Nonequilibrium Physics of Correlated Electron Materials III:

Numerics and Model Systems

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College de France
Oct 5, 2015

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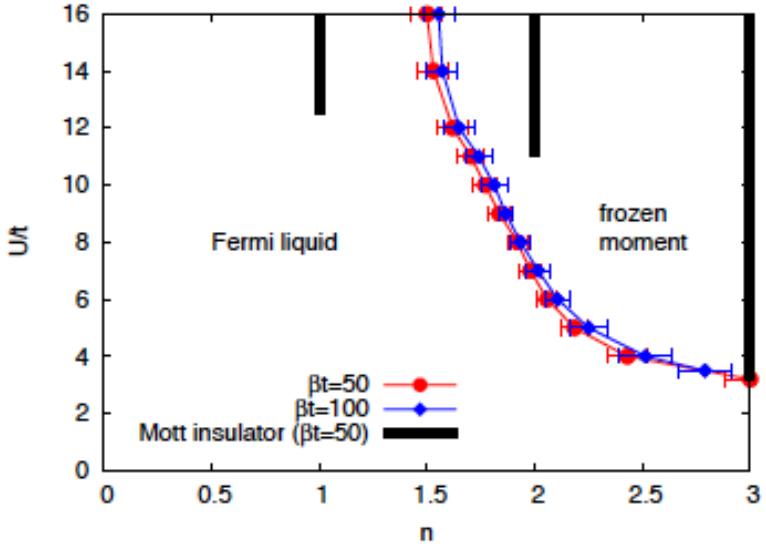
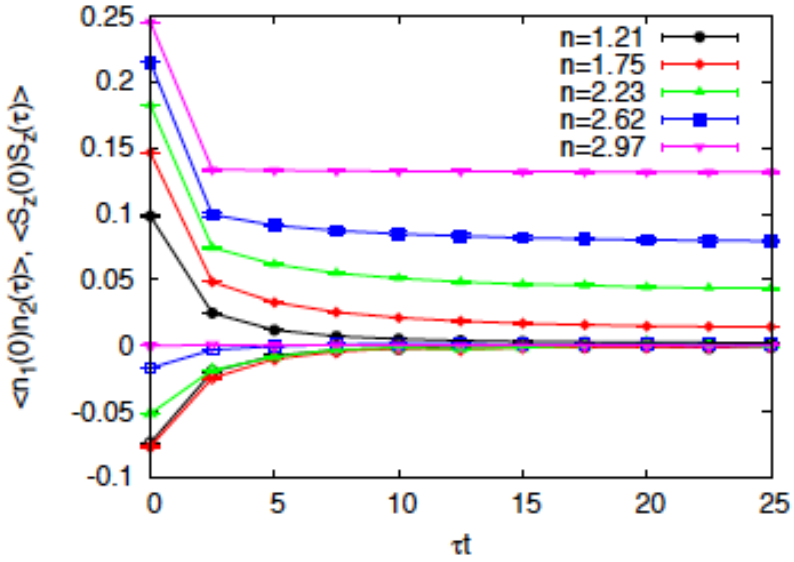
Numerically Exact Methods can bring surprises

Spin Freezing Multiorbital Hubbard Models





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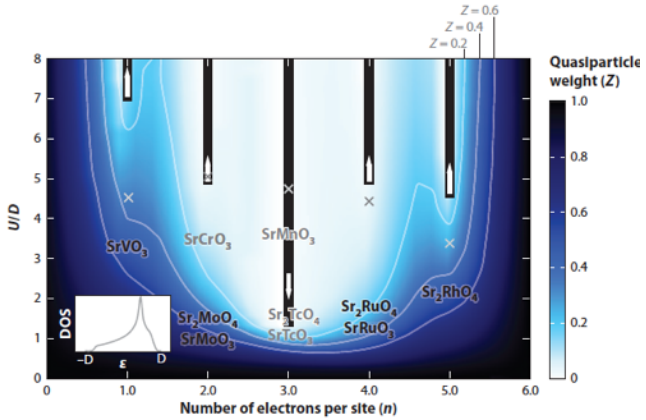
New insights into materials

Strong Correlations from Hund's Coupling

Antoine Georges,[1,4,5] Luca de' Medici,[2,3] and Jernej Mravlje[1,4,6]



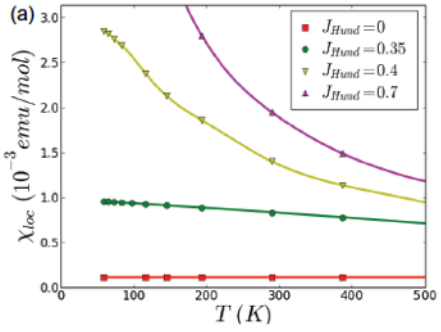
electronic correlations in iron arsendie superconductors

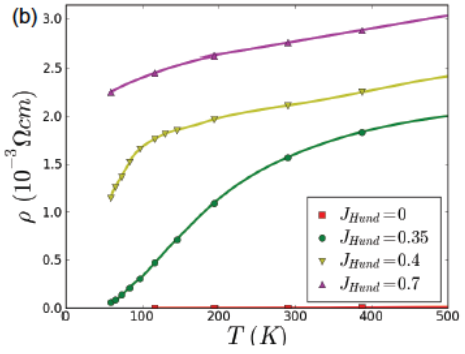
New Journal of Physics
The open-access journal for physics

Coherence–incoherence crossover in the normal state of iron oxypnictides and importance of Hund's rule coupling

K Haule[1] and G Kotliar
Department of Physics, Rutgers University, Piscataway, NJ 08854, USA
E-mail: haule@physics.rutgers.edu

New Journal of Physics **11** (2009) 025021 (13pp)





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Numerically exact methods for nonequilibrium physics needed

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the subject presents two difficulties:

- **The correlated electron part**
- **The nonequilibrium part**

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The correlated electron part: Two (nontrivial) solved problems

1. One dimensional models

   Time evolution of isolated quantum systems

2. Zero dimensional models

   Open interacting systems
   Approximation to lattice systems (DMFT)

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The nonequilibrium part

Correlation function:

$$\chi_{RP}(t_1, t_2) = \mathrm{Tr}\left[e^{-iHt_2} R e^{iH(t_2-t_1)} P e^{-iHt_1} \rho_{init}\right]$$

Typically requires time evolution forward from specified initial state.

Long times required to analyses steady state correlation functions

Direct numerical construction of steady state density matrix not yet much addressed

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Quenches:
Diagonalization and its generalizations

Isolated quantum system started in an specific initial state (e.g. the ground state of a different H)

$$|\psi(\mathbf{t})\rangle = \sum_{\mathbf{n}} \mathbf{e}^{-\mathbf{iE_n t}} |\mathbf{n}\rangle \langle \mathbf{n}|\psi(\mathbf{t}=\mathbf{0})\rangle$$

Approach 1: diagonalize H. Obtain all states and energies

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Rigol, arXiv:0908.3188
Quenches in 1d systems:

$$\hat{H} = \sum_{i=1}^{L} \left\{ -t \left(\hat{f}_i^\dagger \hat{f}_{i+1} + \text{H.c.} \right) + V \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_{i+1} - \frac{1}{2} \right) \right.$$
$$\left. - t' \left(\hat{f}_i^\dagger \hat{f}_{i+2} + \text{H.c.} \right) + V' \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_{i+2} - \frac{1}{2} \right) \right\}$$

Here t', V' are second neighbor couplings that break integrability

Spinless fermions. Can do up to ~ 8 fermions up to ~24 sites

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Rigol, arXiv:0908.3188

Time dependent density matrix

$$\hat{\rho}(t) = \sum_{mn} e^{i(E_n - E_m)t} \psi_n^* \psi_m$$

$$\psi_m = \langle m | \psi(t = 0) \rangle$$

At long times: diagonal?

$$\hat{\rho}_{diag}(t) = \sum_n |\psi_n|^2$$

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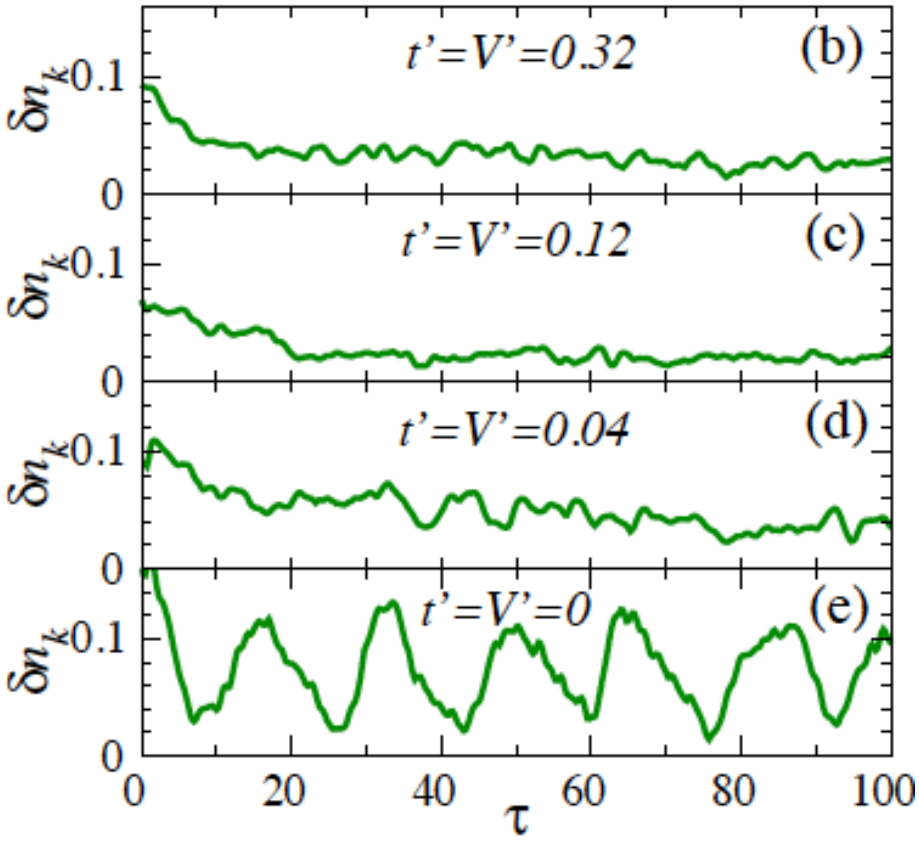
Rigol, arXiv:0908.3188
Quenches in integrable and non-integrable models

Plot: difference between exact result and prediction of diagonal density matrix

$$\delta n_k(\tau) = \frac{\sum_k |n(k,\tau) - n_{diag}(k)|}{\sum_k n_{diag}(k)}$$



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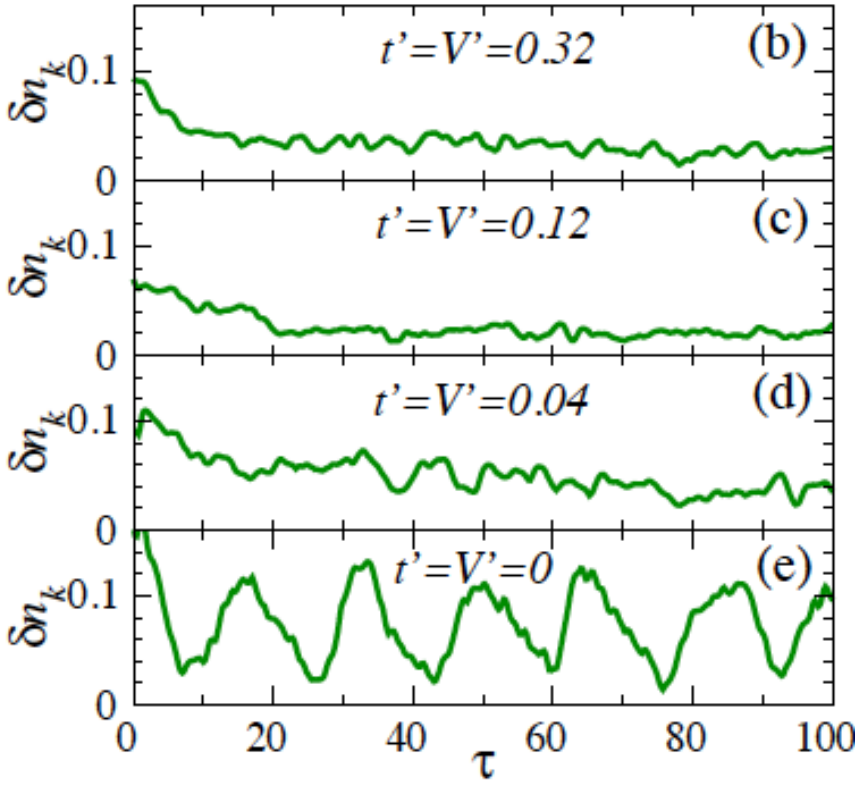
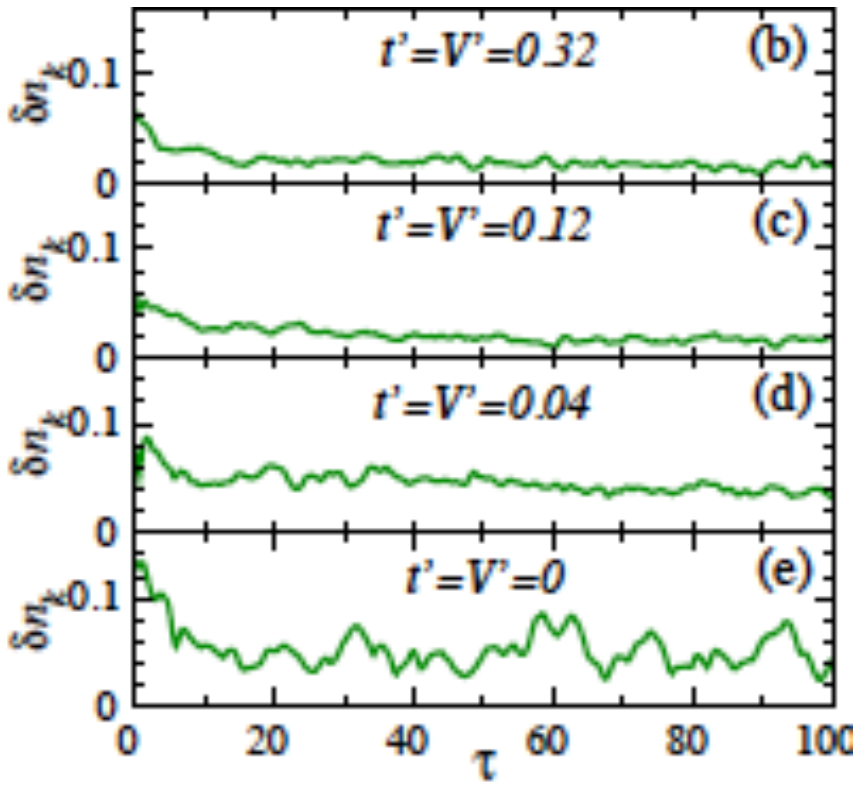
As increase mean energy of quenched state, predictions get closer to those of diagonal ensemble—for non-integrable

$T_{eff}=2$



$T_{eff}=3$



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Direct diagonalization: very suggestive but cant keep enough states to address basic questions

1. How does deviation from diagonal density matrix scale with system size
2. How does crossover from integrable to nonintegrable behavior scale with system size and temperature
3. d>1: need too many states to represent a system of interesting linear dimension

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to improve diagonalization

operate in reduced basis

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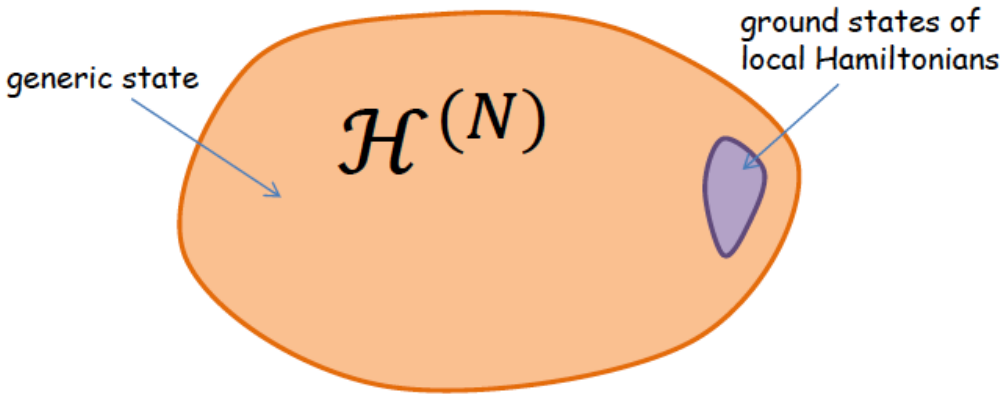
DMRG—MPS

Basic observationL ground states are special

Ground states of local Hamiltonians are special/non-generic states



From G. Vidal

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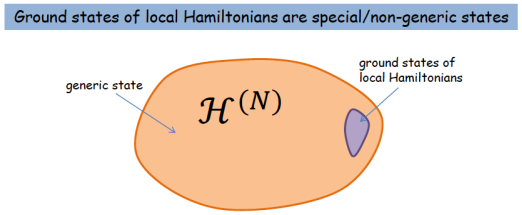
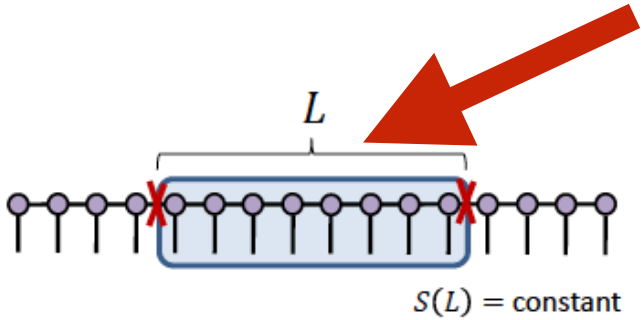
special property of ground states: area law entanglement

(for gapped systems; `pathological' exceptions exist)



Pick a subregion A



reduced density matrix $\hat{\rho}_A = \mathrm{Tr}_{B \not\subset A}\left[\hat{\rho}\right]$

entanglement entropy $S_{A|\not\subset A} = -\mathrm{Tr}\left[\rho_A \ln \rho_A\right]$

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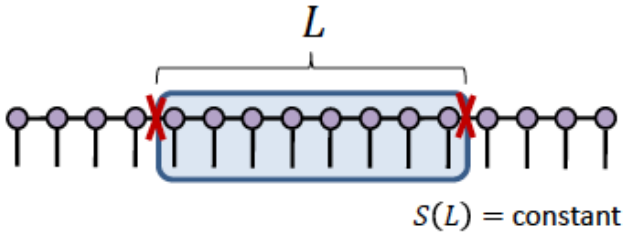
Density matrix eigenvalues

$$S_{A|\not\subset A} = -\sum_{\lambda=1..D_A} w_\lambda \ln w_\lambda$$



Size L=> Hilbert space dimension D for for region A is $D_A=(\text{const})^L$

typical (excited) state of whole system: each eigenvalue. w, of reduced density matrix has magnitude ~$1/D_A$

$$S_{A|\not\subset A} \approx -\ln\frac{1}{D_A} = L\,\ln(\text{cst})$$

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Ground states are different

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Area law for ground states (on reasonable assumptions)

$$S_{A|\not\subset A} \sim L^{d-1}$$

$$S_{A|\not\subset A} = -\sum_{\lambda=1..D_A} w_\lambda \ln w_\lambda$$

Implies reduced density matrix has a non-exponential number of non-neglible eigenvalues (indep of size of L in d=1). Eigenfunctions w big e.v. provide variational basis

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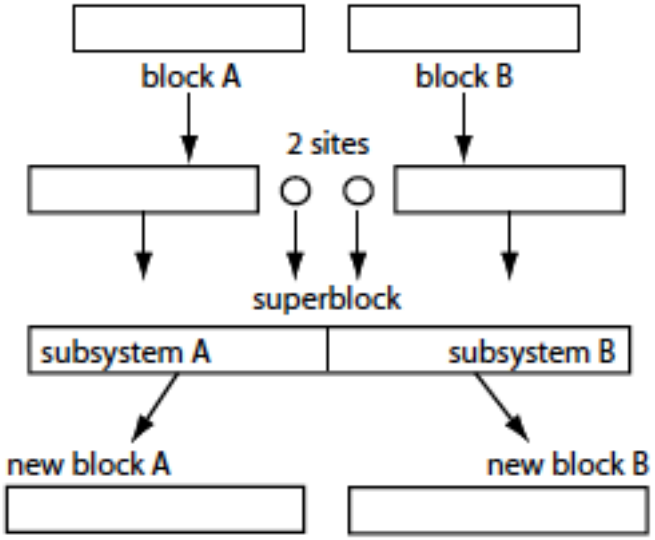
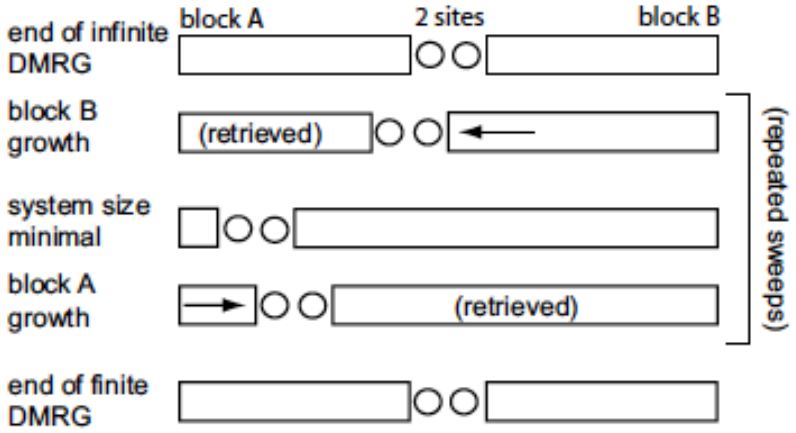
Sketch of Algorithm for Ground State



1. start with variational basis, size 2M
2. partition system
3. add one site to each side
4. recompute reduced density matrix
5. New variational basis: M states with largest eigenvalues

Improvement



1. start with result described above.
2. `sweep: remove sites from one siede, view as new site son other, recompute reduced density matrix.

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Time dependence

If Hamiltonian is sum of local terms:

$$e^{iH\Delta t} \rightarrow 1 + i \sum_i h_i \Delta t$$

Each term in sum is like a term in the `sweep'

=> time dependence can be done with small modification of usual DMRG formalism

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The catch: excited states are `typical'
=>entanglement entropy~ volume

=>typically need exponentially many parameters

1d, typical models have excitations propagating with non-zero velocity=> entanglement increases linearly with time => # of states to represent dynamics needed exponentially with time

Exponential wall: only question is how far can you go before you hit it

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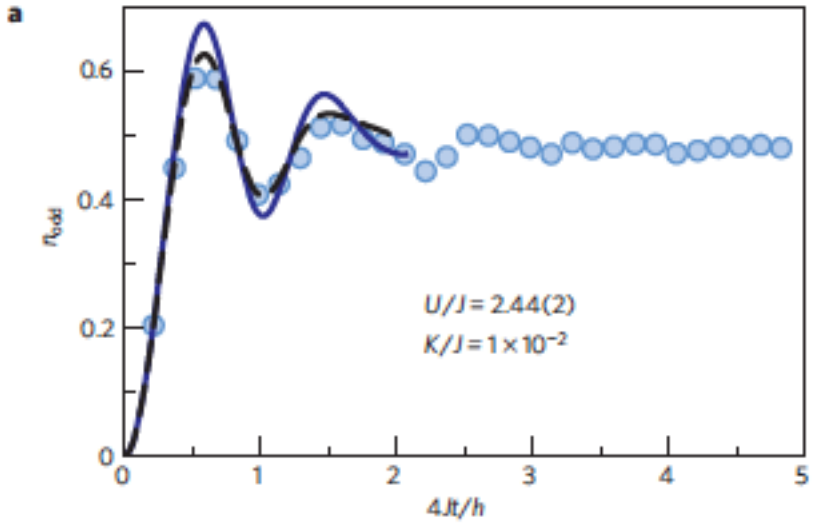
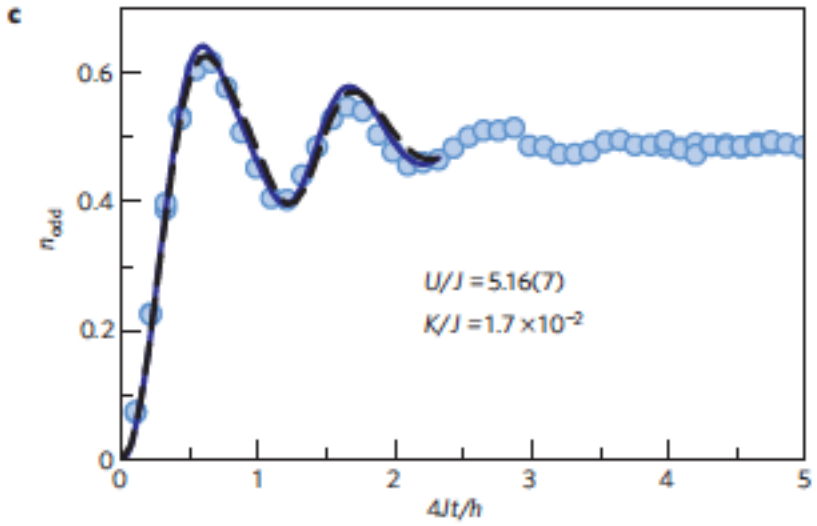
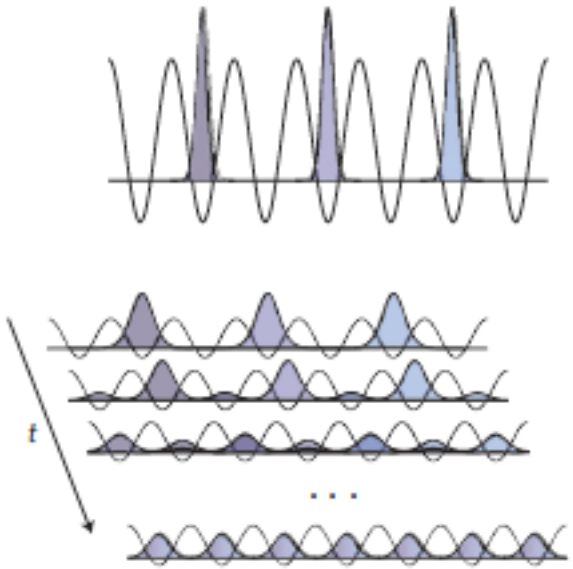
Trotzky et al Nature Physics vol 8 p 325





$$\hat{H} = \sum_i \left[-J\left(\hat{a}_j^\dagger \hat{a}_{j+1} + \text{h.c.}\right) + \frac{U}{2}\hat{n}_j(\hat{n}_j - 1) + \frac{K}{2}\hat{n}_j j^2 \right]$$



Exponential wall at t=2J

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State of the art: lattice systems

Numerics can access short to intermediate times, can address many interesting questions, but exponential wall prevents access to long times.

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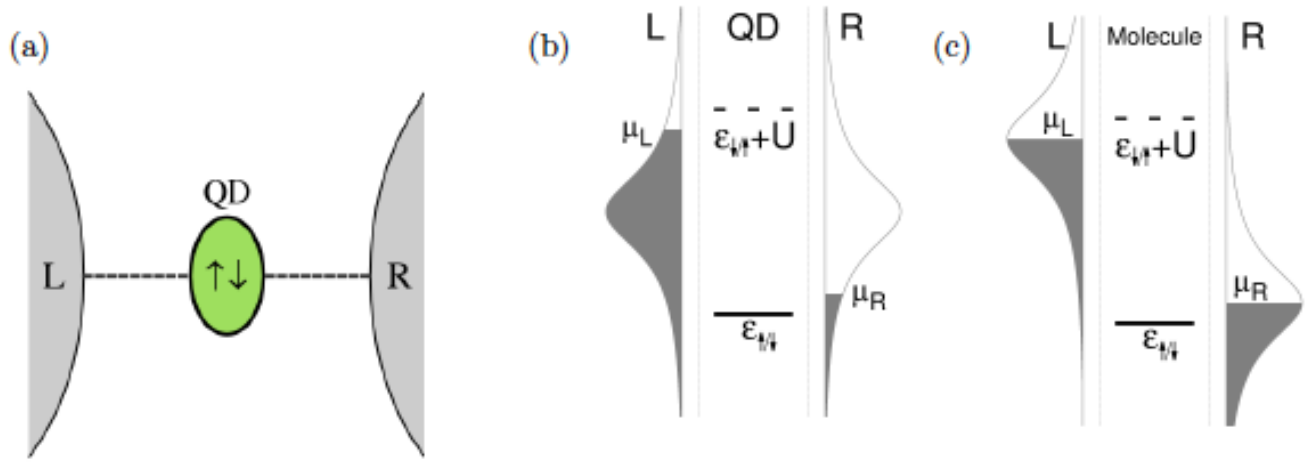
Impurity models and dynamical mean field theory



quantum impurity model: local interacting region sandwiched between two non-interacting leads

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Hamiltonian

$$\mathbf{H} = \sum_{\mathbf{ab}} \mathbf{H^0_{ab}} \mathbf{d^\dagger_a d_b} + \sum_{\mathbf{abcd}} \mathbf{I^{abcd}} \mathbf{d^\dagger_a d^\dagger_b d_c d_d}$$

$$+ \sum_{\mathbf{akb}} \mathbf{V^{akb}} \mathbf{d^\dagger_a c_{kb}} + \mathbf{H.c} + \sum_{\mathbf{kb}} \varepsilon_{\mathbf{kb}} \mathbf{c^\dagger_{kb} c_{kb}}$$

Local levels +interactions, coupled to leads

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Alternative: integrate out bath

Action of 0 (space) +1 (time) d field theory

$$\mathbf{S} = \int \mathbf{dtdt'd_a^\dagger(t)\Delta^{ab}(t,t')d_b(t' + I^{abcd} \int dtd_a^\dagger d_b^\dagger d_c d_d}$$

$$\mathbf{\Delta^{ab} = \left(i\partial_t - H_{ab}^0 - \sum_{kc} V^{akc} G_{kc}(t_1,t_2) V^{bkc} \right)}$$

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Motivation

1. **Model for quantum dots (in and out of equilibrium)**
2. **Auxiliary problem for dynamical mean field theory: approximation for self energy of lattice model from solution of impurity model plus self-consistency condition. In and out of equilibrium**
3. **Test-bed for methods**

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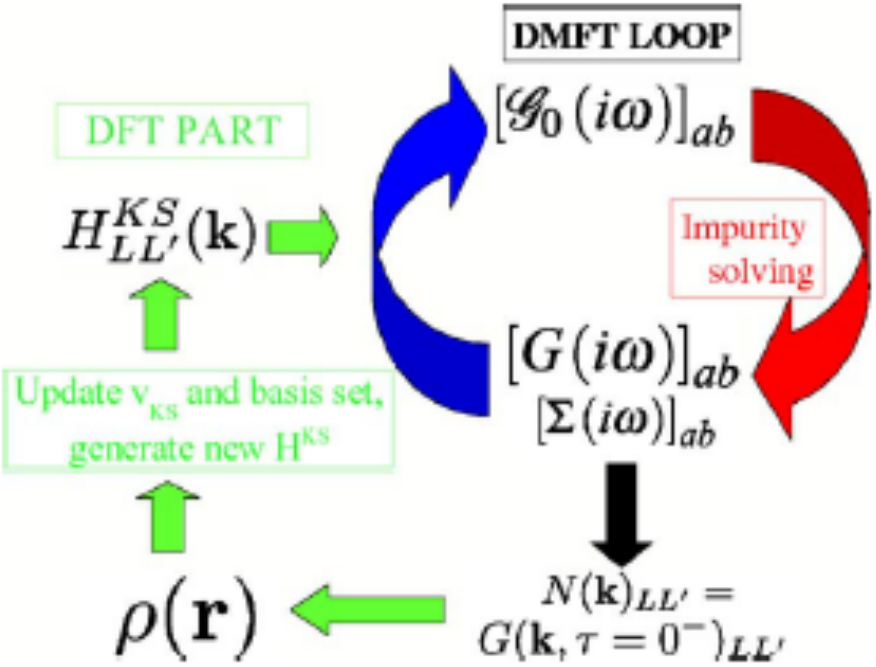
Equilibrium DMFT



Impurity model with self-consistently chosen hybridication functional

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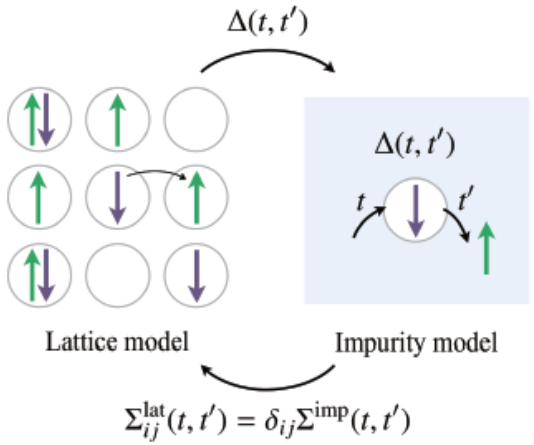
Nonequilibrium DMFT

Original formulation:

- Schmidt and Monien, arXiv:cond-mat/0202046
- Freericks, Turkowski, and Zlatic, PRL 97, 266408

Nice description of modern understandng

Aoki, Tsuji, Eckstein, Kollar, Oka, Werner, arXiv:1310.5329 (RMP 2014)



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Specialize to single-orbital Anderson impurity model

$$\mathbf{H} = \varepsilon \sum_{\sigma} \mathbf{d}_{\sigma}^{\dagger} \mathbf{d}_{\sigma} + \mathbf{U} \mathbf{n}_{\uparrow} \mathbf{n}_{\downarrow}$$

$$+\mathbf{H}_{\mathbf{mix}} \quad +\mathbf{H}_{\mathbf{bath}}$$

Charge density $\mathbf{n} = \mathbf{n}_{\uparrow} + \mathbf{n}_{\downarrow}$

Spin density $\mathbf{m} = \mathbf{n}_{\uparrow} - \mathbf{n}_{\downarrow}$

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Nonequilibrium

1. **Time dependence of parameters in H**
2. **Different chemical potentials for different baths.**

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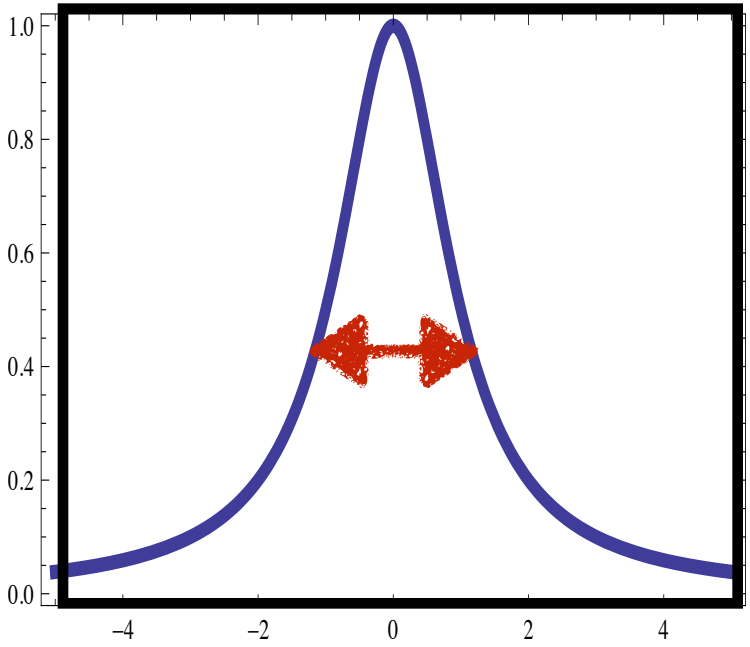
Parameter: bare level width Γ



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To solve impurity model

1. **Approximate methods**
2. **Discretize bath—diagonalize**
3. **Quantum Monte Carlo**

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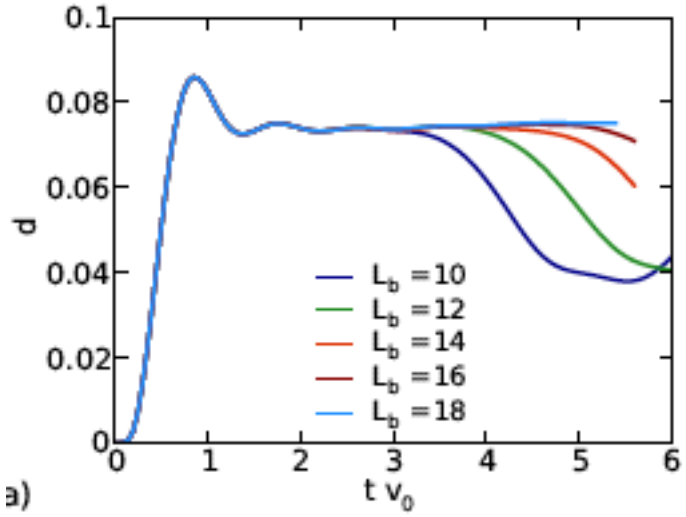
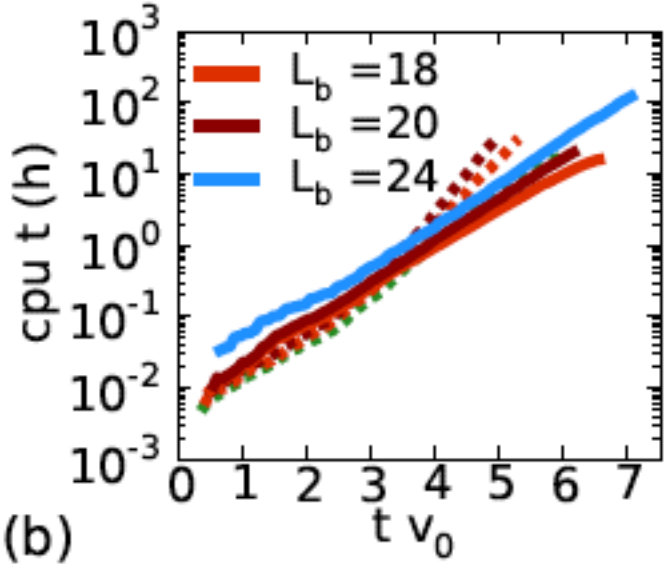
DMRG as real-time impurity solver





Can reach times of order 5 before growth of entanglement wins

Long enough for equilibrium response functions

??Steady state nonequilibrium studies??

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Quantum Monte Carlo

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Equilibrium:
propagation on imaginary time contour

efficiently performed by continuous time quantum Monte Carlo

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Continuous time Monte Carlo:

$$\mathbf{H = H_a + H_b}$$

- **interaction representation with respect to H_b**

$$Z = \mathrm{Tr}\, T_\tau e^{-\beta H_a} \exp\left[-\int_0^\beta d\tau H_b(\tau)\right]$$

- **formal expansion in H_b**

$$= \sum_k (-1)^k \int_0^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^\beta d\tau_k$$
$$\times \mathrm{Tr}\left[e^{-\beta H_a} H_b(\tau_k) H_b(\tau_{k-1}) \ldots H_b(\tau_1)\right]$$

- **sample series stochastically**

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Two expansions

$$\mathbf{H} = \sum_{\mathbf{ab}} \mathbf{H^0_{ab}} \mathbf{d^\dagger_a d_b} + \sum_{\mathbf{abcd}} \mathbf{I^{abcd}} \mathbf{d^\dagger_a d^\dagger_b d_c d_d}$$

$$+ \sum_{\mathbf{akb}} \mathbf{V^{akb}} \mathbf{d^\dagger_a c_{kb}} + \mathbf{H.c} + \sum_{\mathbf{kb}} \varepsilon_{\mathbf{kb}} \mathbf{c^\dagger_{kb}} \mathbf{c_{kb}}$$

In interactions
In hybridization

In equilibrium: both series absolutely convergent at any T>0

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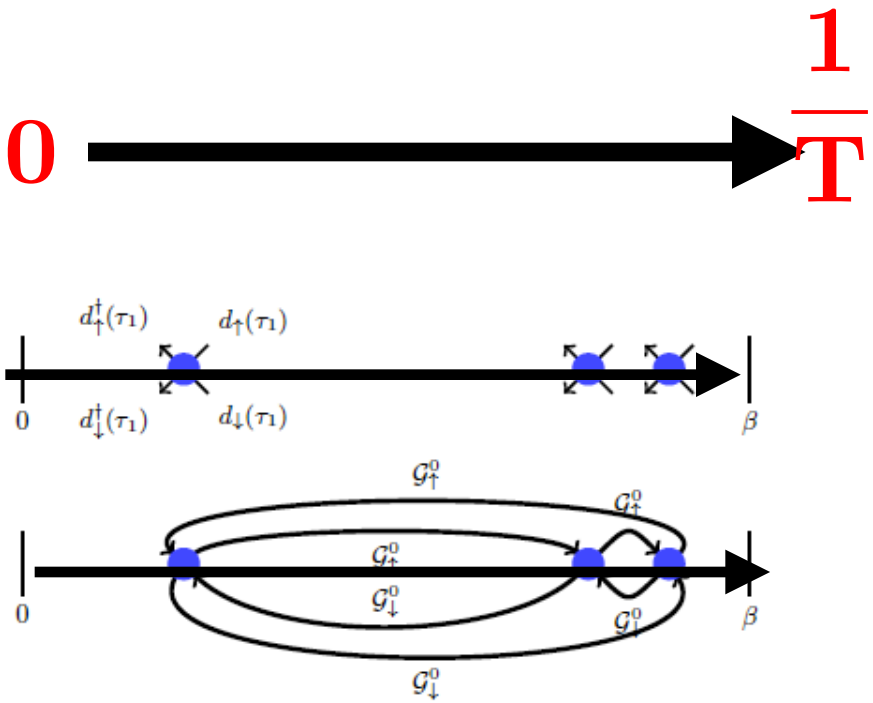
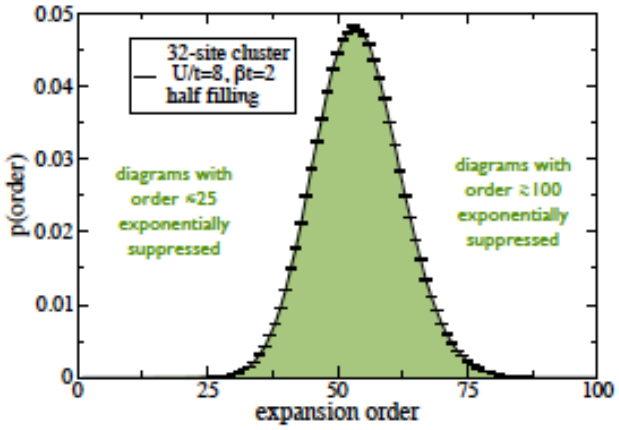
Equilibrium CT-QMC:





Number of vertices needed set by 1/T

Works very well because the method is estimating a real exponential

$$\mathbf{Z = Tr\left[e^{-\beta H}\right]}$$

Method is now very widely used.

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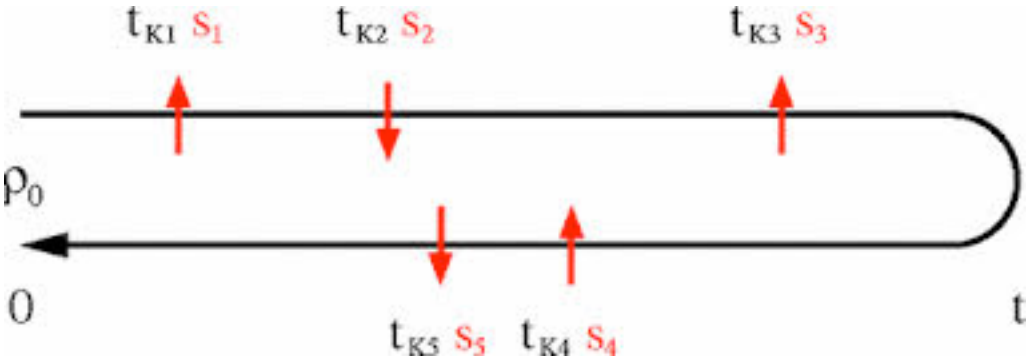
Out of equilibrium

$$\left\langle \hat{\mathcal{O}} \right\rangle_t = Tr\left[\hat{\mathcal{O}}\hat{\rho}(t)\right] = Tr\left[\hat{\mathcal{O}}e^{-i\hat{H}t}\hat{\rho}_0 e^{i\hat{H}t}\right]$$

- **Real time evolution forward from initial condition**
- **Number of vertices ~ time interval**

- **Two time contours required (twice as many vertices)**
- **Convergence by cancellation of oscillations**



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Hybridization vs Interaction Expansion

$$H = \sum_{ab} H^0_{ab} d^\dagger_a d_b + \sum_{abcd} I^{abcd} d^\dagger_a d^\dagger_b d_c d_d$$

$$+ \sum_{akb} V^{akb} d^\dagger_a c_{kb} + H.c + \sum_{kb} \varepsilon_{kb} c^\dagger_{kb} c_{kb}$$

Expand in I: use bare Green functions which include nonequilibrium—expansion can be formulated directly in nonequilibrium steady state

Expand in V: necessarily start in wrong state

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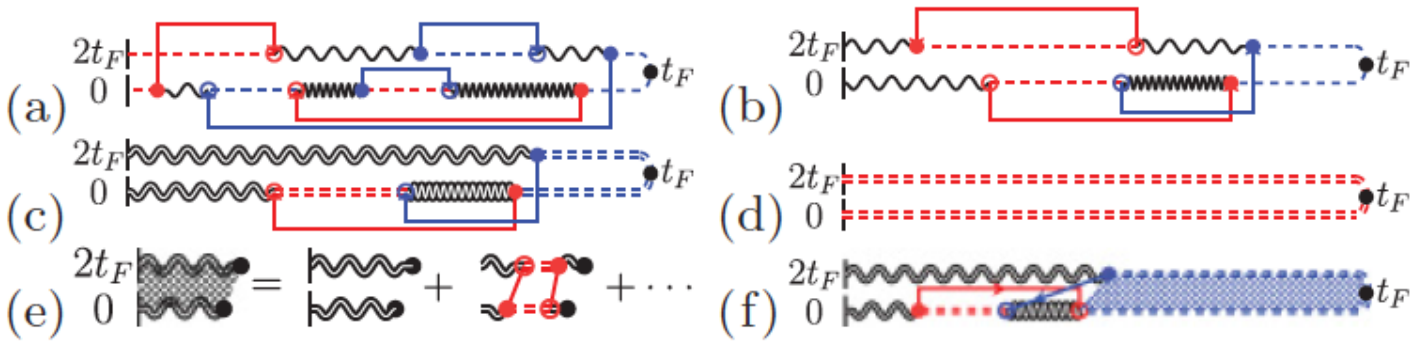
perturbation expansion: diagrammatics on Keldysh contour



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2009: brute force approach

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Real time CT-QMC

(stochastically explore bare perturbation theory)

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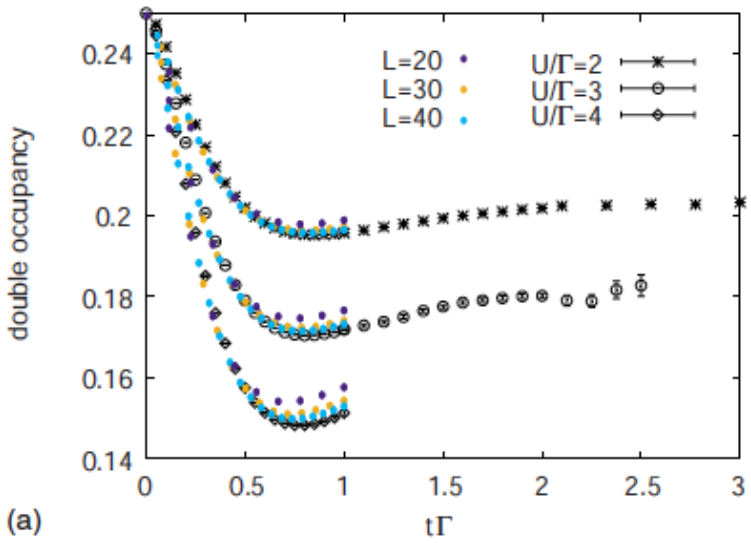
Real time CT-QMC

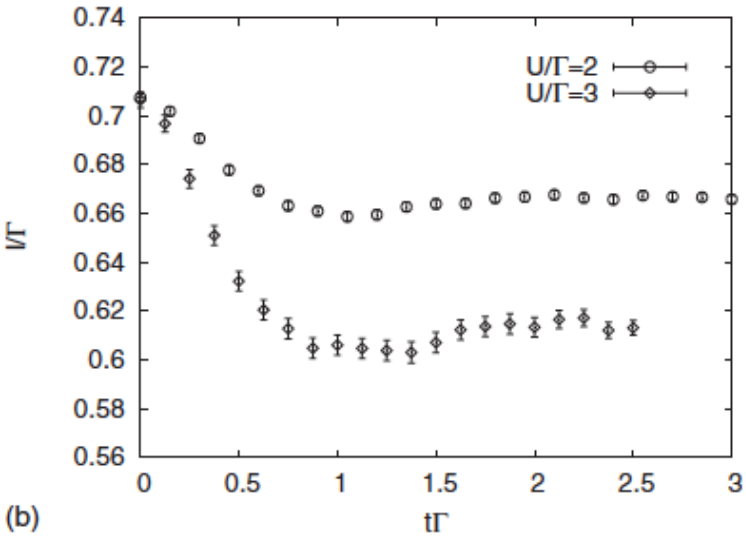
(stochastically explore bare perturbation theory)

Results for Anderson model
(single level quantum dot with 2 leads)

Real time, equilibrium



Current at non-zero voltage



At interesting coupling strengths, method is limited to brutally short times.

Werner-Millis
Rabani-Muhlbacher
Schiro-Fabrizio

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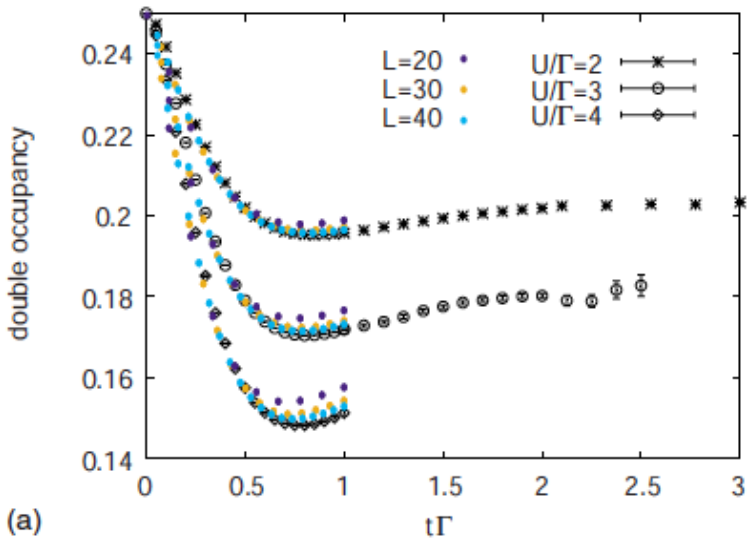
Real time CT-QMC

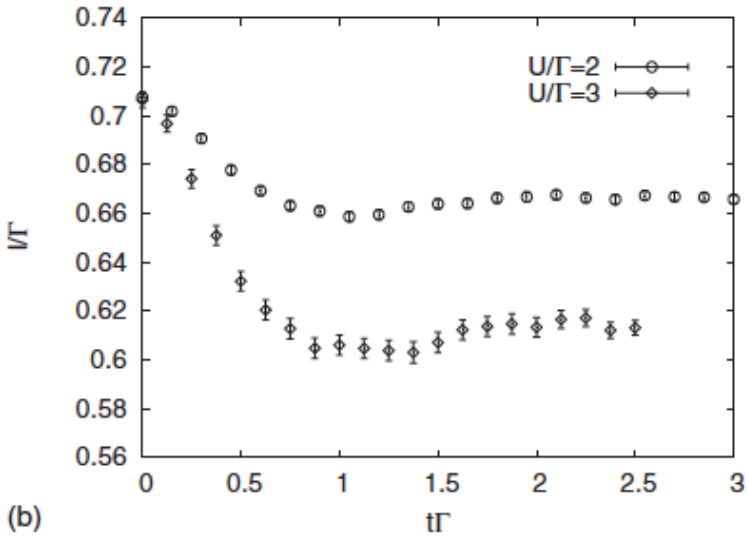
(stochastically explore bare perturbation theory)

Results for Anderson model
(single level quantum dot with 2 leads)

Real time, equilibrium



Current at non-zero voltage



One time quantities (densities) easiest to calculate

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Rabani-Muhlbacher
Schiro-Fabrizio

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Technical point

In real time, convergence with respect to diagram order occurs when sum of all diagrams of a given order decreases rapidly with order.

This cancellation of diagrams (``sign blessing"—N. Prokof'ev) is problematic for Monte Carlo

Solution: put hard wall in calculation (no diagrams of order $n>N_{max}$). Then systematically increase N_{max} until converegence achieved

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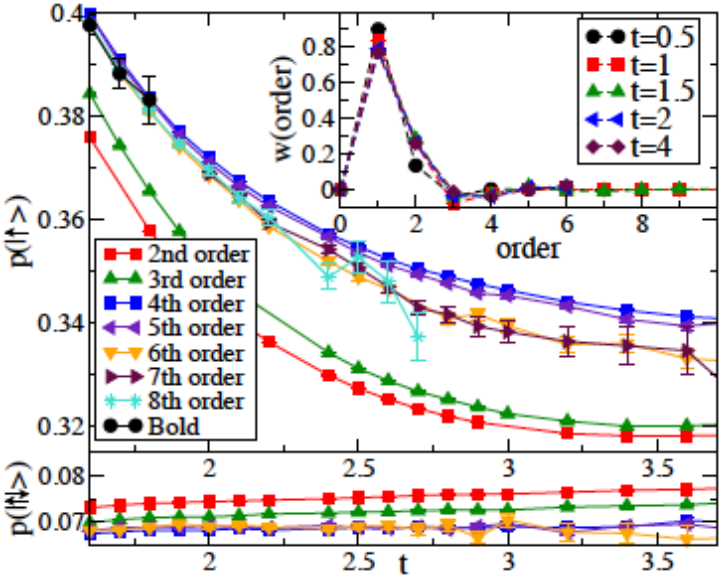
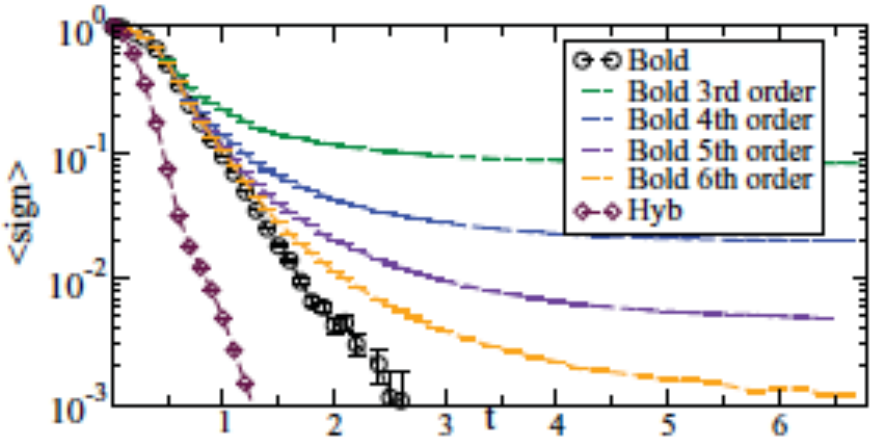
Convergence with respect to order and time





Gull Reichman Milli arXiv:1105.1175s

Method works if calculations converges at a low enough order that the sign does not kill you. Low T and strong interactions are hard to do

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First Improvement: 'Bold' methods

Idea: perform stochastic expansion around partial resummation of diagram series. Partial resummation can be done by solving ``simple" integral equation

What you lose: Wick's theorem

What you gain: fewer corrections needed (if partial resumation is good starting point)

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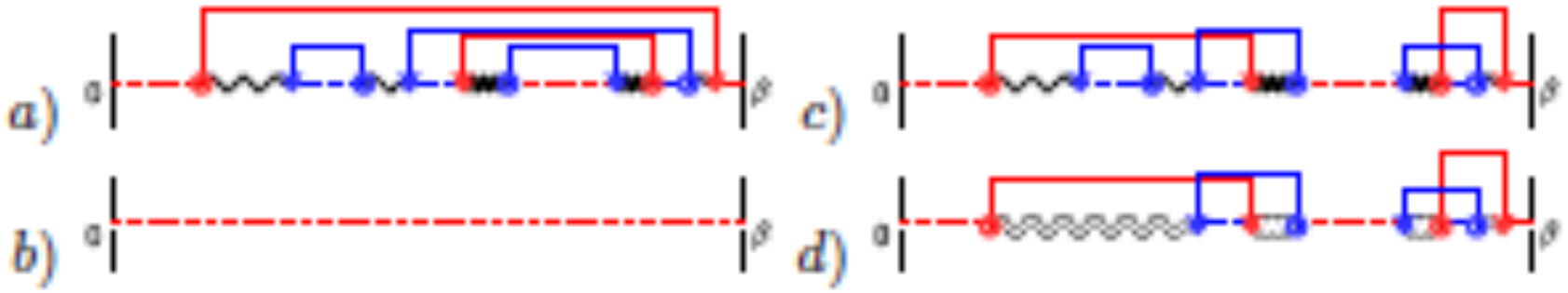
`NCA' (non-crossing approximation): resummation of all diagrams with no crossing hybridization lines or ``OCA" (one crossing approx)



Corrections to NCA by Monte-Carlo

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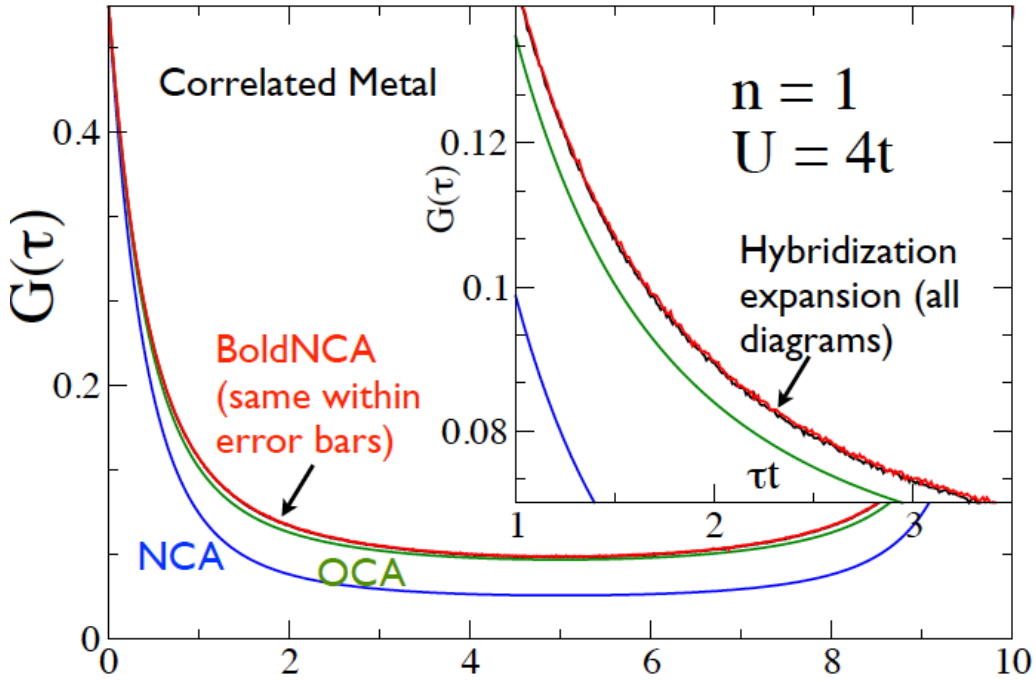
Test in equilibrium

Compare to exact results (here, DMFT, Hubbard model)



NCA: poor in metallic phase (OK in Mott insulator)

OCA good.

Bold—agrees with CT-QMC within error

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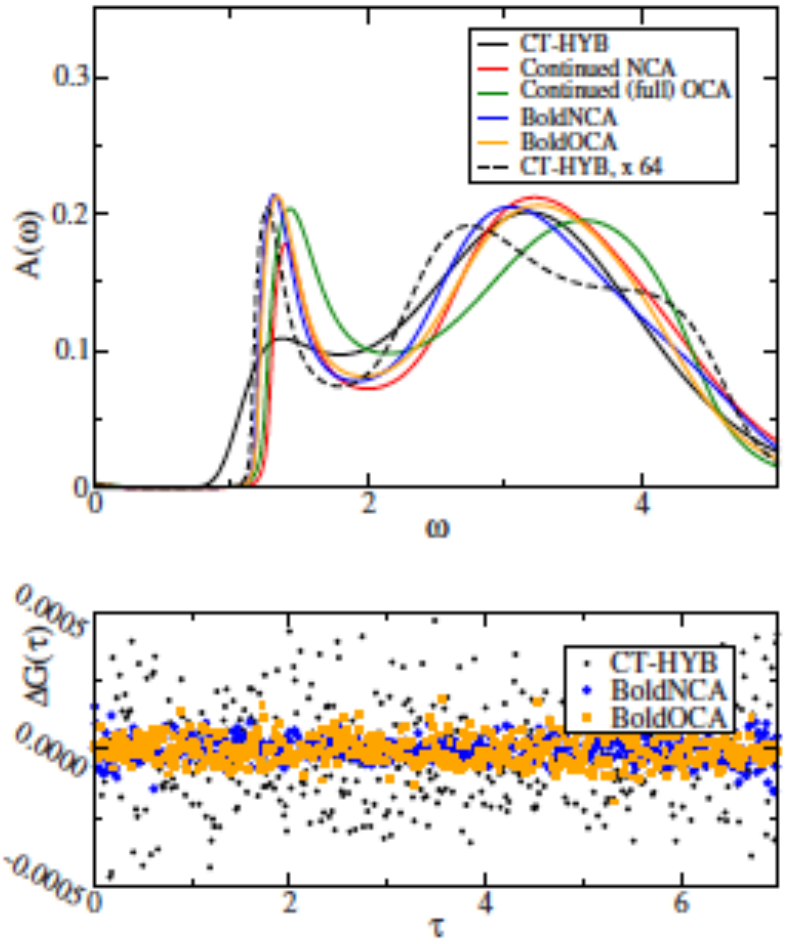
Structure at lower gap edge of Hubbard model



Bold method: significantly higher accuracy=> decent analytical continuation possible—but throwing more CPUs at standard CT-QMC gets same result

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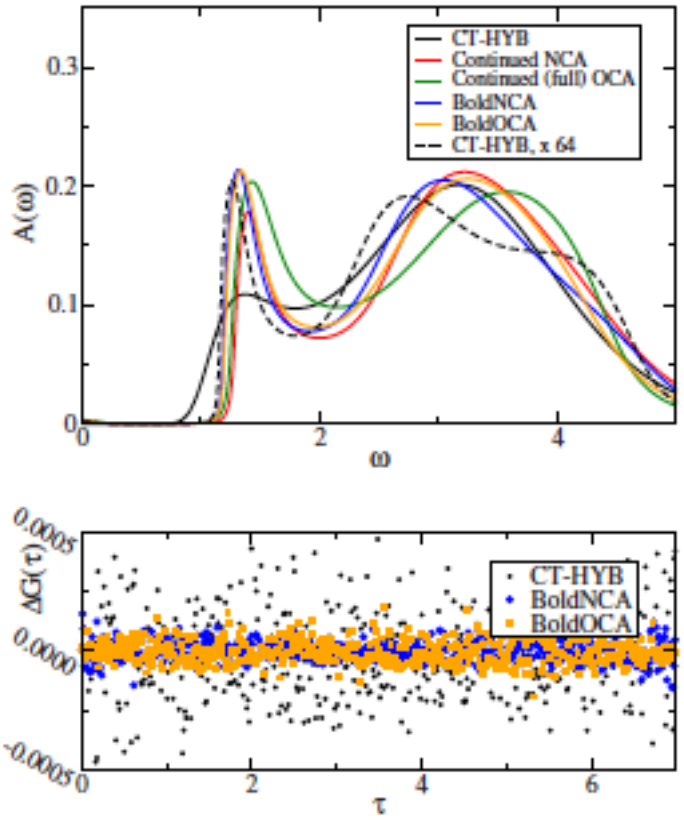
Remark

In equilibrium, bold methods not very useful for the quantum impurity models needed for DMFT

What you gain by expanding around a better starting point is not enough more than what you lose by no Wicks theorem except in a few cases



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Nonequilibrium Results
(quantum dot with voltage drop V)

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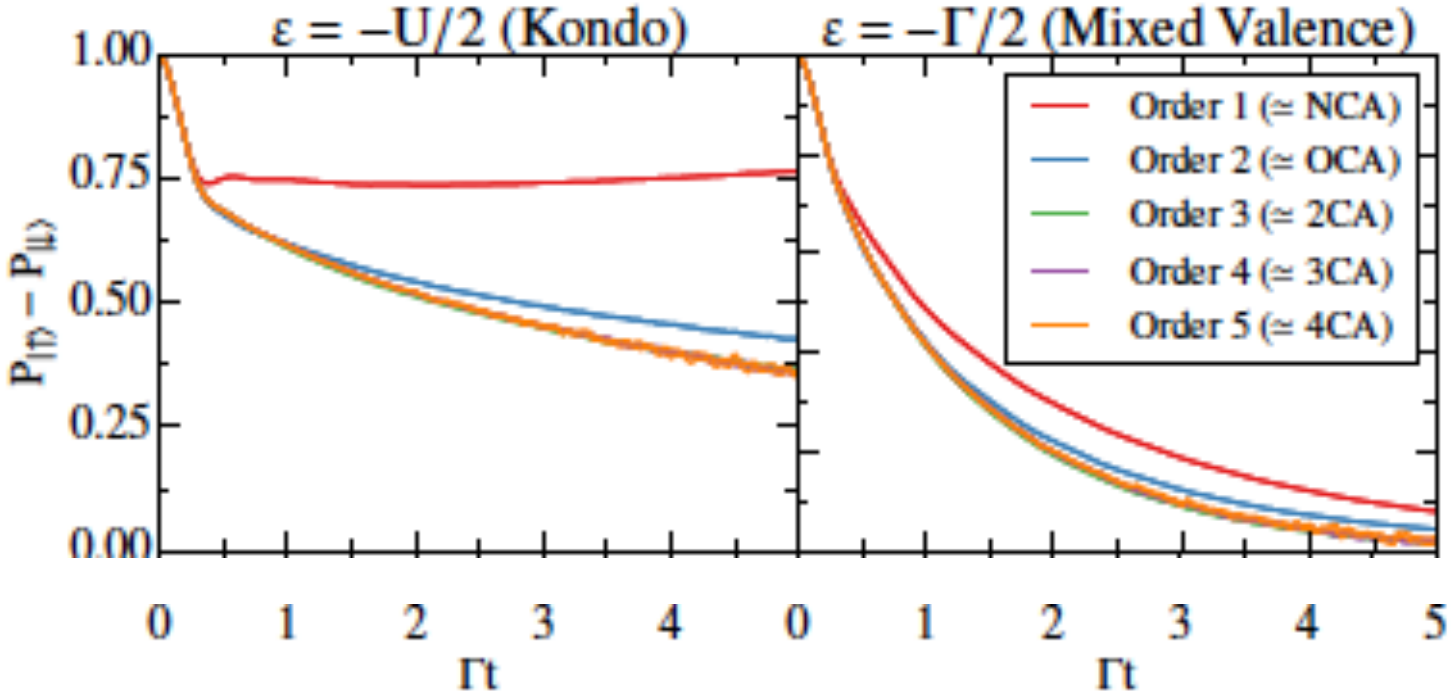
Test out of equilibrium

Magnetization



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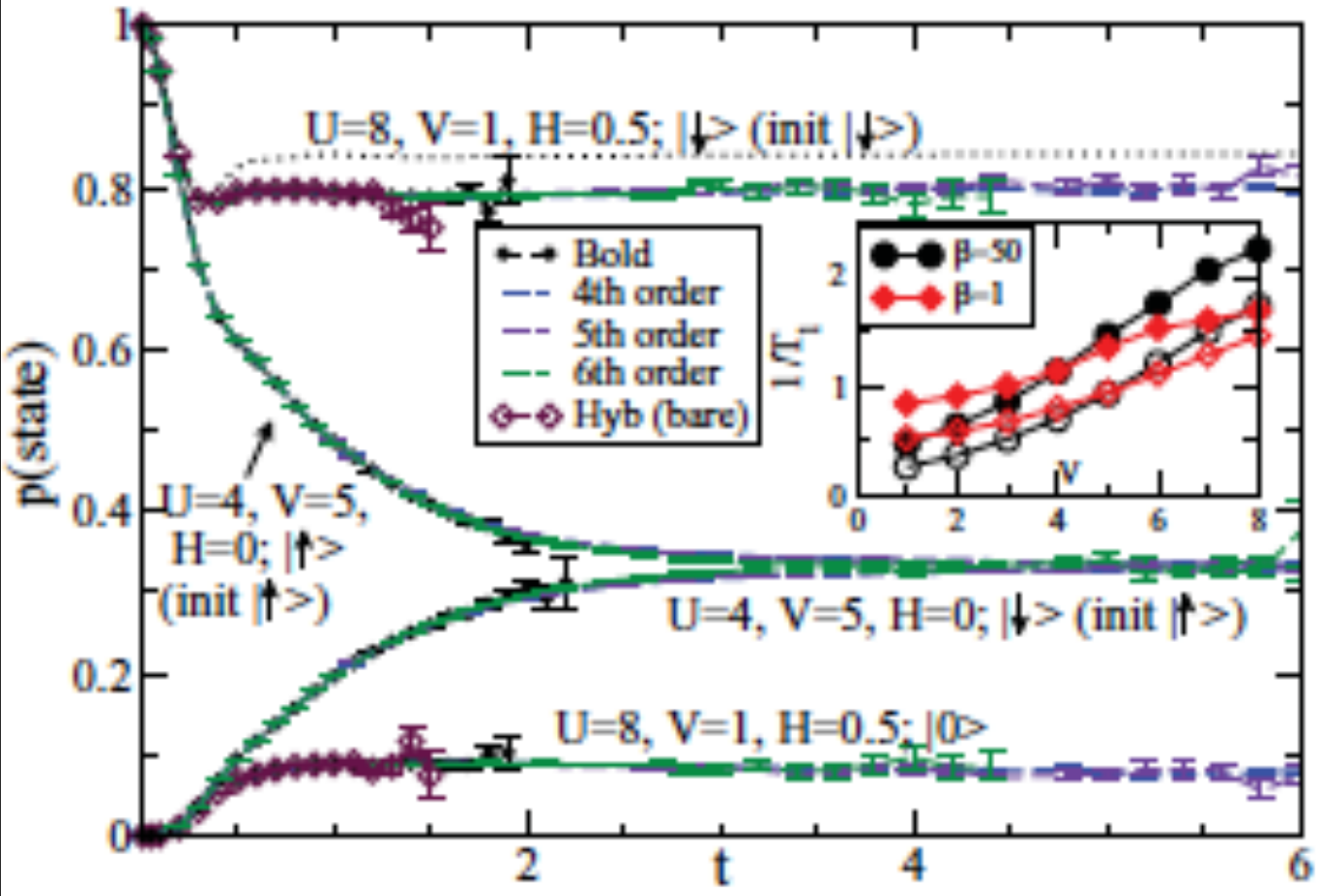
Magnetization relaxation



nb: density is easy to get right. spin dynamics is real test of method

NCA good for elements of density matrix; bad (~factor of 2) for relaxation times

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Bold expansion: accessible region $\sim 5 \times \Gamma$ not long enough!

New refinement (Cohen/Rabani): long timescale comes from small value of relaxation time. But relaxation time is determined by short time physics accessible to bold CT-QMC

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Zwanzig-Mori Memory kernel

Equation for reduced density matrix:

$$\mathbf{i}\frac{\mathbf{d}\sigma}{\mathbf{dt}} = [\mathbf{H_{impurity}},\ \sigma] - \mathbf{i}\int_{\mathbf{0}}^{\mathbf{t}} \mathbf{dt_1}\ \kappa(\mathbf{t_1})\ \sigma(\mathbf{t}-\mathbf{t_1})$$

$\kappa(\mathbf{t_1})$: **relaxation kernel computable by diagrams**

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Idea

Compute relaxation kernel using diagrams up to time t. Then use computed kernel to evaluate physical properties to longer times.

Convergence tests again crucial

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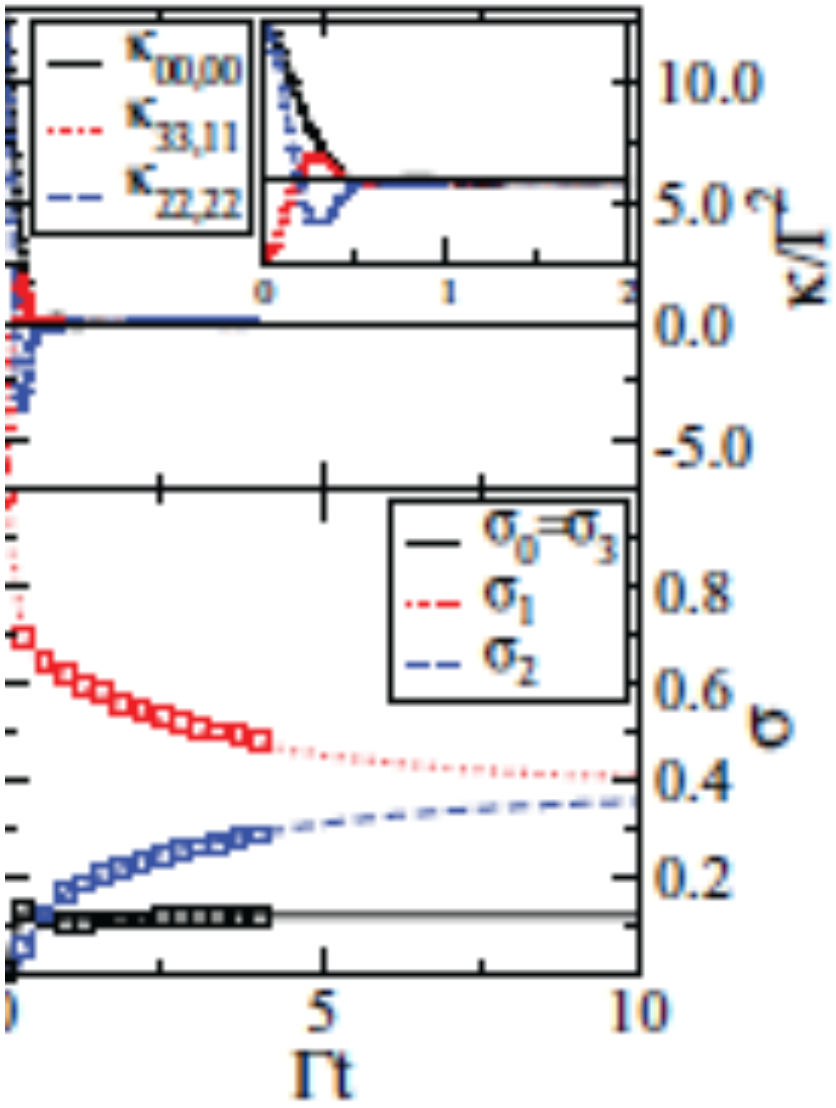
Example



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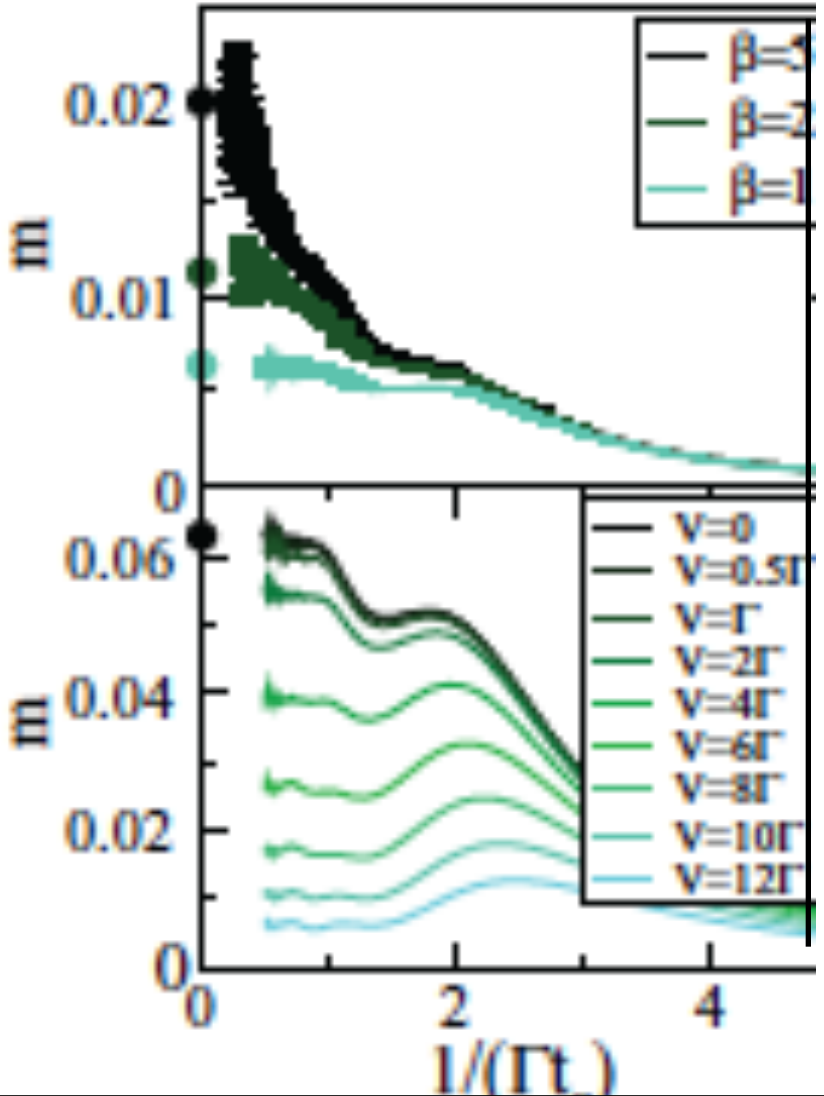
Memory methods: convergence is tricky



Equilibrium

Open question: long-time tail of kernel in FL regime

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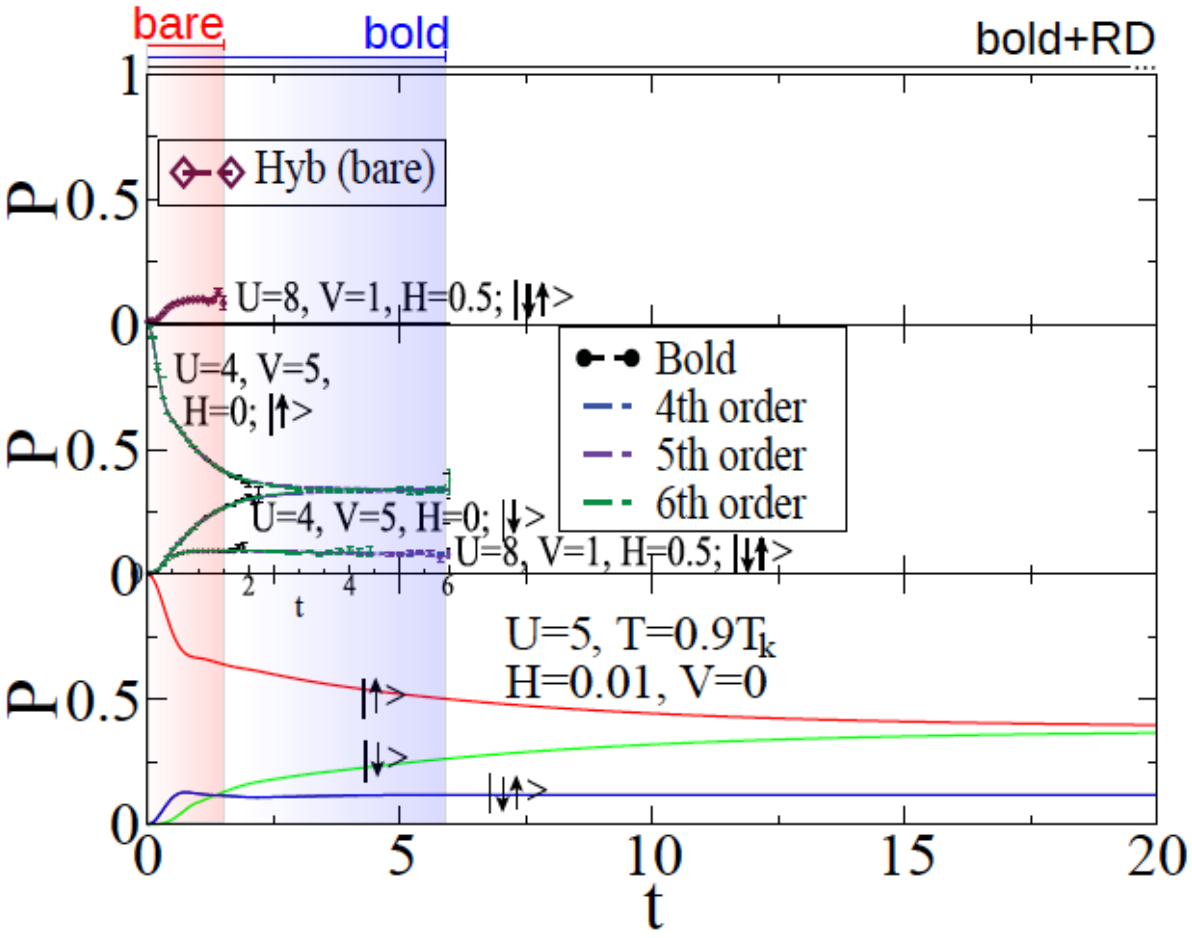
Cc

Memory method: results



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Bold+Memory gets you to long time (at not too low T)

BUT—what it gives you is the density matrix.
How to get the Green function???

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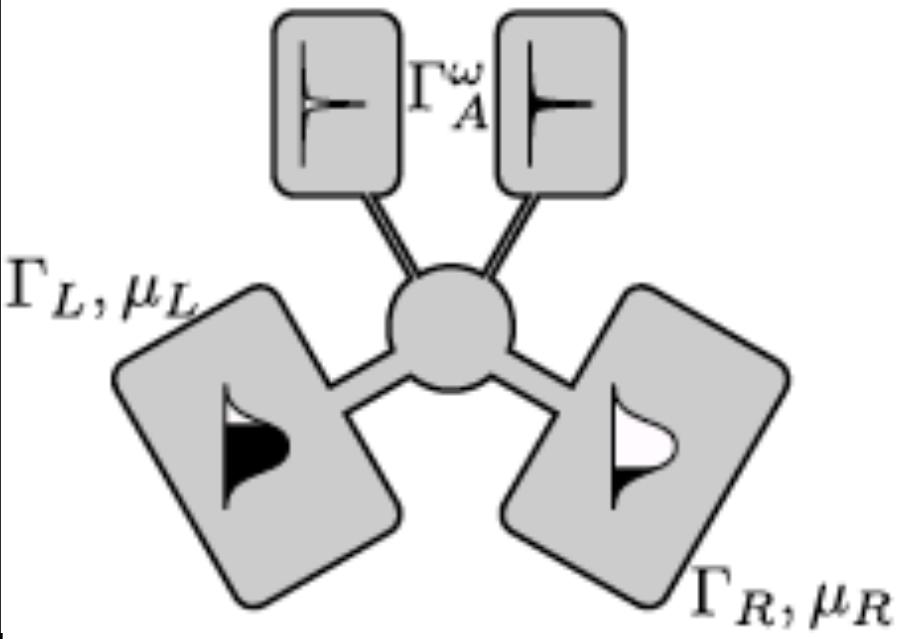
The Greens function (a two-time observable)



Guy Cohen: add two auxiliary leads, one to add and one to remove particles in a narrow energy range

$$A_{\text{aux}}(\omega, t) = \lim_{\eta \to 0} -\frac{2h}{e\pi\eta}\left[I_A^{\text{f}}(\omega, t) - I_A^{\text{e}}(\omega, t)\right]$$

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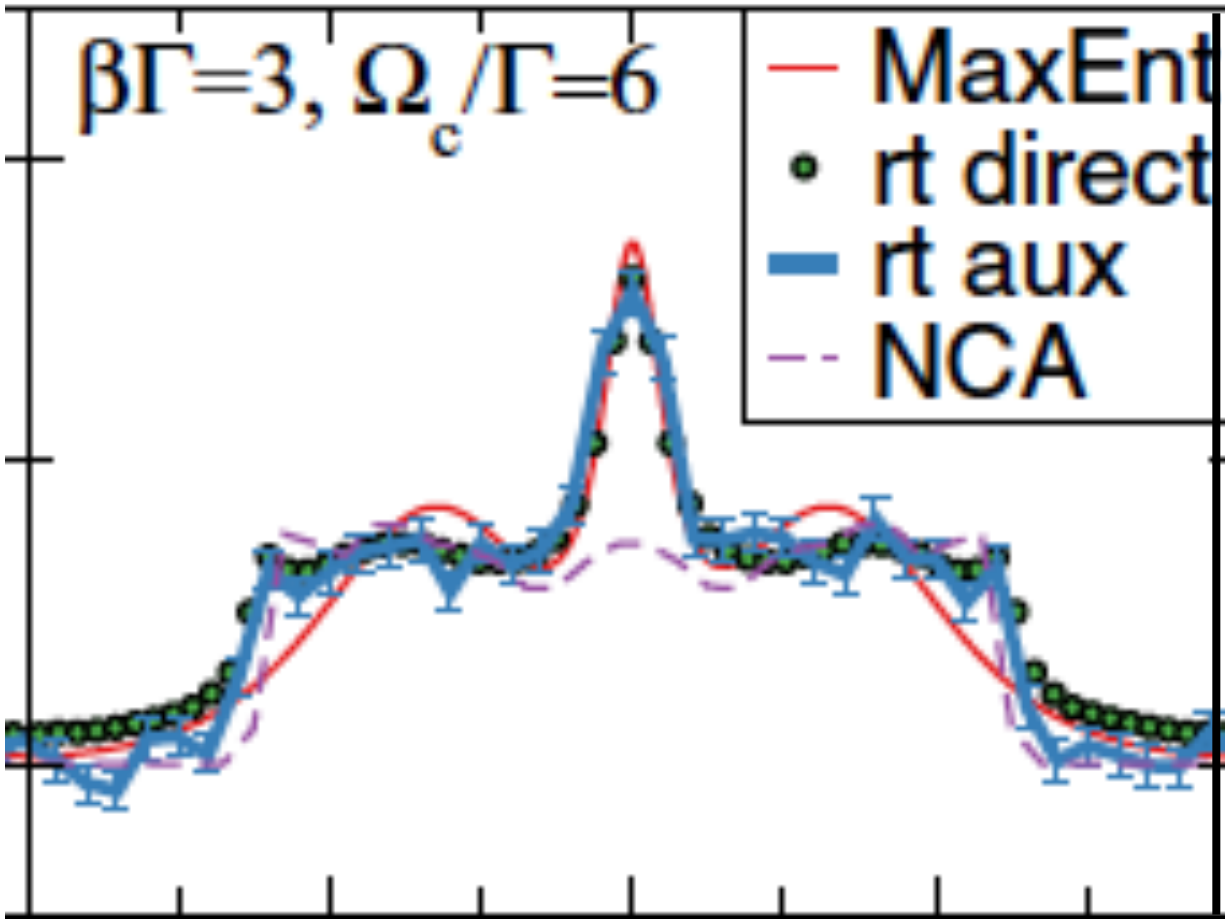
Test: equilibrium spectral function



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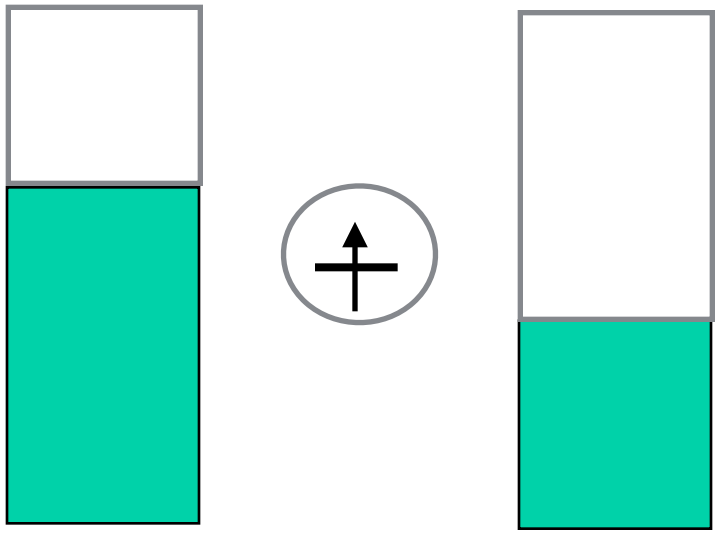
Physics question: nonequilibrium Kondo effect



Kondo effect: bind spin to electron at fermi level of lead.

Out of equilibrium—which lead do you choose?

does the Kondo resonance split?

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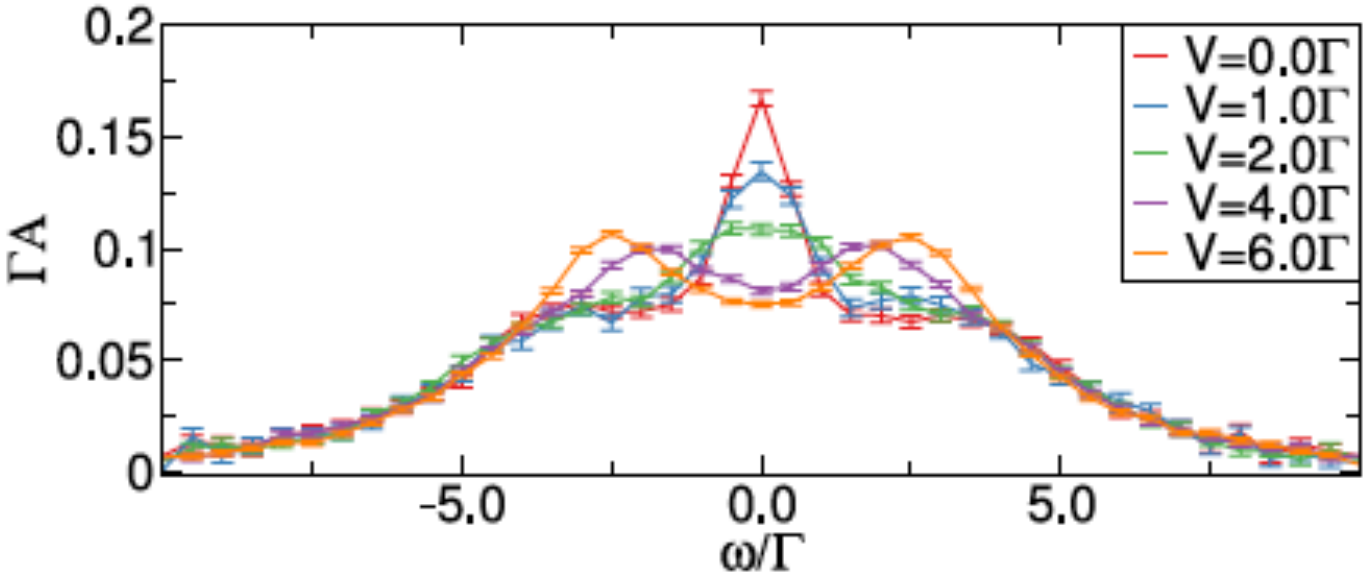
Steady state nonequilibrium spectral function:

Kondo resonance splits (!)



Many people had discussed this; our result provides converged numerics substiating the effect

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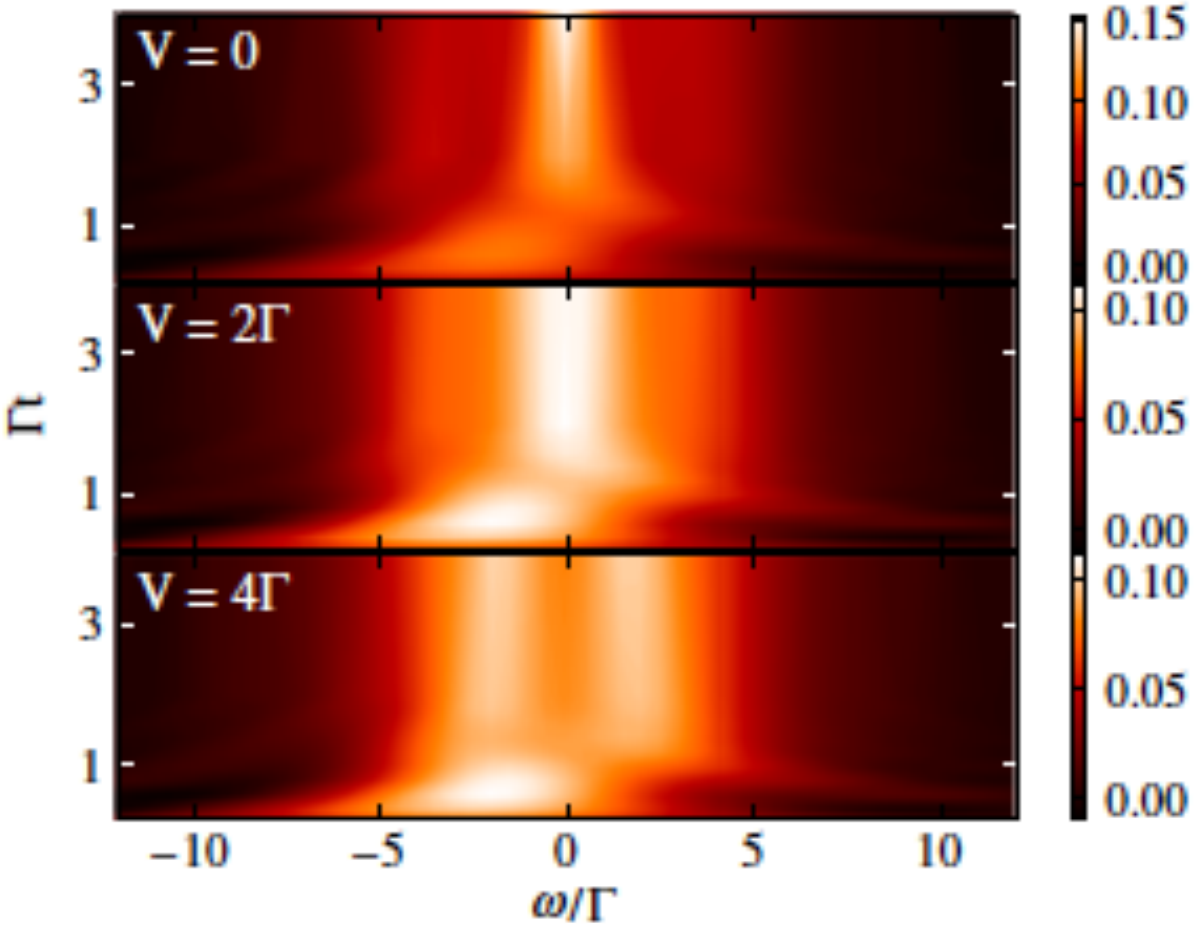
How does it happen in time



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Equation of motion (R. Hartle)

$$i\frac{d\sigma}{dt} = [H_{impurity},\ \sigma] - i\int_0^t dt_1\ \kappa(t_1)\ \sigma(t - t_1)$$

Density matrix (1 time operator obeys an equation involving a kernel (connects 2 times)
Kernel obeys an equation of motion involving a 3 time operator…

Truncate heirarchy at some level=> closed system of equations. Control by increasing level of hierarchy until convergence achieved

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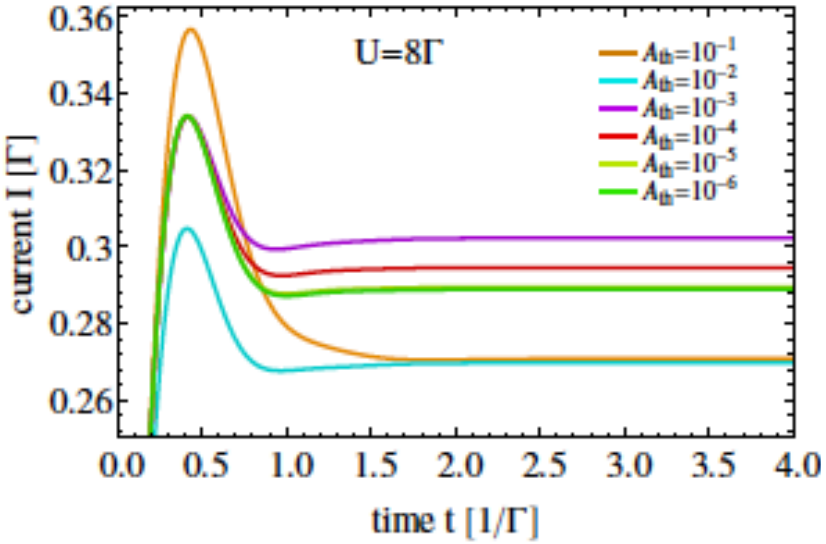
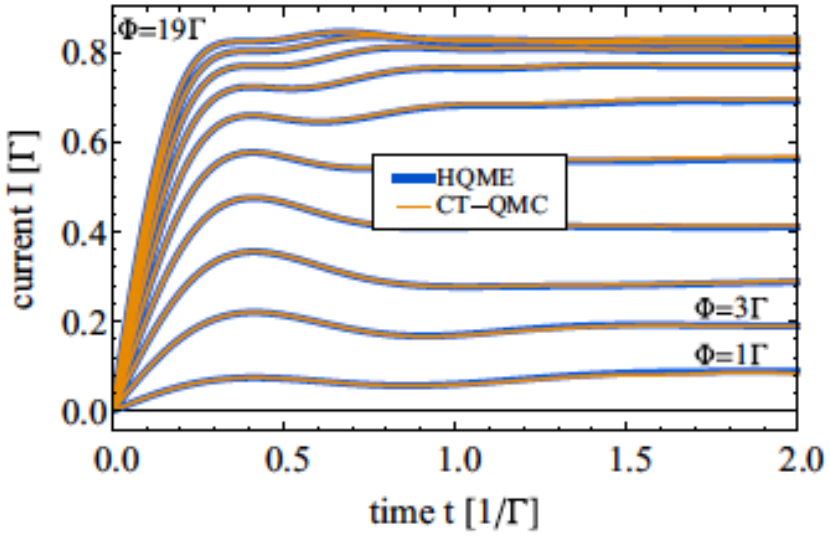
Convergence and comparison

$$T = \frac{\Gamma}{5}$$





R. Hartle, G. Cohen, D. Reichman and AJM PRB 92 085430

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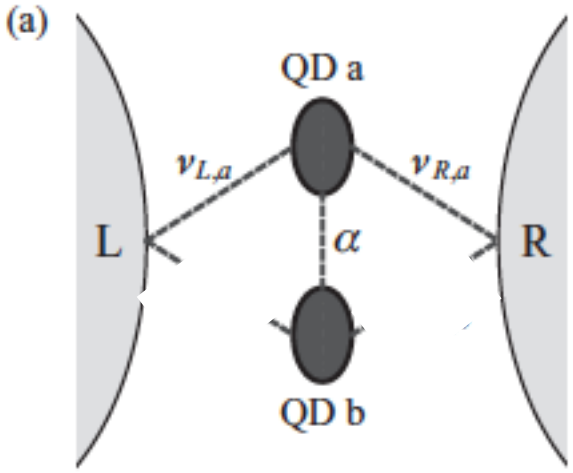
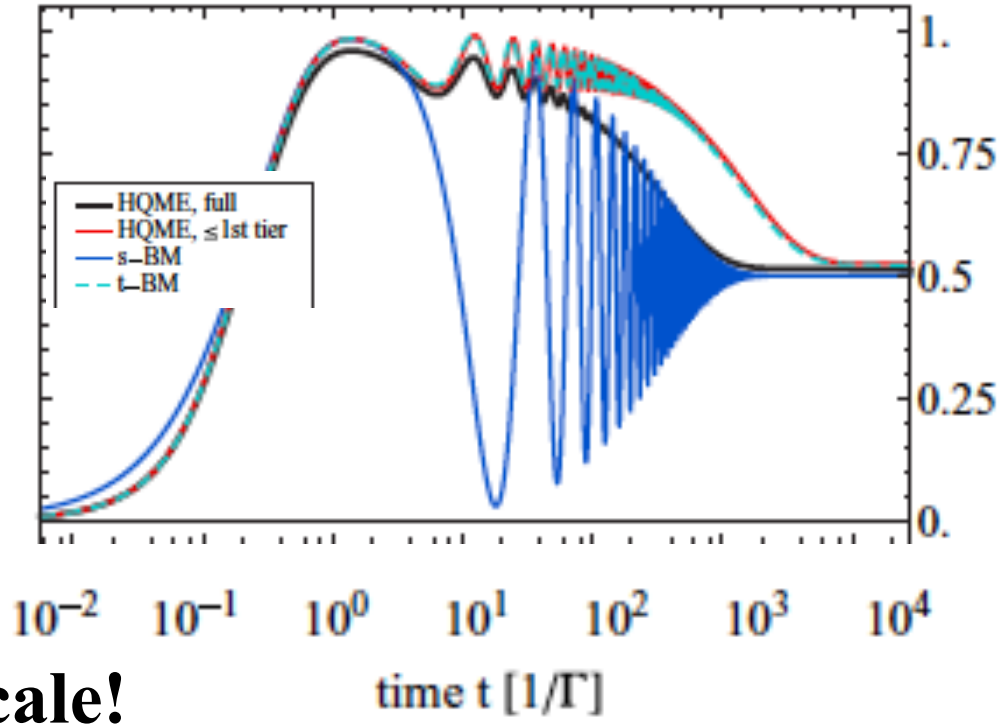
Results: quantum dot with branch not connected to leads





Notice the time scale!

R. Hartle and A. Millis, Phys. Rev. B.90.245426

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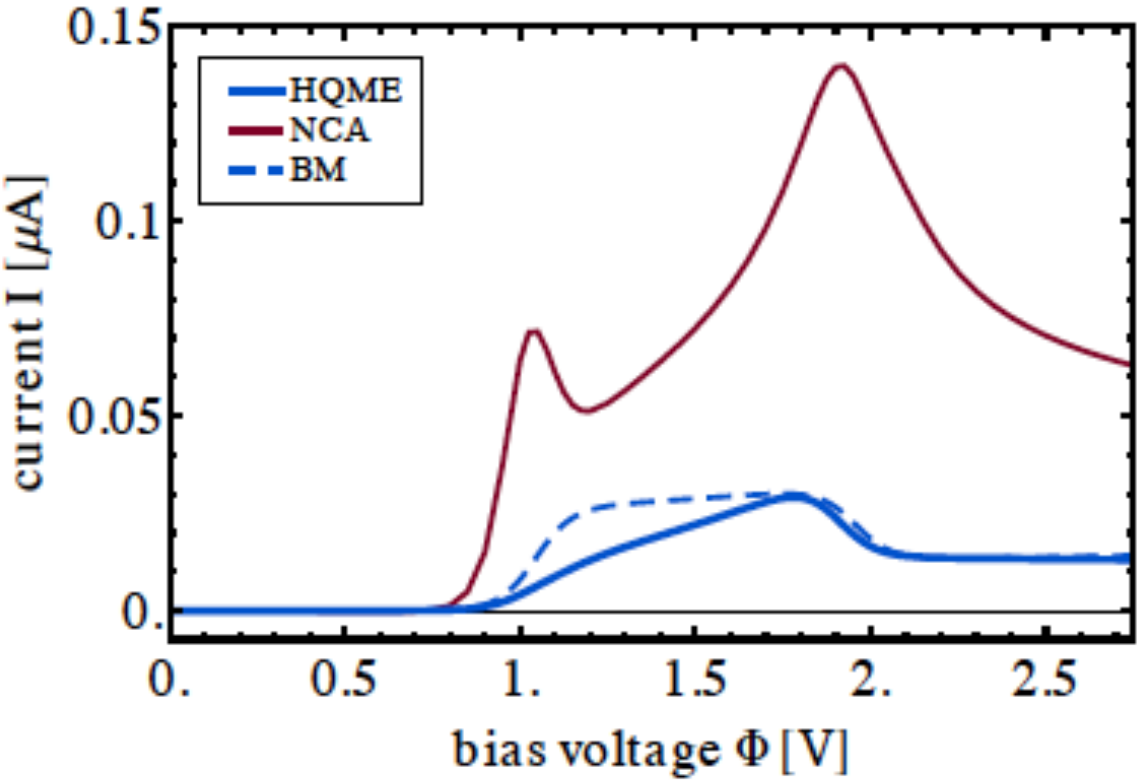
Comparison to other methods



R. Hartle

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Very recent work

Profumo, Groth, Messio, Parcollet Wantal

Key Points

- **Interaction expansion**
- **Impose unitarity (stochastic exploration includes diagram and its `unitarity complement')**
- **Examine convergence of perturbation series**

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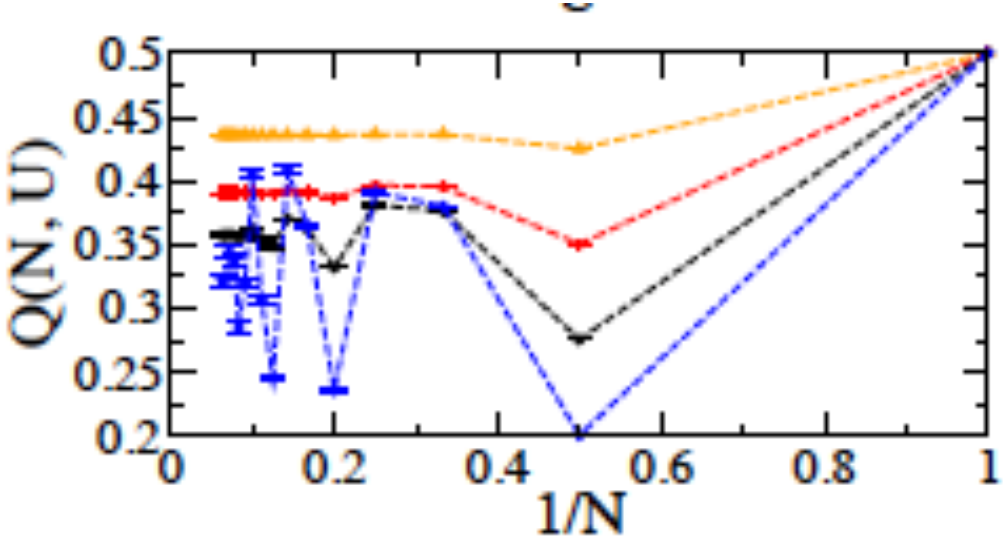
Result:
apparent FINITE radius of convergence in general case

Examine series for charge (Q) term by term

$$Q(N,U) = \sum_{n=0}^{N-1} Q_n U^n$$



U=0.2
U=0.4
U=0.6
U=0.8

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Summary:

At least for simple models methods in place to get long time nonequilibrium response

Simple approximations: quantiatively and sometimes qualitatively wrong.

Convergence ultimately controlled by temperature—convergence properties of T=0 series not yet clear.

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