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Simulating non-equilibrium quantum relaxation in closed interacting quantum many body systems

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Simulating quantum processes and devices

624. Heraeus Seminar, Bad Godesberg, 19.-22.9.2019

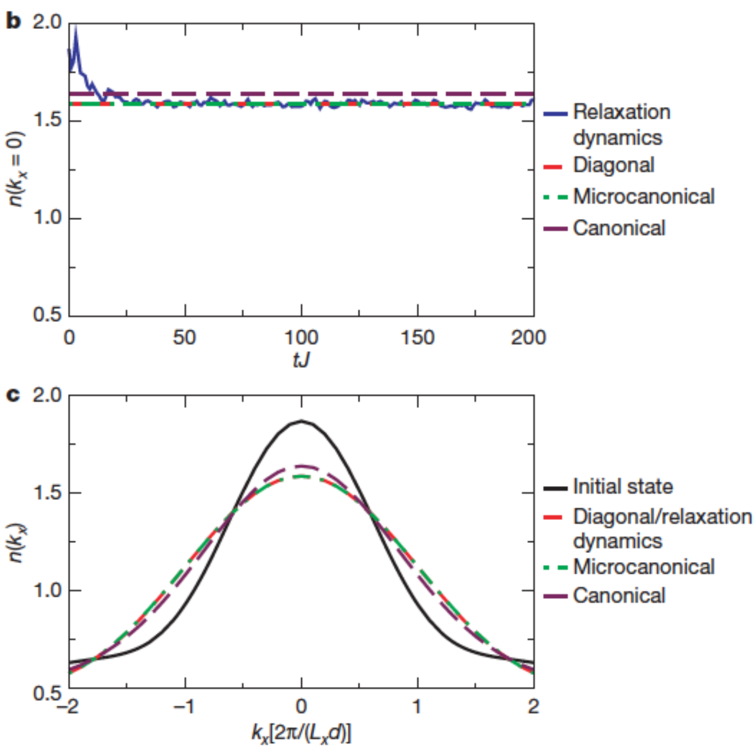
Quantum thermalization – 2008 (numerics)

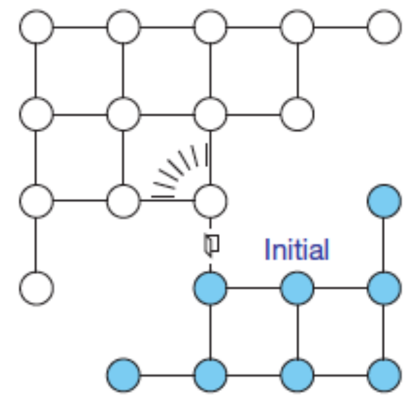
nature
Vol 452|17 April 2008|doi:10.1038/nature06838

LETTERS

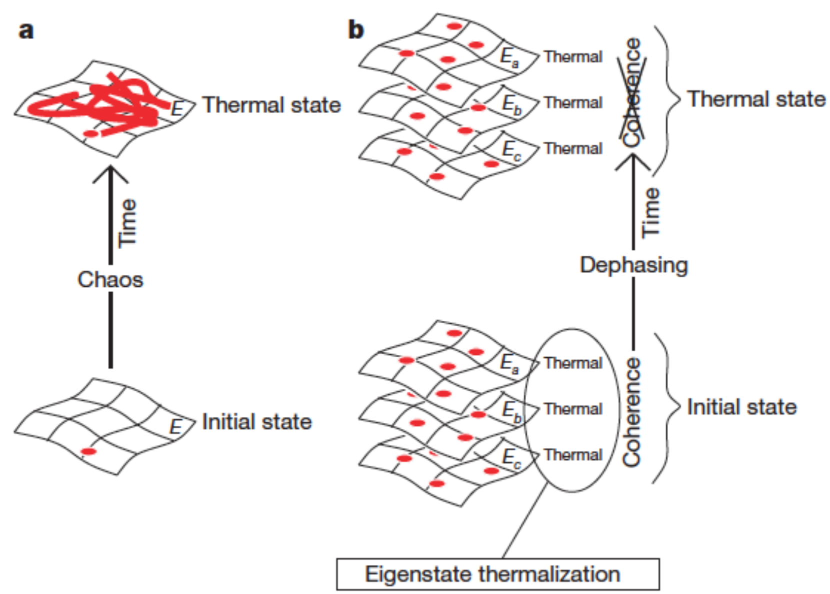
Thermalization and its mechanism for generic isolated quantum systems

Marcos Rigol[1,2], Vanja Dunjko[1,2] & Maxim Olshanii[2]





$H = -\Sigma_{<ij>} J_{ij}(a_i^+ a_j + a_j^+ a_i)$, hard core bosons



Quantum Thermalization – 2016 (experimental)

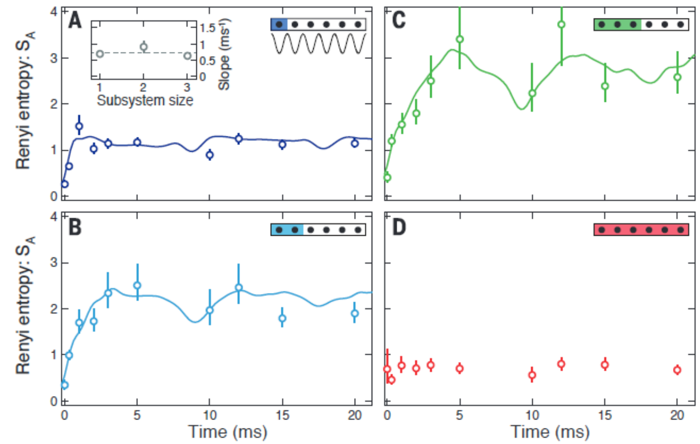
STATISTICAL PHYSICS

Quantum thermalization through entanglement in an isolated many-body system

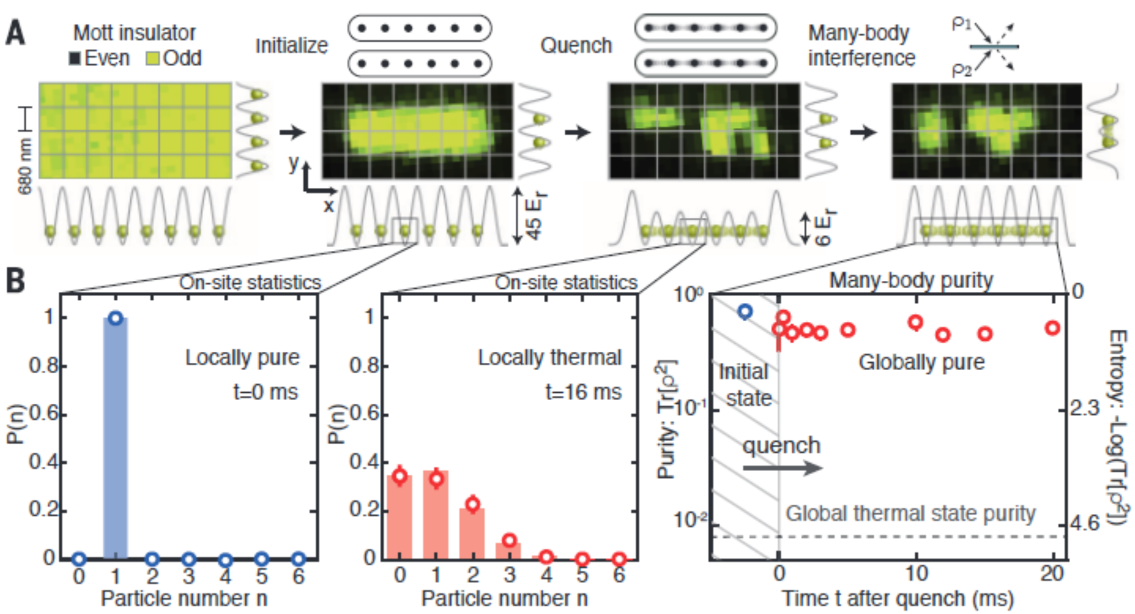
Adam M. Kaufman, M. Eric Tai, Alexander Lukin, Matthew Rispoli, Robert Schittko, Philipp M. Preiss, Markus Greiner*

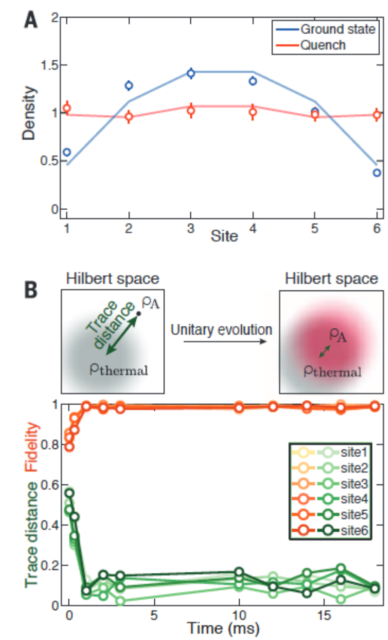
19 AUGUST 2016 • VOL 353 ISSUE 6301

SCIENCE

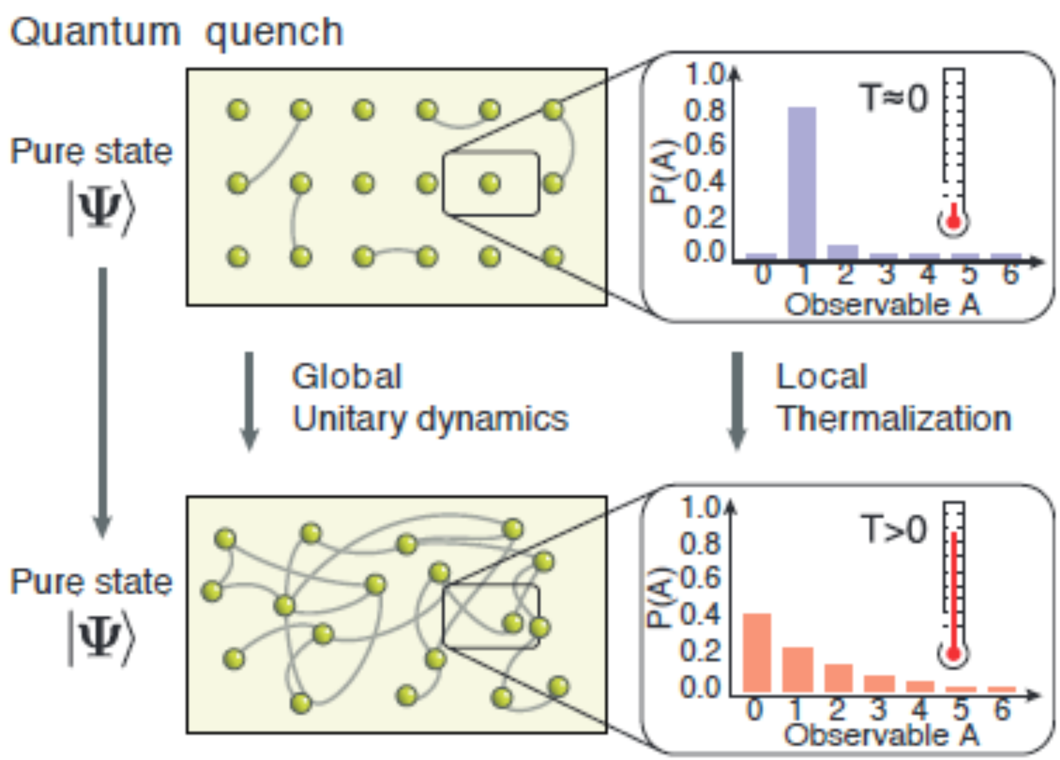


$$H = -\Sigma_{<ij>} J_{ij}(a_i^+a_j + a_j^+a_i) + U\,\Sigma_i n_i(n_i-1)$$





Thermalization in closed systems



Outline

- Focus on transverse Ising model
- 1d : integrable: Generalized Gibbs ensemble (GGE)
- 2d: non-integrable:

  numerical studies of thermalization after quantum quenches

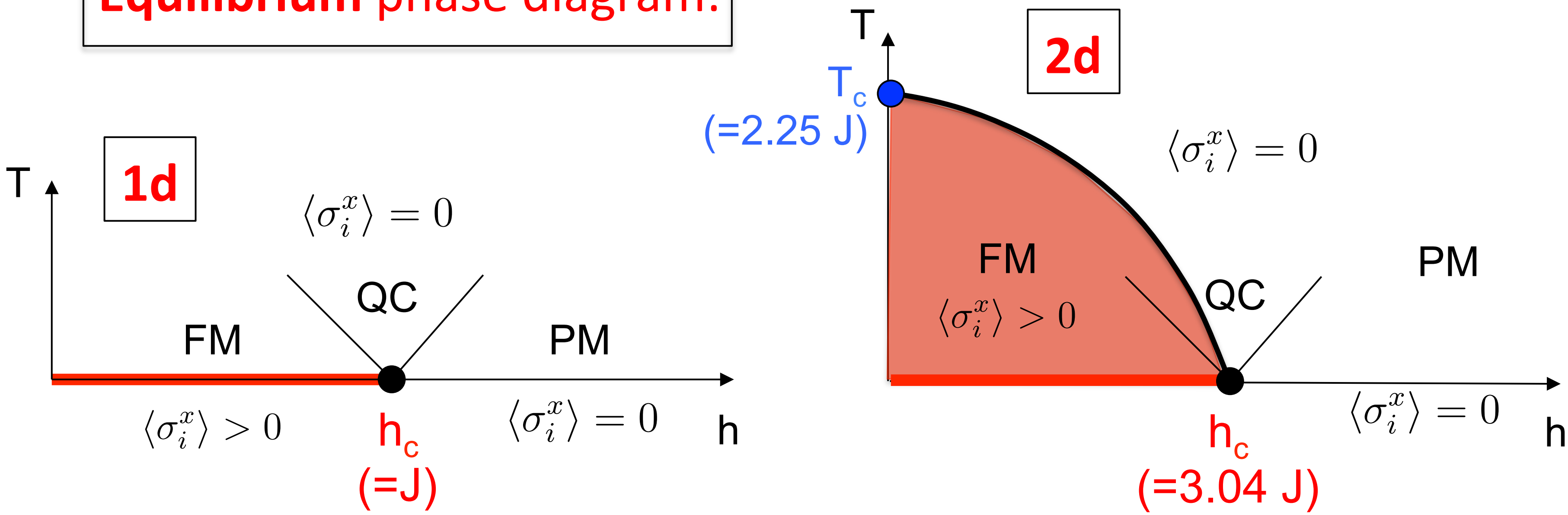
The transverse Ising model

$$H = -J \sum_{(ij)\ n.n.} \sigma_i^x \sigma_i^x - h \sum_i \sigma_i^z$$

σ^x, σ^z Pauli matrices, n.n. = nearest neighbors in d-dimensions, p.b.c.

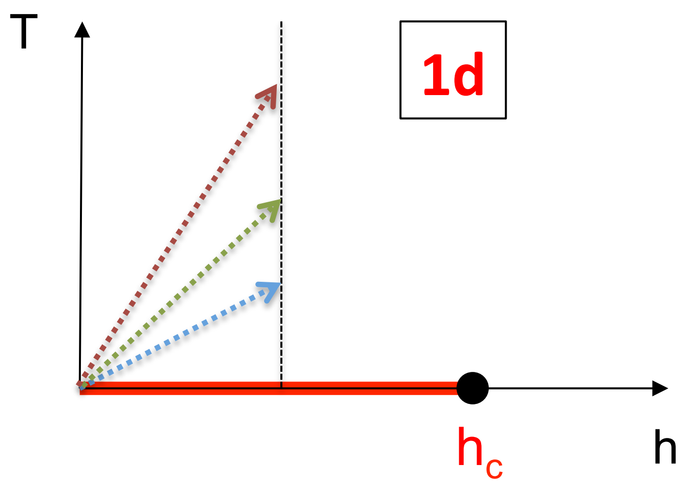
Order parameter: **Magnetization** (not conserved!) $m = \langle \sigma_i^x \rangle$

Equilibrium phase diagram:



Non-equilibrium relaxation with heat bath

Quench from T=0, h=0 to T>0, h>0; heat bath dynamics, thermalization ➔ $\rho \sim e^{-H/T}$



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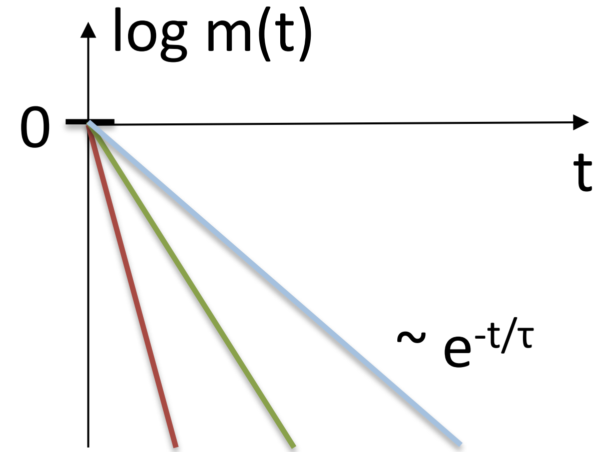

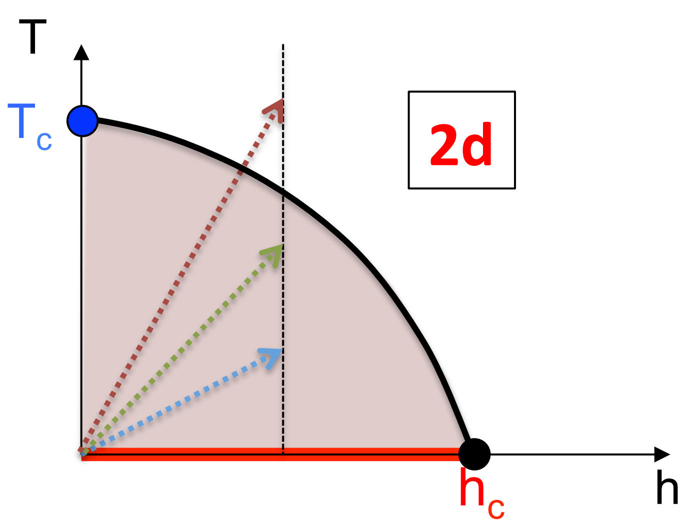

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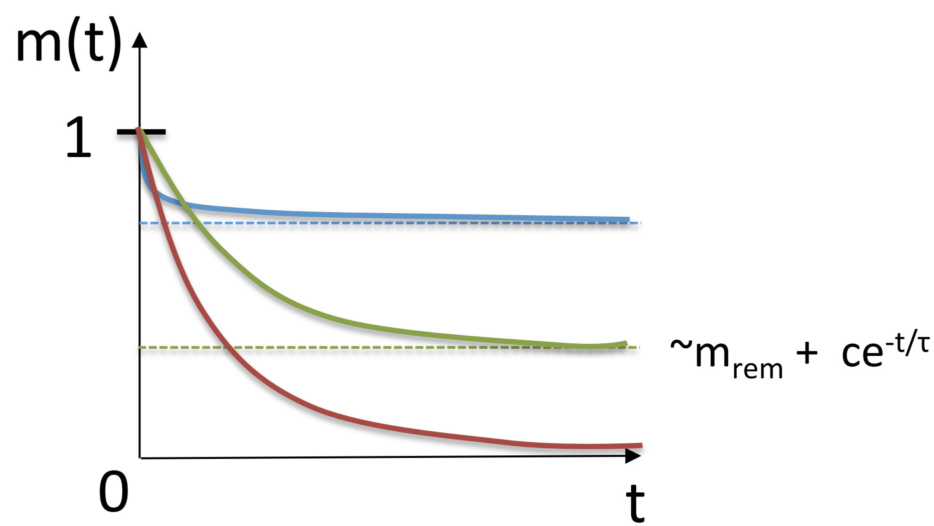
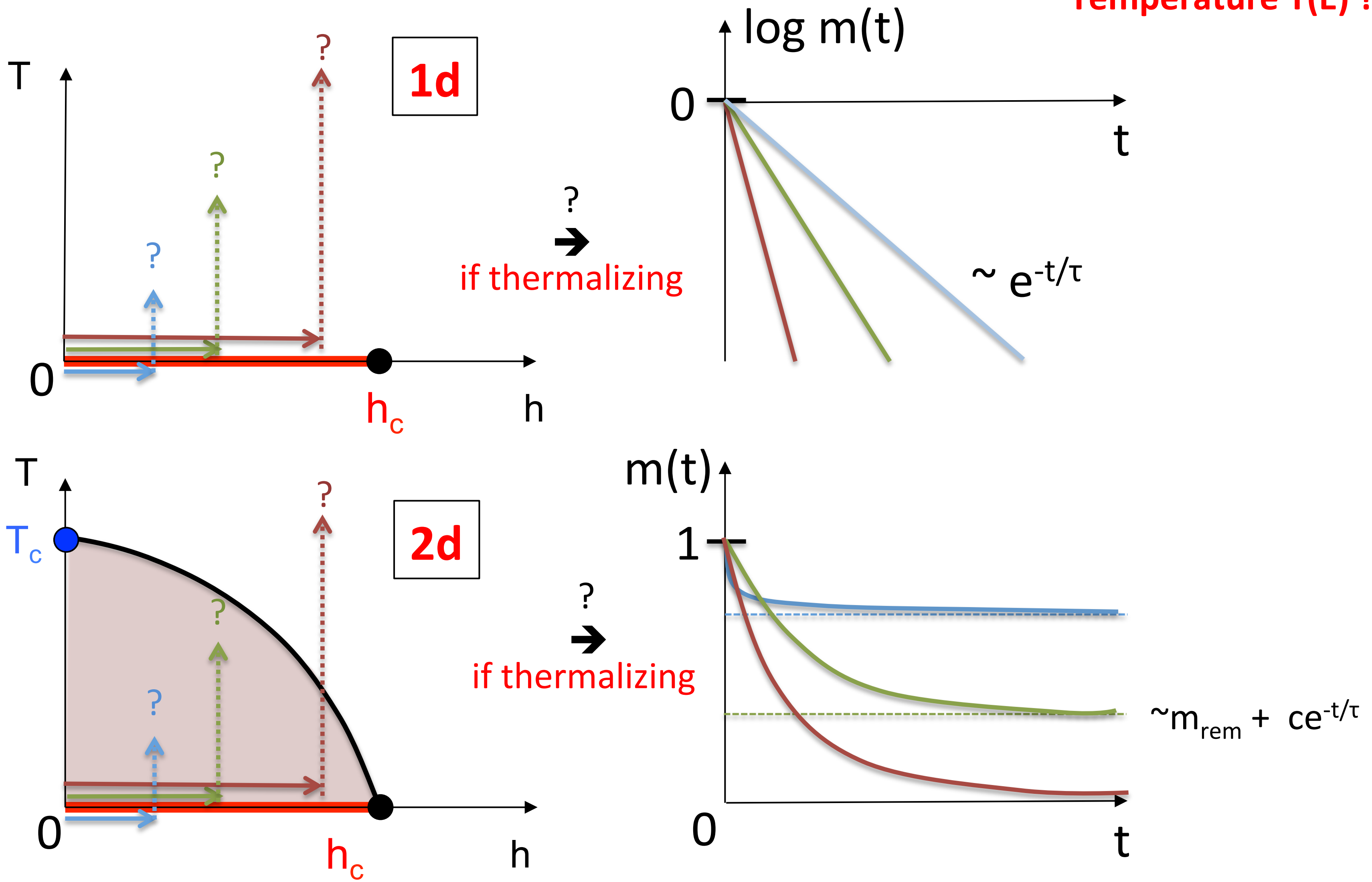


Non-equilibrium dynamics in closed system

Quench from h=0 to h>0;   Schrödinger dynamics (conserved energy E) ➔ **Thermalization ??**
Temperature T(E) ?



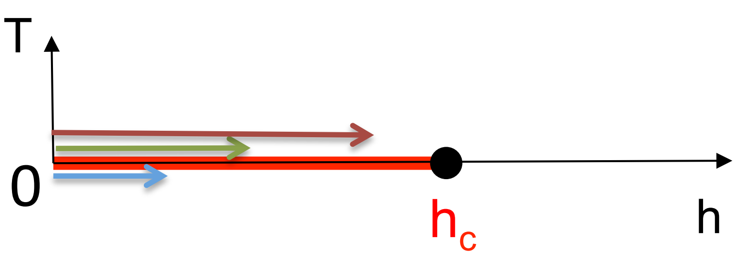
Quantum Quench in the 1d TIM (at T=0)

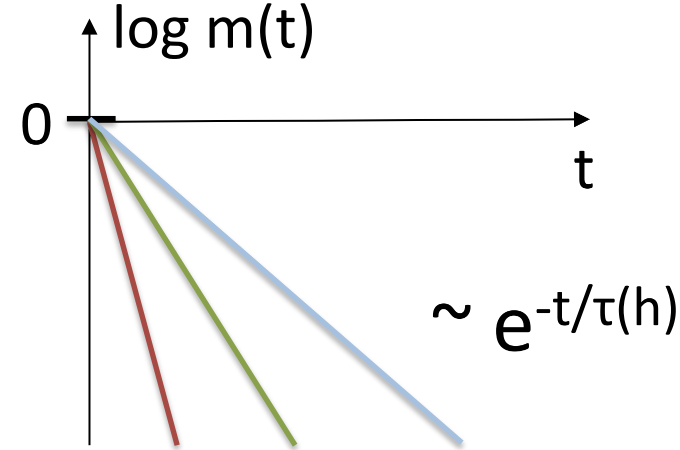
$$H = -\sum_{i=1}^{L}(J\sigma_i^x\sigma_{i+1}^x + h\sigma_i^z) = \sum_p \varepsilon_p \eta_p^+ \eta_p$$

η_p Fermion operators

$$|\psi(t)\rangle = e^{-itH}|\psi_0\rangle$$

Quench:
$|\psi(t=0)>$ GS of H with e.g. h=0,
dynamics for H with h>0 (exactly calculable)





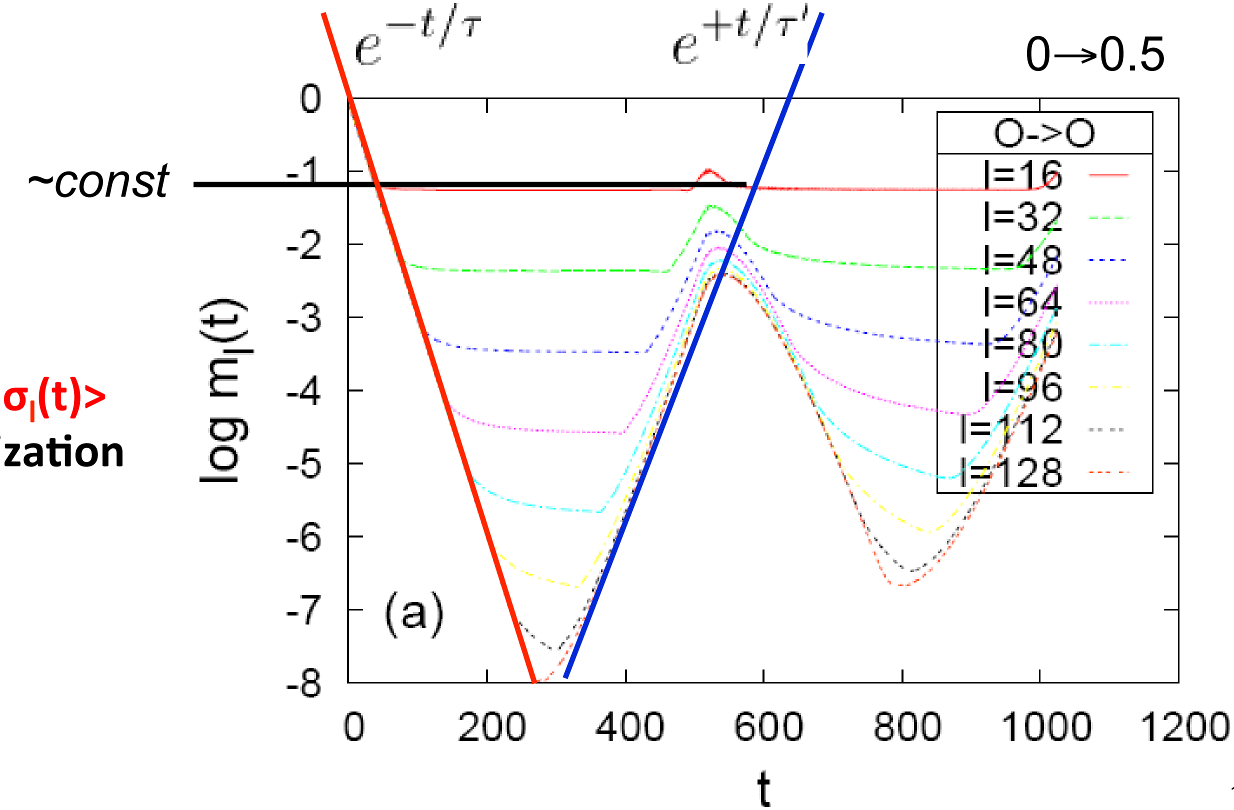
$$m_i(t) = \langle\psi(t)|\sigma_i^x|\psi(t)\rangle \propto \exp(-t/\tau(h))$$ with $$1/\tau(h) = \frac{2}{\pi}\int_0^\pi dp\, v_p \cdot f_p(h_0, h)$$

[Rieger, Iglói 2011]
[Calabrese, Essler, Fagotti 2012]

$$f_p(h, h_0) = \langle\psi_0|\eta_p^+(h)\eta_p(h)|\psi_0\rangle$$ and $$v_p = \frac{\partial\varepsilon_p}{\partial p}$$

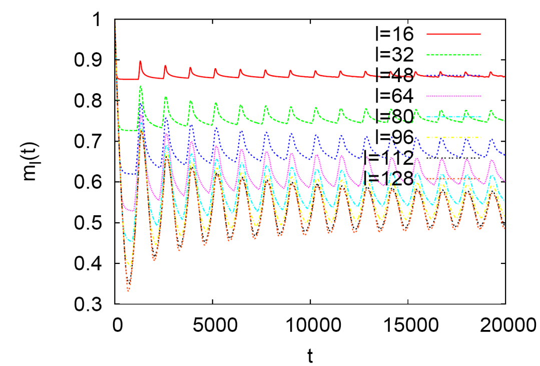
Does the exponential relaxation mean that the system is thermalized?
(no, because $f_p \neq e^{-\beta\varepsilon(p)}$)

Look at finite system – what's going on?



$m_l(t) = \langle \sigma_l(t) \rangle$
magnetization at site l

- **Exponential relaxation**
- **Quasi-stationary regime**
- **Exponential recovery**



Quasi-particles = kinks (in FM phase: h<J)

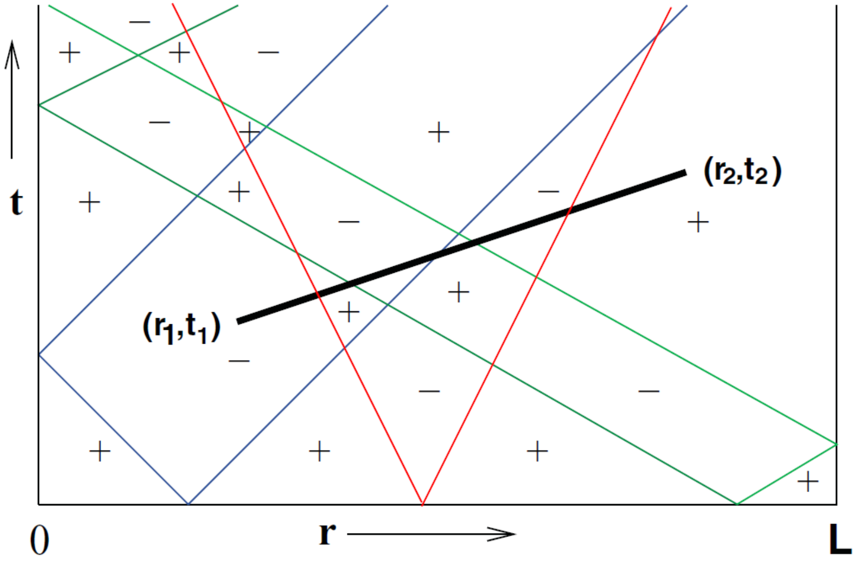
Kinks = non-interacting fermions
are created in pairs (+p,-p)
move with velocity $\pm v_p$

$$\epsilon_p = \sqrt{J^2 + h^2 - 2Jh\cos(p)}$$

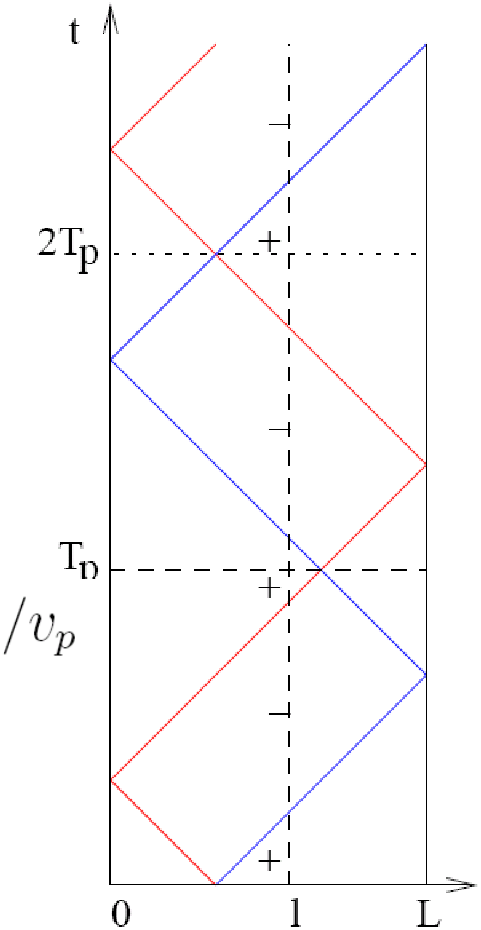
$$v_p = \frac{\partial \epsilon_p}{\partial p} = \frac{Jh\sin(p)}{\epsilon_p}$$

… and will flip spins upon arrival!

E.g. $C(r_1t_1;r_2t_2) = \langle\sigma_{r1}(t_1)\ \sigma_{r2}(t_2)\rangle$:



Finite system:



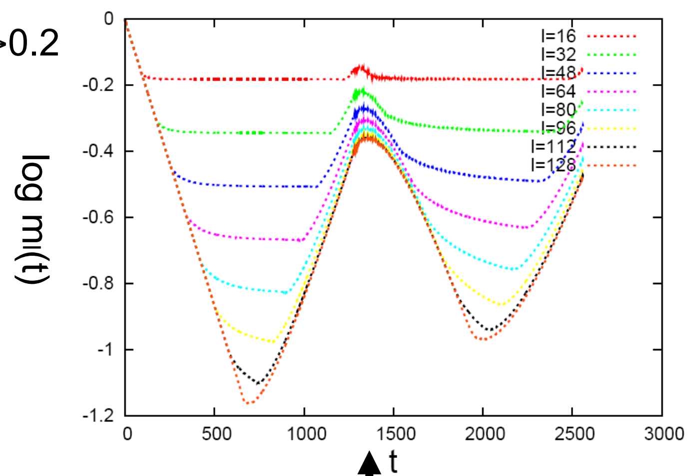
$$T_p = L/v_p$$

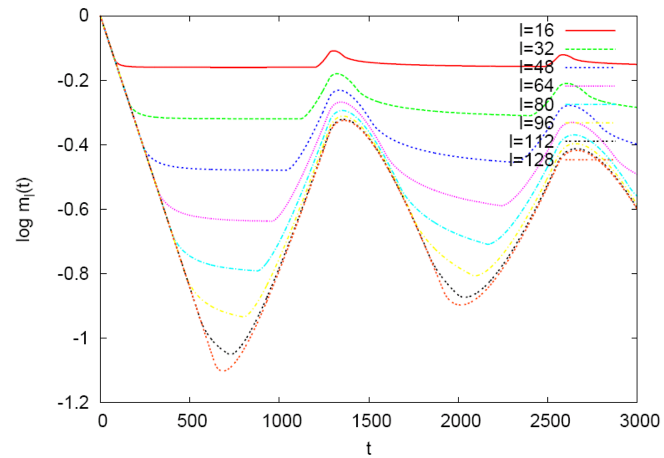
Reflection at the boundaries at i=0 and i=L!

1d TIM does not thermalize

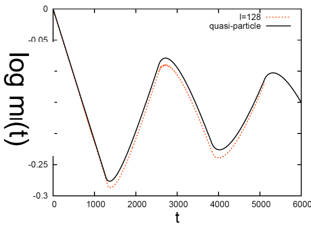
exact | **semi classical**

0→0.2



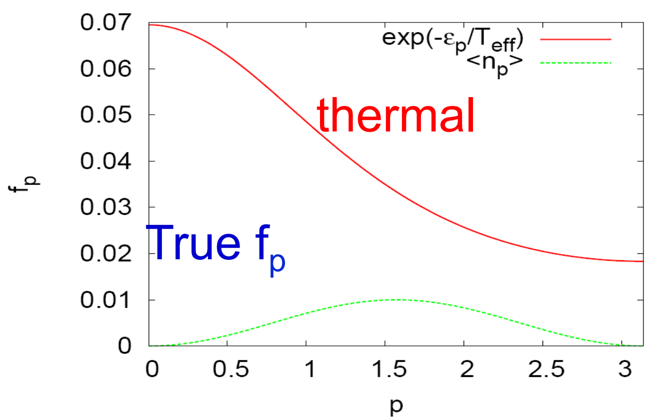


0→0.1, L=256



QP occupation probability:

$$f_p(h_0, h) = \langle\psi_0|\eta_p^+\eta_p|\psi_0\rangle = \frac{1}{4}(h-h_0)^2\sin^2(p)$$



Period:

$T_{period} = L/v_{max} \sim L/h$

$$v_p = \frac{\partial\epsilon_p}{\partial p} = \frac{Jh\sin(p)}{\epsilon_p}$$

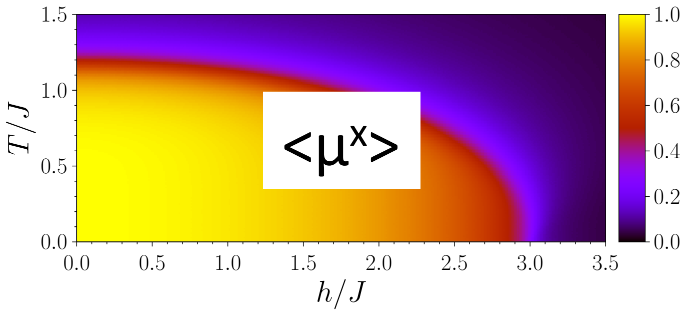
QPs non-interacting,
➔ f_p conserved
➔ no thermalization towards $f_p \sim e^{-\beta\epsilon(p)}$

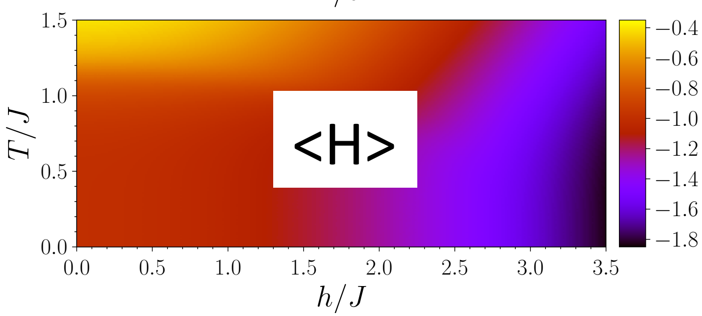
The 2d transverse Ising model: equil. & quenches

$$\hat{H} = -\frac{J}{2} \sum_{<\mathbf{R},\mathbf{R}'>} \hat{\sigma}^x_{\mathbf{R}} \hat{\sigma}^x_{\mathbf{R}'} - \frac{h}{2} \sum_{\mathbf{R}} \hat{\sigma}^z_{\mathbf{R}}$$

$$\hat{\mu}^x = \frac{1}{N} \sum_{\mathbf{R}} \hat{\sigma}^x_{\mathbf{R}} \,.$$

Equilibrium phase diagram





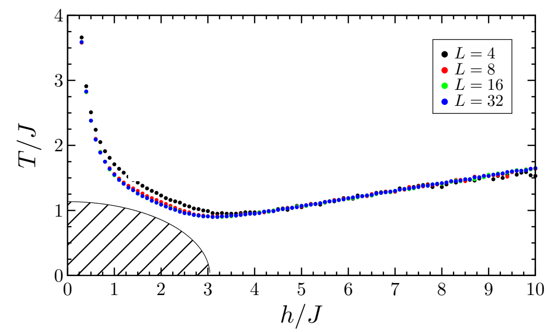
Quenches: $(J_{\rm i}; h_{\rm i}) \to (J_{\rm f}; h_{\rm f})$

Final energy: $E_{\rm f} = \sum_\lambda E_{{\rm f},\lambda} |\langle \Psi_{{\rm i},0} | \Psi_{{\rm f},\lambda} \rangle|^2$

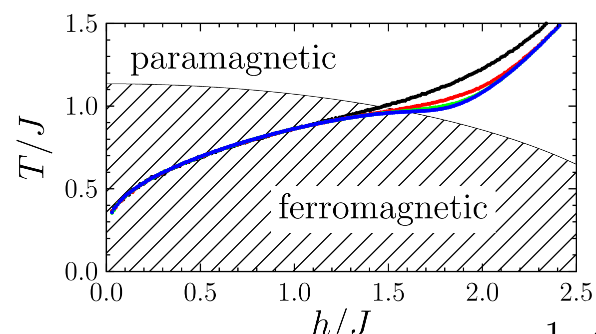
Excess energy: $E_{\rm exc} = E_{\rm f} - E_{{\rm f},0}$

Effective temperature: $\langle \hat{H}_{\rm f} \rangle^{T_{\rm eff}}_{\rm CGE} = E_{\rm f}$

$$|\Psi_{{\rm i},0}\rangle = |\uparrow\uparrow \ldots \uparrow\uparrow\rangle_z = \frac{1}{\sqrt{2^N}} \sum_{\mathbf{x}} |\mathbf{x}\rangle$$



Interaction quenches:
(0,h) -> (J,h)



field quenches:
(J,0) -> (J,h)

$$|\Psi_{{\rm i},0}\rangle = \frac{1}{\sqrt{2}} \left\{ |\uparrow\uparrow \ldots \uparrow\uparrow\rangle_x + |\downarrow\downarrow \ldots \downarrow\downarrow\rangle_x \right\}$$

Time evolution

$$|\Psi(t=0)\rangle = |\Psi_{\mathrm{i},0}\rangle$$

$$|\Psi_{\mathrm{i},0}\rangle = |\uparrow\uparrow\ldots\uparrow\uparrow\rangle_z = \frac{1}{\sqrt{2^N}}\sum_{\mathbf{x}}|\mathbf{x}\rangle$$

$$|\Psi_{\mathrm{i},0}\rangle = \frac{1}{\sqrt{2}}\Big\{|\uparrow\uparrow\ldots\uparrow\uparrow\rangle_x + |\downarrow\downarrow\ldots\downarrow\downarrow\rangle_x\Big\}$$

$$\boxed{|\Psi(t)\rangle = e^{-\imath\hat{H}_{\mathrm{f}}t}|\Psi(t=0)\rangle}$$

$$\langle\hat{\mathcal{O}}\rangle_t = \sum_{\lambda}|c_{\mathrm{f},\lambda}|^2\mathcal{O}_{\lambda\lambda} + \sum_{\lambda\neq\lambda'}c^*_{\mathrm{f},\lambda}c_{\mathrm{f},\lambda'}e^{\imath(E_{\mathrm{f},\lambda}-E_{\mathrm{f},\lambda'})t}\mathcal{O}_{\lambda\lambda'}$$

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\,\langle\hat{\mathcal{O}}\rangle_t = \sum_{\lambda}|c_{\mathrm{f},\lambda}|^2\mathcal{O}_{\lambda\lambda}$$

$$\langle\hat{\mathcal{O}}\rangle_{\mathrm{diag}} = \mathrm{Tr}[\hat{\mathcal{O}}\,\hat{\rho}_{\mathrm{diag}}] \qquad \hat{\rho}_{\mathrm{diag}} = \textstyle\sum_{\lambda} p_{\mathrm{f},\lambda}|\Psi_{\mathrm{f},\lambda}\rangle\langle\Psi_{\mathrm{f},\lambda}|$$

$$p_{\mathrm{f},\lambda} = |c_{\mathrm{f},\lambda}|^2.$$

Techniques for non-integrable systems

$$\hat{H} = -\frac{J}{2} \sum_{<\mathbf{R},\mathbf{R}'>} \hat{\sigma}^x_{\mathbf{R}} \hat{\sigma}^x_{\mathbf{R}'} - \frac{h}{2} \sum_{\mathbf{R}} \hat{\sigma}^z_{\mathbf{R}}$$

L x L square lattice,
p.b.c.

2d TFIM Non-integrable (in particular not a free fermion model as in 1d) !

What can one do to study the (n.eq.) dynamics ? $|\psi(t)\rangle = e^{-itH}|\psi_0\rangle$

1) Mean field theory (or truncated hierarchy of correlations)
2) Exact diaginalization of snall systems (up L=4 or 5)
3) Time series expansion
4) Perturbation theory (e.g. in h)
5) Time dependent variational calculations
6) Real time Quantum Monte Carlo
7) Quantum Boltzmann equation (?)
8) ...

Real Time Dependent Variational Ansatz

Principle:

- Choose set of „physically relevant“ subspace V = span{ $|\Phi_1>$,..., $|\Phi_M>$ }, $M<<2^N$
- Initial state $|\psi_0\rangle = \sum_{k=1}^{M} \alpha_k |\phi_k\rangle$, Ansatz: $|\psi(t)\rangle = \sum_{k=1}^{M} \alpha_k(t) |\phi_k\rangle$
- At each time t minimize distance between $i\frac{\partial}{\partial t}\sum_k \alpha_k(t)|\phi_k\rangle$ and $H\sum_k \alpha_k(t)|\phi_k\rangle$ $\quad \mathcal{D}(t) = \sum_{\mathbf{x}} \left|\dot{\Psi}_{\text{exact}}(\mathbf{x},t) - \dot{\Psi}_{\text{var}}(\mathbf{x},t)\right|^2$
- Resulting differential equation for variational parameters $\alpha_k(t)$:

$$i\frac{\partial}{\partial t}\alpha_k(t) = \sum_{k'} \alpha_{k'}(t)\langle\phi_k|H|\phi_{k'}\rangle$$

- Solve and calculate observales

Interaction quenches (paramagnetic phase)

Jastrow Ansatz
as variational functions

$$|\Psi(t)\rangle = \exp\left(\sum_{\mathbf{r}} \alpha_{\mathbf{r}}(t)\hat{C}^{xx}_{\mathbf{r}}\right)|\uparrow\uparrow\ldots\uparrow\uparrow\rangle_z$$

c.f. Carleo etal
PRA 2014

$$\hat{C}^{xx}_{\mathbf{r}} = \frac{1}{N_{\mathbf{r}}}\sum_{\mathbf{R}} \hat{\sigma}^x_{\mathbf{R}}\hat{\sigma}^x_{\mathbf{R}+\mathbf{r}}$$

Equations of
Motion for α_r

$$\sum_{\mathbf{r}'} \langle \delta\hat{C}^{xx}_{\mathbf{r}}\delta\hat{C}^{xx}_{\mathbf{r}'}\rangle_t\, \dot{\alpha}_{\mathbf{r}'}(t) = -\imath\,\langle E^{\mathrm{local}}_{\mathrm{f}}(t)\delta\hat{C}^{xx}_{\mathbf{r}}\rangle_t$$

$$\delta\hat{\mathcal{O}} = \hat{\mathcal{O}} - \langle\hat{\mathcal{O}}\rangle_t \qquad E^{\mathrm{local}}_{\mathrm{f}}(\mathbf{x},t) = \langle\mathbf{x}|\hat{H}_{\mathrm{f}}|\Psi(t)\rangle \,/\, \langle\mathbf{x}|\Psi(t)\rangle$$

Initial condition $\alpha_{\mathbf{r}}(t=0) = 0$

Expectation values $\langle\hat{\mathcal{O}}\rangle_t = \dfrac{\sum_{\mathbf{x}} |\Psi(\mathbf{x},t)|^2\mathcal{O}(\mathbf{x})}{\sum_{\mathbf{x}} |\Psi(\mathbf{x},t)|^2}$

Calculation via **Monte Carlo**

$$A\left(\mathbf{x}\to\mathbf{x}',t\right) = \min\left[1, Q\left(\mathbf{x}\to\mathbf{x}',t\right)\right]$$

$$Q\left(\mathbf{x}\to\mathbf{x}',t\right) = \exp\left\{2\sum_{\mathbf{r}}\alpha^R_{\mathbf{r}}(t)\left(C^{xx}_{\mathbf{r}}(\mathbf{x}') - C^{xx}_{\mathbf{r}}(\mathbf{x})\right)\right\}$$

Field quenches (ferromagnetic phase)

$$|\Psi(t)\rangle = \sum_{m,n} \alpha_{m,n}(t)\,|\Psi_{m,n}\rangle$$

$$|\Psi_{m,n}\rangle = \frac{1}{\sqrt{N_{m,n}}} \sum_{k=1}^{N_{m,n}} |\Psi^k_{m,n}\rangle$$

Symmetric superposition of all states with n spins up and m kinks

L	4	8	12	16
number of $\alpha_{m,n}$	45	848	4551	14834

Eq. Of motion:

$$\imath\dot{\alpha}_{m,n}(t) = -J\,(N-n)\,\alpha_{m,n}(t) - \frac{h}{2}\sum_{m',n'} t_{m',n';m,n}\,\alpha_{m',n'}(t)$$

$$t_{m',n';m,n} = T_{m',n';m,n}/\sqrt{N_{m',n'}\,N_{m,n}}$$

$T_{m,n;m',n'}$ = number of transitions between $H_{n,m}$ and $H_{n',m'}$ via 1 spin flip.

Initial valuse:

$$\alpha_{m,n}(t=0) = \begin{cases} \frac{1}{\sqrt{2}} & \text{if } (m,n)=(0,0) \text{ or } (N,0) \\ 0 & \text{else} \end{cases}$$

Calculation with rare event sampling **Monte Carlo**

Observables

Time average:

$$\overline{\langle \hat{\mathcal{O}} \rangle_t} = \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} dt \, \mathrm{Tr}[\hat{\mathcal{O}} \, \hat{\rho}(t)] \qquad \hat{\rho}(t) = |\Psi(t)\rangle\langle\Psi(t)|$$

$$\overline{p_t(\mathcal{O}_j)} = \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} dt \, \mathrm{Tr}[\delta(\mathcal{O}_j - \hat{\mathcal{O}}) \, \hat{\rho}(t)]$$

Thermal average:

$$\langle \hat{\mathcal{O}} \rangle_{\mathrm{CGE}}^{T_{\mathrm{eff}}} = \frac{1}{Z_{\mathrm{CGE}}^{T_{\mathrm{eff}}}} \mathrm{Tr}[\hat{\mathcal{O}} e^{-\hat{H}/T_{\mathrm{eff}}}]$$

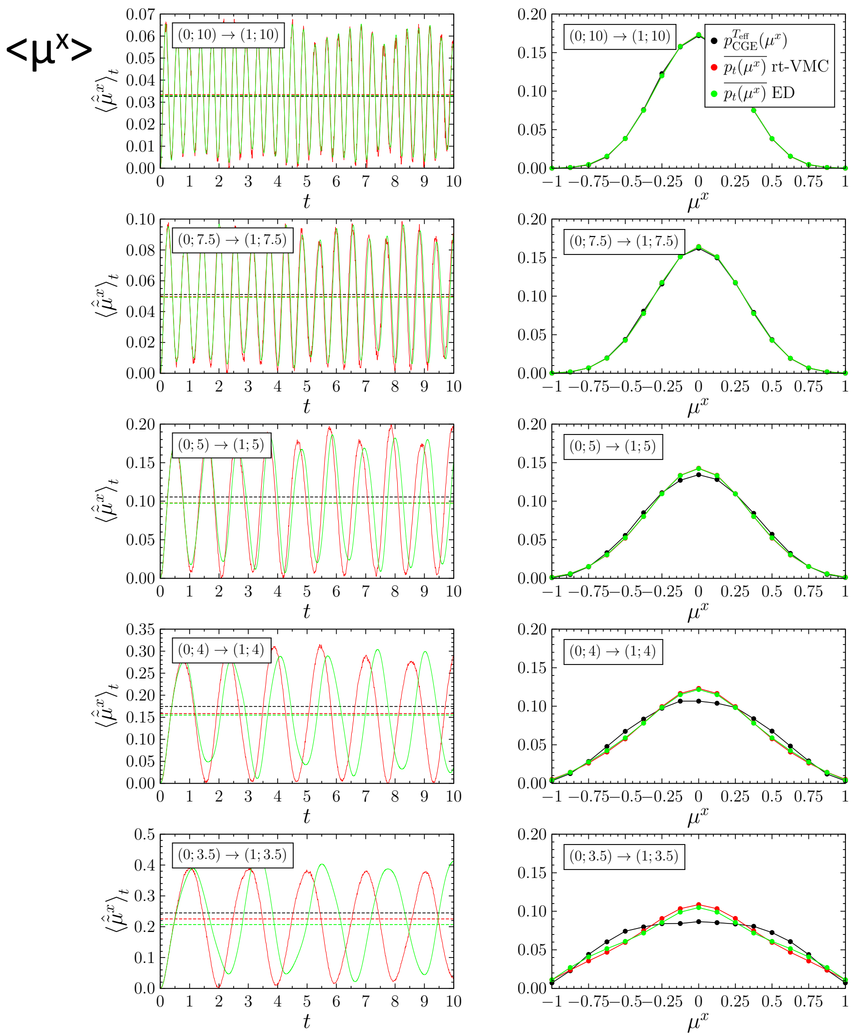
$$p_{\mathrm{CGE}}^{T_{\mathrm{eff}}}(\mathcal{O}_j) = \frac{1}{Z_{\mathrm{CGE}}} \mathrm{Tr}[\delta(\mathcal{O}_j - \hat{\mathcal{O}}) e^{-\hat{H}/T_{\mathrm{eff}}}]$$

Calculated with continuous imaginary time cluster Monte Carlo

Comparison (4x4): thermal, rt-VMC, exact

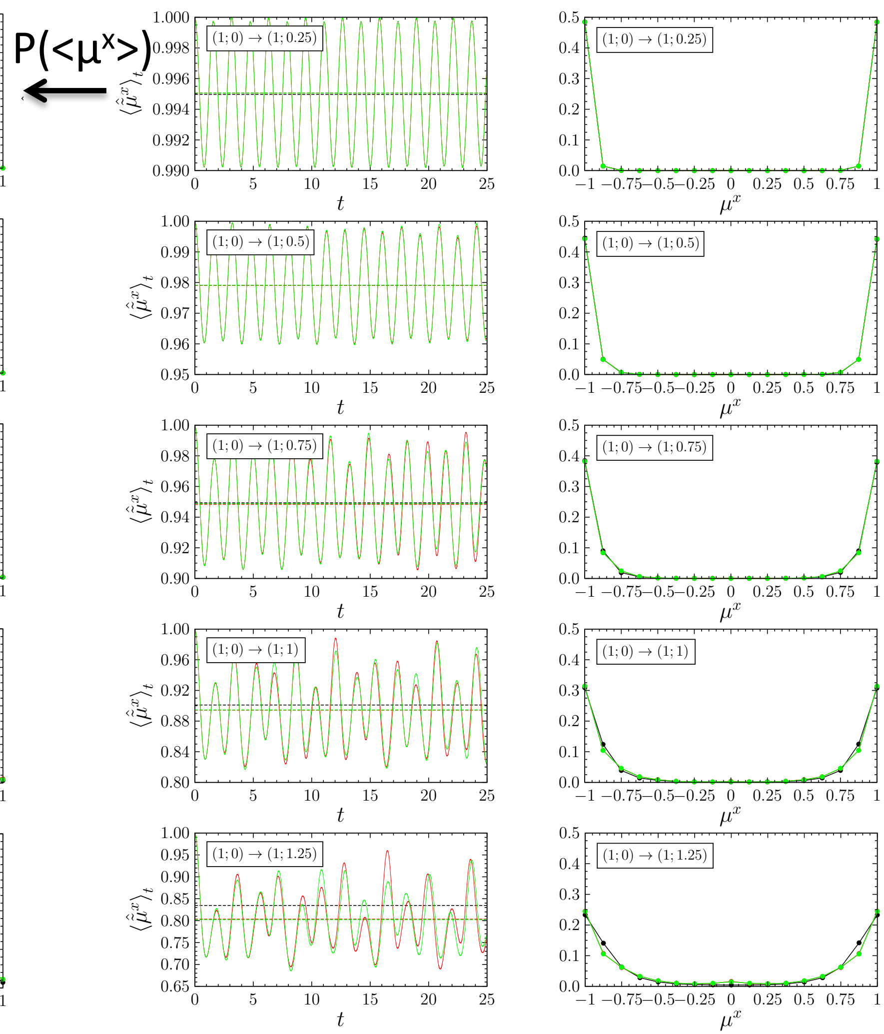
Interaction quench (PM)

$(0; h) \rightarrow (J; h)$



Field quench (FM)

$(J; 0) \rightarrow (J; h)$

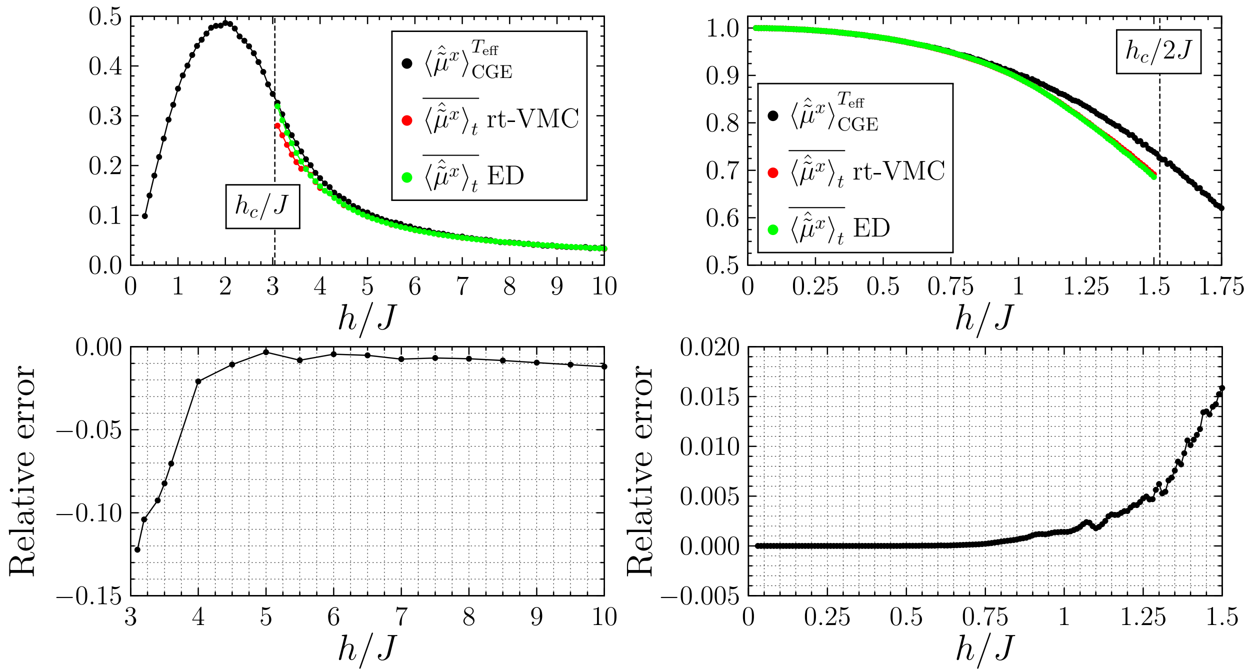


[Blass, Rieger: arXiv 2016]

Comparison (4x4) - magnetization

Interaction quenches $(0; h) \to (J; h)$

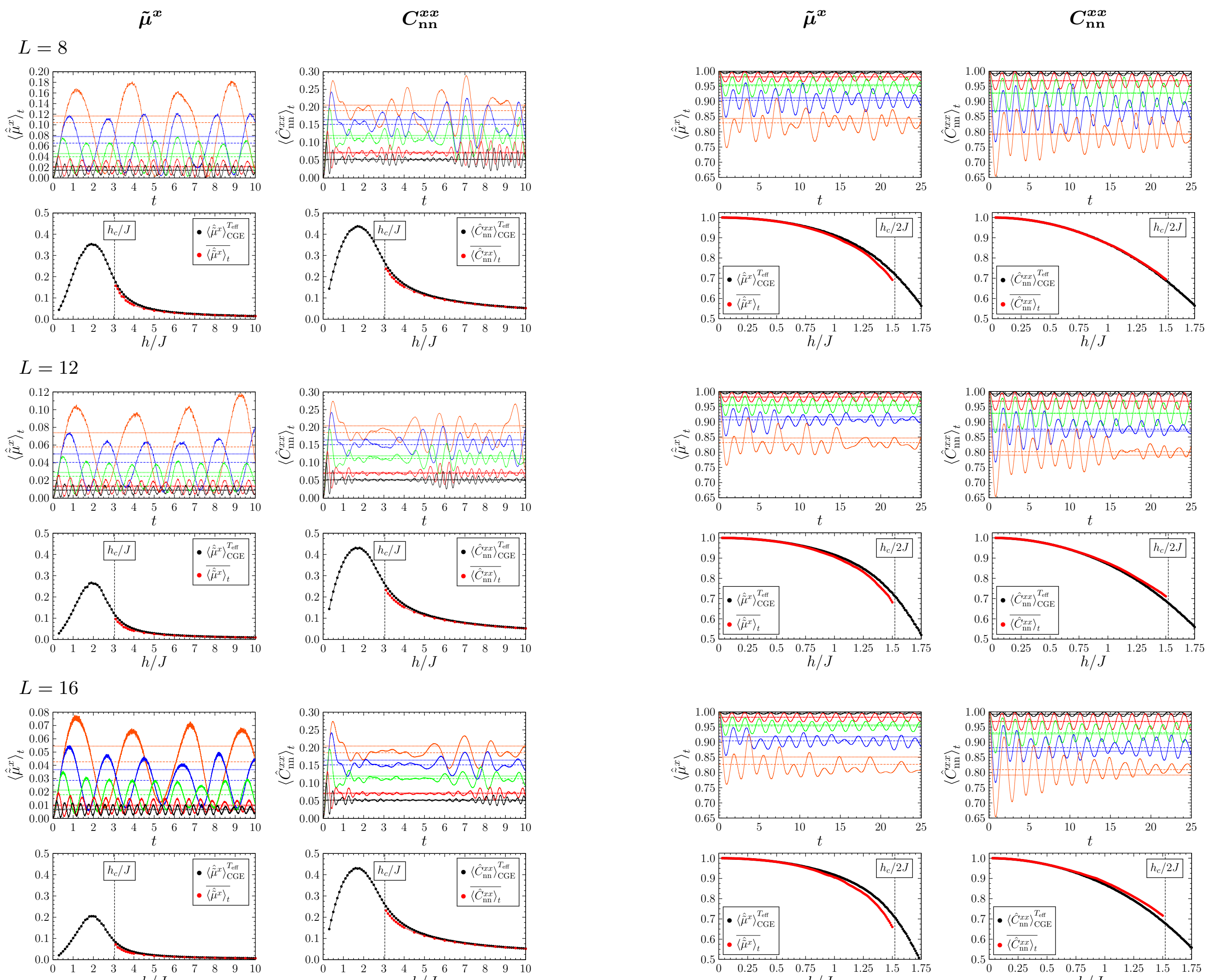
Field quenches $(J; 0) \to (J; h)$



Comparison time (rt-VMC) / thermal average (L=8,12,16)

Interaction quench (PM)

Field quench (FM)

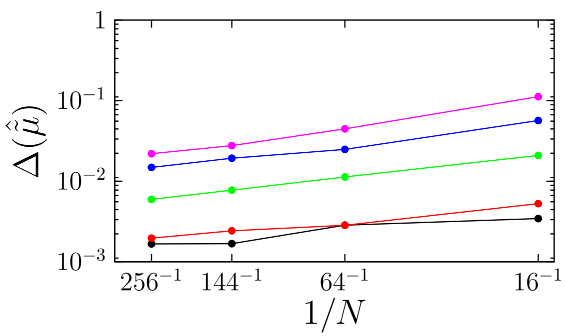


[Blass, Rieger: arXiv 2016]

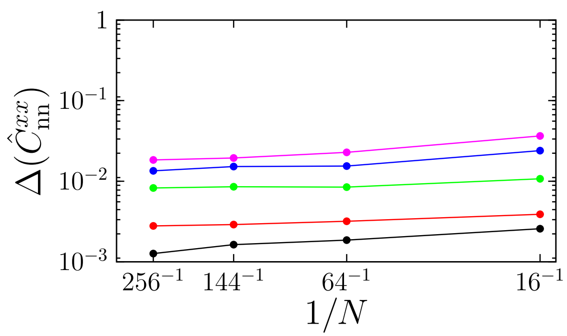
Deviations time - thermal: finite size effects

(a) **Interaction quenches** $(0,h) \to (J,h)$

i. Magnetization

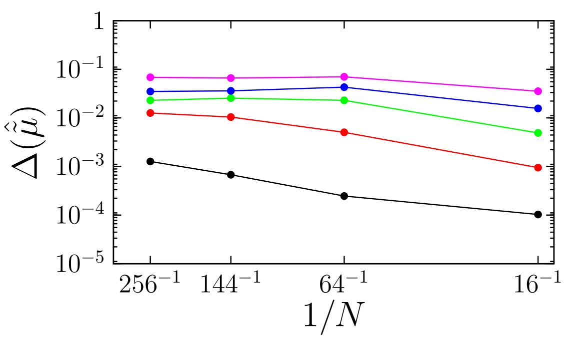


ii. Correlation function

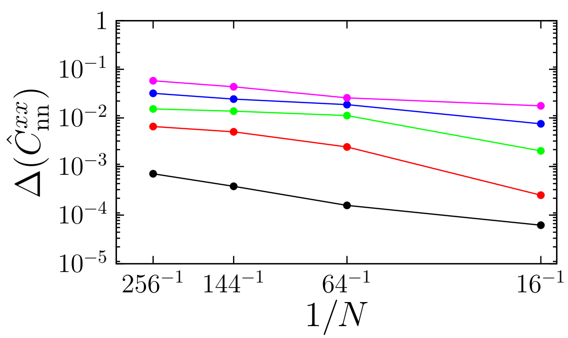


(b) **Field quenches** $(J,0) \to (J,h)$

i. Magnetization

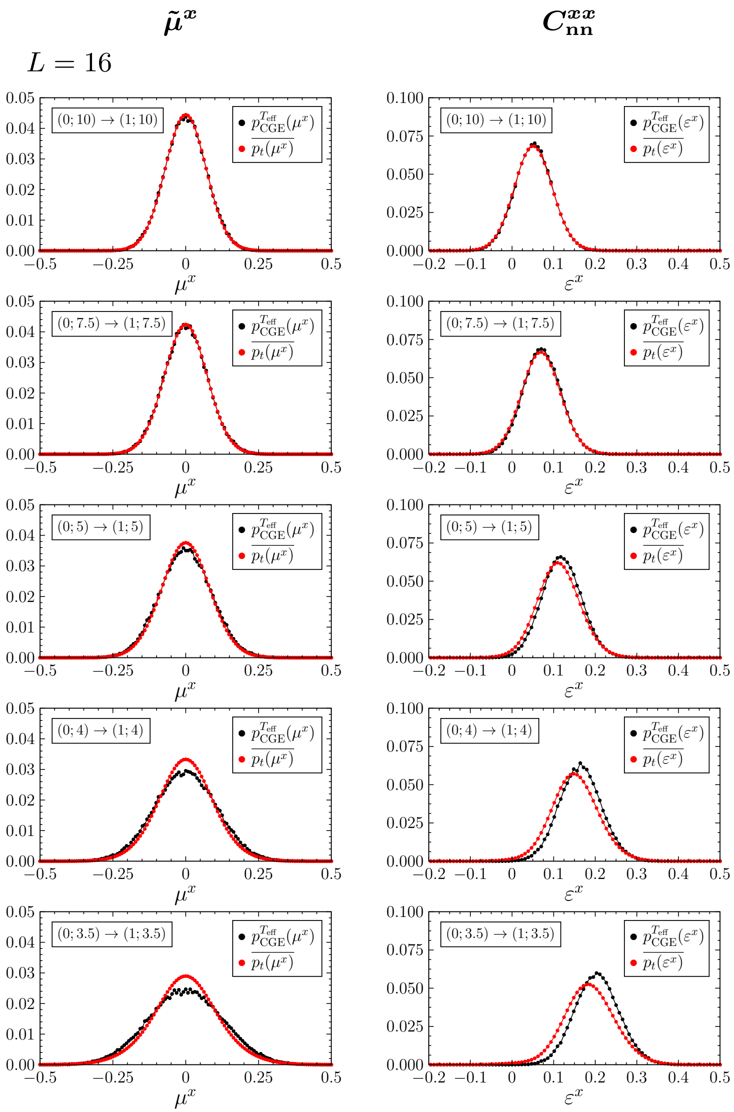


ii. Correlation function

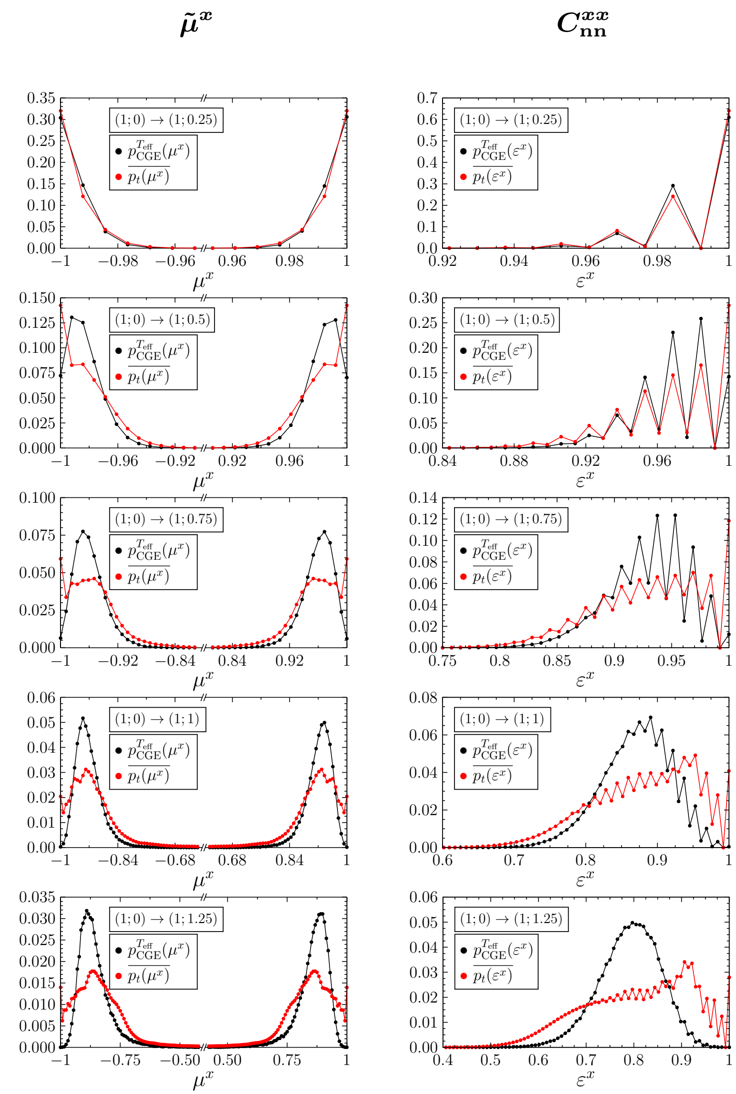


Time / thermal – increasing quench strength (L=16)

Interaction quench (PM)

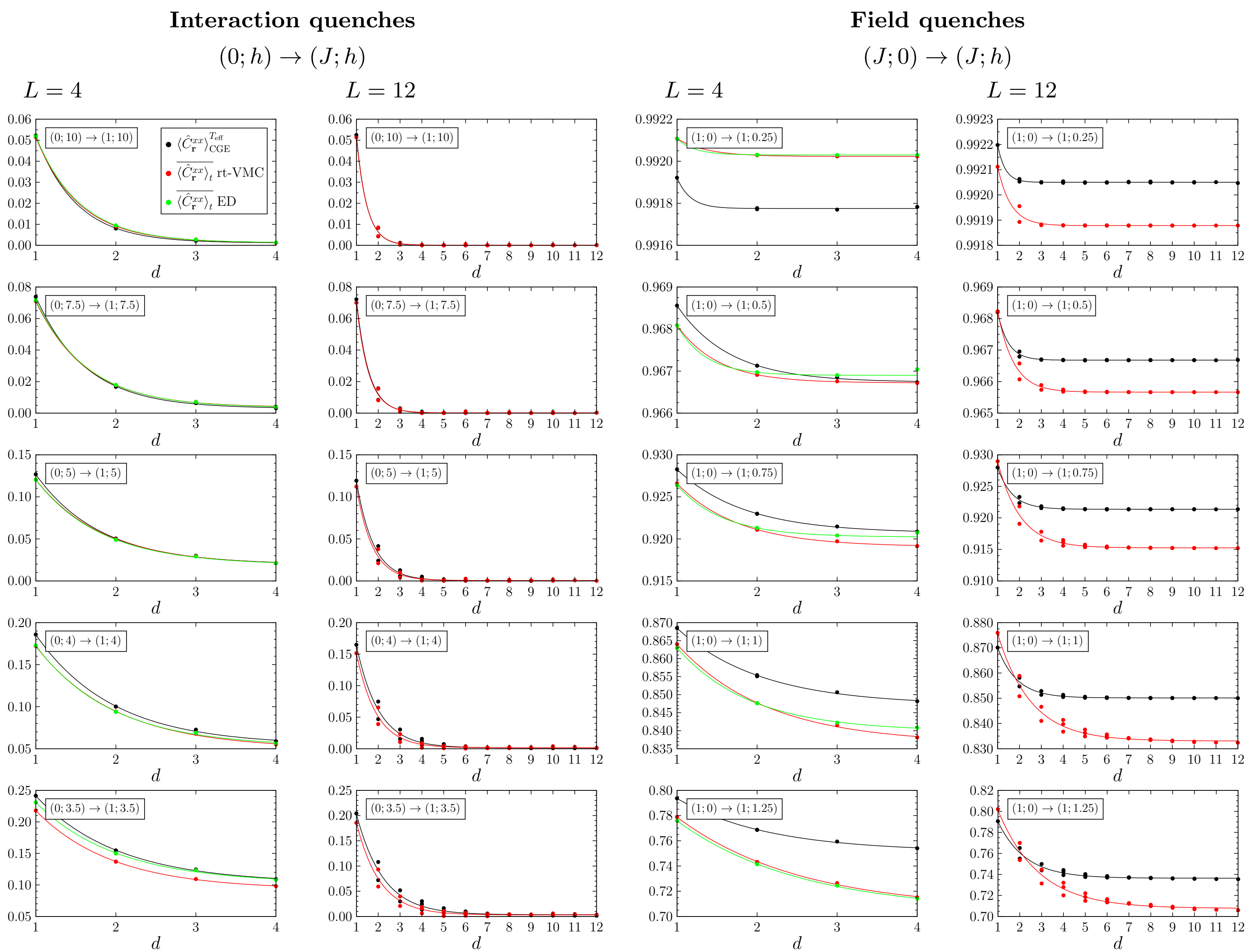


Field quench (FM)



[Blass, Rieger: arXiv 2016]

Correlation functions



[Blass, Rieger: arXiv 2016]

Conclusion

- Quantum relaxation after field quench in 1d TIM:
- No thermalization, quasi particles (kinks) do not interact,
- f_p conserved, reconstruction of magnetization in finite systems

- Quantum relaxation after quenches in 2d TIM
- Time dependent variational calculation (rt-VMC):
- Comparison of time averages with thermal expectation values
- Good agreement for interaction quenches (in the PM phase)
- Absence of thermalization for field quenches (in the FM phase)
- Magnetic correlations do not decay in the FM phase
- Note: FM phase is gapless (-> lack of clustering property?)