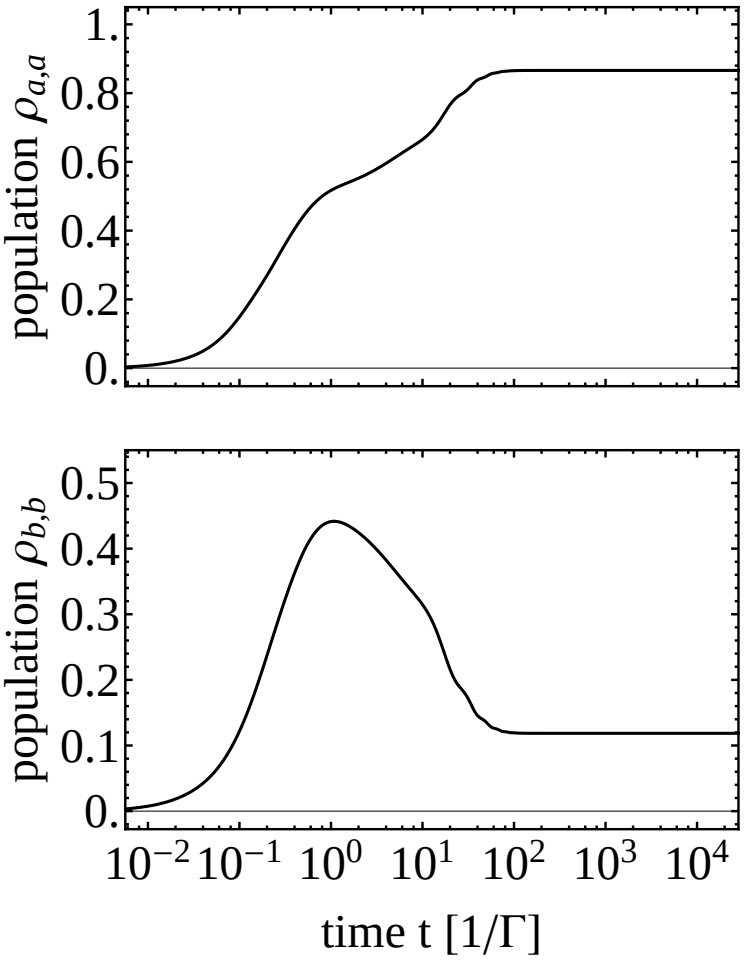
PRB **92**, 085430 (2015)



Current-induced population



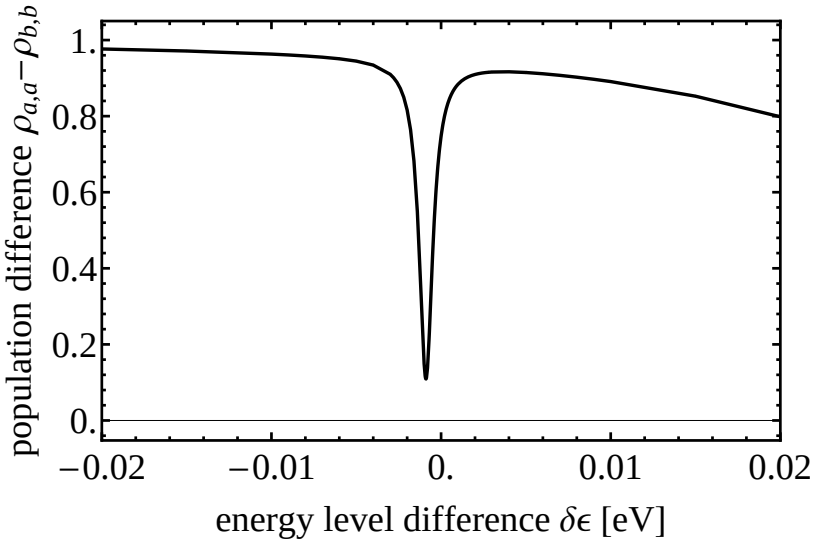


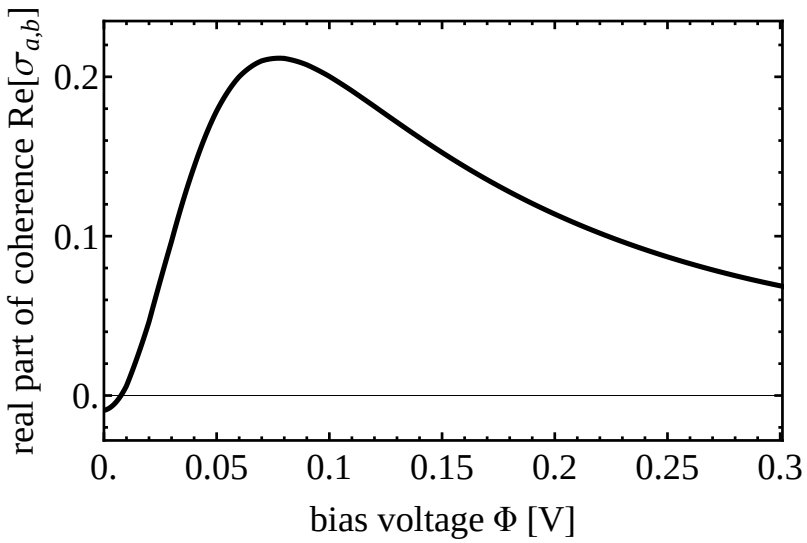


$\rightarrow$ different dot population due to Δ and Re $\left[\rho_{a,b}\right]$

RH, Millis, PRB **90**, 245426 (2014)

Current-induced coherence





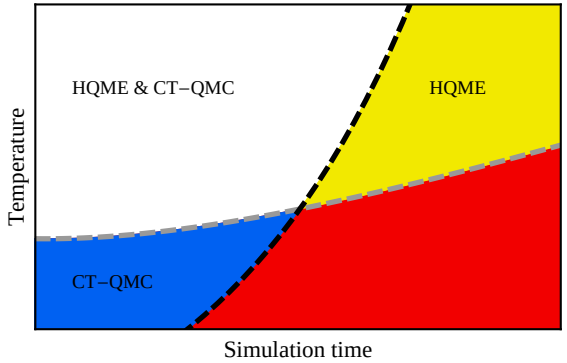
Interaction-induced renormalization:

$$\Delta\epsilon_{m,K} = \frac{\Gamma}{2\pi}\mathrm{Re}\left[\frac{\Psi'\left(\frac{1}{2}+\frac{i(\epsilon_m-\mu_K)}{2\pi k_B T}\right)}{\Psi\left(\frac{1}{2}+\frac{i(\epsilon_m-\mu_K)}{2\pi k_B T}\right)}\right] - \frac{\Gamma}{2\pi}\mathrm{Re}\left[\frac{\Psi'\left(\frac{1}{2}+\frac{i(\epsilon_m+U-\mu_K)}{2\pi k_B T}\right)}{\Psi\left(\frac{1}{2}+\frac{i(\epsilon_m+U-\mu_K)}{2\pi k_B T}\right)}\right]$$

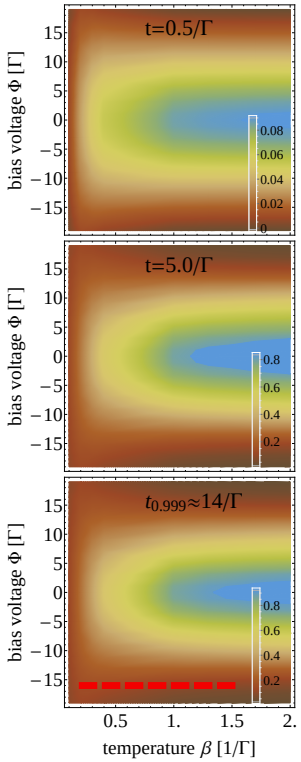
RH, Millis, PRB **90**, 245426 (2014)

Conclusions

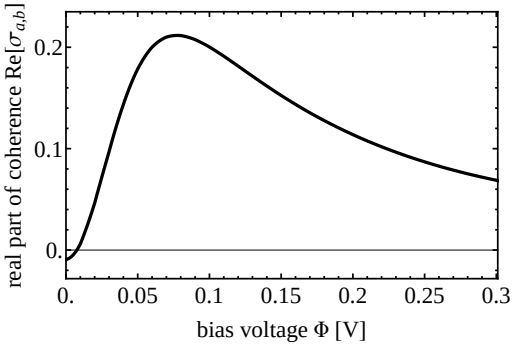
- Usability of HQME and CT-QMC in practical calculations



- Magnetization dynamics (up to $100/\Gamma$)
  $\longrightarrow$ non-monotonous temperature dependence



- Electical current establishes coherence



PRB **90**, 245426 (2014), PRB **92**, 085430 (2015),