Expansion in large coordination number for the quantum Ising model

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Quantum "bucket" challenge

How to deal with quantum dynamics of large size systems!

"Large coordination number expansion" method

VERSUS

- Quantum computers: D-wave, Nasa, Google, ...
- Theory methods: DMRG, QMC, DMFT, ...

to be applied to:

- Quantum Ising model

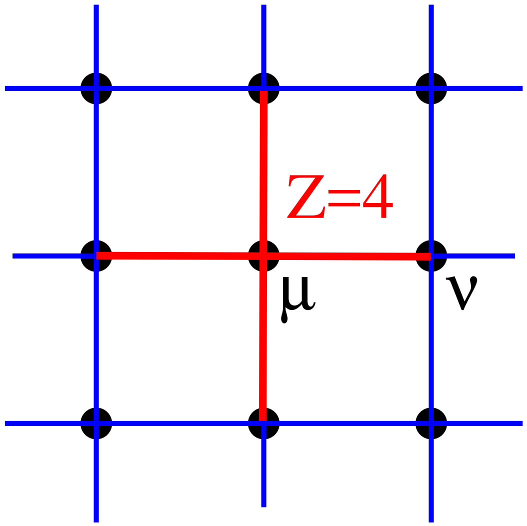
Large coordination number expansion

Benchmark test for this method:

Bose-Hubbard model

$$\hat{H} = -\frac{J}{Z}\sum_{\mu\nu} T_{\mu\nu}\hat{b}^\dagger_\mu \hat{b}_\nu + \frac{U}{2}\sum_\mu \hat{n}_\mu(\hat{n}_\mu - 1)$$

Hopping matrix: $T_{\mu\nu}$ nearest neighbour interactions
Coordination number: $Z = 2D$



Large coordination number expansion

P. Navez, R. Schützhold, Phys. Rev. A **82**, 063603 (2010)

Density Matrix: $\hat{\rho} \equiv \hat{\rho}_{\mu_1 \mu_2 \dots \mu_N}$

$$i\partial_t \hat{\rho} = [\hat{H}, \hat{\rho}] = \frac{1}{Z}\sum_{\mu\nu} [\hat{H}_{\mu\nu}, \hat{\rho}] + \sum_{\mu} [\hat{H}_{\mu}, \hat{\rho}] = \frac{1}{Z}\sum_{\mu\nu} \mathcal{L}_{\mu\nu}\hat{\rho} + \sum_{\mu} \mathcal{L}_{\mu}\hat{\rho}$$

Reduced density matrices:

$$\hat{\rho}_{\mu} = \text{Tr}_{\not{\mu}}(\hat{\rho}) \qquad \hat{\rho}_{\mu\nu} = \text{Tr}_{\not{\mu}\not{\nu}}(\hat{\rho}) \qquad \hat{\rho}_{\mu\nu\kappa} = \text{Tr}_{\not{\mu}\not{\nu}\not{\kappa}}(\hat{\rho}) \qquad \dots$$

Scaling on correlated parts: large Z limit

$$\hat{\rho}_{\mu} \sim \mathcal{O}(Z^0) \quad \rightarrow \text{on} - \text{site correlations}$$

$$\hat{\rho}^{\text{corr}}_{\mu\nu} = \hat{\rho}_{\mu\nu} - \hat{\rho}_{\mu}\hat{\rho}_{\nu} \sim \mathcal{O}(Z^{-1}) \quad \rightarrow \text{off} - \text{site correlations}$$

$$\hat{\rho}^{\text{corr}}_{\mu\nu\kappa} = \hat{\rho}_{\mu\nu\kappa} - \hat{\rho}^{\text{corr}}_{\mu\nu}\hat{\rho}_{\kappa} - \hat{\rho}^{\text{corr}}_{\mu\kappa}\hat{\rho}_{\nu} - \hat{\rho}^{\text{corr}}_{\nu\kappa}\hat{\rho}_{\mu} - \hat{\rho}_{\nu}\hat{\rho}_{\kappa}\hat{\rho}_{\mu} \sim \mathcal{O}(Z^{-2})$$

$$\dots$$

$$\hat{\rho}^{\text{corr}}_{\mathcal{S}} \sim 1/Z^{n-1} \qquad \mathcal{S} = \{\mu_1 \dots \mu_n\}$$

Hierarchy equations for $\widehat{\rho}_{\mathcal{S}}^{\text{corr}} = \widehat{\rho}_{\mu_1 \ldots \mu_n}^{\text{corr}}$

$$i\partial_t \widehat{\rho}_{\mathcal{S}}^{\text{corr}} = \frac{1}{Z} \sum_{\mu,\nu \in \mathcal{S}} \sum_{\mathcal{P} \subseteq \mathcal{S} \setminus \{\mu,\nu\}}^{\mathcal{P} \cup \bar{\mathcal{P}} = \mathcal{S} \setminus \{\mu,\nu\}} \left\{ \mathcal{L}_{\mu\nu}\, \widehat{\rho}_{\{\mu\} \cup \mathcal{P}}^{\text{corr}}\, \widehat{\rho}_{\{\nu\} \cup \bar{\mathcal{P}}}^{\text{corr}} - \text{Tr}_{\nu} \left[\mathcal{L}_{\mu\nu}^{S} \Big(\widehat{\rho}_{\{\mu,\nu\} \cup \bar{\mathcal{P}}}^{\text{corr}} + \sum_{\mathcal{Q} \subseteq \bar{\mathcal{P}}}^{\mathcal{Q} \cup \bar{\mathcal{Q}} = \bar{\mathcal{P}}} \widehat{\rho}_{\{\mu\} \cup \mathcal{Q}}^{\text{corr}}\, \widehat{\rho}_{\{\nu\} \cup \bar{\mathcal{Q}}}^{\text{corr}} \Big) \right] \widehat{\rho}_{\{\nu\} \cup \mathcal{P}}^{\text{corr}} \right\}$$

$$+ \sum_{\mu \in \mathcal{S}} \mathcal{L}_{\mu} \widehat{\rho}_{\mathcal{S}}^{\text{corr}} + \frac{1}{Z} \sum_{\mu,\nu \in \mathcal{S}} \mathcal{L}_{\mu\nu}\, \widehat{\rho}_{\mathcal{S}}^{\text{corr}} + \frac{1}{Z} \sum_{\kappa \notin \mathcal{S}} \sum_{\mu \in \mathcal{S}} \text{Tr}_{\kappa} \left[\mathcal{L}_{\mu\kappa}^{S} \widehat{\rho}_{\mathcal{S} \cup \kappa}^{\text{corr}} + \sum_{\mathcal{P} \subseteq \mathcal{S} \setminus \{\mu\}}^{\mathcal{P} \cup \bar{\mathcal{P}} = \mathcal{S} \setminus \{\mu\}} \mathcal{L}_{\mu\kappa}^{S} \widehat{\rho}_{\{\mu\} \cup \mathcal{P}}^{\text{corr}}\, \widehat{\rho}_{\{\kappa\} \cup \bar{\mathcal{P}}}^{\text{corr}} \right]$$

$$\mathcal{L}_{\mu\nu}^{S} = \mathcal{L}_{\mu\nu} + \mathcal{L}_{\nu\mu}$$

$\rightarrow$ **Iterative procedure:** **Order**$= n$, **Size**$= L$ $\rightarrow$ **Computer size** $\sim L^{n-1}$

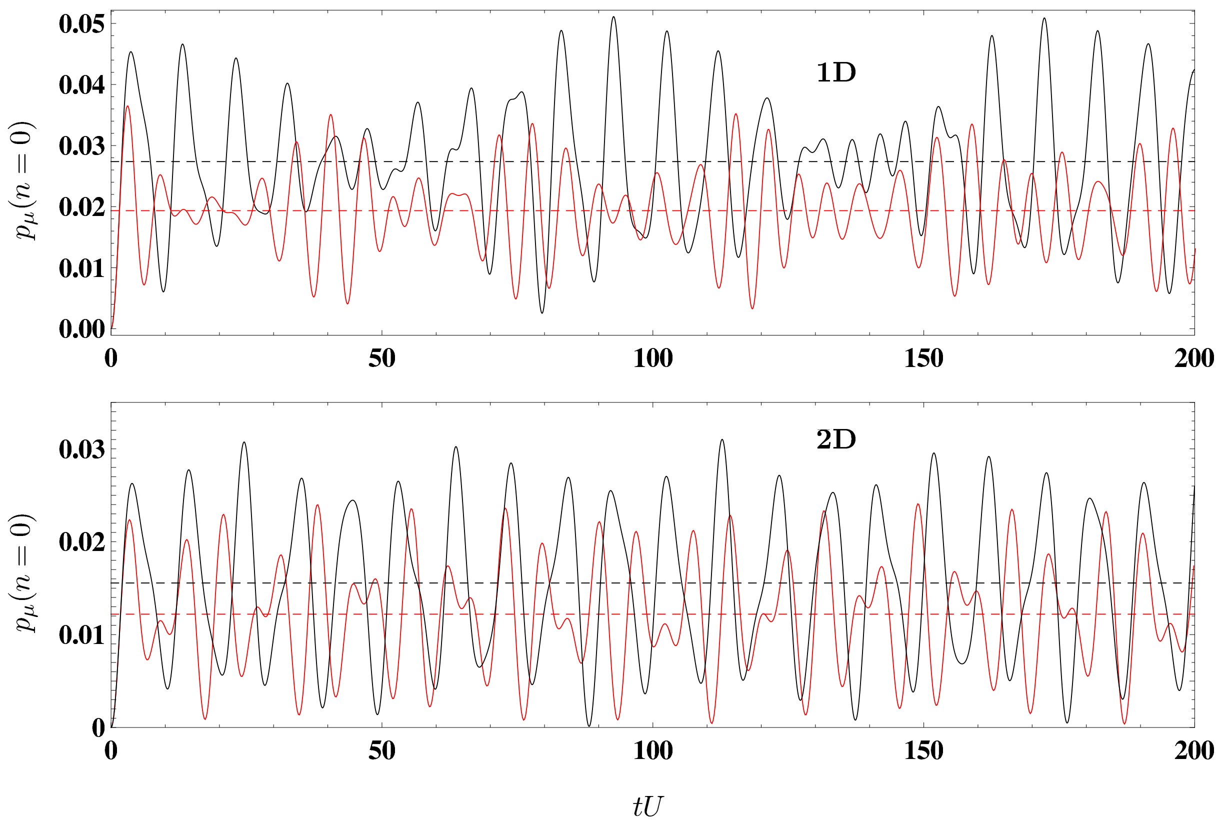
we expect fast convergence for $n \leq 5$ assuming $L = 1024$

Accuracy test: hole probability to order $1/Z$

K. Krutitsky et al. , EPJ Quantum Technology, 1:12 (2014)

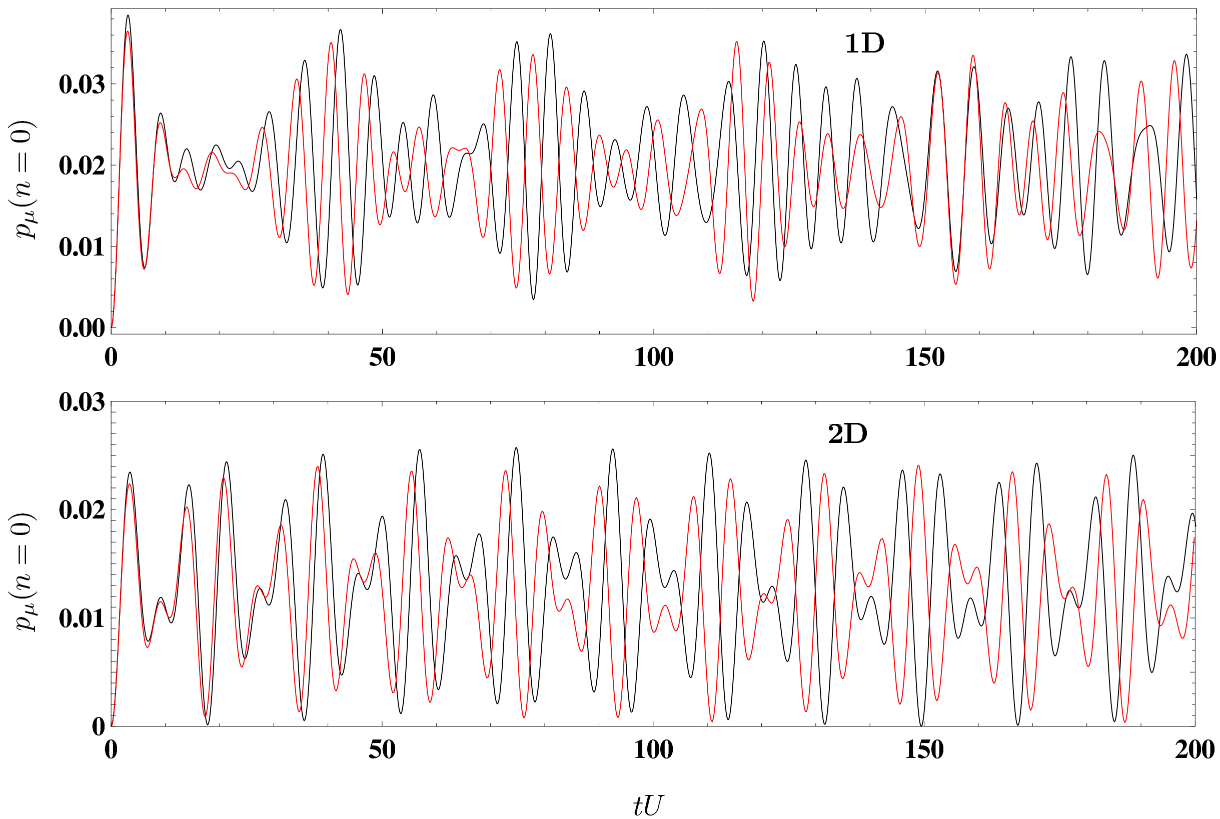
Mott phase: $\hat{\rho}_\mu(t=0) = |1\rangle_\mu\langle 1| \rightarrow$ particle and hole creation

$J/U = 0 \rightarrow 0.1$ 1D: 11 sites 2D: 3×3 sites red: exact



Accuracy test: hole probability to order $1/Z^2$

$J/U = 0 \to 0.1$ 1D: 11 sites 2D: 3×3 sites red: exact



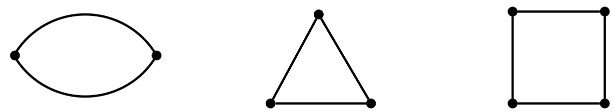
Convergence to the exact solution !

Accuracy test: phase diagram for unit filling in 3D

P. Navez, F. Queisser, R. Schützhold, `arXiv:1601.06302`, accepted in PRA

1st order: Ring diagram resummation

a)

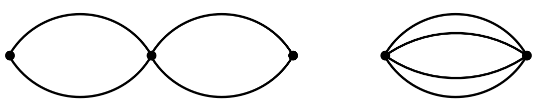


$$\sum_{\mu,\nu}\frac{T_{\mu\nu}T_{\nu\mu}}{Z^2} \qquad \sum_{\mu,\nu,\lambda}\frac{T_{\mu\nu}T_{\nu\lambda}T_{\lambda\mu}}{Z^3} \qquad \sum_{\mu,\nu,\lambda,\kappa}\frac{T_{\mu\nu}T_{\nu\lambda}T_{\lambda\kappa}T_{\kappa\mu}}{Z^4}$$

b)

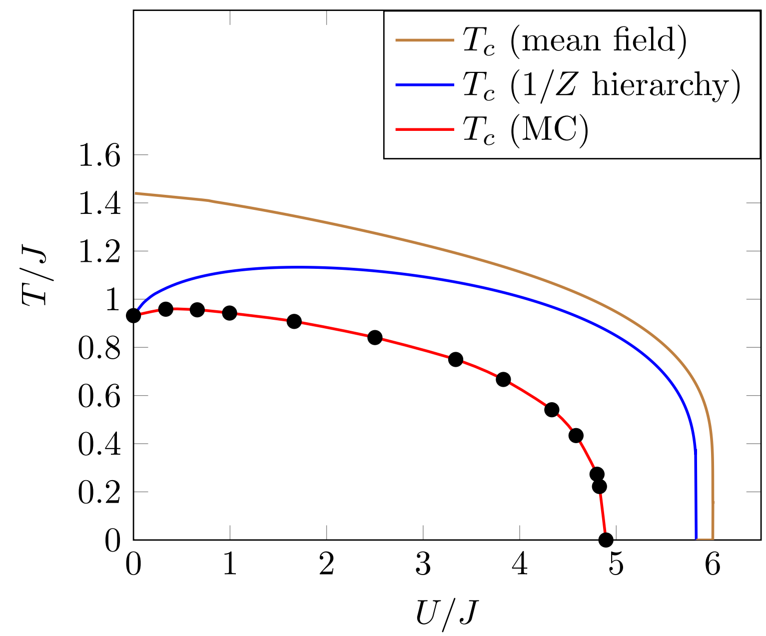
$$-\sum_{\mu,\nu,\lambda}\frac{T_{\mu\nu}^2T_{\nu\lambda}^2}{Z^4} \qquad \sum_{\mu,\nu}\frac{T_{\mu\nu}^4}{Z^4}$$

c)



$$\sum_{\mu,\nu,\lambda}\frac{T_{\mu\nu}^2T_{\nu\lambda}^2}{Z^4} \qquad \sum_{\mu,\nu}\frac{T_{\mu\nu}^4}{Z^4}$$

Phase diagram superfluid-normal phase



Improvement beyond mean field !

Quantum Ising model: quantum fluctuations propagation

P. Navez, G. Tsironis, A. Zagoskin, arXiv:1603.04465

$$\hat{H} = -J \sum_{\mu\nu} \frac{T_{\mu\nu}}{Z} \hat{S}^z_\mu \hat{S}^z_\nu - \sum_\mu B \hat{S}^x_\mu$$

- $T_{\mu\nu}$ interaction matrix, $Z = \sum_\mu T_{\mu\nu}$ coordination number
- J interaction responsible for ferromagnetism
- B transverse magnetic field (magnetic moment set to 1)

e.g. hypercubic lattice:

- dimension D
- $T_{\mu\nu} = 1$ for nearest neighbours and 0 otherwise
- periodic boundary conditions

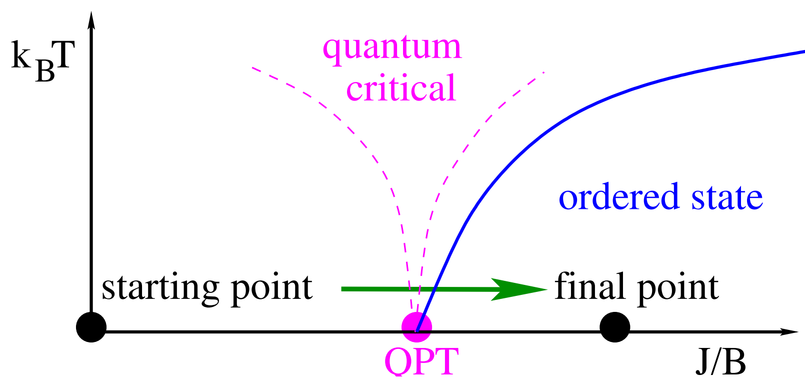
One of the simplest quantum model for test!

Motivations: quantum transition in quench process

Equilibrium: Quantum transition

≡ Abrupt change of the ground state due to its quantum (spin) fluctuations

$$|\psi\rangle \stackrel{J\to 0}{=} |\rightarrow\rightarrow\rightarrow\cdots\rightarrow\rightarrow\rightarrow\rangle \text{ to } |\psi\rangle \stackrel{B\to 0}{=} \frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\ldots\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\ldots\downarrow\downarrow\downarrow\rangle)$$



Non equilibrium: Sweep (quench)

Fast quantum transition from paramagnetic state to a ferromagnetic order at $J/B \sim 1$

Analog to Kibble-Zurek Mechanism ! ⇒ Domain Formation

From paramagnetic to quantum transition up to first order

Equations for spin and quantum correlations:

$$S_\mu^i = \langle \widehat{S}_\mu^i \rangle \qquad M_{\mu\nu}^{ij} = \langle \delta\widehat{S}_\mu^i \delta\widehat{S}_\nu^j \rangle \qquad i,j = x,y,z$$

Need to solve the system of equations:

$$\begin{aligned}
\partial_t S_\mu^x &= \tfrac{2J}{Z} \textstyle\sum_{\nu\neq\mu} T_{\mu\nu} M_{\mu\nu}^{yz} \\
\partial_t M_{\mu\nu}^{zz} &= -BM_{\mu\nu}^{yz} - BM_{\mu\nu}^{zy} \\
\partial_t M_{\mu\nu}^{yz} &= -BM_{\mu\nu}^{yy} + BM_{\mu\nu}^{zz} - \tfrac{2J}{Z} \textstyle\sum_{\kappa\neq\mu} T_{\kappa\nu} M_{\mu\kappa}^{zz} S_\nu^x - \tfrac{2J}{Z} T_{\mu\nu} \tfrac{1}{4} S_\nu^x \\
\partial_t M_{\mu\nu}^{yy} &= BM_{\mu\nu}^{yz} + BM_{\mu\nu}^{zy} - \tfrac{2J}{Z} \textstyle\sum_{\kappa\neq\nu} T_{\mu\kappa} M_{\nu\kappa}^{yz} S_\mu^x - \tfrac{2J}{Z} \textstyle\sum_{\kappa\neq\mu} T_{\kappa\nu} M_{\mu\kappa}^{yz} S_\nu^x
\end{aligned}$$

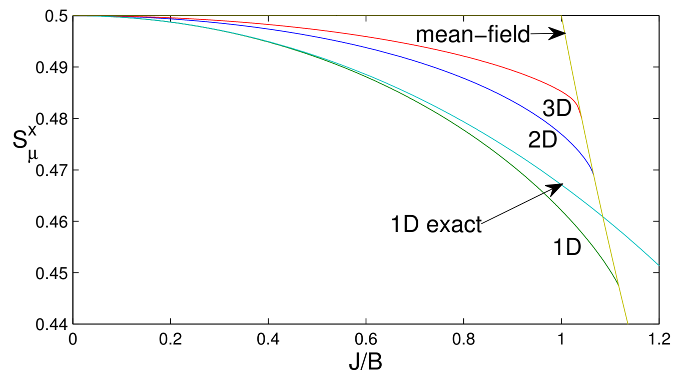
Ground state at transition:

- adiabatic switching $J(t) = J_c \exp(\epsilon t) \qquad t \in]-\infty, 0]$ and $\epsilon \to 0$
- initial condition: $S_\mu^x = \frac{1}{2}$, $M_{\mu\nu}^{ij} = 0$

Ground state calculation: order $1/Z$

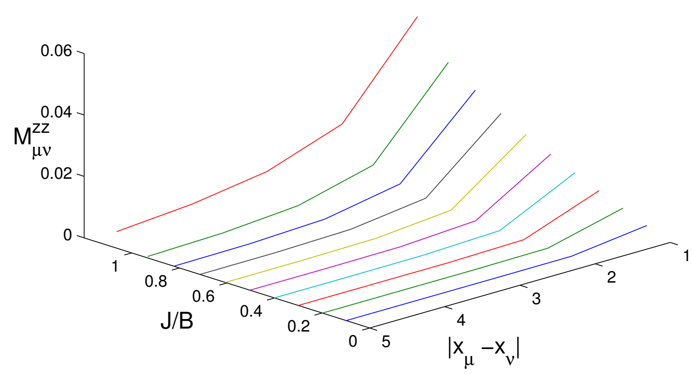
Adiabatic switching techniques: paramagnetic spin component

test of convergence for 1D:



For $D = 2$, critical value $(J/B)_c = 1.075$ approaches QMC result $(J/B)_c = 1.314$

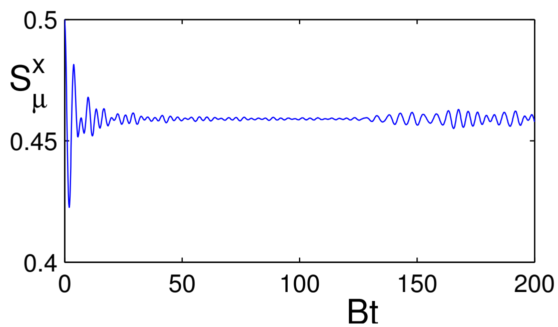
Quantum fluctuations $M_{\mu\nu}^{zz}$ in 2D becomes long range

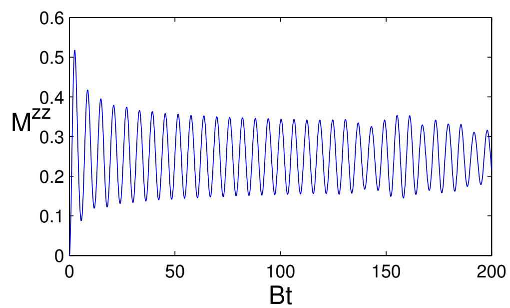


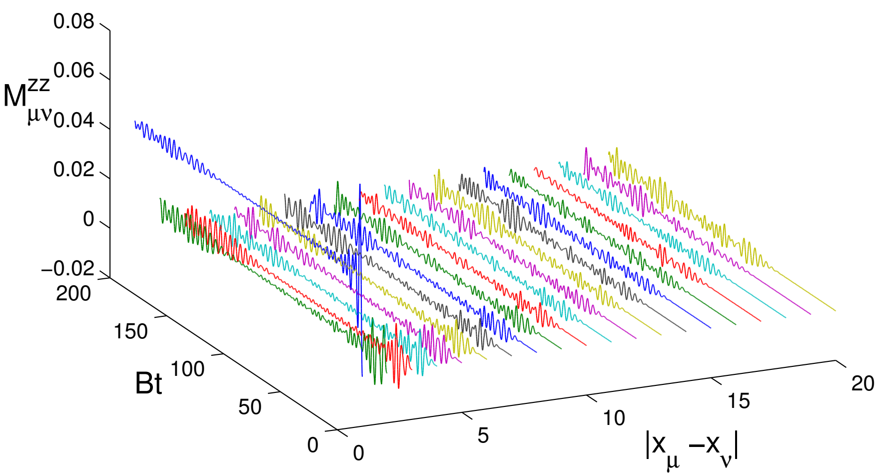
Quench in the paramagnetic regime

Sudden quench: $0 \to J/B = 0.8$ in 2D for 40×40 sites

Low oscillating total correlation: $M^{zz} = \sum_{\mu \neq \nu} M^{zz}_{\mu\nu} = \sum_{\mu \neq \nu} \langle \delta \widehat{S}^z_\mu \delta \widehat{S}^z_\nu \rangle$







Excitation production in pair!

group velocity: $c = 2\text{Max}\dfrac{\partial \omega_{\mathbf{k}}}{\partial k_x}$

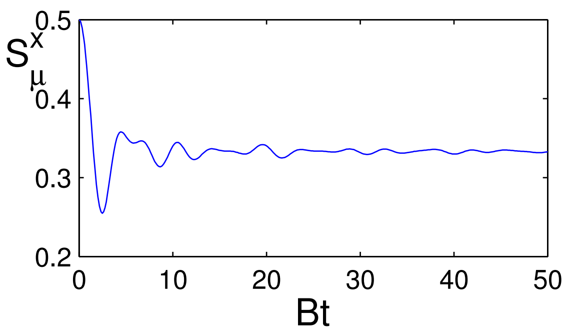
$$\omega_{\mathbf{k}} = \sqrt{B^2 - BJT_{\mathbf{k}}}$$

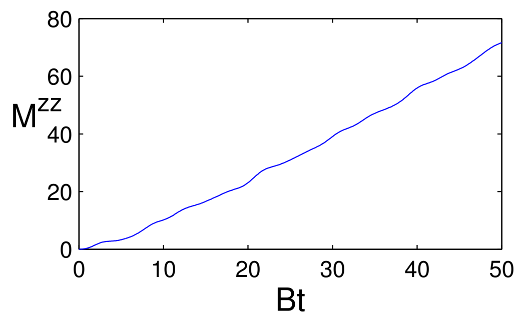
Wave pulse-like propagation of quantum correlations! $\to$ **Test of "quantumness"**

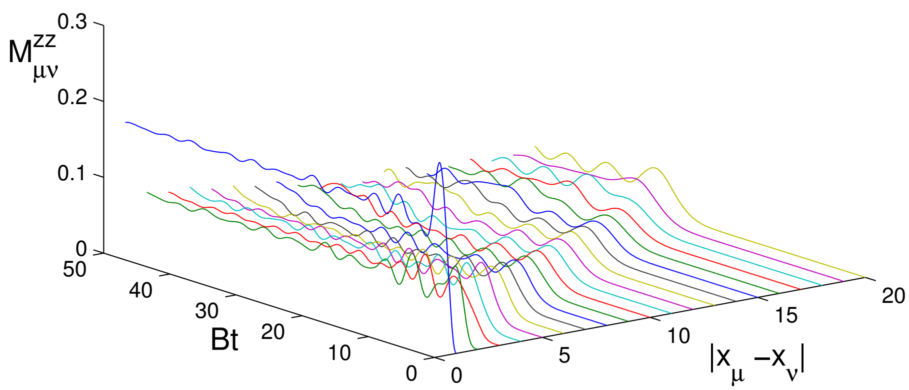
Quench in the Ferromagnetic regime

Growing total correlation: $M^{zz} = \sum_{\mu\neq\nu} M^{zz}_{\mu\nu} = \sum_{\mu\neq\nu} \langle \delta\widehat{S}^z_\mu \delta\widehat{S}^z_\nu \rangle$

Sudden quench: $0 \to J/B = 1.5$ in 2D for 40×40 sites







Interdistance quantum correlations generation → growing domains

Conclusions and Perspectives

General method applicable for any quantum lattice system:

$1/Z$ EXPANSION: hierarchy in multipartite correlations (entanglement)

- Lowest order Z^0: Phase transition, Excitation spectrum, On-site correlations
- Higher order Z^{-n}: Off-site correlations e.g. $\langle \delta \widehat{S}^z_{\mu_1} \ldots \delta \widehat{S}^z_{\mu_n} \rangle \to$ computer size $\sim L^{n-1}$
- Non equilibrium: Quench, Sauter-Schwinger effect, ...
- Equilibrium: Ring diagram resummation
- Synthetic: includes Bogoliubov, Holstein-Primakov and Hubbard approximations
- Comprehensive: allows analytics as well as numerics

PERSPECTIVES:

- Still need to collect more evidences: equilibrium, equilibration, ...
- Quantum Ising model, quantum metamaterials,
  ... and why not high T_c superconductors, lattice QCD