TEBD simulation of quantum quenches in the S=1 Heisenberg chain: numerical test of the semiclassical approximation

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(BME Dept. Theor. Phys.)

ELTE seminar 07/03/2018

Outline

- Quantum quenches in 1D systems.
- Matrix Product States, the TEBD algorithm
- Quantum quenches in gapped systems: the semiclassical description
- Half chain spin fluctuations after the quench: semi-classics vs. TEBD simulations.
- Generalization of semi classics

Quantum quenches in 1D

Dynamical properties of correlated quantum systems?

$$i\partial_t |\Psi\rangle = \hat{H} |\Psi\rangle$$

Many-body wave function

$$|\Psi(t=0)\rangle = |\Psi_0\rangle$$

Initial state: Usually the ground state of some $\hat{H}_0$

We initialize the g.s. of $\hat{H}_0$,
then at $t = 0$ we switch to $\hat{H}$

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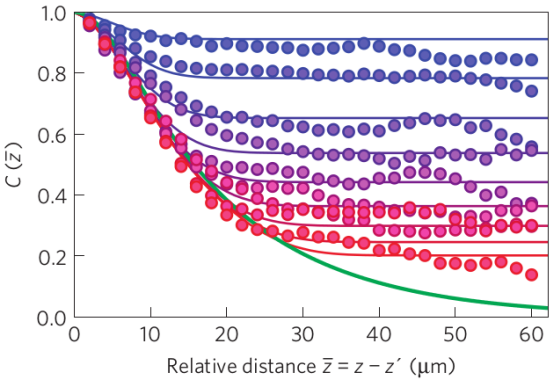
Experimental realization with cold atoms



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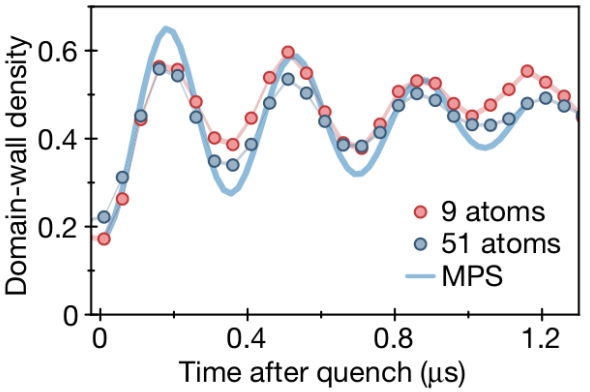

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Questions

- Does there exist a post-quench stationary state? Can we describe it?
- Is it a thermal state?
- Can we describe the relaxation dynamics?

Hard numerical problem

$$\dim \mathcal{H} \propto d^V$$

- Integrable models, exact solutions
- **1D models: powerful methods for slightly entangled states**

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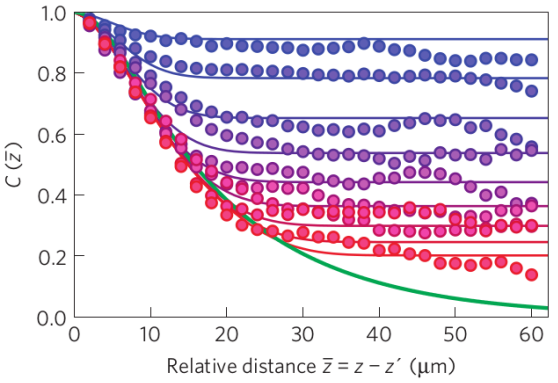

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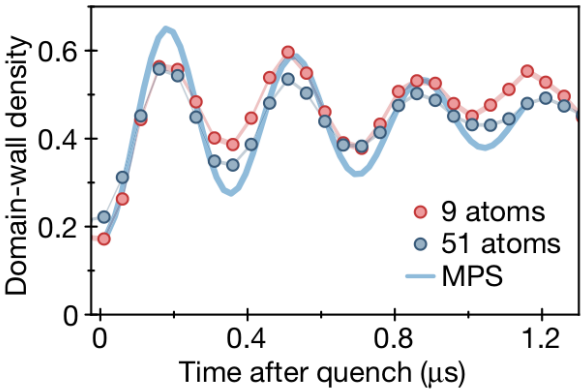

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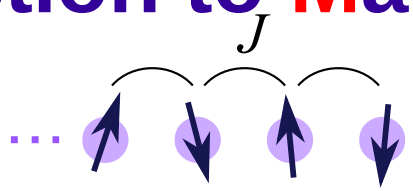
Short Introduction to Matrix Product States

$$\hat{H} = J \sum_i \vec{S}_i \vec{S}_{i+1}$$



$$|\Psi\rangle = \sum_{\mu_1,\ldots,\mu_L} C_{\mu_1 \mu_2 \ldots \mu_L} |\mu_1\rangle \cdots |\mu_L\rangle$$

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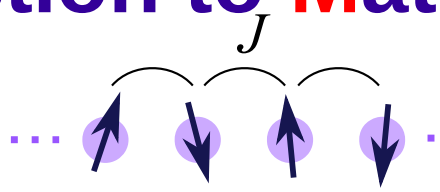

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Schmidt decomposition

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$$

$$|\Psi\rangle = \sum_{i,j} \Psi_{ij} |i_A\rangle |j_B\rangle$$

Singular **V**alue **D**ecomposition:

$$\Psi_{ij} = \sum_{\alpha} U_{i,\alpha} \lambda_\alpha V^*_{j,\alpha}$$

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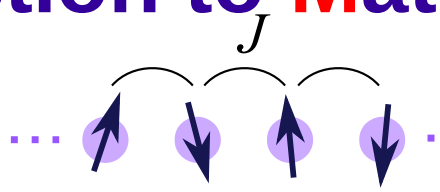

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Schmidt values

Schmidt states

Normalization: $\langle \Psi | \Psi \rangle = 1 = \sum_\alpha \lambda_\alpha^2$

Wave function compression: truncation

$$|\Psi\rangle = \sum_{\alpha} \lambda_\alpha |\alpha_A\rangle |\alpha_B\rangle$$

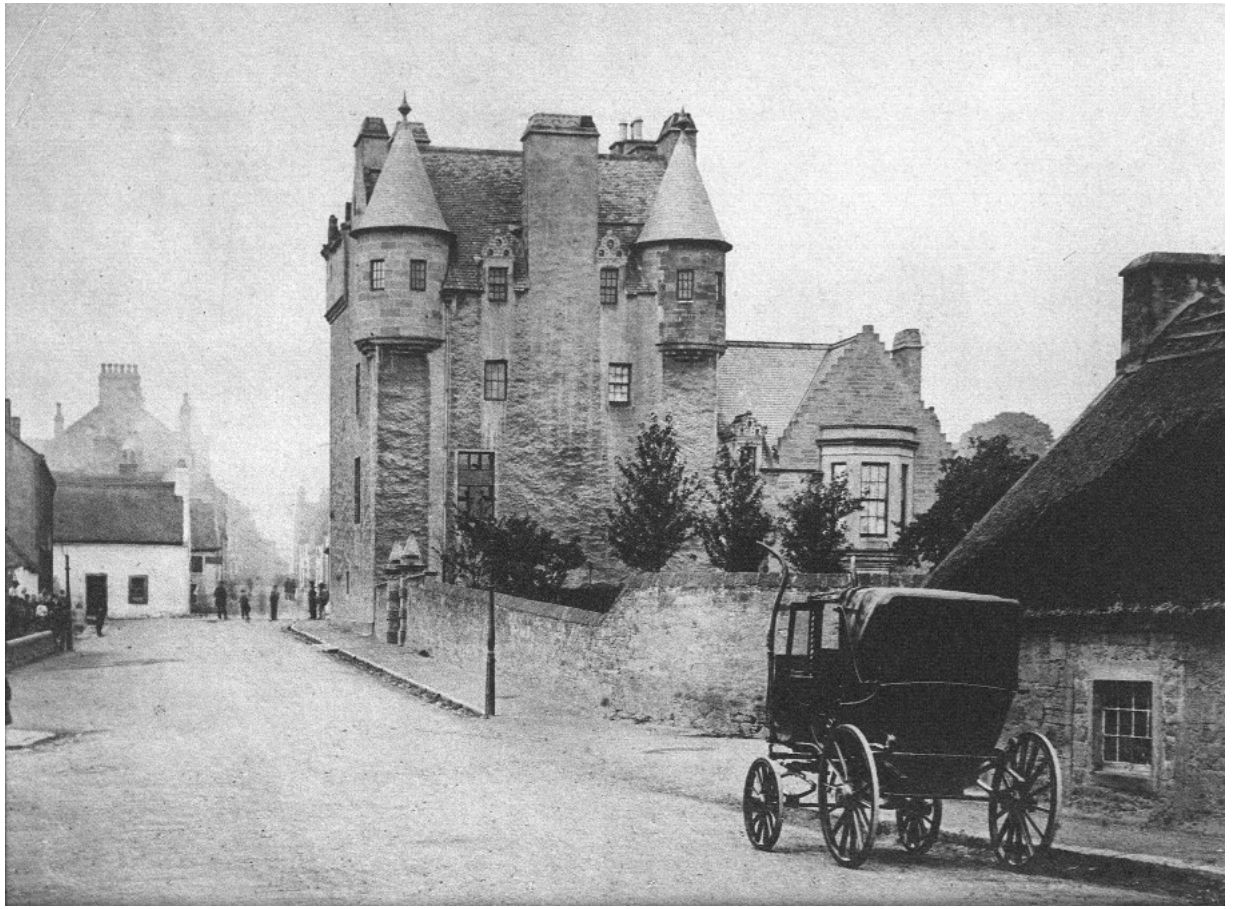
The number of Schmidt pairs generally:

$$\dim\lambda_\alpha = \min(\dim\mathcal{H}_A, \dim\mathcal{H}_B)$$

In practice we don't need all of them

Truncation: keep only M Schmidt pairs with the largest Schmidt values!

"Bond dimension": $M \ll \min(\dim\mathcal{H}_A, \dim\mathcal{H}_B)$



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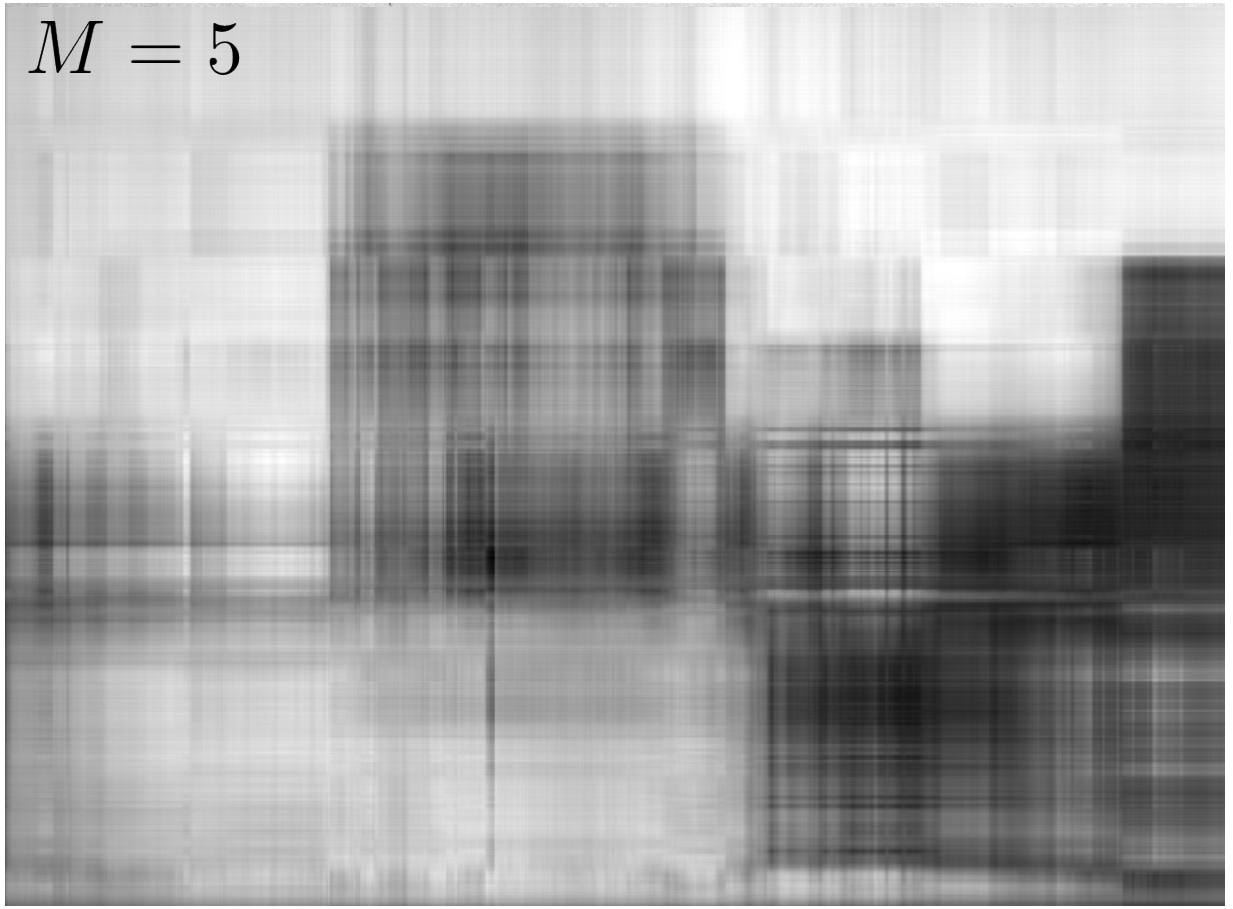

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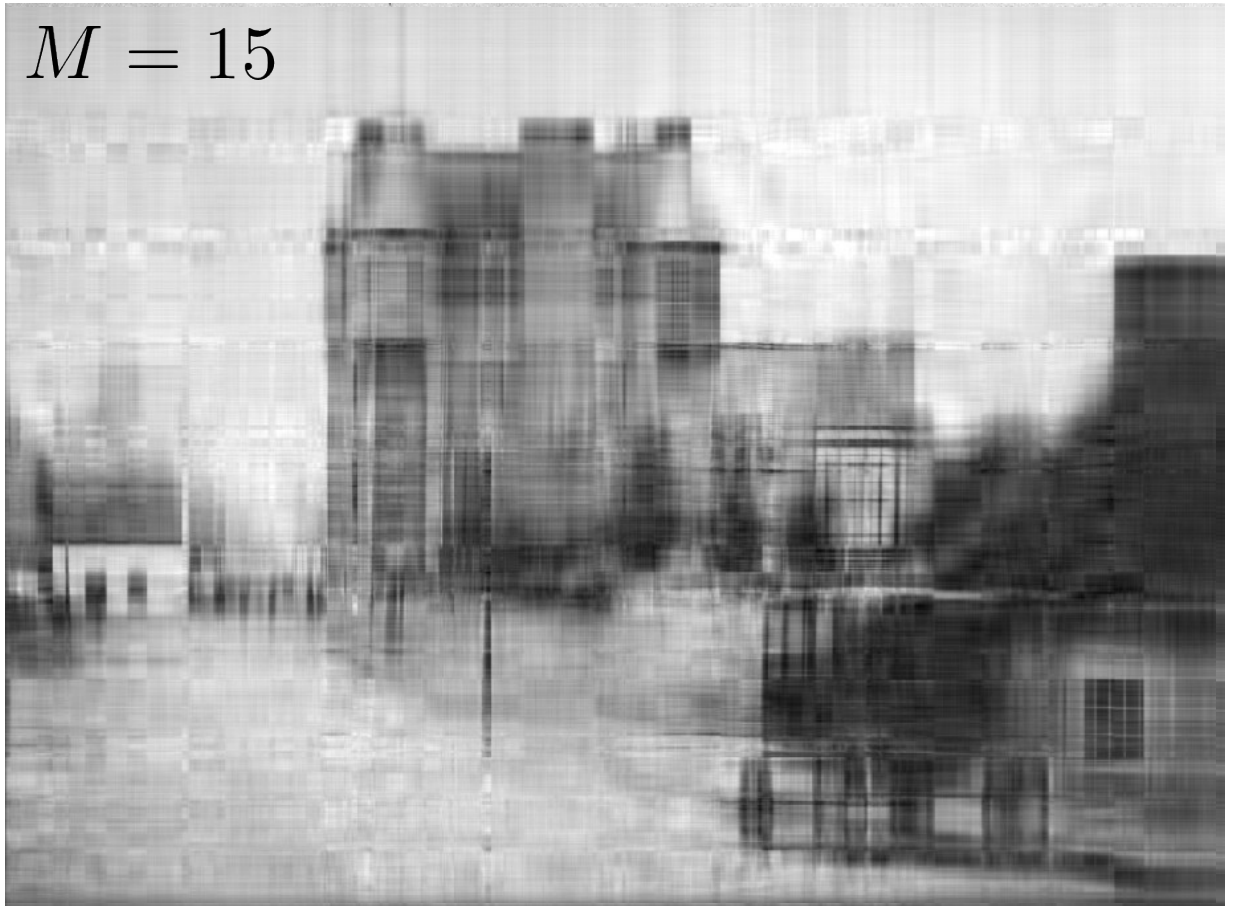

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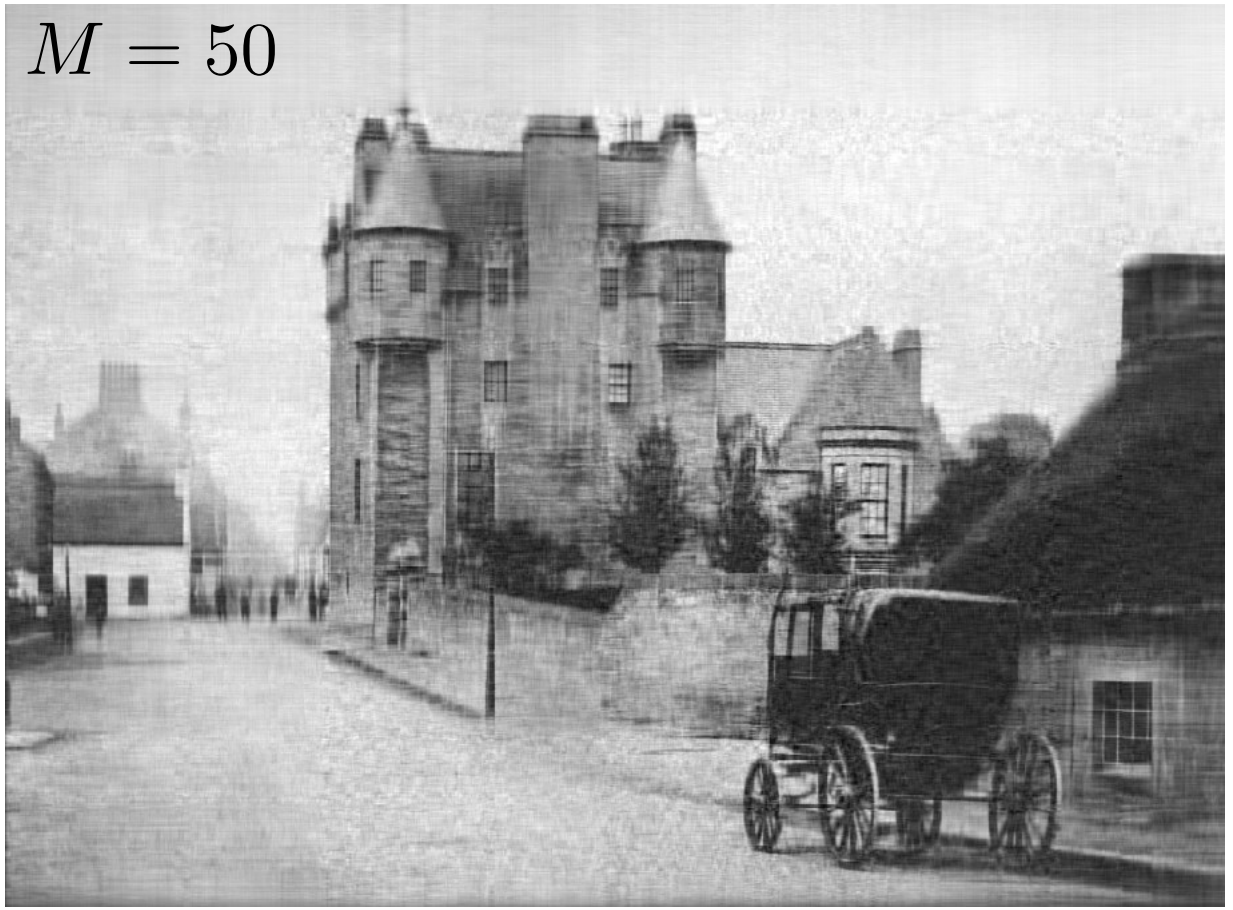

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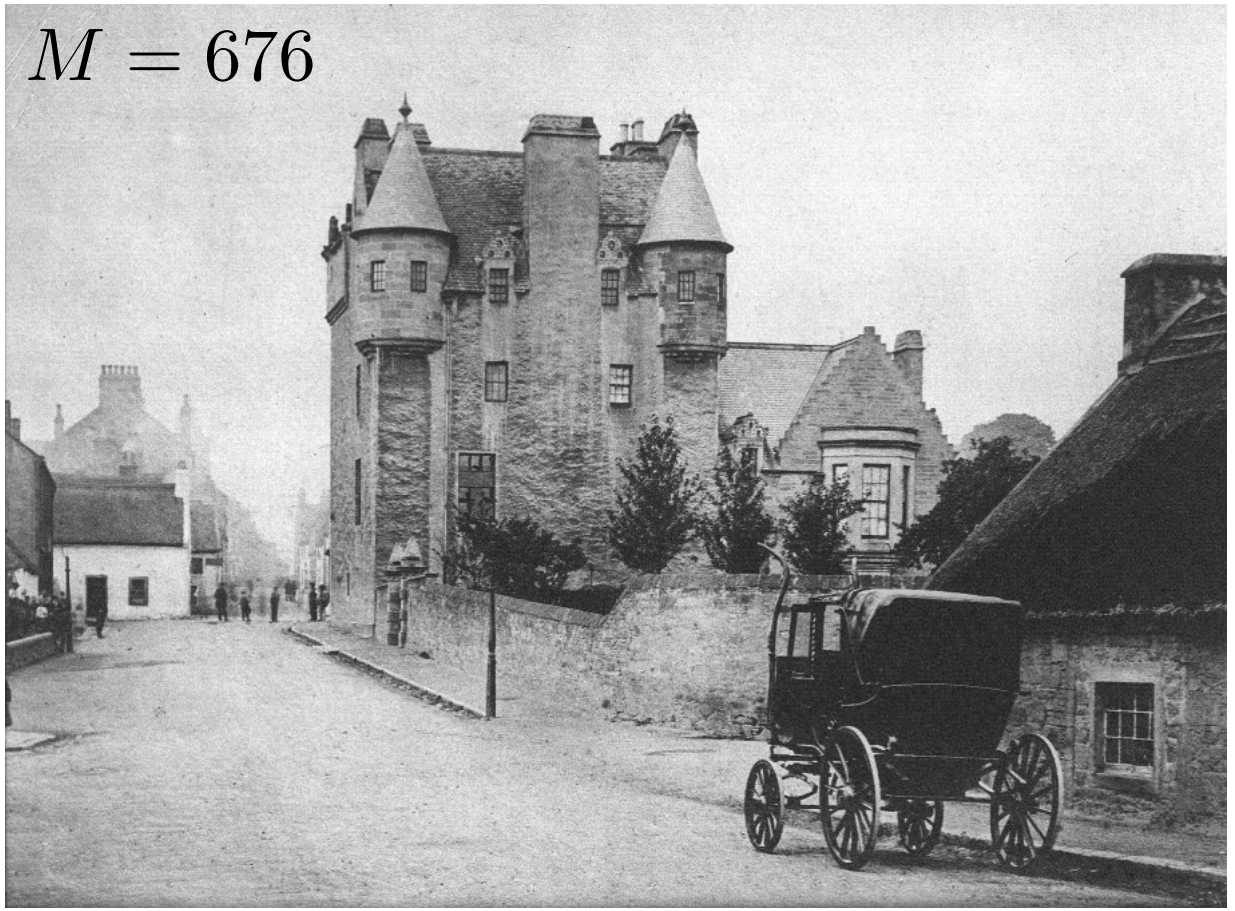

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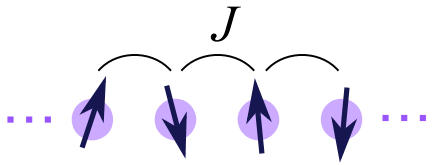
Construction of Matrix Product States

1D chain of sites



Local Hilbert space $\mathcal{H}_1 \quad \dim\mathcal{H}_1 = d$

Cut the chain after between sites l and $l+1$

$A = [1, \ldots, l] \qquad B = [l+1, \ldots, L]$

Schmidt-decomposition:

$$|\Psi\rangle = \sum_{\alpha_l} \lambda_{\alpha_l}^{[l]} \, |\alpha_l\rangle_{\text{left}} \, |\alpha_l\rangle_{\text{right}}$$

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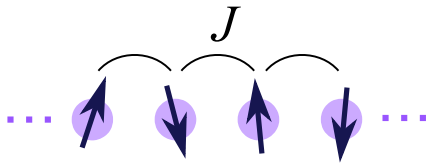

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Now cut between *l-1* and *l*

$$|\Psi\rangle = \sum_{\alpha_{l-1}} \lambda^{[l-1]}_{\alpha_{l-1}} |\alpha_{l-1}\rangle_{\text{left}} |\alpha_{l-1}\rangle_{\text{right}}$$

Connection between the Schmidt states:

$$|\alpha_l\rangle_{\text{left}} = \sum_{\alpha_{l-1},\mu_l} \lambda^{[l-1]}_{\alpha_{l-1}} \Gamma^{[l],\mu_l}_{\alpha_{l-1}\,\alpha_l} |\alpha_{l-1}\rangle_{\text{left}} |\mu_l\rangle$$

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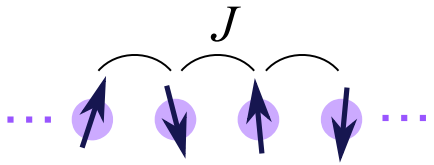

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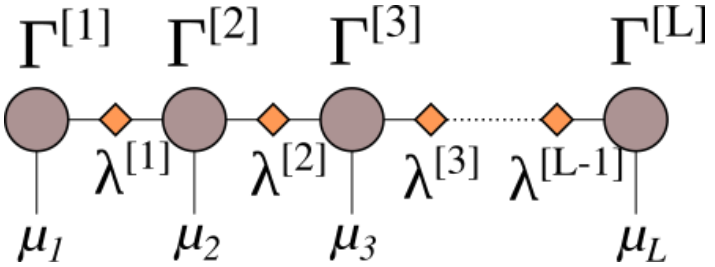
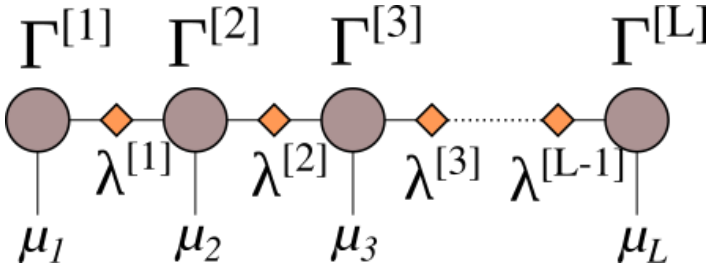
MPS factorization of the wave function coefficients

$$C_{\mu_1\mu_2\ldots\mu_L} = \sum_{\alpha_1\ldots\alpha_{L-1}} \Gamma^{[1]\mu_1}_{\alpha_1} \lambda^{[1]}_{\alpha_1} \Gamma^{[2]\mu_2}_{\alpha_1\,\alpha_2} \lambda^{[2]}_{\alpha_2} \ldots \Gamma^{[L]\mu_L}_{\alpha_{L-1}}$$



Truncation: discard small Schmidt values!

MPS based algorithms



Why is MPS a powerful ansatz?

Ground states are slightly entangled

Entanglement entropy: $S_{vN} = -\sum_{\alpha} \lambda_{\alpha}^2 \ln \lambda_{\alpha}^2$

Gapped model: Area Law

$S_{vN} \propto \text{const.}$

Finite M even in the TDL

Critical model:

$S_{vN} \propto \log L$

Ground state algorithm:

Density Matrix Renormalization Group

- MPS as a variational ansatz
- Iterative optimization of the matrices
- Finite and infinite chain
- Wide field of applications (cond. mat., Qchem, stat. phys.)

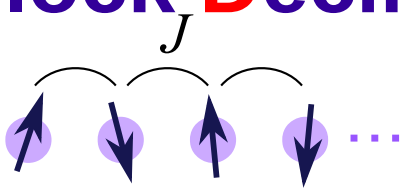
Real time dynamics:

Various algorithms

- **TEBD or tDMRG: conceptionally simple, only for short-ranged interactions**
- MPO-based time evolution
- Time Dependent Variational Principle: most accurate, similar to the standard DMRG algorithm
- Entropy bottleneck → accurate results only for short times

Time Evolving Block Decimation

$$\hat{H} = J \sum_i \vec{S}_i \vec{S}_{i+1}$$



Nearest neighbor Hamiltonian:

$$\hat{H} = \sum_i \hat{h}_{i,i+1} = \hat{H}_e + \hat{H}_o = \sum_k \hat{h}_{2k,2k+1} + \sum_k \hat{h}_{2k+1,2k+2}$$

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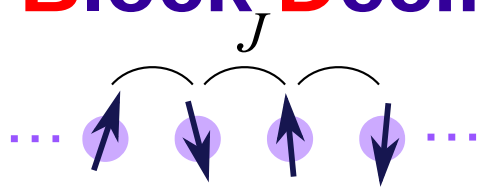

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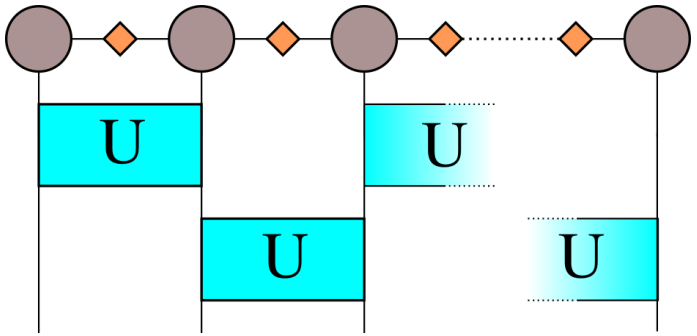
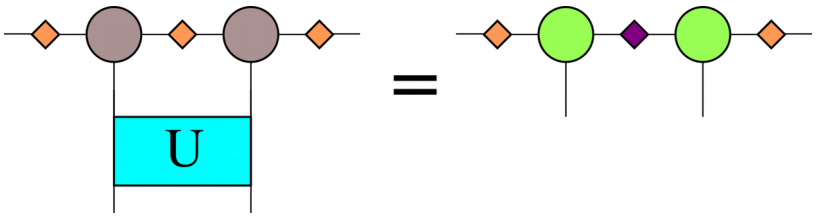
Suzuki-Trotter expansion:

$$e^{-i\hat{H}\Delta t} = e^{-i\hat{H}_e \Delta t} e^{-i\hat{H}_o \Delta t} + O(\Delta t^2)$$



$$U = e^{-i\hat{h}\Delta t}$$

TEBD step



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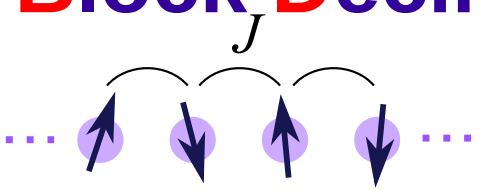

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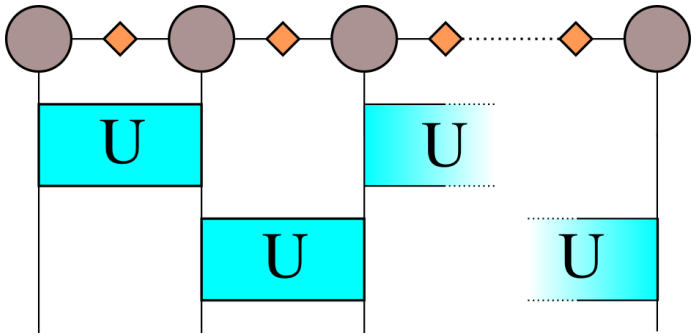

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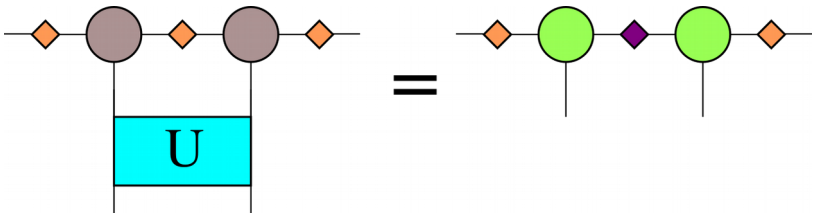
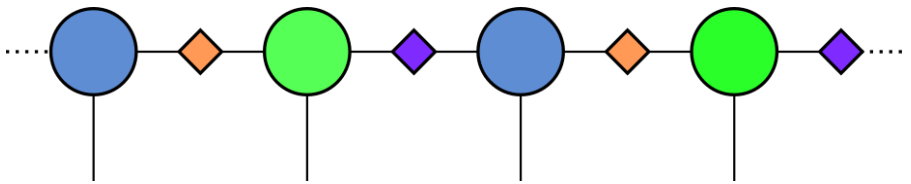


- Evolution in imaginary time: convergence to the ground state $U_{im} = e^{-\hat{h}\Delta t}$
- Infinite chain, translational invariant state



Non-Abelian MPS, spin fluctuations

If $|\Psi\rangle$ is a “singlet” state:

Schmidt states are “spin” eigenstates: $|\alpha\rangle = |t, S, M\rangle$

Schmidt values are degenerate within multiplets: $\lambda_{t,S,\cancel{M}} = \frac{1}{\sqrt{2S+1}} \Lambda_{S,t}$

Non singlet states: auxiliary site trick

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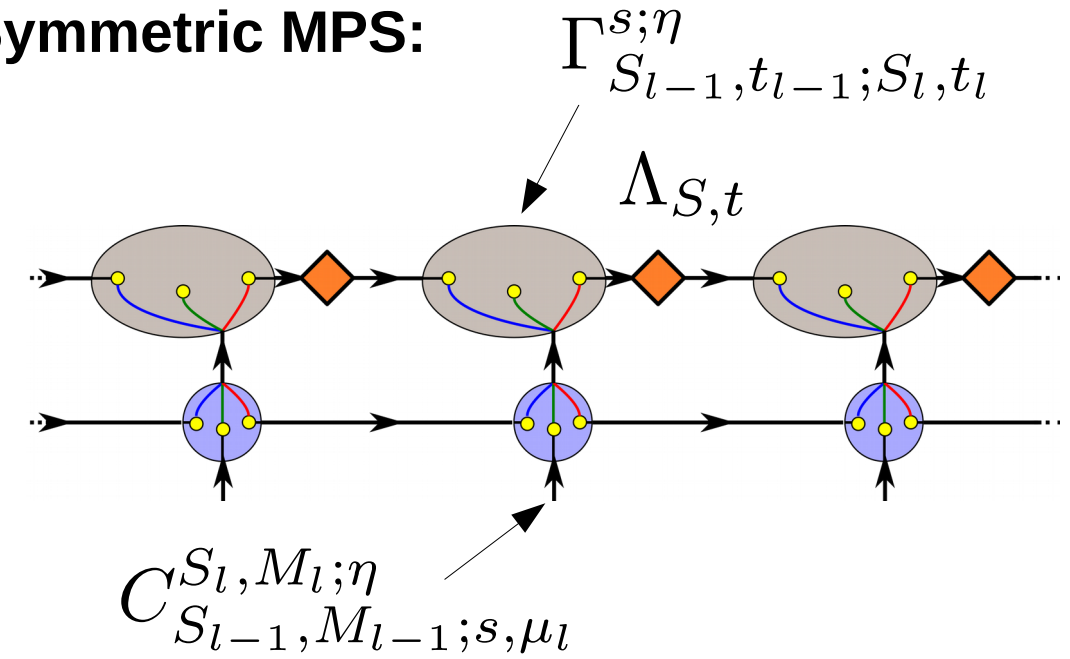

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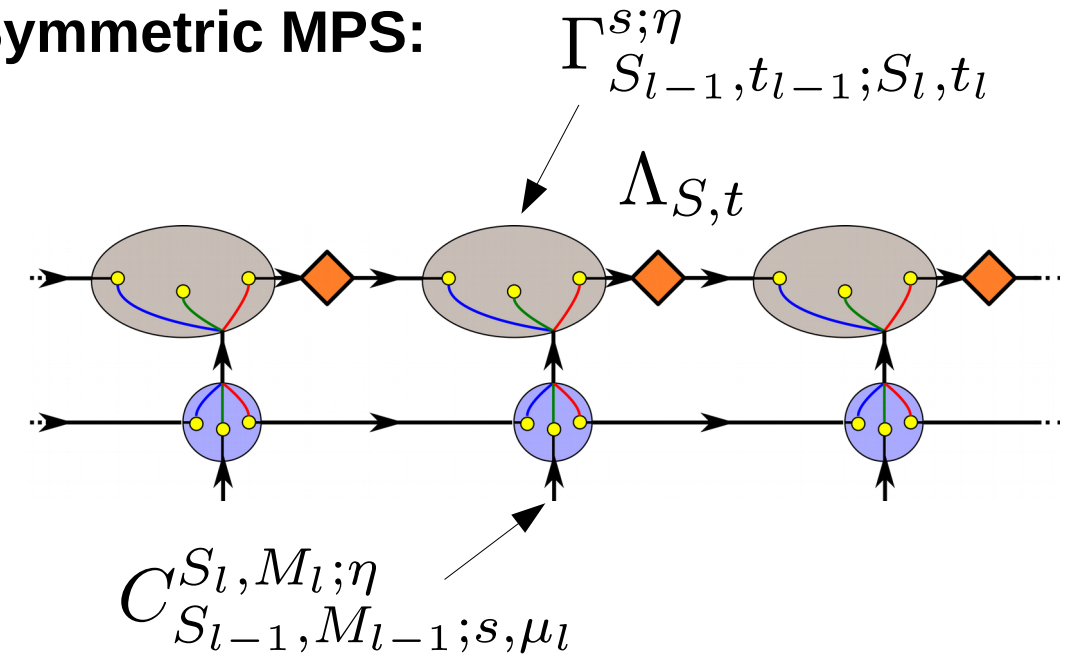
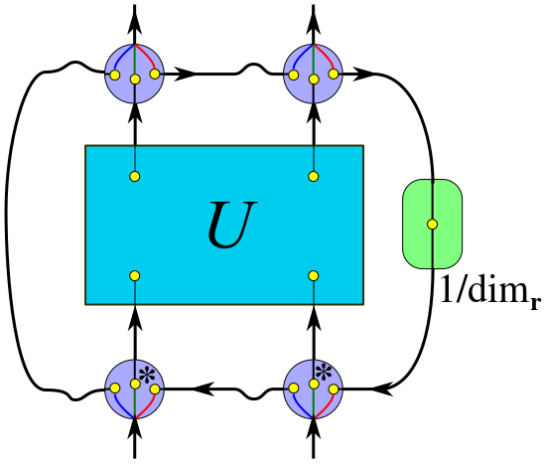


Clebsch-Gordan coefficient tensor

Idea: the Clebsch-layer is constant: "cut" them before the simulation.

Symmetrized evolver: can be calculated before the simulation

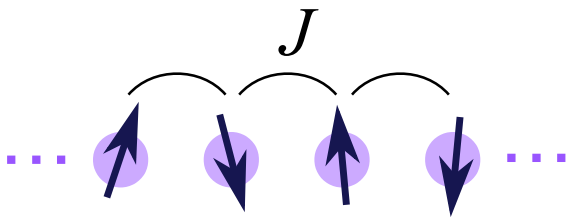


Symmetric iTEBD algorithm:

- Speedup
- Higher bond dimensions
- Well defined spins for Schmidt states (no "spin contamination")

The S=1 Heisenberg model

$$\hat{H} = J \sum_i \vec{S}_i \vec{S}_{i+1}$$



$$S_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

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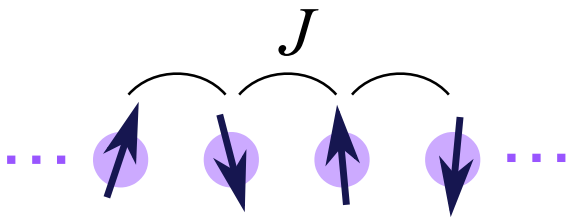

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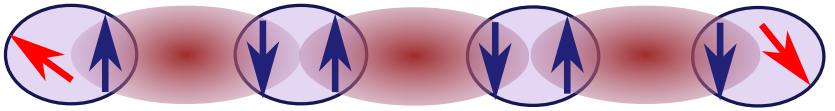
$J > 0 \longrightarrow$

- Symmetric ($S_{tot} = 0$), gapped ground state

- GS from the AKLT class, topological order

$$S = 1 \Leftarrow 1/2 + 1/2$$



I. Affleck et al., PRL 59, 799 (1987)

Free S=1/2 edge spins

The S=1 Heisenberg model

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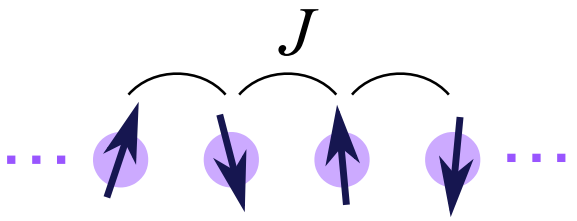

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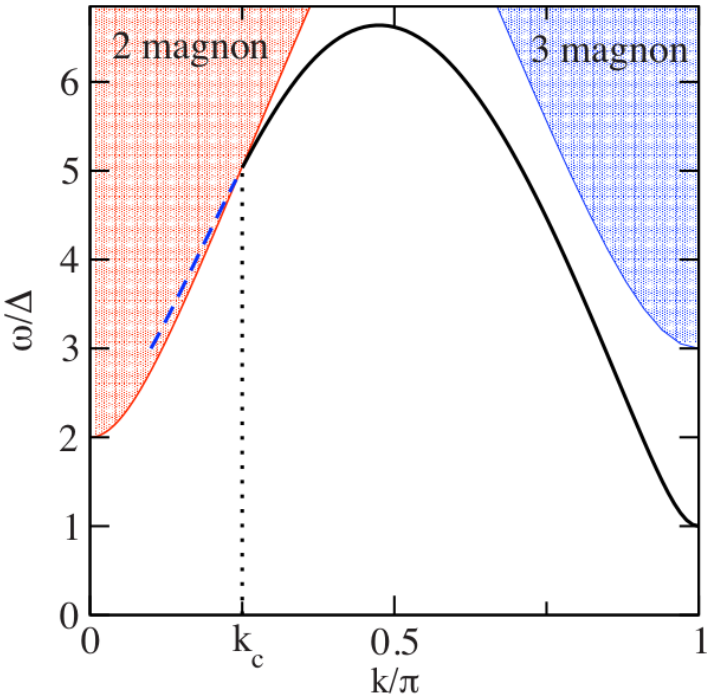
• S=1 magnon excitations



S.R.White & I. Affleck, PRB 77, 134437 (2008)

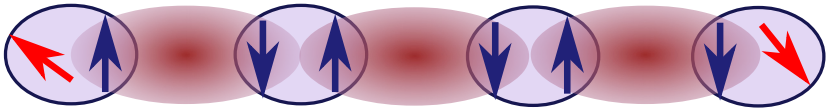
$$\varepsilon_k \approx \sqrt{\Delta^2 + v^2 (k - \pi)^2}$$

$$\Delta \approx 0.41 \qquad (J = 1)$$

$$v \approx 2.472$$

• GS from the AKLT class, topological order

$$S = 1 \Leftarrow 1/2 + 1/2$$



I. Affleck et al., PRL 59, 799 (1987)

Free S=1/2 edge spins

Semi-classical approach

$$\hat{H} = \sum_i \vec{S}_i \vec{S}_{i+1}$$

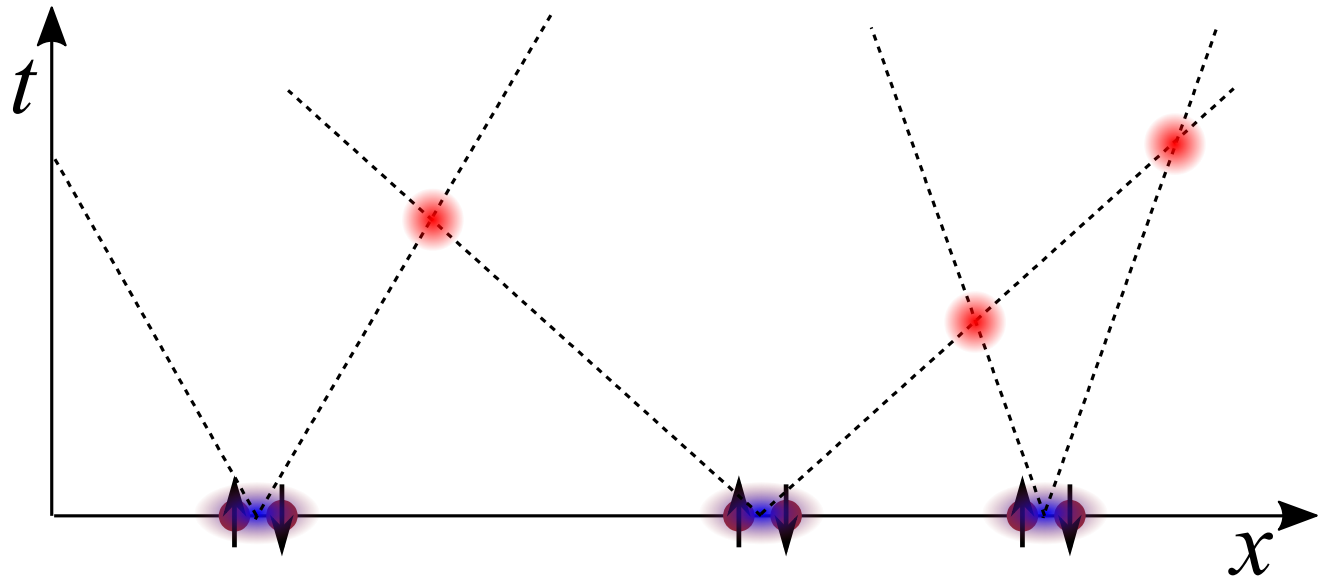
Small quench: $\hat{H}_0$ is close to $\hat{H}$

The post-quench state is a dilute gas of quasiparticles

$|\Psi_0\rangle$: singlet state, $\hat{H}_0,\ \hat{H}$ are symmetric under spin rotation and translation

The total spin remains zero

$|\Psi_0\rangle$ local, entangled magnon pairs with zero spin and momentum

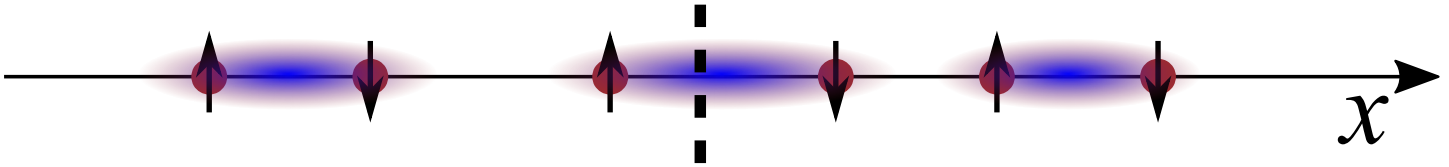


H. Rieger and F. Iglói, Phys. Rev. B **84,** 165117 (2011)

M. Kormos and G. Zaránd, Phys. Rev. E **93,** 062101 (2016).

Spin fluctuations in the SC approach

Dilute and cold gas (slow particles): total reflection at collisions → No spin exchange



Measured quantity: the total spin of the half chain

Quasiparticle spin fluctuation is described by $Q(S)$

- Singlet bond is cut: S = 1
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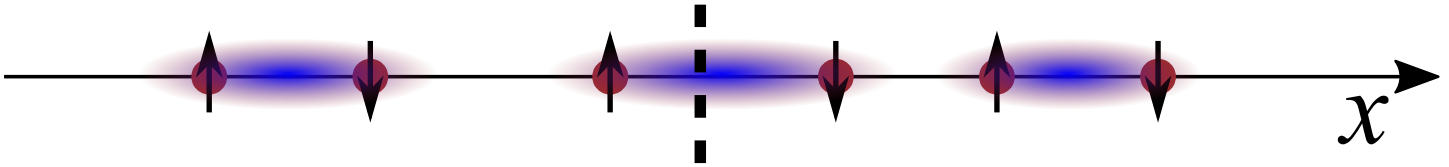

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Singlet bond is cut, if $n_+ + n_- = \mathrm{odd}$

$$p(n_+, n_-) = \frac{1}{n_+! n_-!} q^{n_+ + n_-} e^{-2q}$$

$$q = \rho \int_0^\infty dv\, vt\, f(v)$$

$$\tau^{-1} = 4\rho \int_0^\infty dv\, v\, f(v)$$

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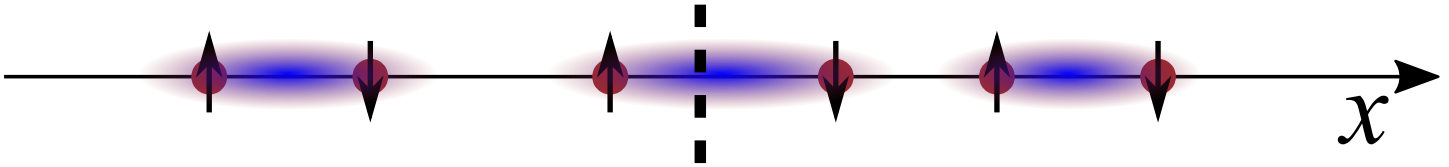

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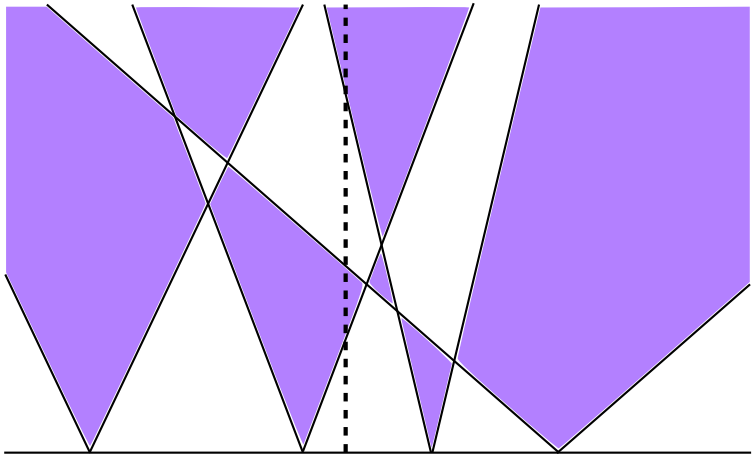

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$$Q(0) = 0.5(1 + e^{-4q}) = 0.5(1 + e^{-t/\tau})$$

$$Q(1) = 0.5(1 - e^{-4q}) = 0.5(1 - e^{-t/\tau})$$

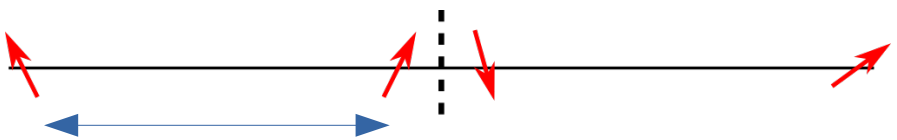
$$\tau^{-1} = 4\rho \int_0^\infty dv\, v\, f(v)$$

Vacuum spin fluctuations, edge states

In the vacuum (ground state): $P_0(S)$:

$$P_0(0) = 0.2425 \sim 1/4$$
$$P_0(1) = 0.7388 \sim 3/4$$
$$P_0(2) = 0.0187$$
$$P_0(S \geq 3) < 10^{-5}$$

Simple picture:



No correlation:

↓

3 triplet and 1 singlet states are equally probable. + small additional bulk fluctuations

S=0	S=1	S=2	S=3	S=4
4.9228702E-01	4.9228702E-01	6.0881107E-02	1.0520127E-03	2.5818472E-06
1.4151521E-02	6.0881107E-02	4.0800539E-03	6.8257833E-05	1.6331054E-07
7.8246749E-04	1.4151521E-02	1.1779856E-03	8.2430136E-06	
2.9018983E-04	4.0800537E-03	1.0520127E-03	5.1223619E-06	
4.7950931E-05	1.1779855E-03	2.1739493E-04	3.2660856E-06	
3.5072218E-05	7.8246815E-04	6.8257662E-05	2.5818387E-06	
1.5838368E-05	2.9019016E-04	5.7805128E-05	1.2637007E-06	
4.6165916E-06	2.1739339E-04	4.2446541E-05	3.8317511E-07	
2.4027291E-06	5.7804057E-05	1.3476745E-05	2.9467783E-07	
1.3505714E-06	4.7952665E-05	9.2379614E-06	1.6325501E-07	
1.0401261E-06	4.2445092E-05	8.2426060E-06	1.4642239E-07	
7.6242411E-07	3.5077961E-05	5.1218804E-06	6.3829175E-08	
3.1681501E-07	1.5840889E-05	3.2649586E-06		
1.4492712E-07	1.3471007E-05	3.1019949E-06		
	9.2325894E-06	2.3983826E-06		
	4.6179224E-06	1.7767720E-06		
	3.0930996E-06	1.2631173E-06		
	2.4230632E-06	7.5467978E-07		
	2.3959958E-06	6.4590484E-07		
	1.7640945E-06	3.9103949E-07		
	1.3728415E-06	3.8204660E-07		
	1.0405764E-06	2.9308016E-07		
	7.6411093E-07	2.8267484E-07		
	7.4289465E-07	1.6243716E-07		
	6.4470865E-07	1.4477185E-07		
	3.8145556E-07	9.6909966E-08		
	3.2023064E-07	8.2649639E-08		
	2.8093760E-07	6.8747636E-08		
	1.5180697E-07	6.2568432E-08		

Edge states & Schmidt values

Exact degeneracies beyond SU(2)

$$\Lambda_{t,S} = \Lambda_{\tilde{t},\tilde{S}}$$

↓

Pairs only for $\tilde{S} = S \pm 1$

↓

Edge state: $S_{\text{edge}=1/2}$

Quench protocols

$$\hat{H}_0^D = \sum_k \left(\frac{2+\gamma}{2} \vec{S}_{2k} \cdot \vec{S}_{2k+1} + \frac{2-\gamma}{2} \vec{S}_{2k+1} \cdot \vec{S}_{2k+2} \right)$$

Phase transition to a dimerized phase at $\gamma \sim 0.52$

Unit cell is doubled: 2 sublattices

Only a moderate change in the GS till the phase boundary

$$\rho_E/\Delta \approx 0.1\frac{1}{a} \quad \text{at} \quad \gamma = 0.5$$

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$$\hat{H}_0^{\mathrm{biq}} = \sum_i cos(\theta) \vec{S}_i \cdot \vec{S}_{i+1} + \sin(\theta) \left(\vec{S}_i \cdot \vec{S}_{i+1} \right)^2$$

SU(3) symmetric critical point at $\theta = \frac{\pi}{4}$

Homogeneous quench

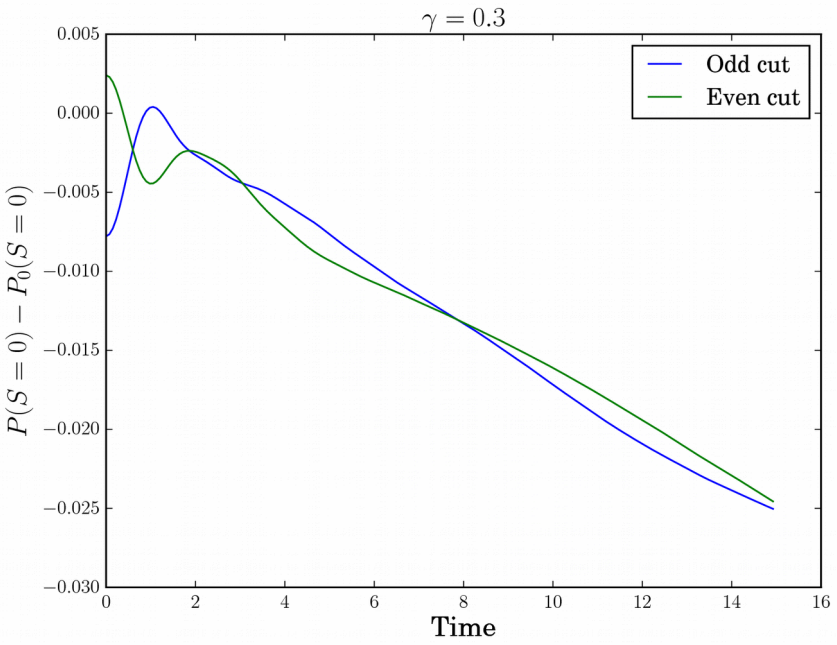
Larger change in the GS till the phase boundary

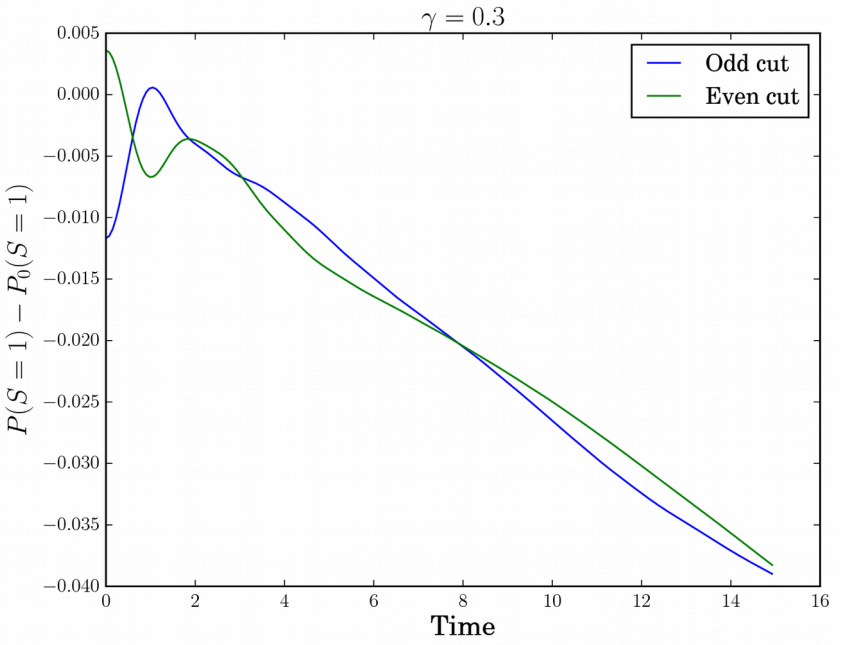
$$\rho_E/\Delta \approx 3 \frac{1}{a} \quad \text{at} \quad \theta = 0.7$$

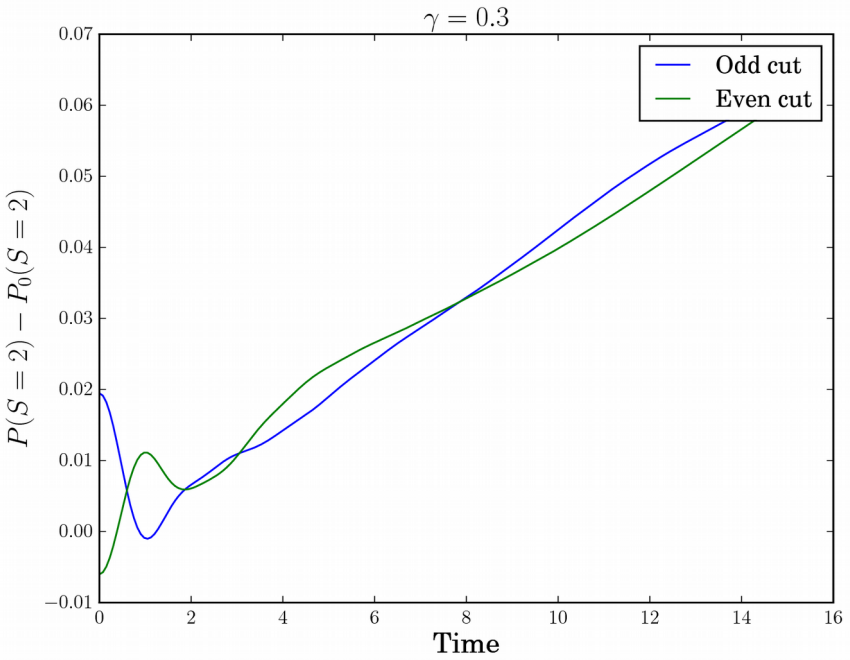
Post-quench spin fluctuations

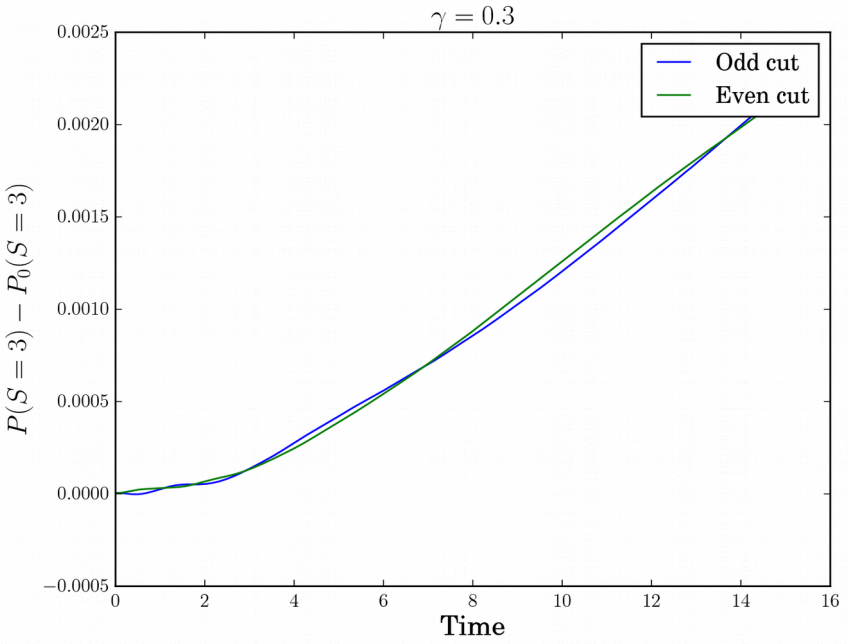
$$P(S) = \sum_{t \in S} \Lambda^2_{t,S}$$

Spin fluctuations after a sudden (“D”-type” quench):









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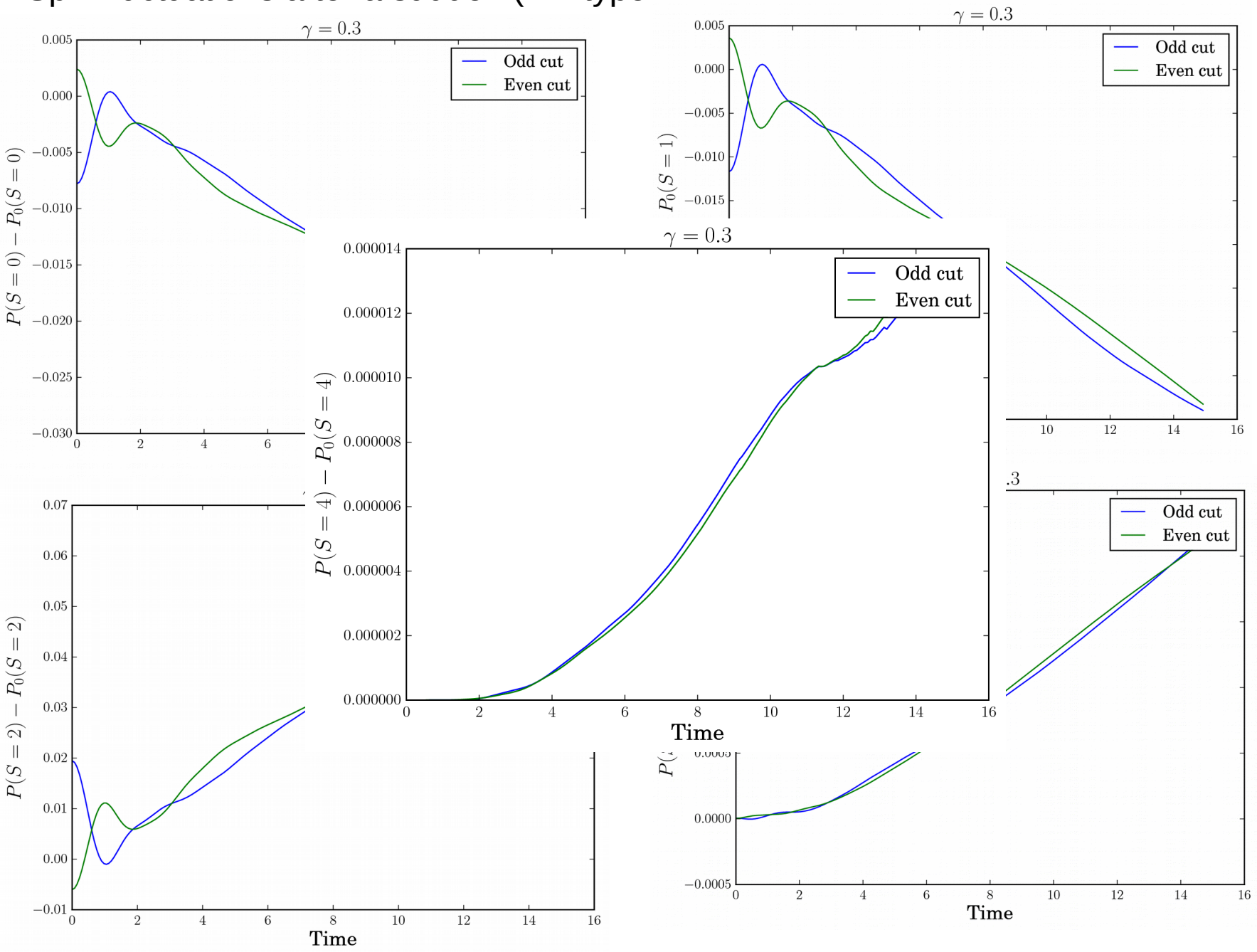


Post-quench spin fluctuations: semi-classics

Idea: $"P(S,t) = P_0(S) + Q(S,t)"$

Vacuum

Quasiparticles

"Uncorrelated" spin addition:

$$P(S) = \sum_{S_q} \sum_{S_v} \frac{P_0(S_v)}{2S_v+1} \frac{Q(S_q)}{2S_q+1} (2S+1)$$

$$|S_q - S_v| \leq S \leq S_q + S_v$$

$$Q(0) = \frac{1}{2} + \frac{1}{2} e^{-t/\tau}$$

$$Q(1) = \frac{1}{2} - \frac{1}{2} e^{-t/\tau}$$

$$P_0(0) = 0.2425$$

$$P_0(1) = 0.7388$$

$$P_0(2) = 0.0187$$

$$P(S=0,t) = P_0(0)Q(0) + \frac{P_0(1)Q(1)}{9} = 0.1623 + 0.0802\, e^{-t/\tau}$$

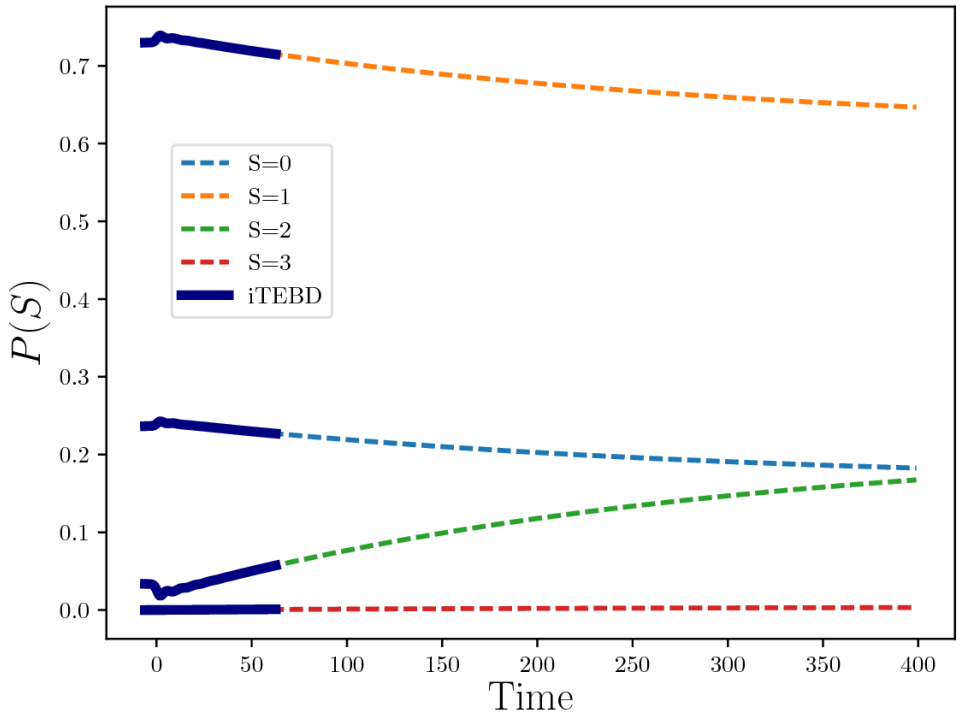
$$P(S=1,t) = \ldots = 0.6157 + 0.1231\, e^{-t/\tau}$$

$$P(S=2,t) = \ldots = 0.2177 - 0.1990\, e^{-t/\tau}$$

$$P(S=3,t) = \ldots = 0.0044 - 0.0044\, e^{-t/\tau}$$

$$P(S=4,t) < 3 \cdot 10^{-6}$$

MPS test: short times

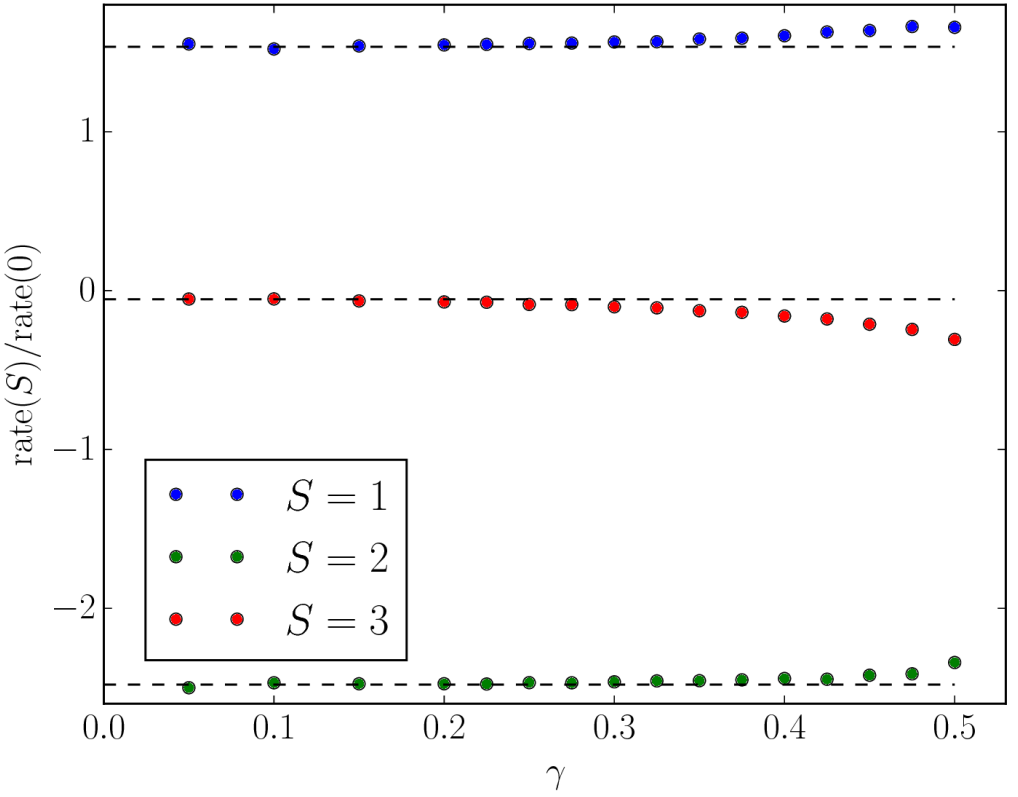


The initial rates are well described by SC!

$$\text{rate}(S) = \left.\frac{dP(S,t)}{dt}\right|_{t=0}$$

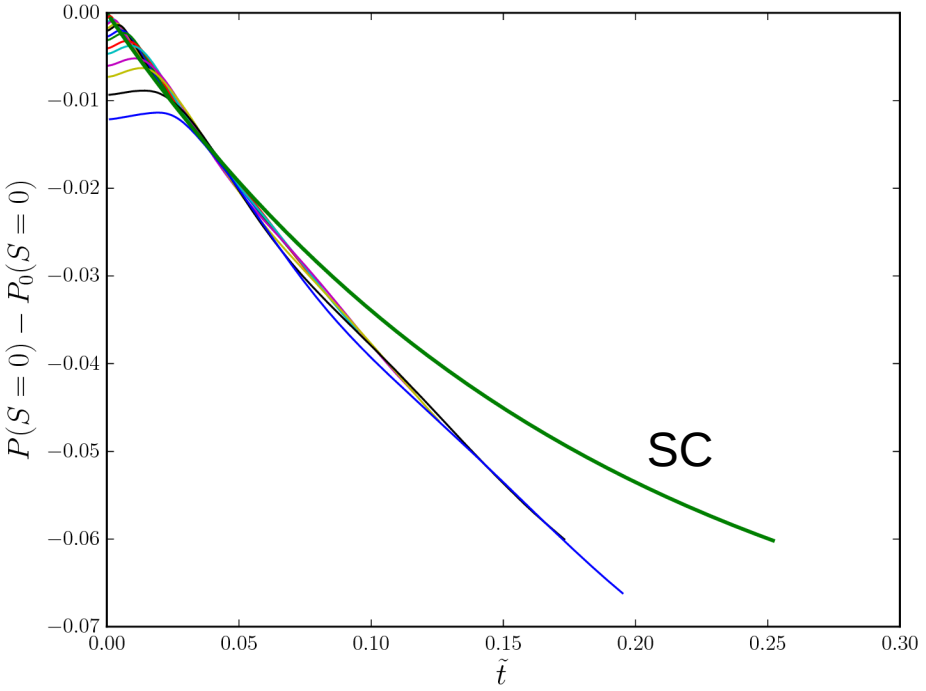
$$\frac{\text{rate}(1)}{\text{rate}(0)} = 1.535 \quad \frac{\text{rate}(2)}{\text{rate}(0)} = -2.481$$

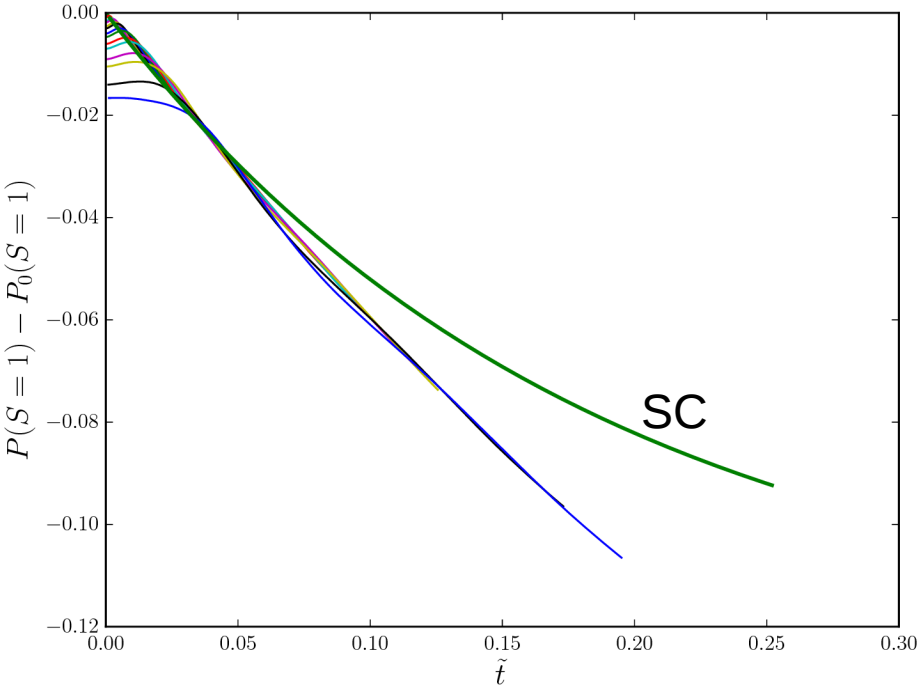
$$\frac{\text{rate}(3)}{\text{rate}(0)} = -0.055$$

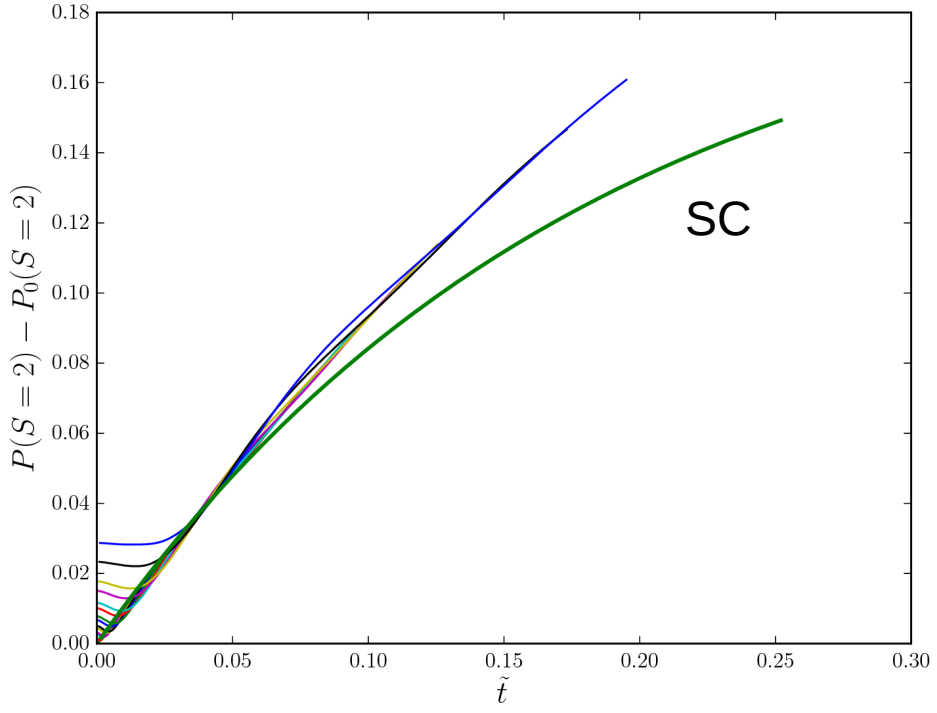


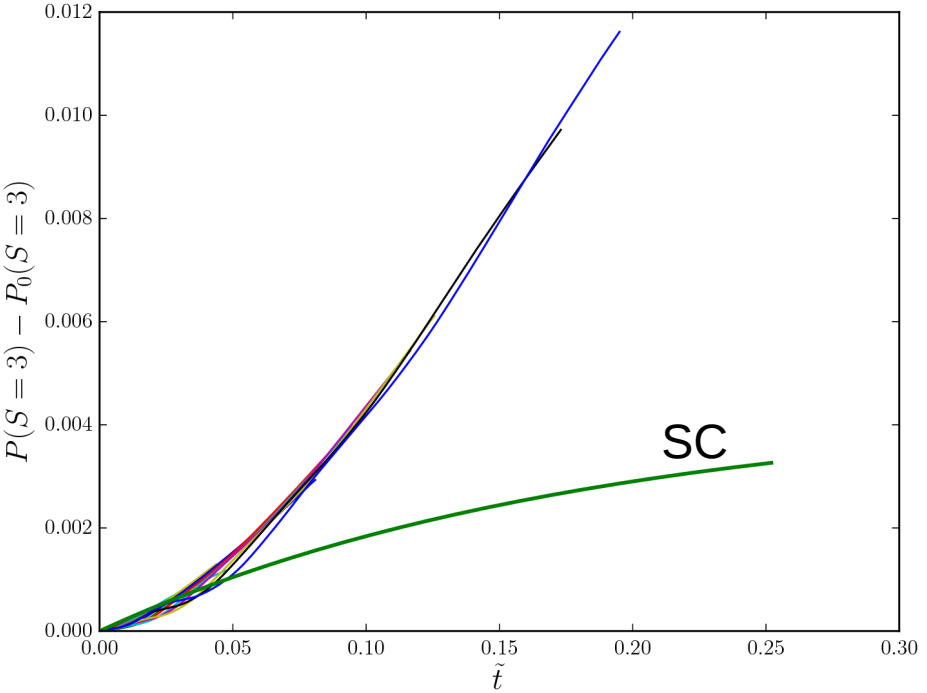
MPS test: long times

$\tilde{t} = t/\tau$









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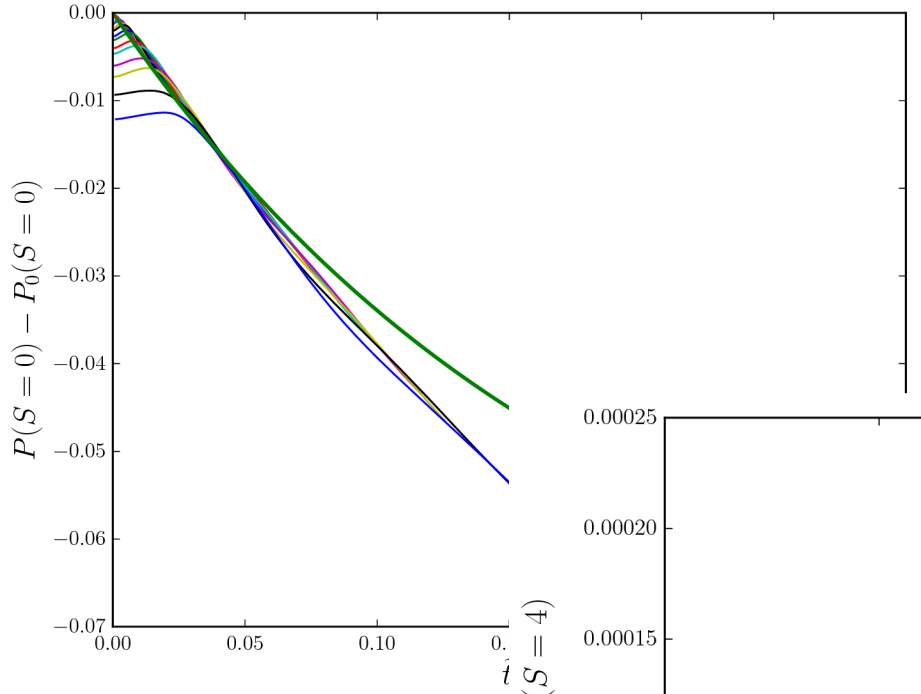
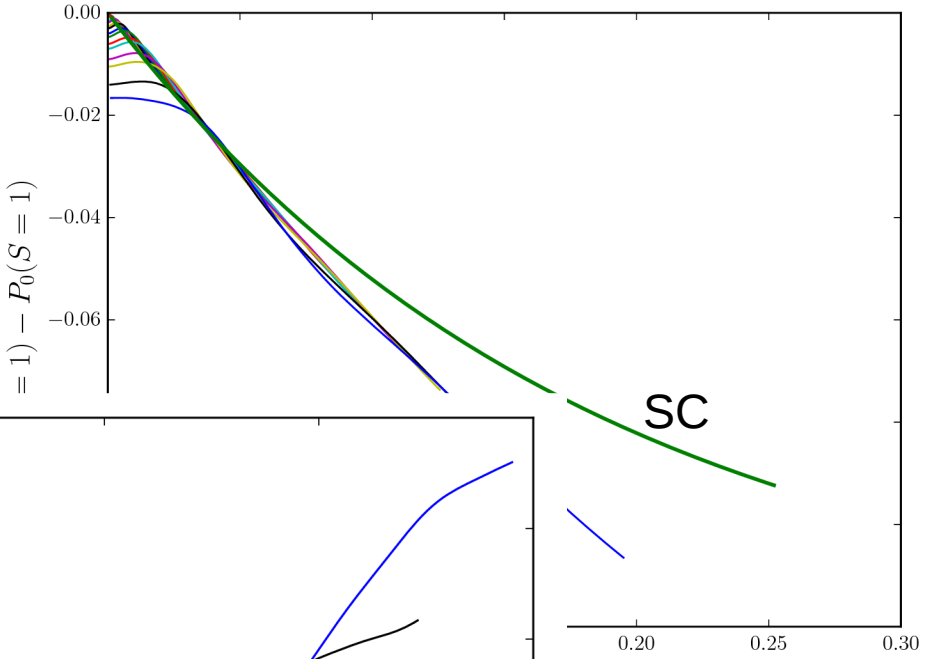
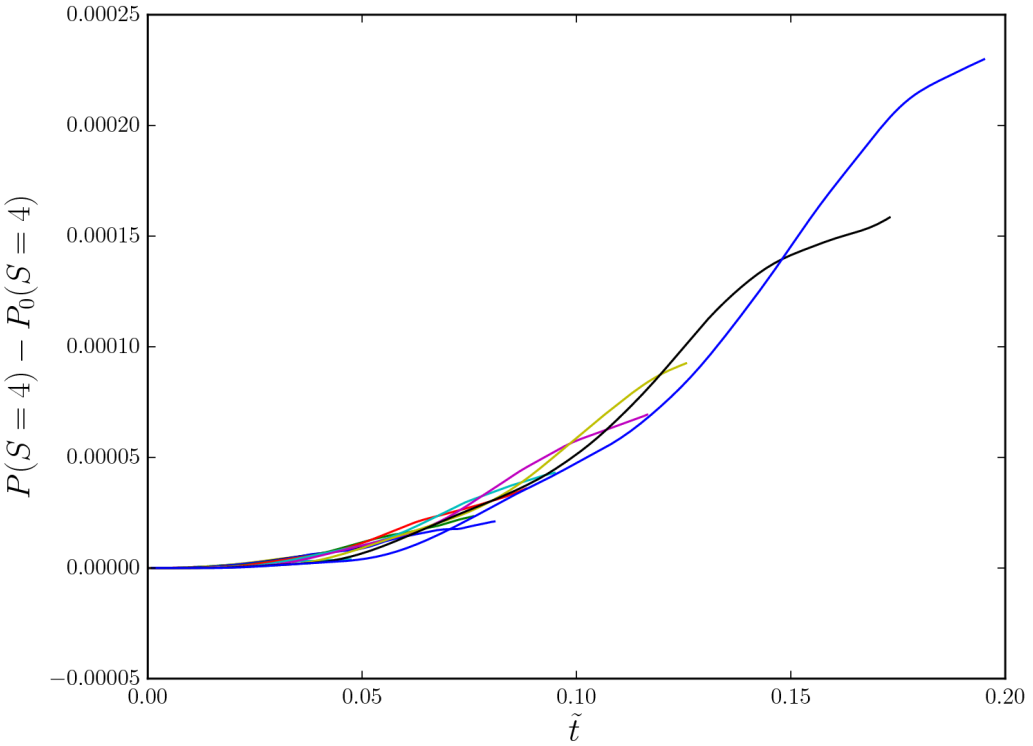
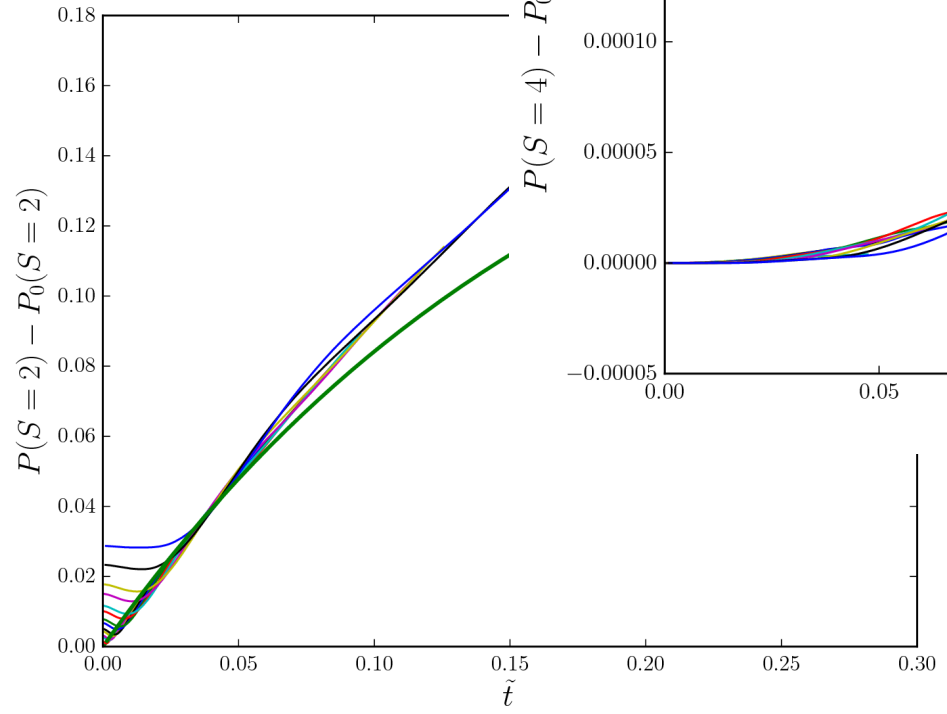
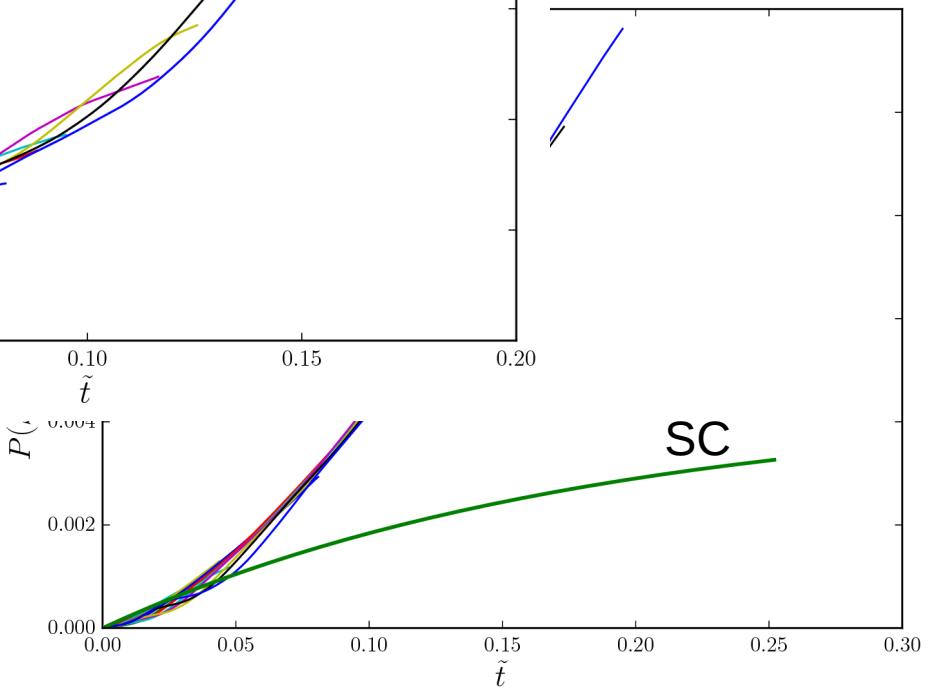








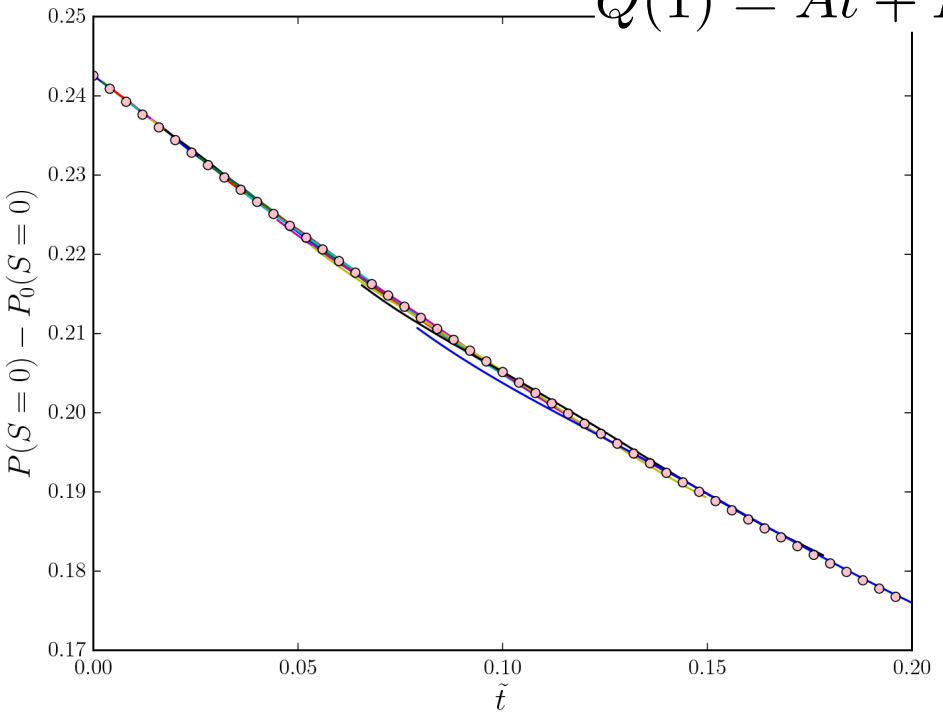


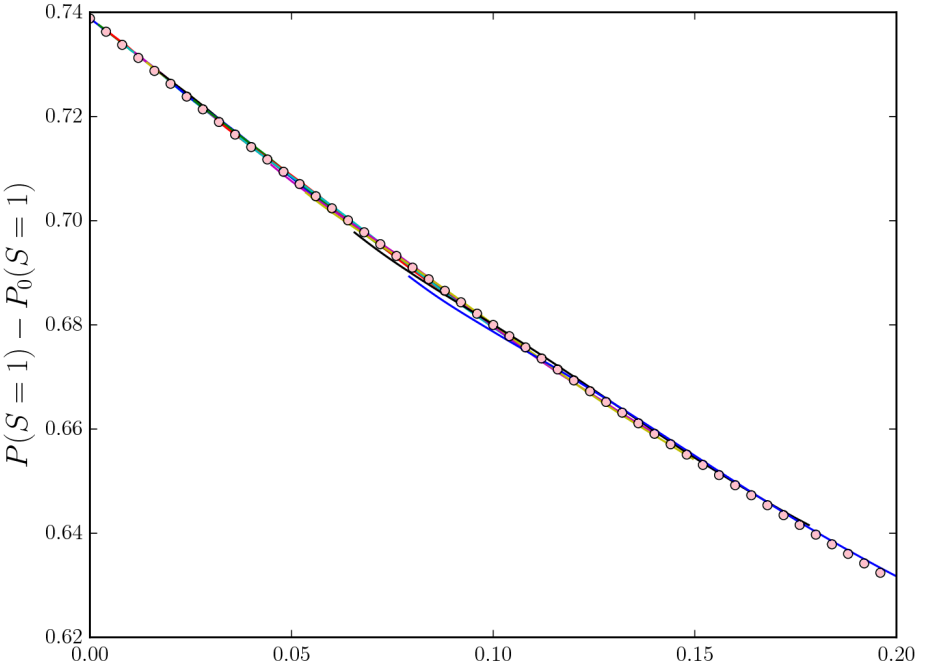
Beyond SC

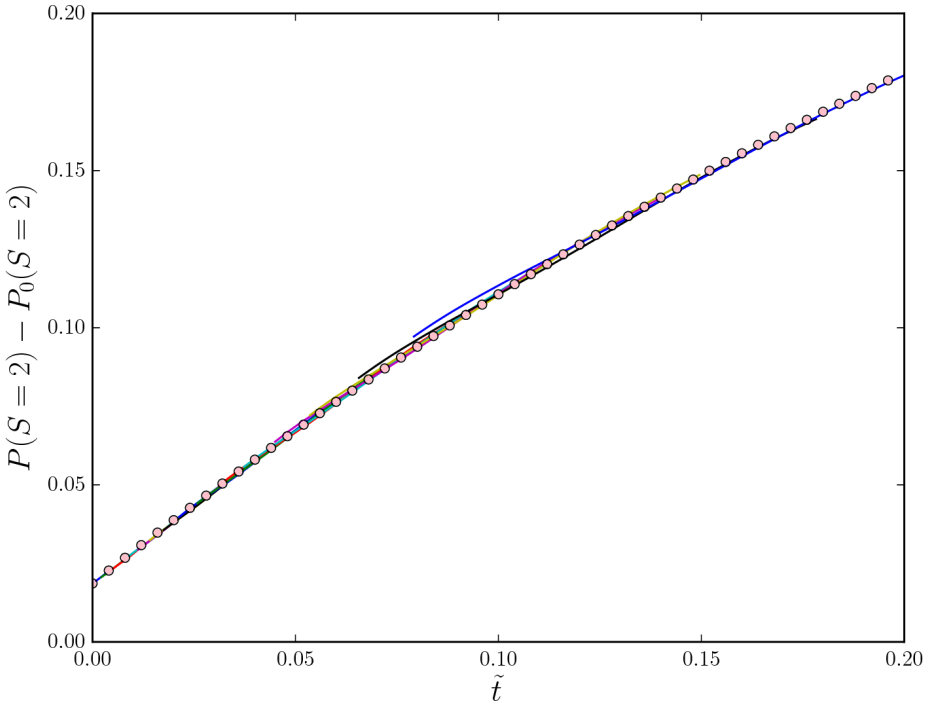
$$Q(0) = 1 - At - (B + C)t^2$$

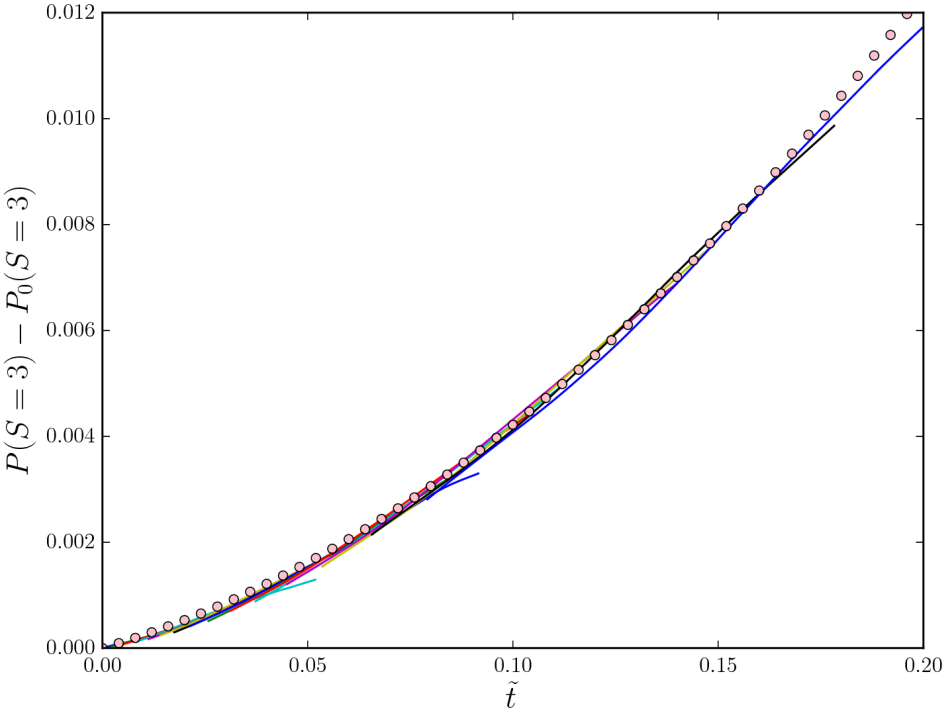
$$Q(1) = At + Bt^2$$

$$Q(2) = Ct^2$$







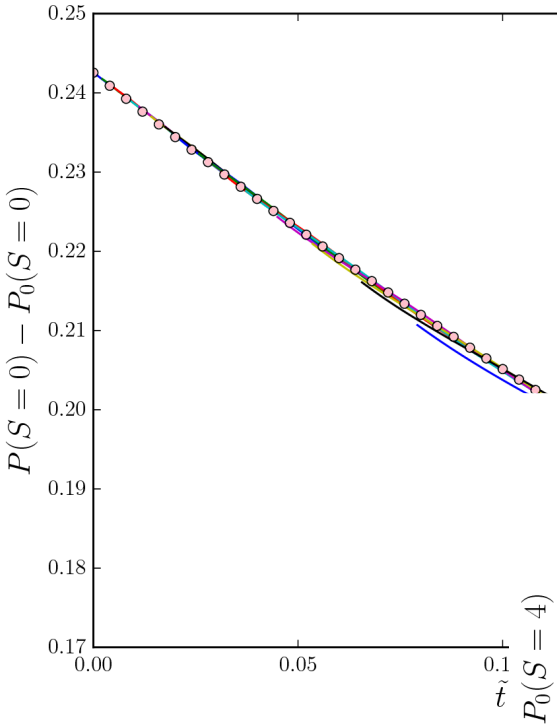


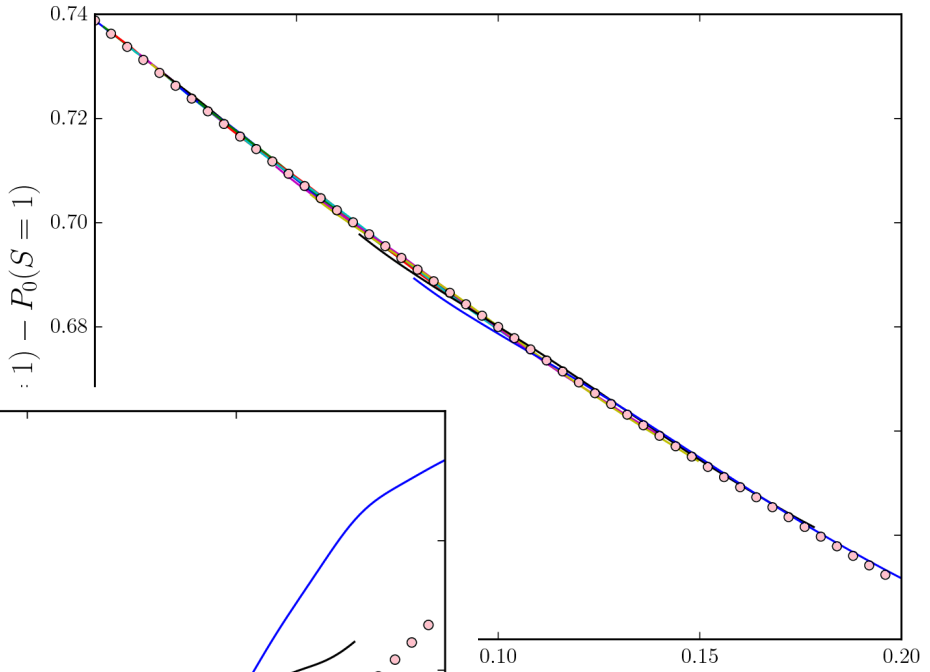
Beyond SC

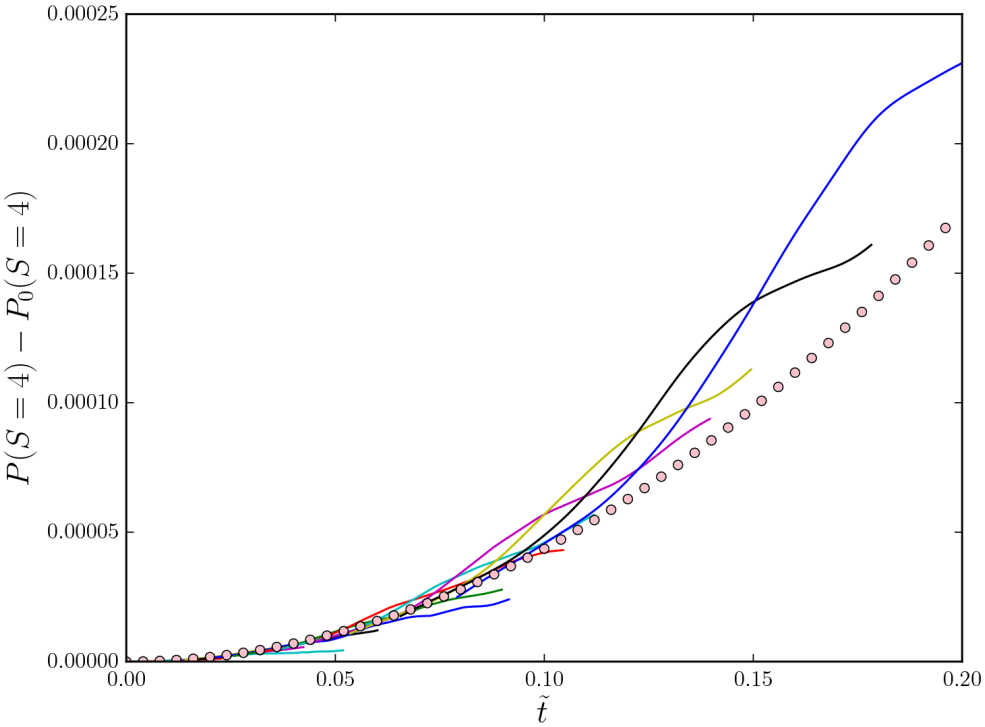
$$Q(0) = 1 - At - (B + C)t^2$$

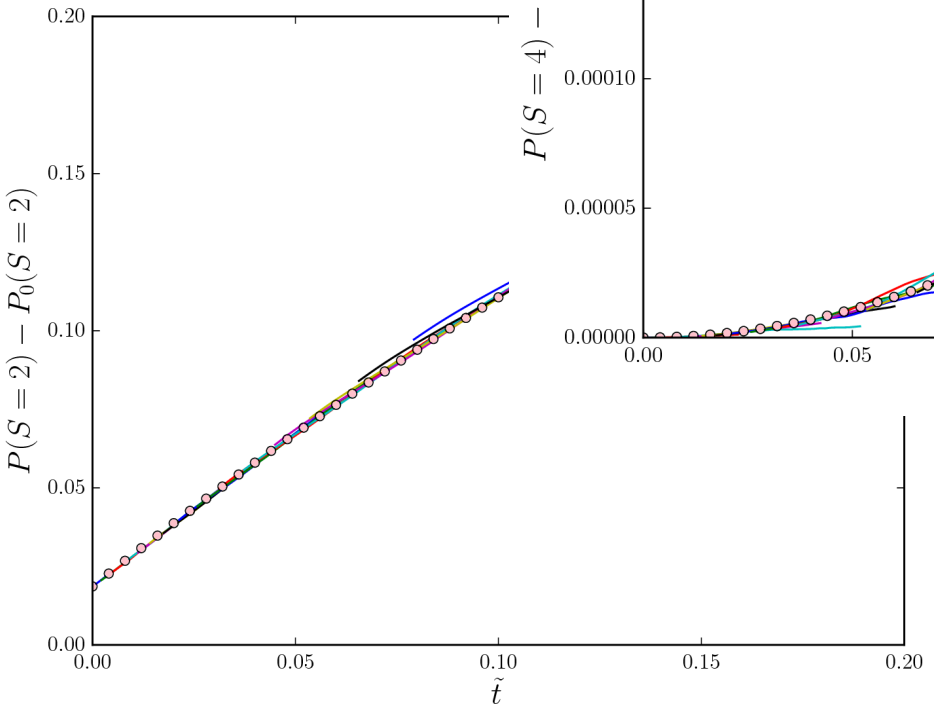
$$Q(1) = At + Bt^2$$

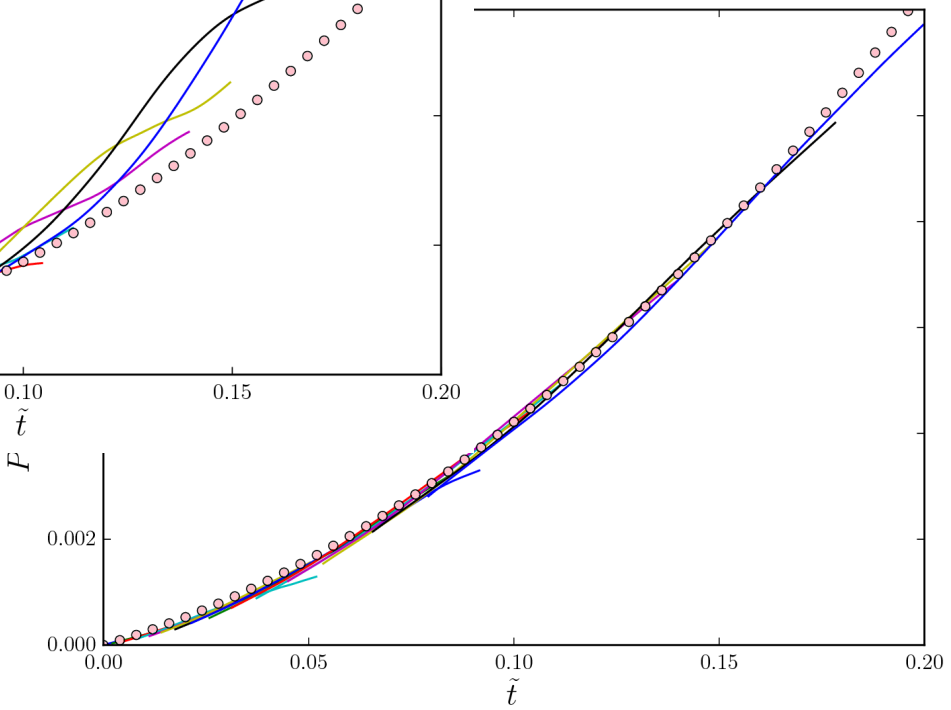
$$Q(2) = Ct^2$$





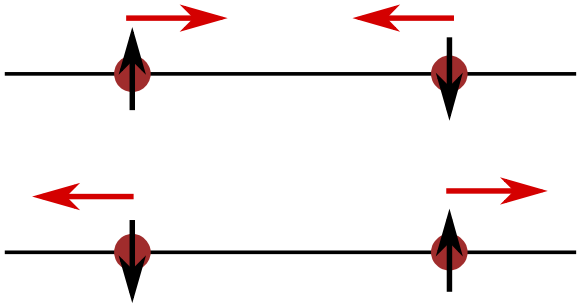






Beyond semi-classics: semi-semi-classics

Semi-classics: dilute, **cold** gas ⟷ Sudden quench: fast particles



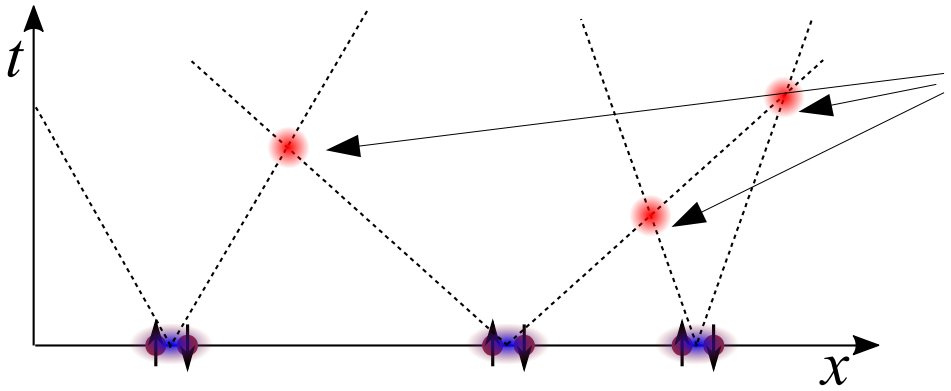
- Spin flip processes
- Singlet bonds are broken

$$Q(S>1)>0$$

Semi-semi classical description: Classical orbital + quantum spin

$$|\Psi\rangle = \sum_{m_1,m_2,\ldots,m_N} C_{m_1 m_2 \ldots m_N} |m_1, m_2, \ldots, m_N\rangle$$

$$|\Psi_{SC}\rangle = |\uparrow\downarrow\rangle\,|\uparrow\downarrow\rangle \ldots |\uparrow\downarrow\rangle$$



Use the S-matrix!

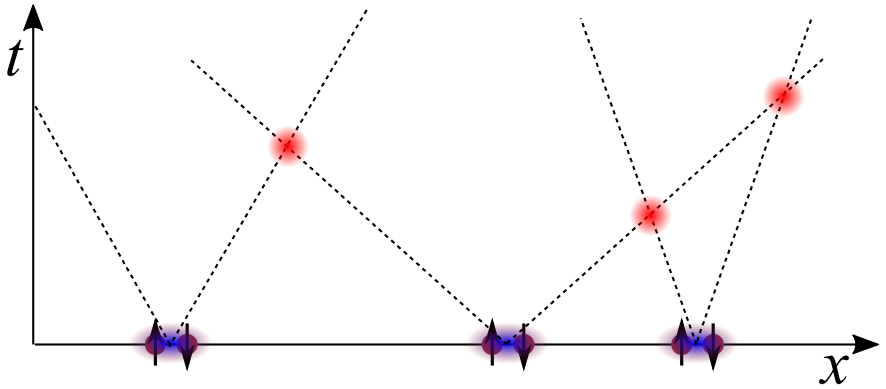
- Classical MC on trajectories
- MPS simulation on spins

C.P.Moca, M. Kormos & G. Zaránd (2017)

Semi-semi classics

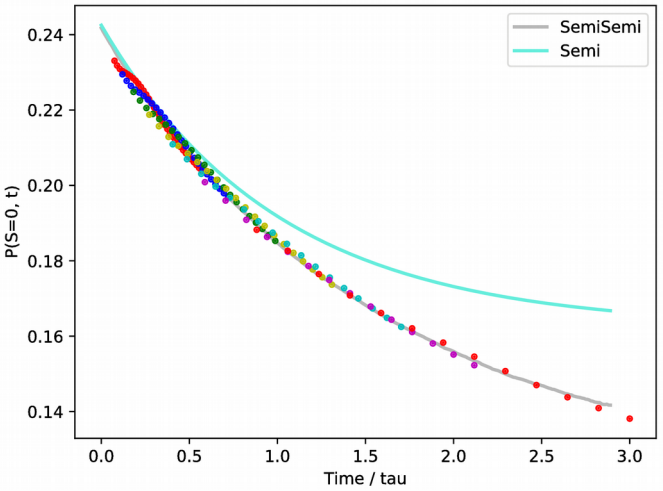
Semi-semi classical description: Classical orbital + quantum spin

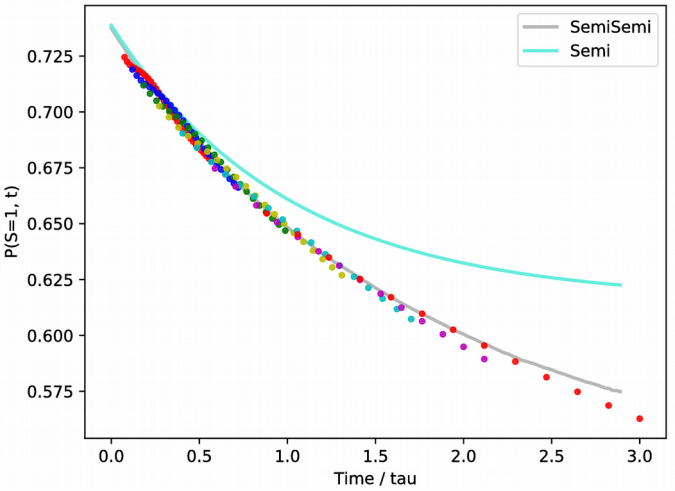
$$|\Psi\rangle = \sum_{m_1, m_2, \ldots, m_N} C_{m_1 m_2 \ldots m_N} \, |m_1, m_2, \ldots, m_N\rangle$$

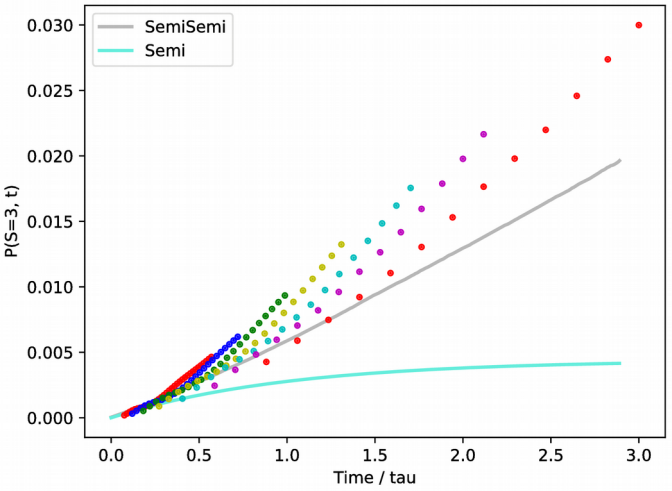


- TEBD for the particles' spin
- Two-particle evolver: the S-matrix
- Classical Monte-Carlo for the trajectories

Preliminary results:







Summary

- Semi-classical and semi-semi-classical description of quenches
- Half chain spin fluctuations from semi-classics
- Matrix Product States, TEBD simulations
- Vacuum spin-fluctuations and edge states
- Success of semi-classics for short times
- Breakdown of semi-classics for long times

Acknowledgment

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Thank You for the attention!