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Transient dynamics of the Ohmic two-state system via the time-dependent numerical renormalization group method

December 6, 2016 | Theo Costi: IAS Symposium 2016 |

Acknowledgements/Coworkers

- Joint DFG Research Training Group RWTH/FZJ:
  - "Quantum Many-Body Methods in Condensed Matter Systems"
- Supercomputer support:
  - Juropa/Jureca (NIC/FZJ)
  - Compute cluster (RWTH)
- Collaborators:
  - Dr Hoa Nghiem (PGI-2/IAS-3) :TDNRG $\Rightarrow$ Poster-21
  - Dr Dante Kennes (RWTH): TD-DMRG
  - Dipl. Phys. C. Klöckner (RWTH/FUB) : Functional RG
  - Prof. Volker Meden (RWTH) : Functional RG

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[1] H. T. M. Nghiem, D. M. Kennes, C. Klöckner, V. Meden and T. A. Costi, Phys. Rev. B 93, 165130 (2016).

Outline

- Introduction to the Ohmic two-state system
- Motivation
- Results for $P(t) = \langle \sigma_z(t) \rangle_{\rho_{TLS}}, \quad \rho_{TLS} = |\uparrow\rangle\langle\uparrow|$
  - Comparisons: TDNRG vs NIBA
  - Comparisons: TDNRG vs TD-DMRG
  - Comparisons: TDNRG vs FRG
- Conclusions

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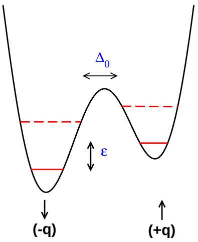
[1] H. T. M. Nghiem, D. M. Kennes, C. Klöckner, V. Meden and T. A. Costi, Phys. Rev. B 93, 165130 (2016).
[2] H. T. M. Nghiem and T. A. Costi, Phys. Rev. B 89, 075118 (2014).

The dissipative two-state system

- e.g., TL atoms, qubits,...



Spectral function: $J(\omega) = \sum_i \lambda_i^2 \delta(\omega - \omega_i)$

Ohmic dissipation: $J(\omega) = 2\pi\alpha\omega, \quad \omega \ll \omega_c$

- Generic model

$$H_{\mathrm{SBM}} = \underbrace{-\frac{1}{2}\Delta_0\sigma_x + \frac{1}{2}\epsilon\sigma_z}_{H_{\mathrm{TLS}}} \underbrace{+ \frac{1}{2}\sigma_z \sum_i \lambda_i (a_i + a_i^\dagger)}_{H_{\mathrm{int}}} \underbrace{+ \sum_i \omega_i (a_i^\dagger a_i + 1/2)}_{H_{\mathrm{bath}}}$$

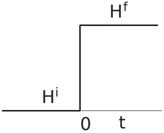
A. J. Leggett et al., Rev. Mod. Phys. 1987

U. Weiss, Quantum dissipative systems, 1999

Motivation: develop methods for time-evolution

The time-dependent numerical renormalization group method (TDNRG)

- Quantum quench: $H(t) = \theta(-t)H_i(\epsilon = -\infty) + \theta(t)H_f(\epsilon = 0)$



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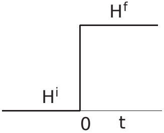
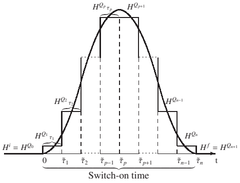


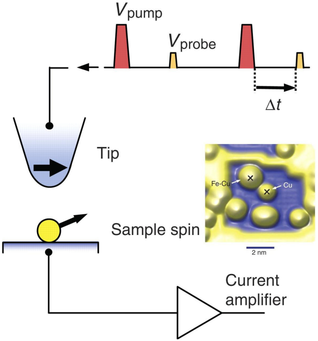
- General pulse or periodic driving field



- Parallelization: $N_{\mathrm{cores}} = n_{\mathrm{quenches}} \times n_z$

Motivation: experiments in the time-domain

- STM with pump-probe techniques[1]



[1] S. Loth *et al.*, Science 329, 1868 (2010).

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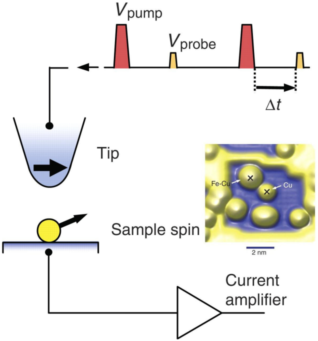

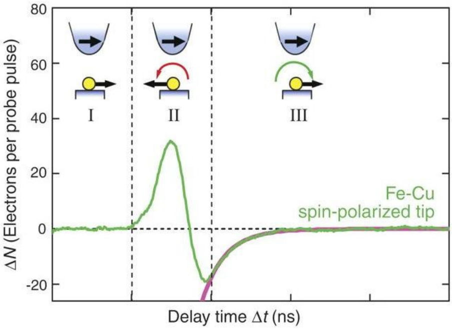

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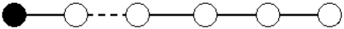
Numerical renormalization group[1]

see Poster-21



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[3] A. Weichselbaum and J. von Delft, Phys. Rev. Lett. 99, 076402 (2007).

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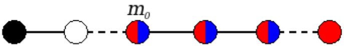

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Numerical renormalization group[1]

see Poster-21

- Complete basis set[2], $\sum_{m=m_0}^{N} \sum_{le} |lem\rangle\langle lem| = 1$
- Full density matrix[3], $\rho = \sum_{m=m_0}^{N} \sum_{le} |lem\rangle \frac{e^{-\beta E_l^m}}{\tilde{Z}_m} w_m \langle lem|$
- Only approximation: $H|rem\rangle \approx H_m|rem\rangle = E_r^m|rem\rangle$

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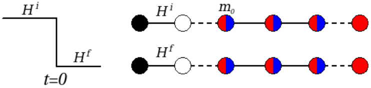
TDNRG for a single quench at finite temperature

see Poster-21

- Time evolution[1]: $O(t \geq 0) = \mathrm{Tr}[\rho(t)\hat{O}]$, $\rho(t) = e^{-iH_f t}\rho_i e^{iH_f t}$



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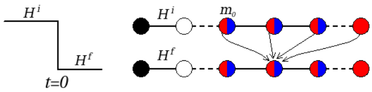

FDM: $\rho_i = \sum_{m'=m_0}^{N} \sum_{l'e'} |l'e'm'\rangle_i \frac{e^{-\beta E_{l'}^{m'}}}{\tilde{Z}_{m'}} w_{m'i} \langle l'e'm'|$

$$O(t) = \sum_{m=m_0}^{N} \sum_{rs \notin KK'} \underbrace{\left(\sum_{e} {}_f\langle sem| \overbrace{\rho_i} |rem\rangle_f \right)}_{\rho_{sr}^{i\to f}(m)} e^{-i(E_s^m - E_r^m)t} O_{rs}^m$$

- Projected (reduced full) density matrix[2]

$$\rho_{sr}^{i\to f}(m) = \underbrace{\rho_{sr}^{++}(m)}_{m'>m} + \underbrace{\rho_{sr}^{0}(m)}_{m'=m} + \underbrace{\rho_{sr}^{--}(m)}_{m'<m}$$

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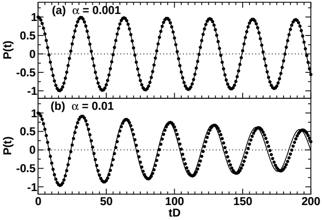
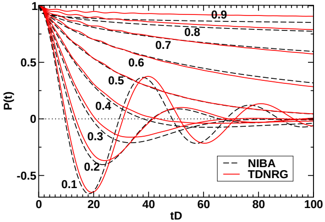
P(t): TDNRG vs NIBA

- $\alpha \ll 1,\ \Delta_0/\omega_c = 0.1$



- $0.1 \lesssim \alpha \lesssim 0.9,\ \Delta_0/\omega_c = 0.1$

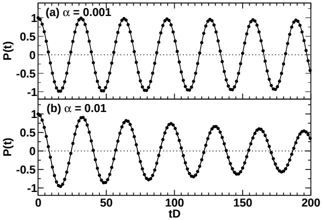


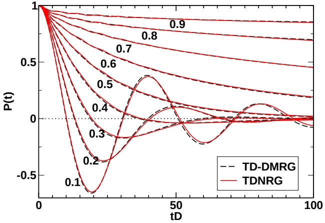
- Noninteracting-blip-approximation (NIBA) [1]: $P(t) = E_{2-2\alpha}(-(t\Delta_{\rm eff}(\alpha))^{2-2\alpha})$
- $\Delta_{\rm eff}(\alpha) = (\Gamma(1-2\alpha)\cos(\pi\alpha))^{1/2(1-\alpha)}\,\Delta_{\rm r}(\alpha),\ \ \Delta_r(\alpha)/\omega_c = (\Delta_0/\omega_c)^{1/(1-\alpha)}$
- NIBA oscillations lag behind TDNRG with increasing α
- NIBA/TDNRG differences up to 30% at $t \sim 1/\Delta_{\rm eff}(\alpha)$

[1] A. J. Leggett et al, Rev. Mod. Phys. 59, 1 (1987).

P(t): TDNRG vs TD-DMRG

- $\alpha \ll 1,\ \Delta_0/\omega_c = 0.1$
- $0.1 \lesssim \alpha \lesssim 0.9,\ \Delta_0/\omega_c = 0.1$





- TD-DMRG for $L = 200$ sites, numerically exact for not too long times.
- TDNRG/TD-DMRG agreement quantifies limitations of NIBA
- TDNRG/TD-DMRG agreement indicates that TDNRG remains accurate up to $1/\gamma_r(\alpha)$, $\gamma_r(\alpha) \sim \alpha\Delta_{\mathrm{eff}}(\alpha)$

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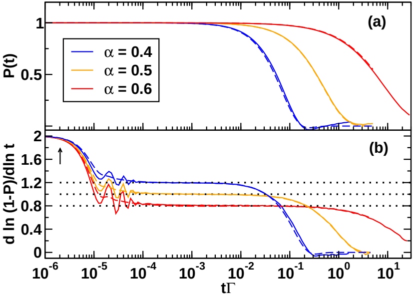
$P(t)$: TDNRG vs FRG



- Short-time limit: $1 - P(t) \sim (\Delta_{\mathrm{eff}}(\alpha)t)^{2(1-\alpha)}$, $1/D \ll t \ll 1/\Delta_{\mathrm{eff}(\alpha)}$
- Ultra-short time limit: $1 - P(t) \sim c_{\alpha_i}(Dt)^2$, $0 < t \ll 1/D$

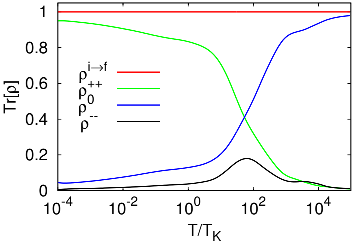
Conclusions

- TDNRG/TD-DMRG/FRG comparisons indicate that
  - TDNRG quantitatively accurate up to times $t \lesssim 1/\gamma_r(\alpha)$
  - NIBA quantitatively wrong even at $\alpha \ll 1$
- Future extensions/improvements/applications:
  - Improve long time limit of TDNRG
  - Applications to non-equilibrium transport in nanodevices
  - Applications to pump-probe experiments

Thanks for your attention !

Exact results and errors in TDNRG[1]

- $Tr\rho^{i\to f} = 1$



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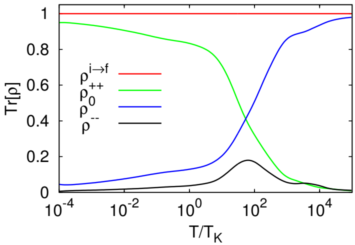

- $O(t \to 0^+) = O_i$

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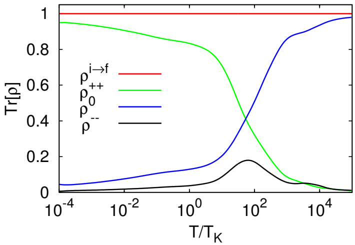

- $O(t \to 0^+) = O_i$

- $O(t \to \infty) \neq O_f$!

α	$1/\Delta_{\mathrm{eff}}(\alpha)$	$1/T_0(\alpha)$	$P(\infty)$
0.001	5.008	5.018	0.000003
0.01	5.089	5.18	0.00016
0.1	6.11	6.97	0.0045
0.2	7.915	9.79	0.0092
0.3	11.098	14.38	0.0143
0.4	17.34	22.82	0.0186
0.5	31.83	40.92	0.0414
0.6	75.9	89.2	0.0407
0.7	288.6	270.4	0.049
0.8	3232	1541.9	0.0556
0.9	1032584	38800.0	0.066

Table: $P(t) = \langle \sigma_z(t) \rangle_{\rho_i}$

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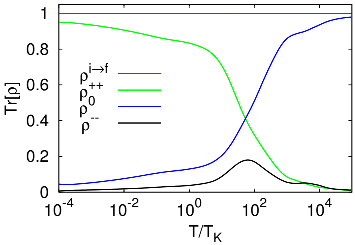

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- Motivation [2]: accuracy of TDNRG at $0 < t < \infty$?

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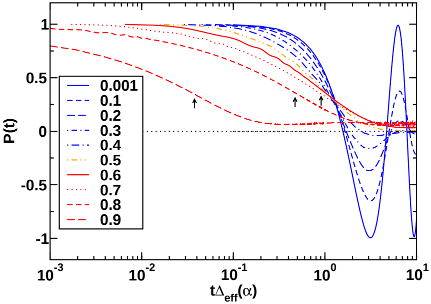
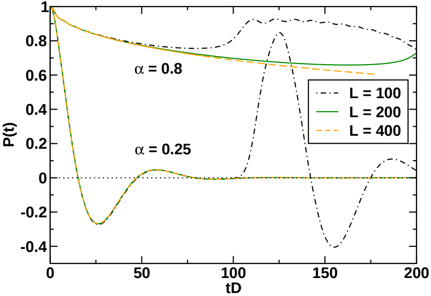
[2] H. T. M. Nghiem, D. M. Kennes, C. Klöckner, V. Meden and T. A. Costi, Phys. Rev. B 93, 165130 (2016).

Long-time TDNRG results



- TDNRG stable to infinite times !
- However, finite errors at $t = \infty$

L-dependence of TD-DMRG results



- TD-DMRG are for finite chains $L = 100, 200, 400$
- Results up to $tD = 100$ independent of L