# Numerical approaches to dissipative quantum phase transitions

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*“Many-body physics with light – denselight15”*

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# Framework

Focus on **strong local correlations** in quantum many-body systems

( quantum phase transitions, quantum magnetism, high-Tc superconductivity, … )

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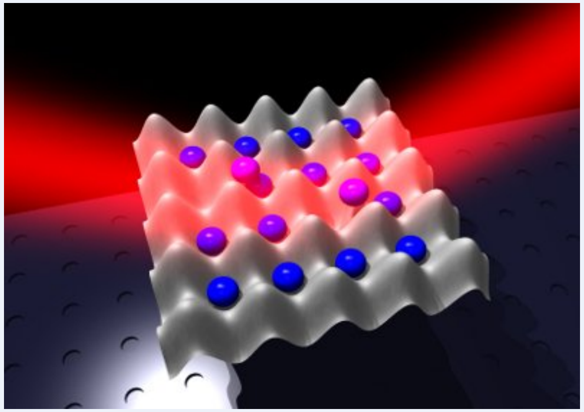
( quantum phase transitions, quantum magnetism, high-Tc superconductivity, … )

## Quantum simulators

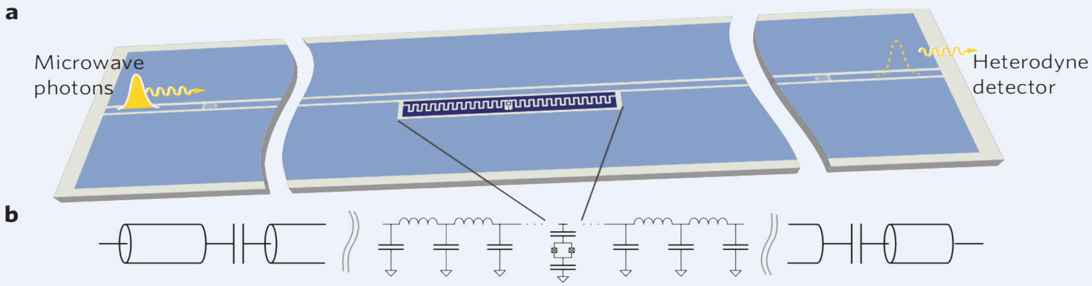
Feynman, *Int. J. Theor. Phys.* **21**, 467 (1982)
*Nature Physics Insight*, Vol. **8**, No. 4 (2012)



- Josephson junctions arrays
- Optically confined atoms/molecules
- Ion traps
- Nanopatterned semiconductors
- …

→ novel platforms recently devised

Tureci, Wallraff …



# Outline of the talk

## $Z_2$–symmetry breaking dissipative phase transitions

- ✔ Quantitative numerical study for a system of interacting spin-1/2 particles on a *lattice*
- ✔ Beyond mean-field predictions
- ✔ Scaling of correlation functions
- ✔ Role of dimensionality

# *Numerical* strategies

***Established methods:***

– Mean-field → crude treatment of interactions

– Cluster mean-field

See *e.g.* Tomadin *et al.*, *Phys. Rev. A* **81**, 061801(R) (2010)

– Quantum trajectories → severely limited to small sizes (L ~ 10)

See Daley, *Adv. Phys.* **63**, 77 (2014)

– DMRG-based simulations → basically work only in 1D

See Verstraete *et al.* *PRL* **93**, 207204 (2004); Zwolak & Vidal, *PRL* **93**, 207205 (2004)

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***Novel approaches:***

– Mean-field + quantum trajectories

– Perturbative expansions, linked clusters, …

– Tensor networks (refined MPOs, PEPO, …)

– …

*Hartmann, Koch, Ciuti, Bañuls, Eisert, Keeling, Savona, Weimer, …*

# A spin-system toy model:

We consider a spin-1/2 XYZ anisotropic Heisenberg model

$$\mathcal{H} = \sum_{\langle i,j \rangle} \left( J_x \sigma_i^x \sigma_j^x + J_y \sigma_i^y \sigma_j^y + J_z \sigma_i^z \sigma_j^z \right)$$

in the presence of incoherent dissipative spin-flips (*z axis*)

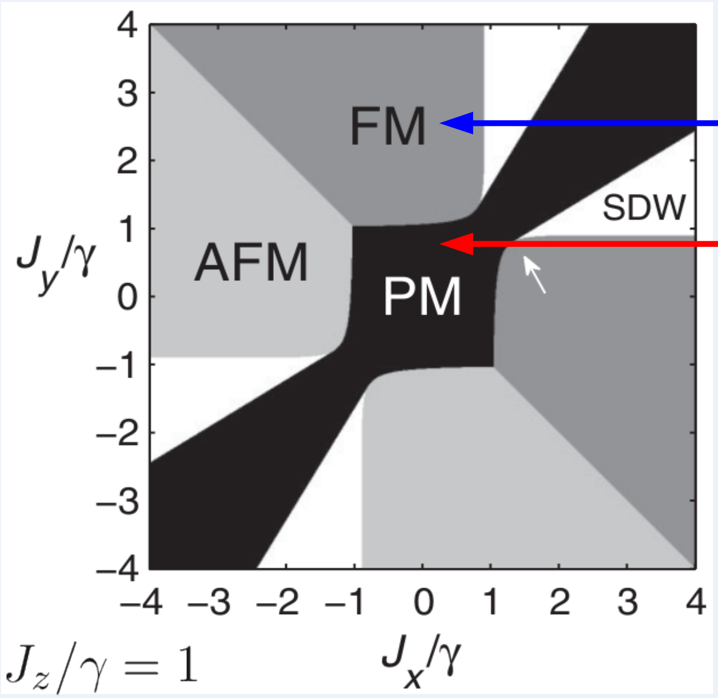
$$\partial_t \rho = -i[\mathcal{H}, \rho] + \gamma \sum_i \left( \sigma_i^- \rho \sigma_i^+ - \frac{1}{2}\{\sigma_i^+ \sigma_i^-, \rho\} \right)$$

- *x-y* Hamiltonian anisotropy generates a **competition** between coherent dynamics & dissipative effects
- experimentally implementable with trapped ions
- mean-field study performed in
  T.E. Lee, S. Gopalakrishnan, M.D. Lukin, *Phys. Rev. Lett.* **110**, 257204 (2013)

The master equation has a $\mathbb{Z}_2$ symmetry $\sigma_j^x, \sigma_j^y \to -\sigma_j^x, -\sigma_j^y$

which may **spontaneously break** in *ordered phases*

(*e.g.*: the paramagnetic / ferromagnetic transition in the *Ising model*)




**Mean-field phase diagram**

T.E. Lee, S. Gopalakrishnan, M.D. Lukin, *Phys. Rev. Lett.* **110**, 257204 (2013)

We study the paramagnet (PM) / ferromagnet (FM)

**steady-state phase transition**

**Q.** What happens *beyond mean-field* ?

– infinite MPO
– cluster mean-field
– mean-field + quantum trajectories

# One-dimensional geometry

- Due to extremely reduced dimensionality, mean field should **fail**
- Reminiscence of features predicted by mean field
- Presumably no phase transition

Lee, Gopalakrishnan, Lukin (2013)

→ We target the steady state using

- Runge-Kutta (RK) integration of small clusters ($L \leq 10$)
- Quantum trajectories (QT) up to slightly larger sizes ($L \leq 16$)
- Infinite-MPO (i-MPO) for the thermodynamic limit

→ finite-size scaling (RK, QT)

# A few words on the methods …

# Stochastic unraveling of the master equation

$$\partial_t \rho = \boxed{-i[\mathcal{H},\rho] - \frac{1}{2}\gamma \sum_j \{\sigma_j^+ \sigma_j^-, \rho\}} + \boxed{\gamma \sum_j \sigma_j^- \rho \sigma_j^+}$$

effective non-hermitian Hamitonian

quantum jumps

$$\mathcal{H}_{\text{eff}} = \mathcal{H} - \frac{i}{2}\gamma \sum_j \sigma_j^+ \sigma_j^- \qquad \mathrm{d}p_j = \langle \phi(t_0)| \, \sigma_j^+ \sigma_j^- \, |\phi(t_0)\rangle$$

$$\rho(t_0) = |\phi(t_0)\rangle \langle \phi(t_0)|$$

$t_0 \rightarrow t_0 + \delta t$

time evolution $\delta t$

collapse to

$$\rho(t_0 + \delta t) = \Big(1 - \sum_j \mathrm{d}p_j\Big) |\phi_0\rangle \langle \phi_0| + \sum_j \mathrm{d}p_j \, |\phi_j\rangle \langle \phi_j| \longrightarrow |\phi_j\rangle \quad j = 0, 1, 2, \ldots$$

$$|\phi_0\rangle = \frac{e^{-i\mathcal{H}_{\text{eff}}\delta t} \, |\phi(t_0)\rangle}{\sqrt{1 - \sum_j \mathrm{d}p_j}} \qquad |\phi_j\rangle = \frac{\sigma_j^- \, |\phi(t_0)\rangle}{\| \sigma_j^- \, |\phi(t_0)\rangle \, \|}$$

J. Dalibard, Y. Castin, K. Mølmer, *Phys. Rev. Lett.* **68**, 580 (1992)

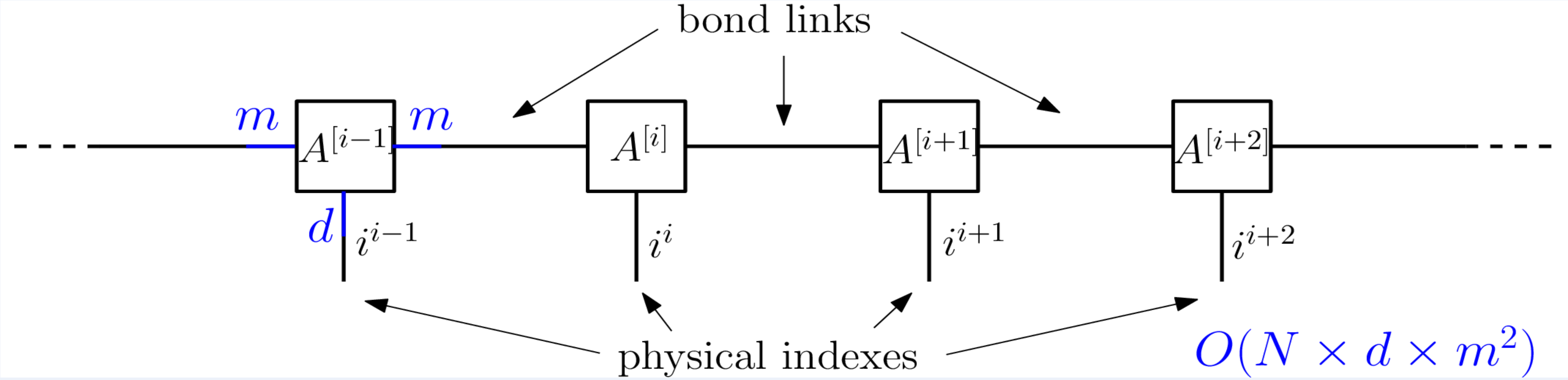
# DMRG-based approach

Digression on the non-dissipative framework:

DMRG ⟷ variational approach on Matrix Product States (MPS)

$$|\psi\rangle = \sum_{i_1, i_2, \cdots, i_N} \mathrm{Tr}\left(A^{[1]i_1} \cdot A^{[2]i_2} \cdot \ldots \cdot A^{[N]i_N}\right) |i_1, i_2, \ldots, i_N\rangle$$

area-law entanglement



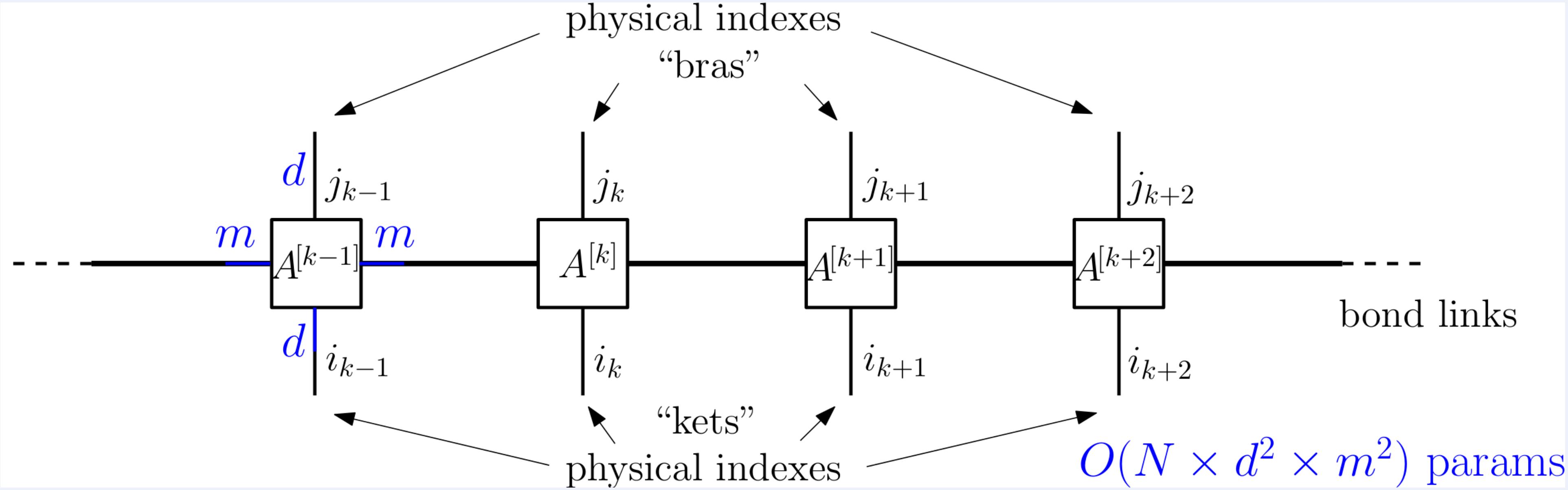

J.I. Cirac and F. Verstraete, *J. Phys. A* **42**, 504004 (2009)
F. Verstraete, J.I. Cirac, and V. Murg, *Adv. Phys.* **57**, 143 (2008)
U. Schollwoeck, *Ann. Phys.* **326**, 96 (2011)

## DMRG-based approach

With dissipation one should target the zero eigenmode of the Liouvillian (tricky!!)

→ We just employ the TEBD method on a Matrix Product Operator (MPO)

$$\rho = \sum_{i_1,\cdots,i_N} \sum_{j_1,\cdots,j_N} \mathrm{Tr}\left(A^{[1]i_1,j_1} \cdot \ldots \cdot A^{[N]i_N,j_N}\right) |i_1,\ldots,i_N\rangle \langle j_1,\ldots,j_N|$$




F. Verstraete, J.J. García Ripoll, J.I. Cirac, *Phys. Rev. Lett.* **93**, 207204 (2004)

M. Zwolak and G. Vidal, *Phys. Rev. Lett.* **93**, 207205 (2004)

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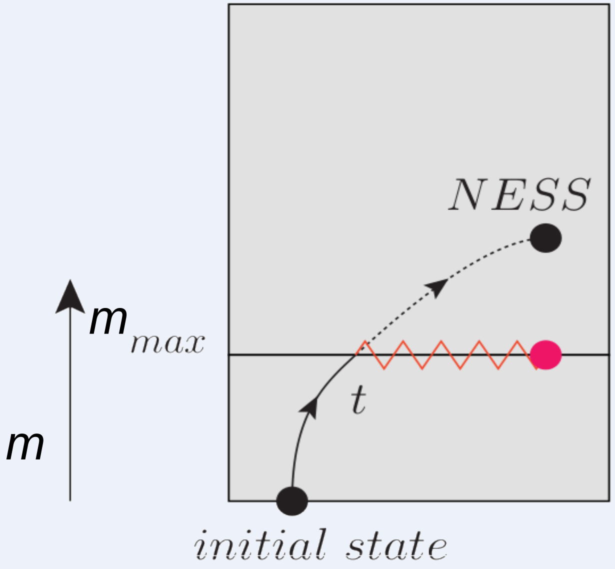
$$\rho(t) = e^{\mathcal{L}t}\rho(0)$$ trotterize the evolution super-operator, …

A subtle problem:
*uncontrolled* bond-link growth
in approaching the steady state

Q. Area-law violation ?



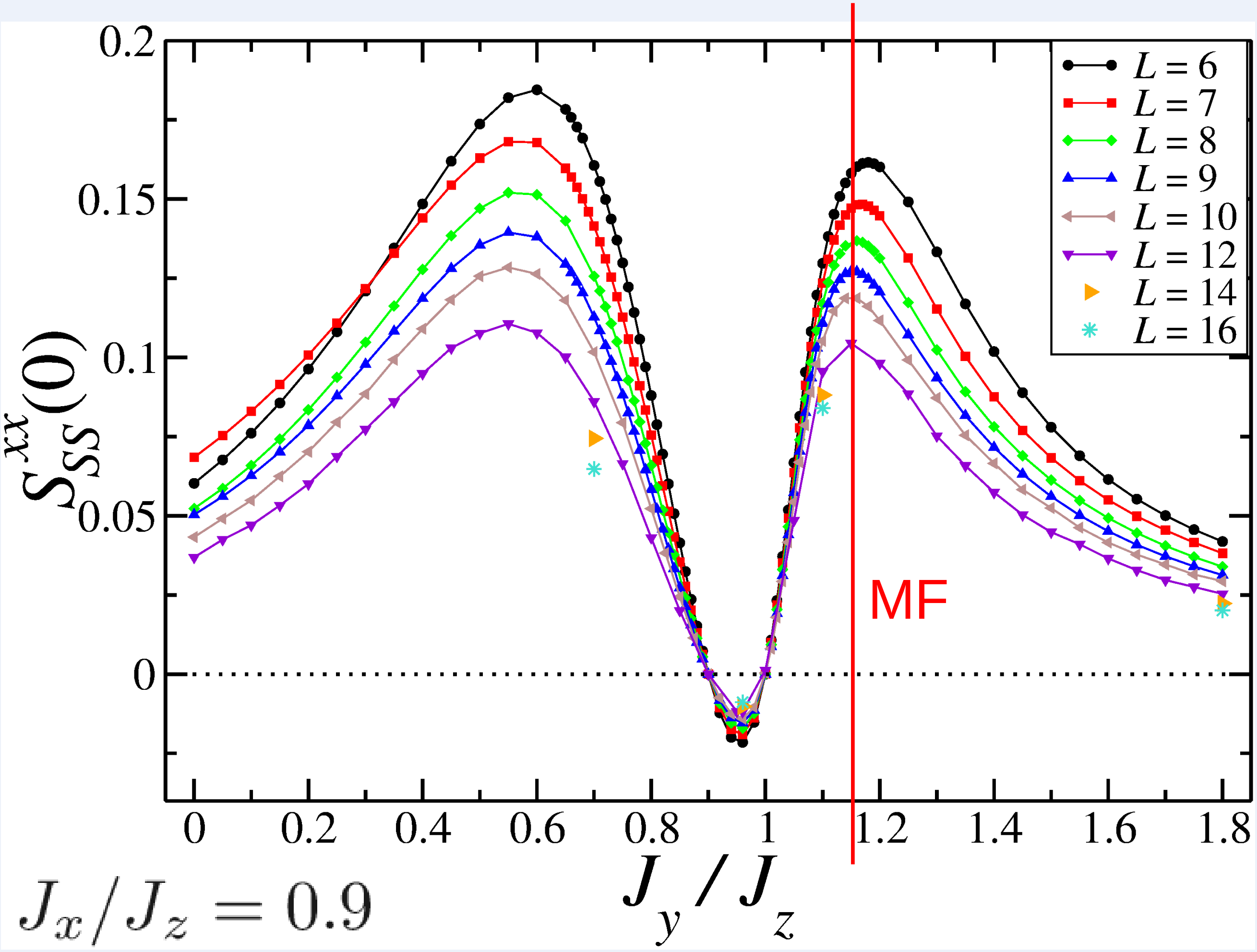
# Results

# One-dimensional geometry

Spin ordering signaled
by the **structure factor**

($k$ = 0 ↔ FM  $k$ = π ↔ AFM)

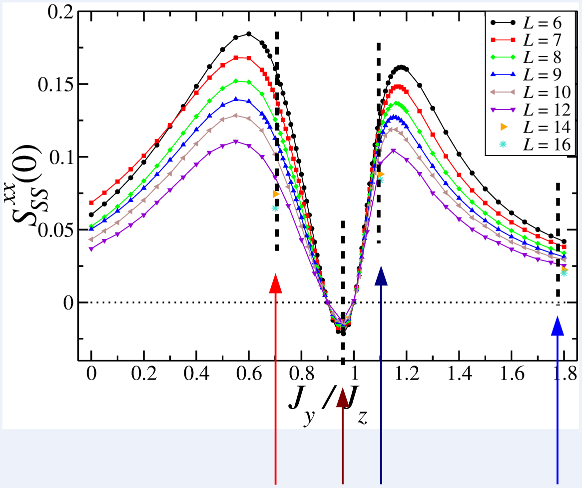
$$S^{xx}_{\rm SS}(k) = \frac{1}{L^2}\sum_{j,l} e^{-ik(j-l)}\langle\sigma^x_j\sigma^x_l\rangle_{\rm SS}$$

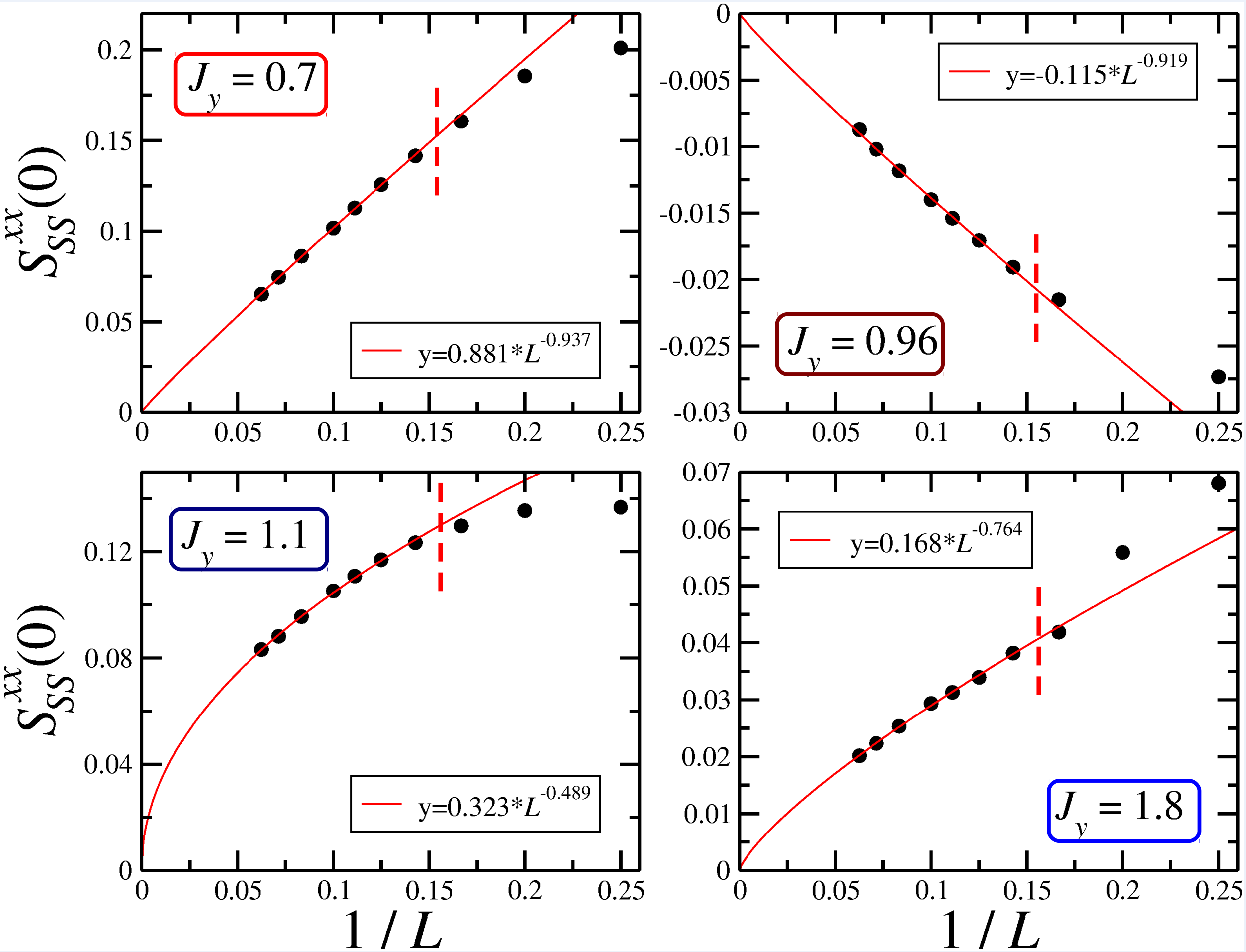



Mean field prediction:
*PM–to–FM transition*

$$\frac{J^c_y}{J_z} = \frac{37}{12} \approx 1.156$$

# One-dimensional geometry




**Finite-size scaling**

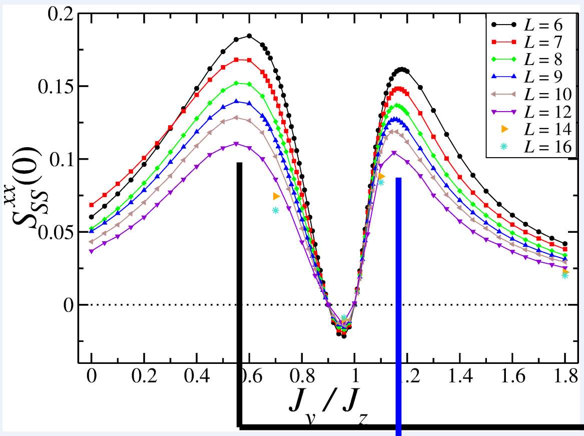
of numerical data along the four cuts

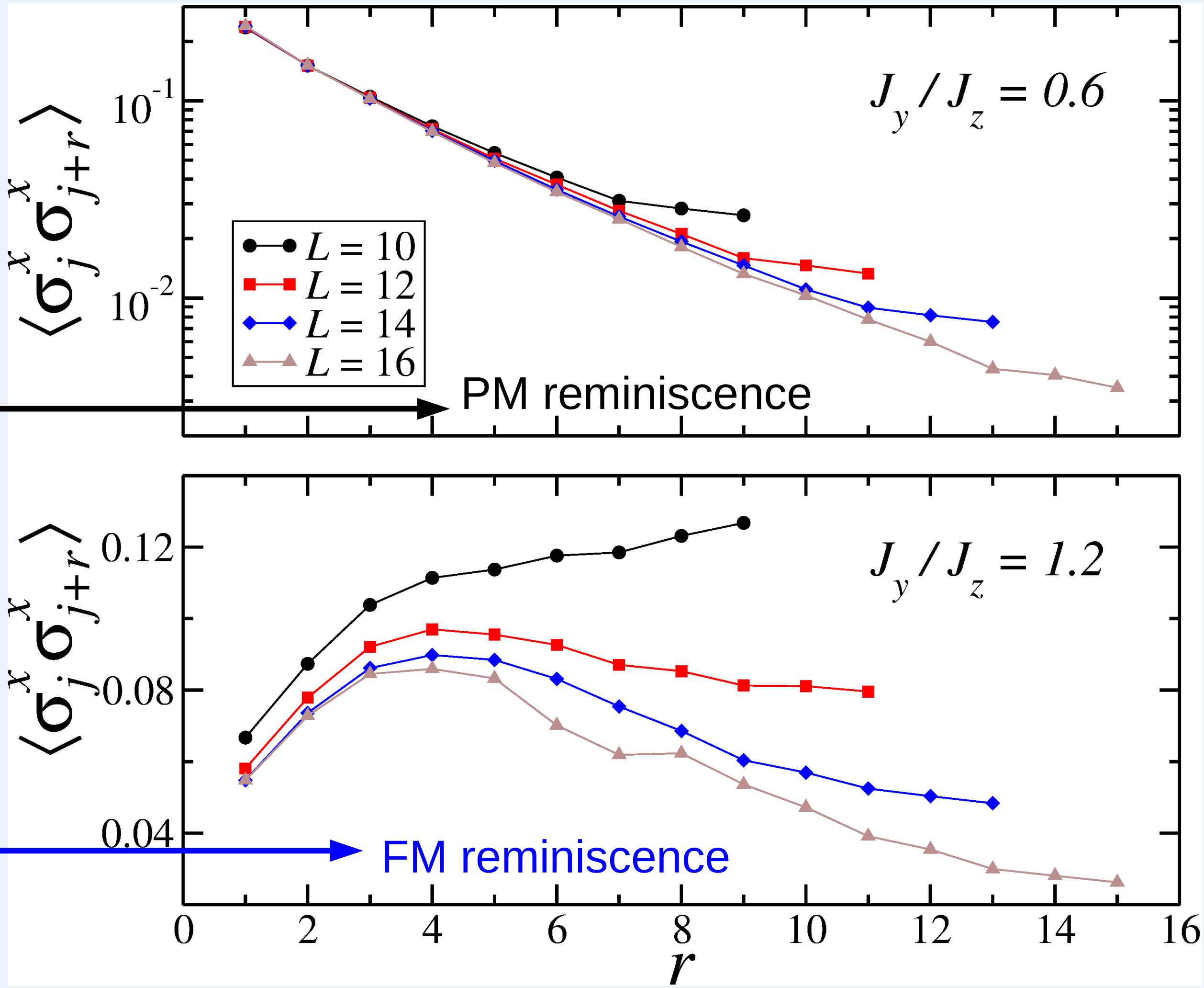
→ power-law decay

$$S^{xx}_{\rm SS}(0) \sim \kappa L^{-\gamma}$$

the exponent decreases when approaching the MF critical point $J^c_y \approx 1.156$

# One-dimensional geometry



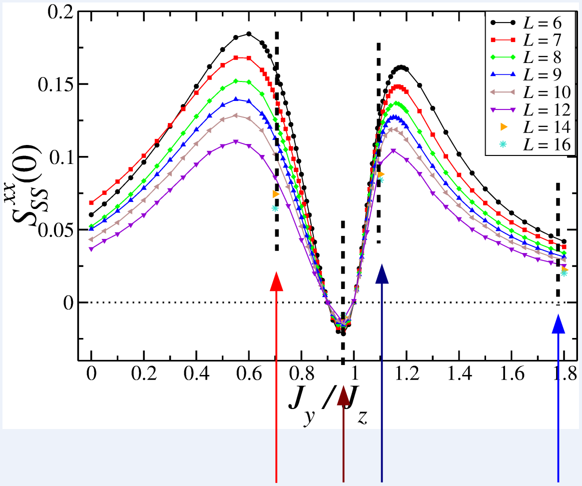




*xx* correlators:

$J_y < J_y^c$
exponential decay

$J_y > J_y^c$
not clear

# One-dimensional geometry

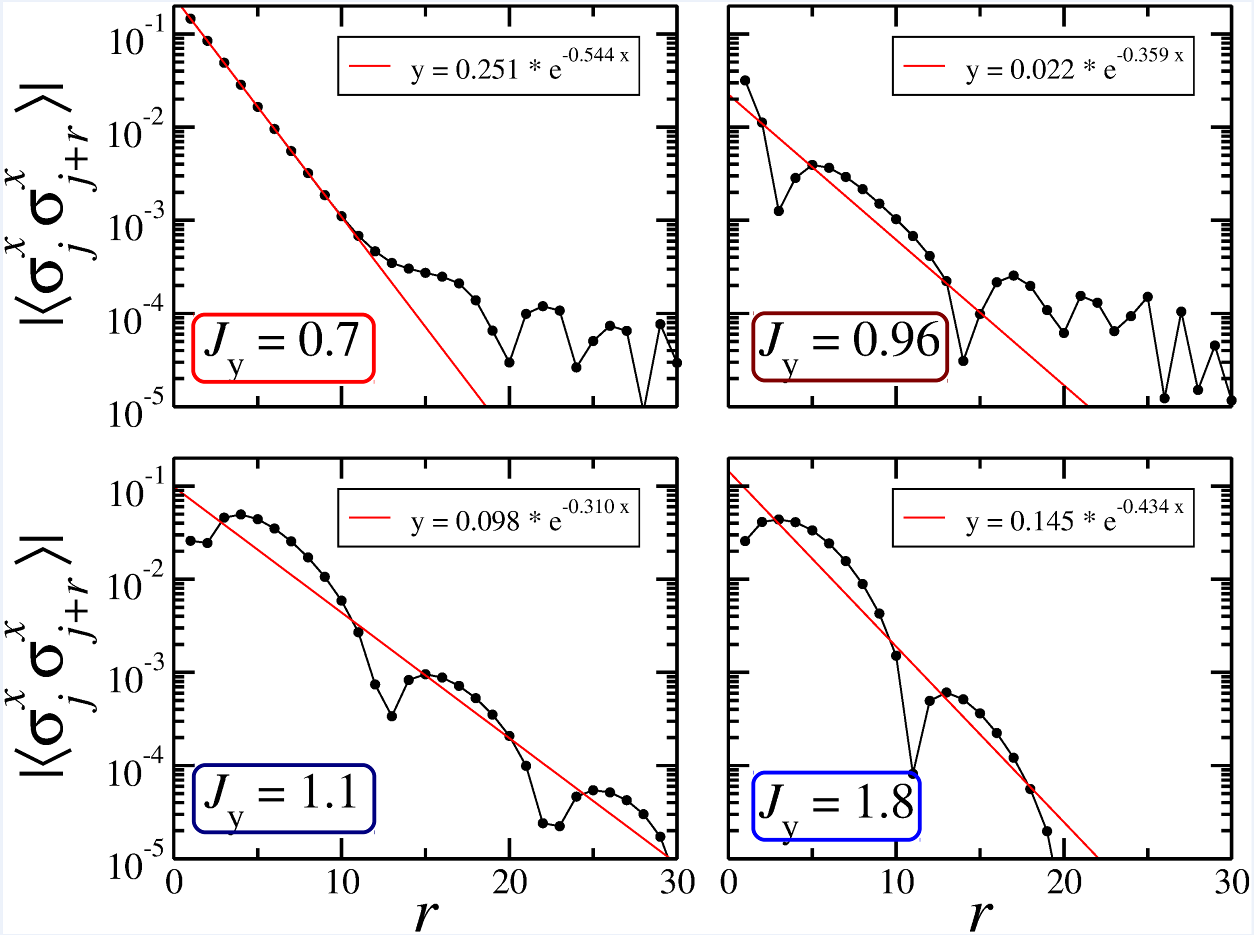



infinite-MPO

↓

thermodynamic limit

always a clear exponential decay



# Two-dimensional geometry

- What is the fate of mean field?
- Presumably **there is** a symmetry-broken phase

→ We target the steady state using the **cluster mean-field**

- standard cluster-mean field (CMF) approach (L ≤ 3x3)
- quantum trajectories + cluster mean-field (L ≤ 4x4)

finite-size scaling ?

# A few words on the methods again …

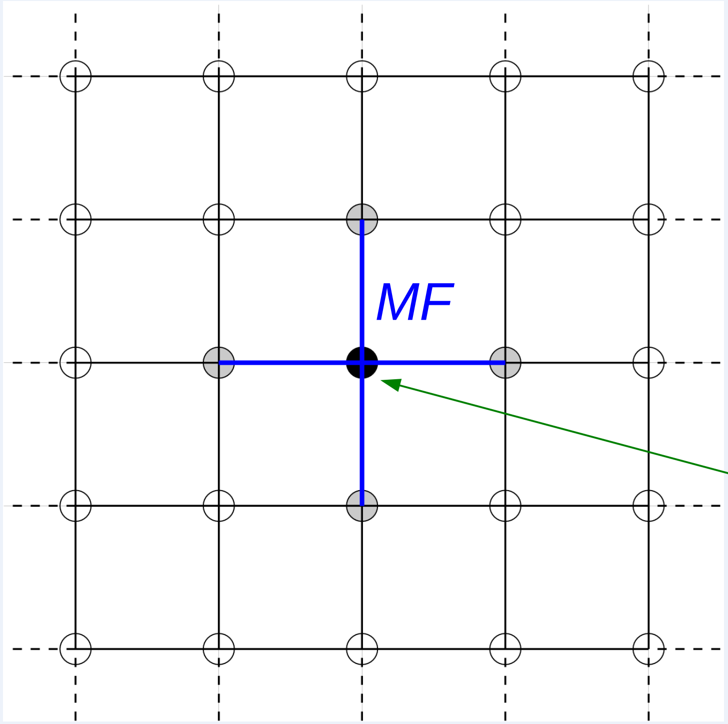
## Single-site mean-field

$$z^{-1}\sum_{\langle i,j\rangle}\sigma_i^\alpha\sigma_j^\alpha \longrightarrow \boxed{\langle\sigma^\alpha\rangle}\sum_j \sigma_j^\alpha$$

($z$: coordination number)

mean field

One completely **decouples** the lattice sites in a minimal structure:




$$\rho_{\mathrm{MF}}(t) = \prod_{j=1}^{L}\rho_j$$

$$\partial_t\rho_j = -i[\mathcal{H}_j,\rho_j] + \mathcal{L}_j[\rho_j]$$

$$\mathcal{H}_j = z\left[J_x\langle\sigma^x\rangle\sigma_j^x + \langle\sigma^y\rangle\sigma_j^y + \langle\sigma^z\rangle\sigma_j^z\right]$$

$$\text{with}\quad \langle\sigma^\alpha\rangle = \mathrm{Tr}(\sigma^\alpha\rho_j)$$

→ *single-site* problem!

## Single-site mean-field

$$\partial_t \rho_j = -i[\mathcal{H}_j, \rho_j] + \mathcal{L}_j[\rho_j]$$

(note that *j* is irrelevant here)

The mean-field values $\langle\sigma^\alpha\rangle$ are determined self-consistently by

$$\langle\sigma^\alpha\rangle = \mathrm{Tr}\left[\sigma^\alpha \rho_j(t)\right] \quad \star$$

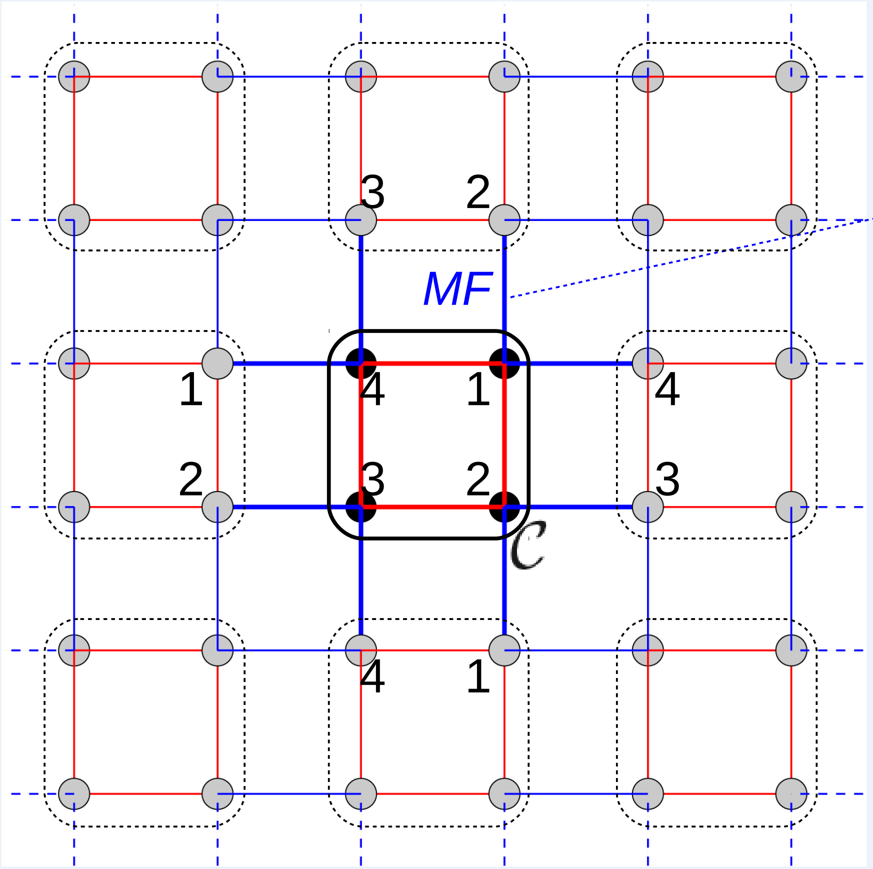
- Integrate the single-site differential equation for a small time step
- At time intervals δ*t*, enforce the self-consistence condition ★
- Steady-state solution: *long-time limit* starting from a generic initial state…

# Refining the mean-field: <u>cluster mean-field</u>

$$\mathcal{H}_{\rm CMF} = \mathcal{H}_{\mathcal{C}} + \mathcal{H}_{\mathcal{C}-\mathcal{C}'}$$

exact Hamiltonian of a cluster

interactions between neighbor clusters (mean field)




for example this link gives a term $\langle\sigma_2^\alpha\rangle\sigma_1^\alpha$ in the Hamiltonian for *C*–*C′* interactions

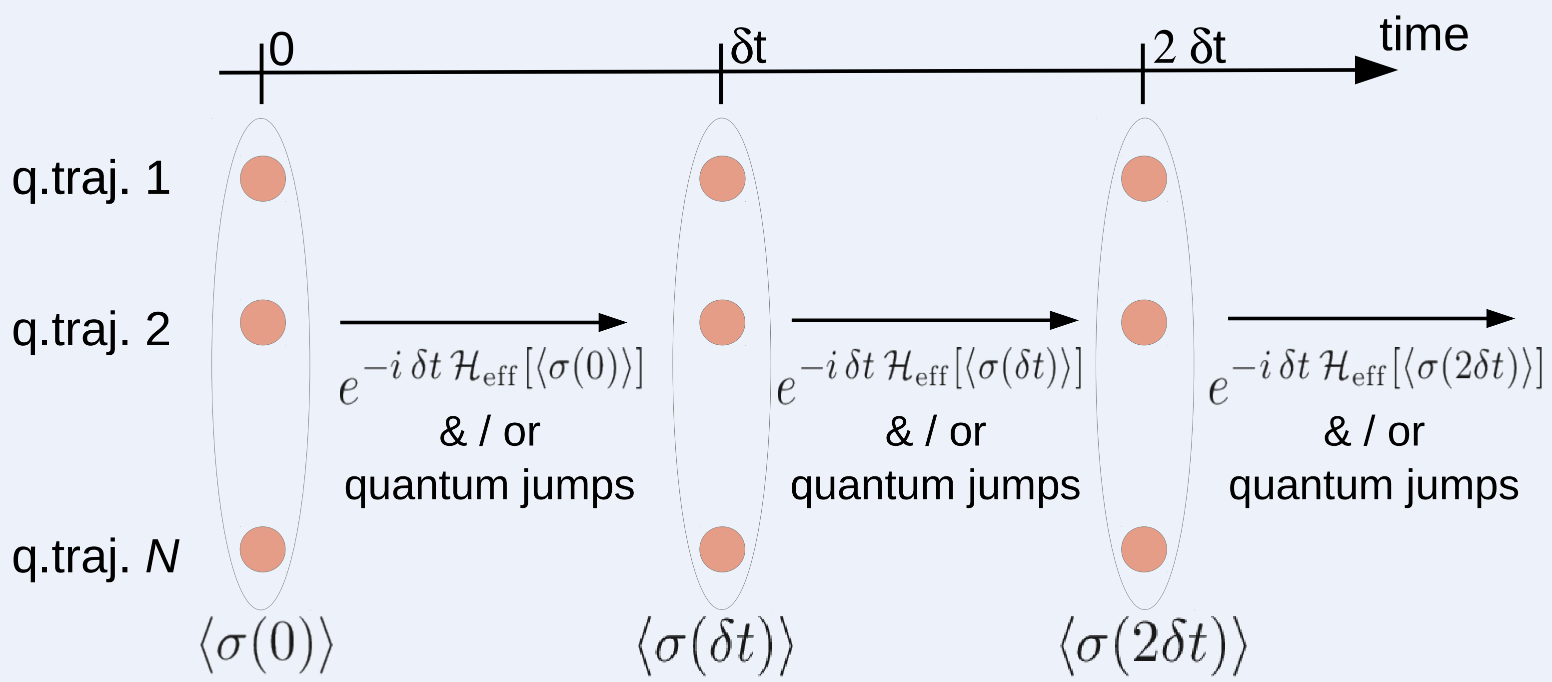
One **decouples** the whole lattice into a cluster structure:

$$\rho_{\rm CMF}(t) = \prod_{\mathcal{C}} \rho_{\mathcal{C}}$$

# Stochastic unraveling of the master equation
# + mean-field coupling to adjacent clusters

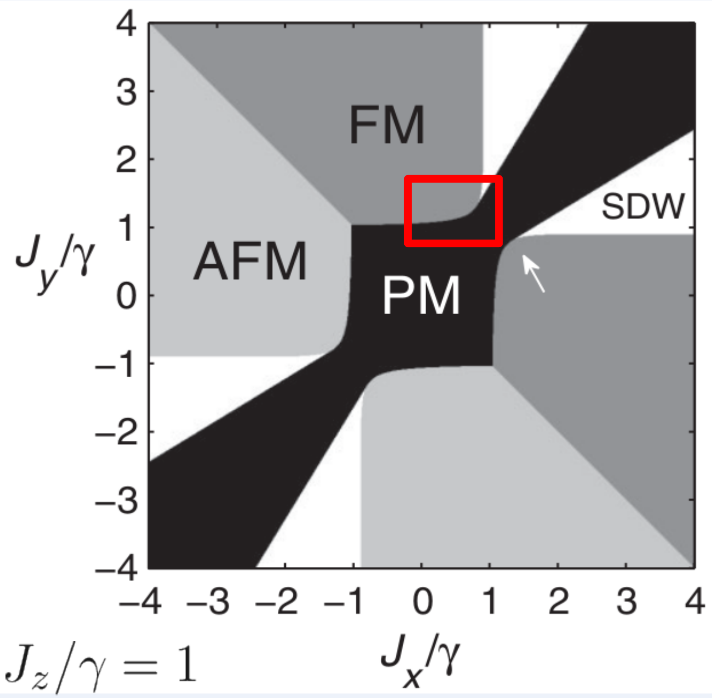
$$\mathcal{H}_{\text{eff}}[\langle\sigma(t)\rangle] = \mathcal{H}_{\text{CMF}}[\langle\sigma(t)\rangle] - \frac{i}{2}\gamma\sum_j \sigma_j^+\sigma_j^-$$

$$\mathcal{H}_{\text{CMF}}[\langle\sigma(t)\rangle] = \mathcal{H}_C + \mathcal{H}_{C-C'}[\langle\sigma(t)\rangle]$$



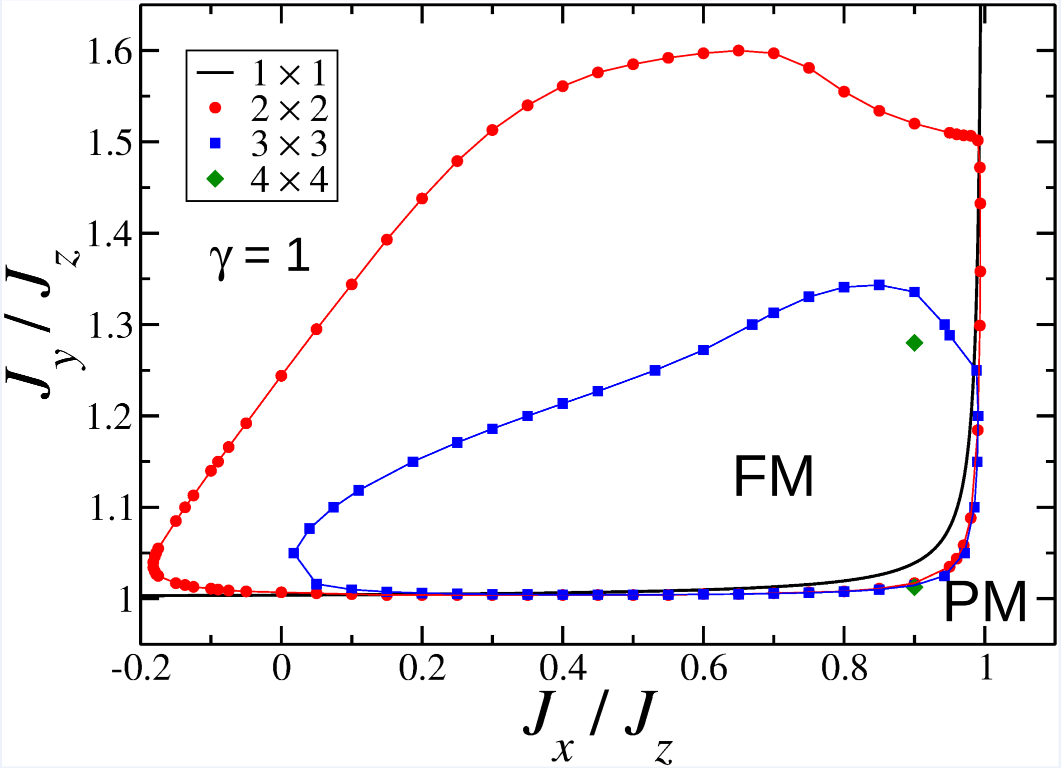
# Results

# Two-dimensional geometry




**Mean-field phase diagram**

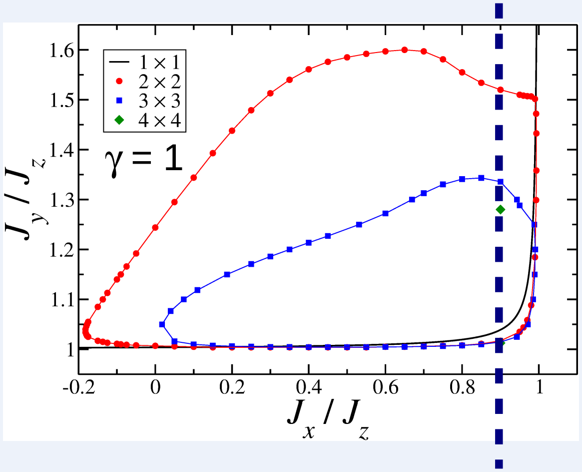
!




**Cluster mean-field on a 2D square lattice**

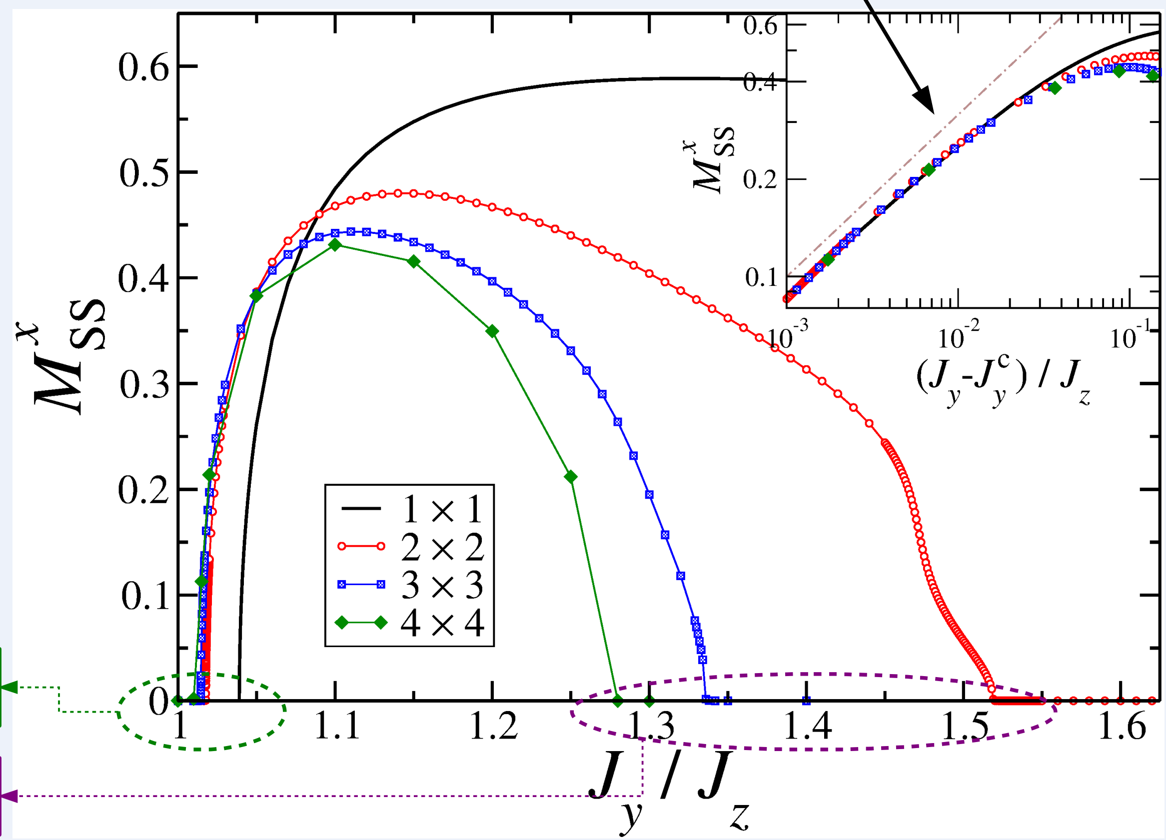
- We analyze a square-lattice geometry
- Up to *4x4 clusters*, the symmetry-broken phase (FM) <u>survives</u>
- Its extension <u>drastically reduced</u>: significant deviations from mean field

# Two-dimensional geometry




$$M^x_{\mathrm{SS}} = \frac{1}{\ell^2}\sum_{j=1}^{\ell^2}\langle\sigma^x_j\rangle_{\mathrm{SS}}$$

$$M^x_{\mathrm{SS}} \sim m\sqrt{\frac{J_y - J_y^c}{J_y^c}}$$

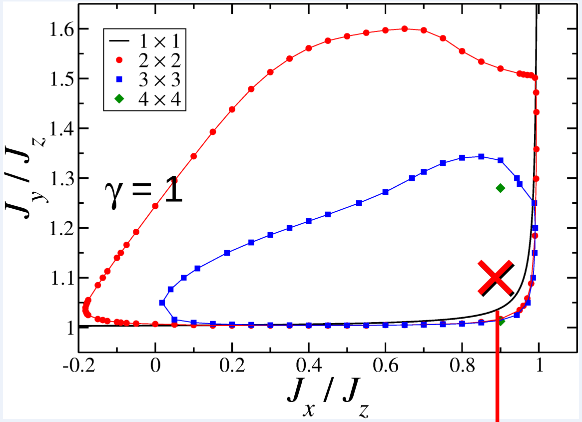



$$J_y^{c,1} \approx 1.010 + 0.030\,\ell^{-1}$$

$$J_y^{c,2} \approx 1.194 + 1.341\,\ell^{-1}$$

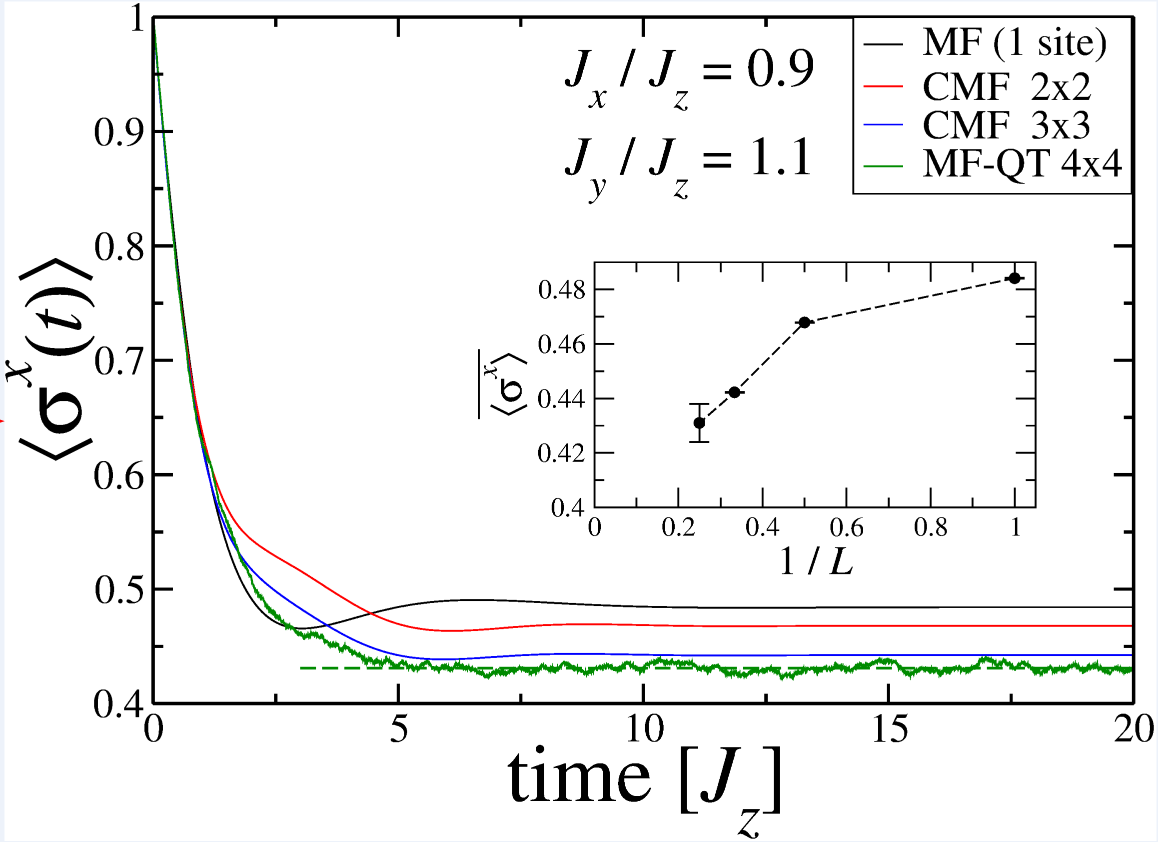
A rough finite-size scaling confirms the stabilization of a FM phase

# Two-dimensional geometry

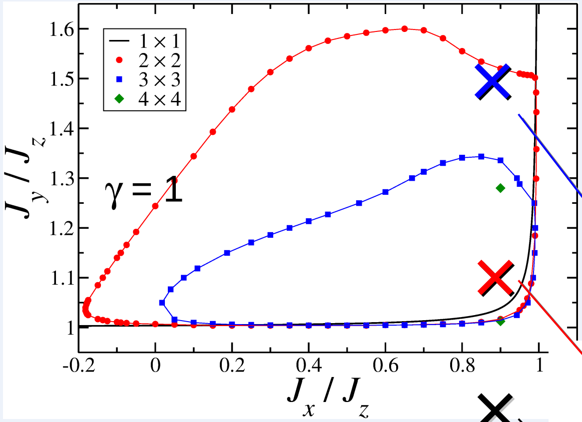



Robust indication of a finite magnetization

(no need to evaluate correlators with mean field: The system spontaneously breaks the symmetry)

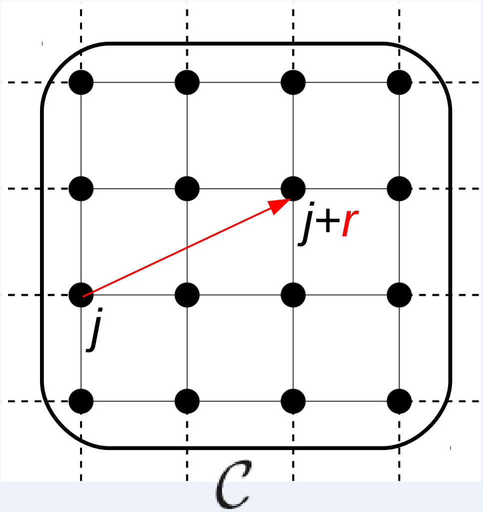


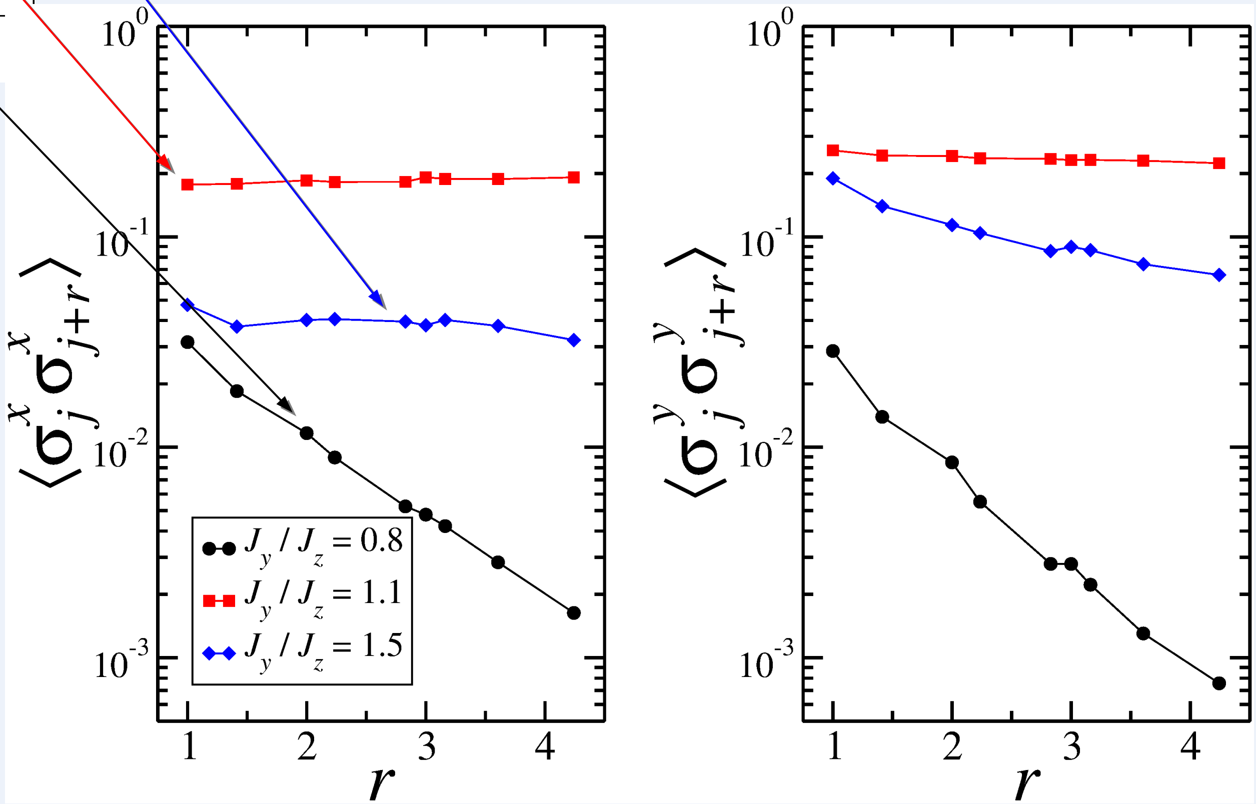
# Two-dimensional geometry



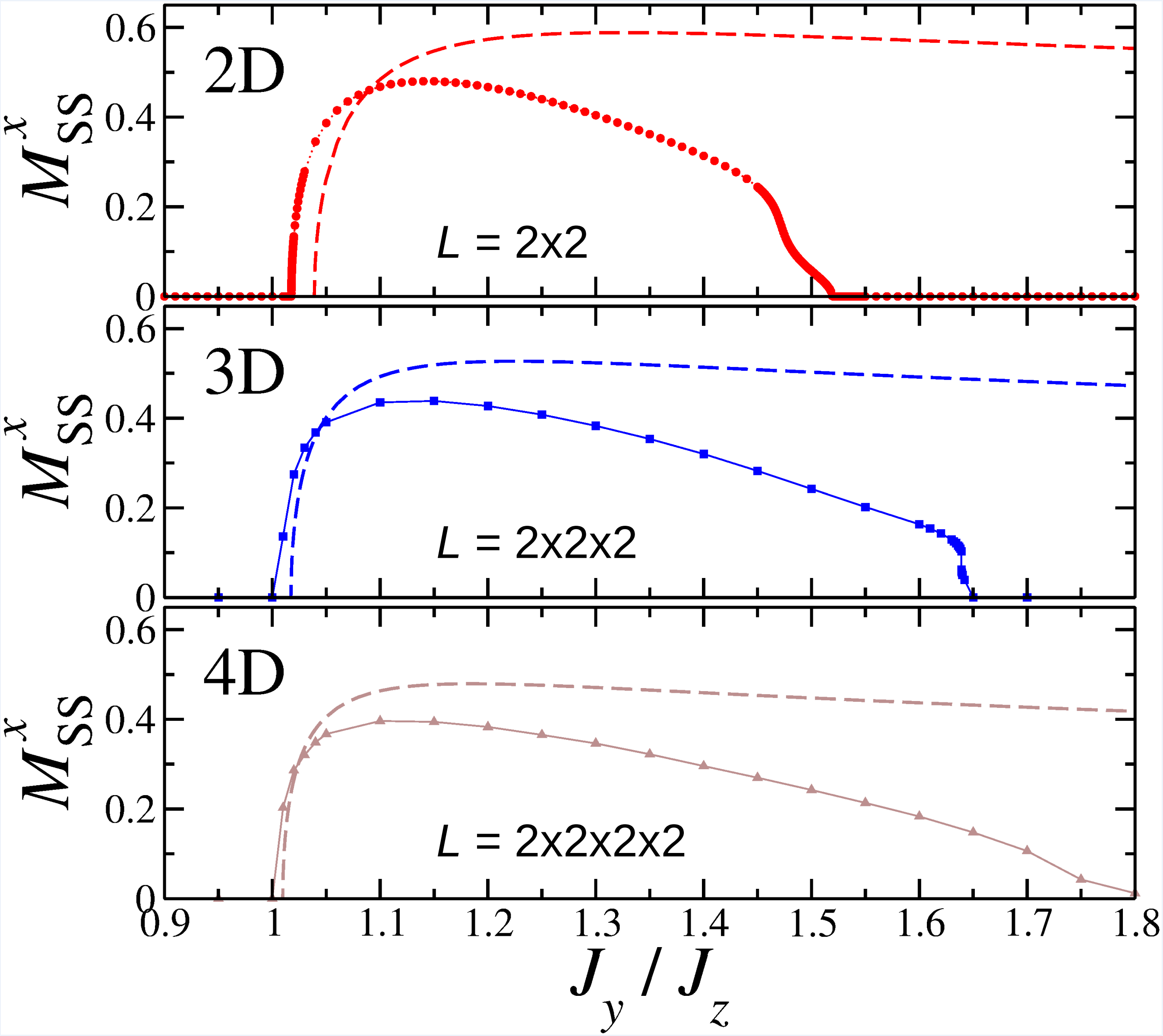

FM phase corroborated by the correlation functions:

→ PM phase: exponential decay
→ FM phase: saturation
→ crossover region: unclear at small size



# Higher dimensionalities




**cluster mean-field**

MF results approached if the dimensionality is increased

BUT a **finite** extension of the FM phase is predicted even in 4D

Upper critical dimension > 4 ???

# Numerical linked-cluster method ?

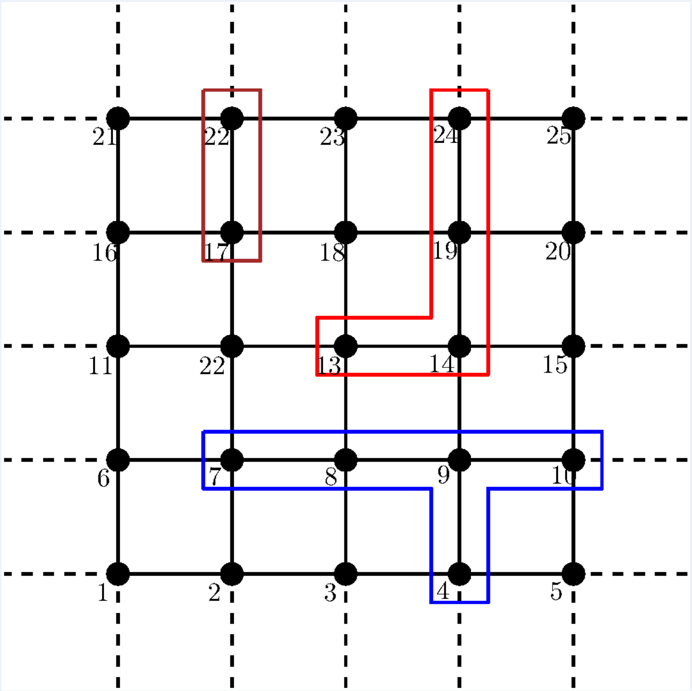
Lattice constant

counts # of "embeddings"

$$P/L = \sum_{\mathcal{G}} l(\mathcal{G}) W_{[P]}(\mathcal{G}) \, .$$

Cluster weight

$$W_{[P]}(\mathcal{C}) = P_{\mathcal{C}} - \sum_{\mathcal{S} \subset \mathcal{C}} W_{[P]}(\mathcal{S})$$




→ disconnected clusters have vanishing weight

→ if expansion is up to order R,
then only clusters at most of size R shall be considered

Results directly at the *thermodynamic limit*

→ finite-size scaling substituted by **series extrapolation**

M. Rigol, T. Bryant, R. Singh, *Phys. Rev. Lett.* **97**, 187202 (2006)

M. Rigol, *Phys. Rev. Lett.* **112**, 170601 (2014)

# Summary

Non-equilibrium phase transitions
of quantum dissipative many-body systems

A $\mathbb{Z}_2$ symmetry breaking (Ising-like) phase transition

***mean-field*** results reveal their ***fragility*** to a more accurate analysis

- 1D: ***no*** *symmetry-broken phase*
- 2D: the ordered phase *drastically shrinks*
- 3D – 4D: mean-field predictions approached

*XYZ* Heisenberg
+
incoherent spin-flips

– Matrix product operators (MPO)
– Cluster mean-field (CMF)
– Cluster mean-field with quantum trajectories (CMF+QT)
– Numerical linked cluster expansions (NLCE) → perspective

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