Wormhole quantum Monte Carlo for quantum dissipative spin systems

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Workshop on the sign problem in QCD and beyond

January 21, 2025

TECHNISCHE UNIVERSITÄT DRESDEN

ct.qmat Complexity and Topology in Quantum Matter

Outline

(1) Introduction

(2) Wormhole quantum Monte Carlo method

(3) SU(2)-symmetric spin-boson model

(4) Dissipation-induced order in the $S = 1/2$ quantum spin chain

(5) Conclusions

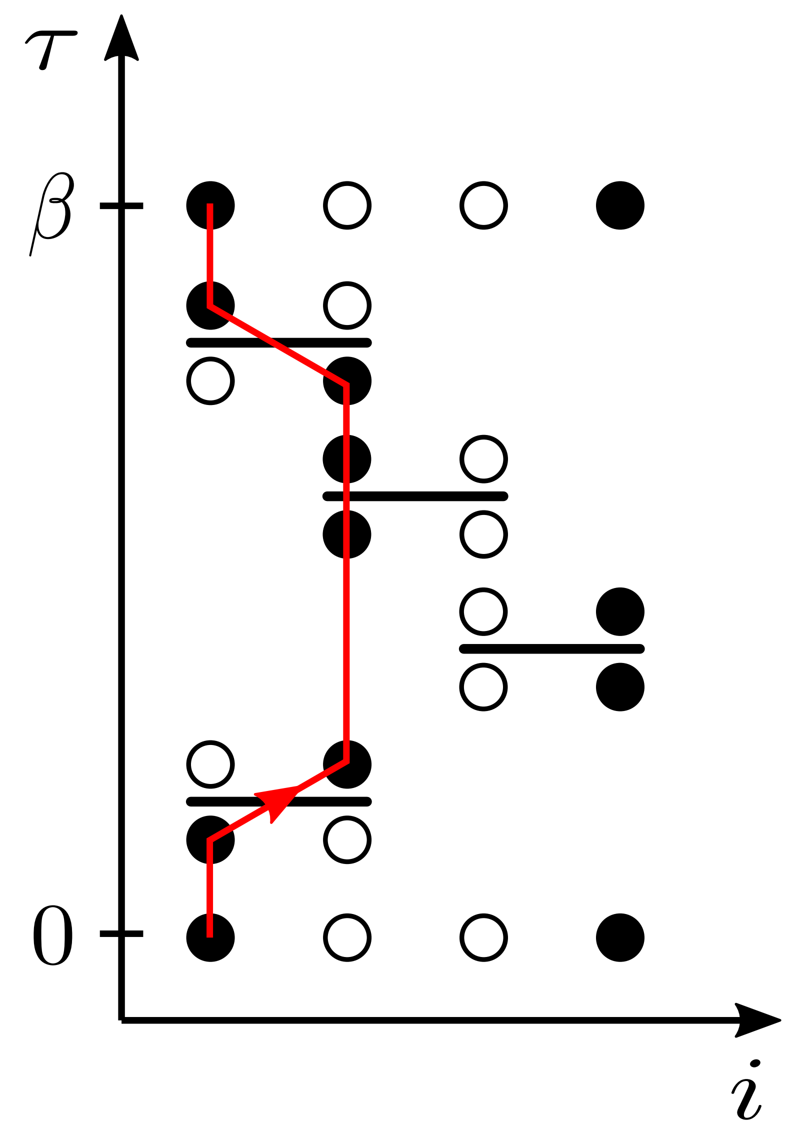
Introduction

Success of world-line QMC methods

Worm/directed-loop algorithms scale linearly in system parameters and represent the state-of-the-art for a large class of quantum many-body systems:

- (anti)ferromagnetic spin systems on (bipartite) lattices
- Bose-Hubbard models on any lattice
- electronic systems in one dimension
- long-range Ising models in a transverse magnetic field
- certain frustrated models
- exotic quantum phase transitions between different orders
- many more …

Prokof'ev, Svistunov, Tupitsyn, JETP (1998);
Syljuåsen, Sandvik, PRE (2002)



⟶ It is highly desirable to extend the scope of these methods to new interaction types!

In this talk:

- no solution to the sign problem, but
- efficient simulation of **spin-boson interactions**: quantum dissipation, light-matter coupling, …

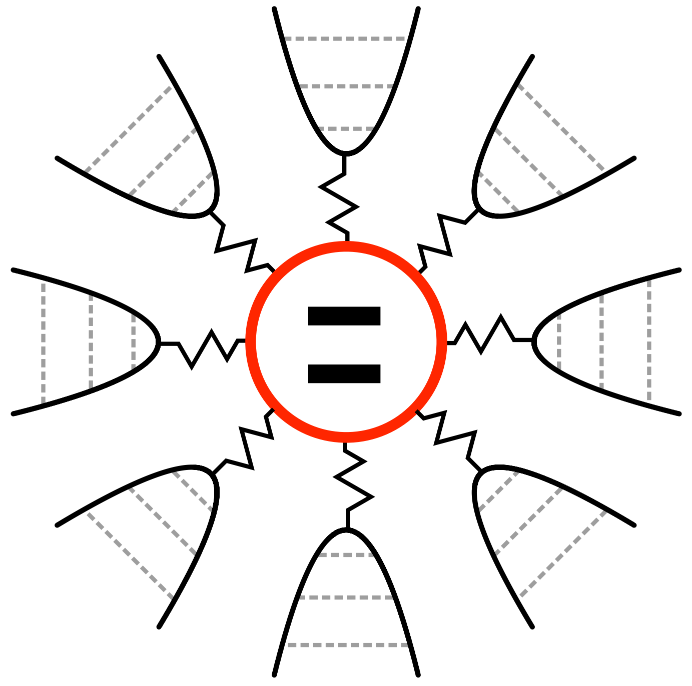
Spin-boson model

Two-level system coupled to bosonic bath:

$$\hat{H} = -h_x \hat{S}_x + \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q + \sum_q \gamma_q \left(\hat{a}_q^\dagger + \hat{a}_q\right) \hat{S}_z$$

⟶ Caldeira-Leggett model for dissipation

⟶ originally studied as a nonequilibrium tunneling problem Leggett et al., Rev. Mod. Phys. (1987)

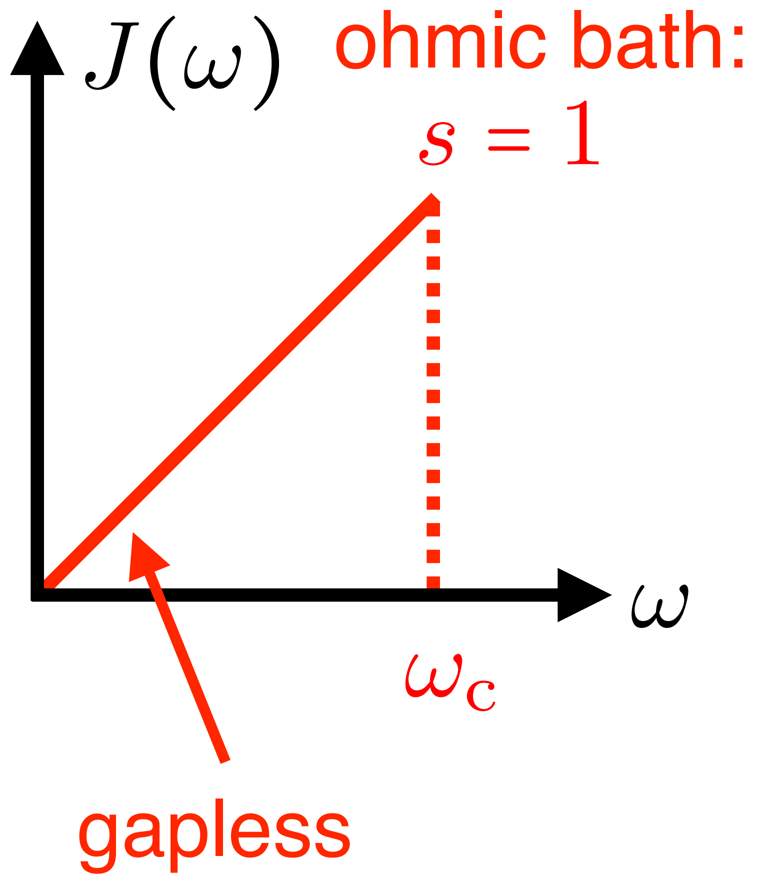


bath spectral function:

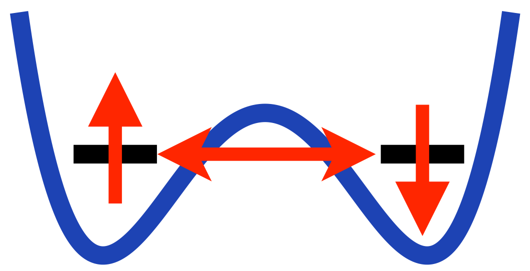
$$J(\omega) = \pi \sum_q \gamma_q^2 \, \delta(\omega - \omega_q)$$

$$= 2\pi\alpha\, \omega_c^{1-s} \omega^s$$

power law

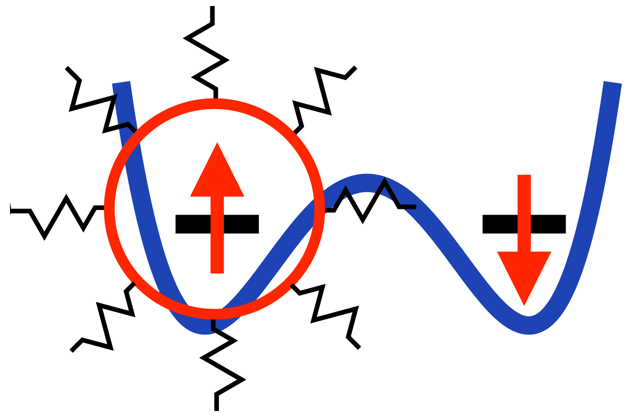


Possible ground states:



delocalized:

spin points along x direction, level splitting

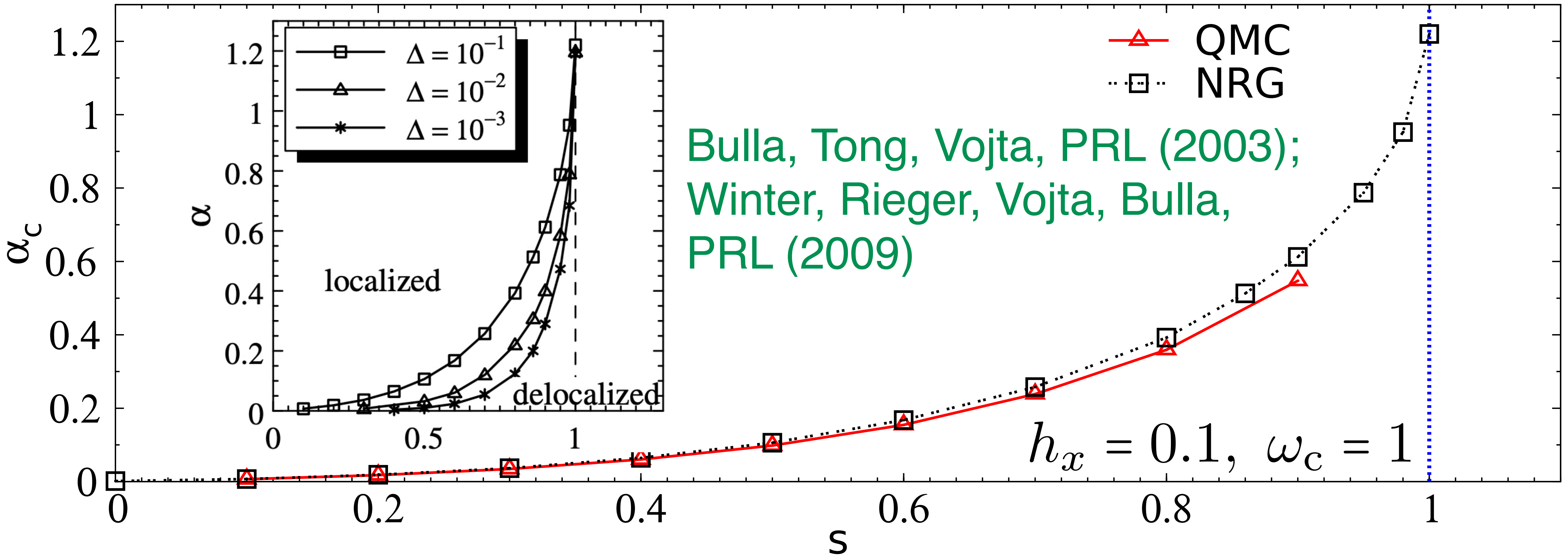


localized:

bath "measures" spin, spontaneous breaking of Z_2 symmetry

$$\hat{S}_z \to -\hat{S}_z \quad , \quad \hat{a}_q \to -\hat{a}_q$$

Quantum phase transition:



Quantum-to-classical correspondence:

same universality class as 1D long-range Ising model

Spin-boson model with multiple baths

We couple each spin component to an independent bath:

$$\hat{H} = -\sum_{\ell} h_\ell \hat{S}_\ell + \sum_{q\ell} \omega_q \hat{a}^\dagger_{q\ell} \hat{a}_{q\ell} + \sum_{q\ell} \gamma_{q\ell} \left(\hat{a}^\dagger_{q\ell} + \hat{a}_{q\ell} \right) \hat{S}_\ell$$

→ competing dissipation channels can lead to nontrivial phenomena even at $h_\ell = 0$

$\alpha_x = \alpha_y,\ \alpha_z = 0:$ two-bath spin-boson model with U(1) symmetry

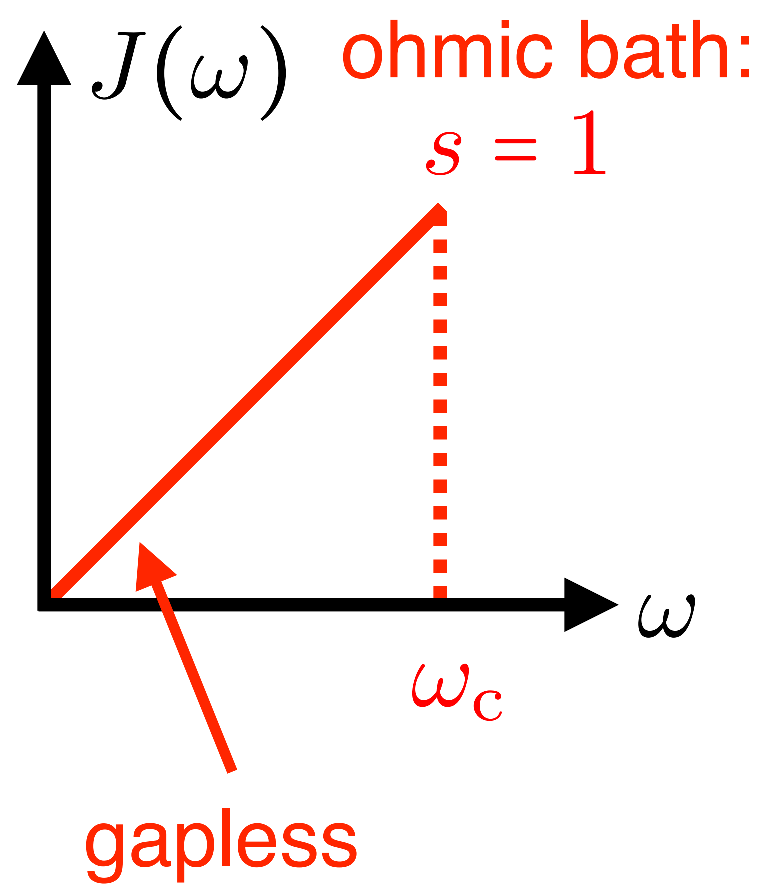
$\alpha_x = \alpha_y = \alpha_z \equiv \alpha:$ three-bath spin-boson model with SU(2) symmetry (Bose Kondo model, spin in a fluctuating magnetic field)

bath spectral function:

$$J_\ell(\omega) = \pi \sum_q \gamma^2_{q\ell}\, \delta(\omega - \omega_q)$$

$$= 2\pi \alpha_\ell\, \omega_c^{1-s} \omega^s$$

power law



Why is the SU(2)-symmetric spin-boson model relevant?

In many solid-state systems, the relevant degrees of freedom couple in an isotropic way to bosonic modes (magnons, particle-hole fluctuations in itinerant magnetism)

→ magnetic moments in critical antiferromagnets — Sachdev, Buragohain, Vojta, Science (1999)

→ SYK models — Sachdev, Ye, PRL (1993); Chowdhury, Georges, Parcollet, Sachdev, Rev. Mod. Phys. (2022)

→ self-consistent treatment of bosonic fluctuations in extended DMFT

→ Kondo-breakdown transitions in heavy-fermion metals — Si, Rabello, Ingersent, Smith, Nature (2001)

→ **here:** interesting scenario of fixed-point annihilation and pseudo-criticality

Wormhole quantum Monte Carlo for spin-boson interactions

MW, Phys. Rev. B **105**, 165129 (2022)

Stochastic series expansion

High-temperature expansion of the partition function:

Sandvik, Kurkijärvi, PRB (1991)

$$Z = \sum_\alpha \langle\alpha| e^{-\beta \hat{H}} |\alpha\rangle = \sum_\alpha \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{S_n} \langle\alpha| \prod_{p=1}^{n} \hat{H}_{a_p,b_p} |\alpha\rangle \qquad \hat{H} = -\sum_{a,b} \hat{H}_{a,b}$$

Configuration space consists of: (i) initial state $|\alpha\rangle$

(ii) expansion order n

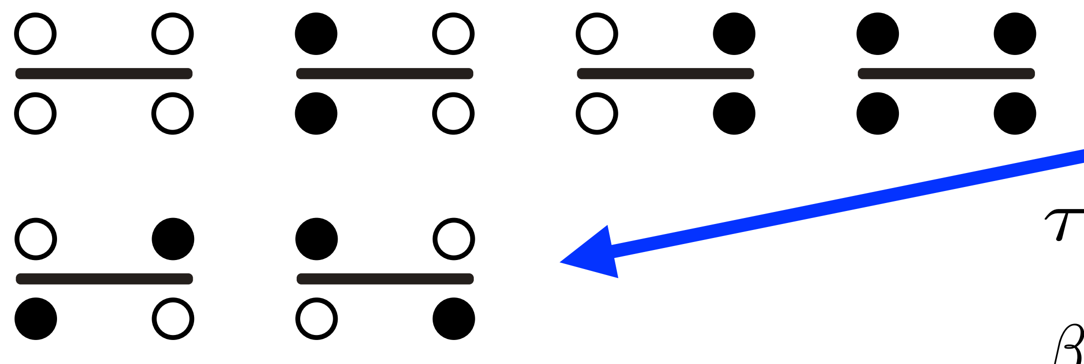
(iii) index sequence $S_n = \{[a_1, b_1], \ldots, [a_n, b_n]\}$

operator type (a_1) — bond variable (b_n)

Introduce **graphical representation** of operators using the example of the Heisenberg model:

$$\hat{H}_{2,b} = C - J \hat{S}^z_{i(b)} \hat{S}^z_{j(b)} \quad \longrightarrow$$

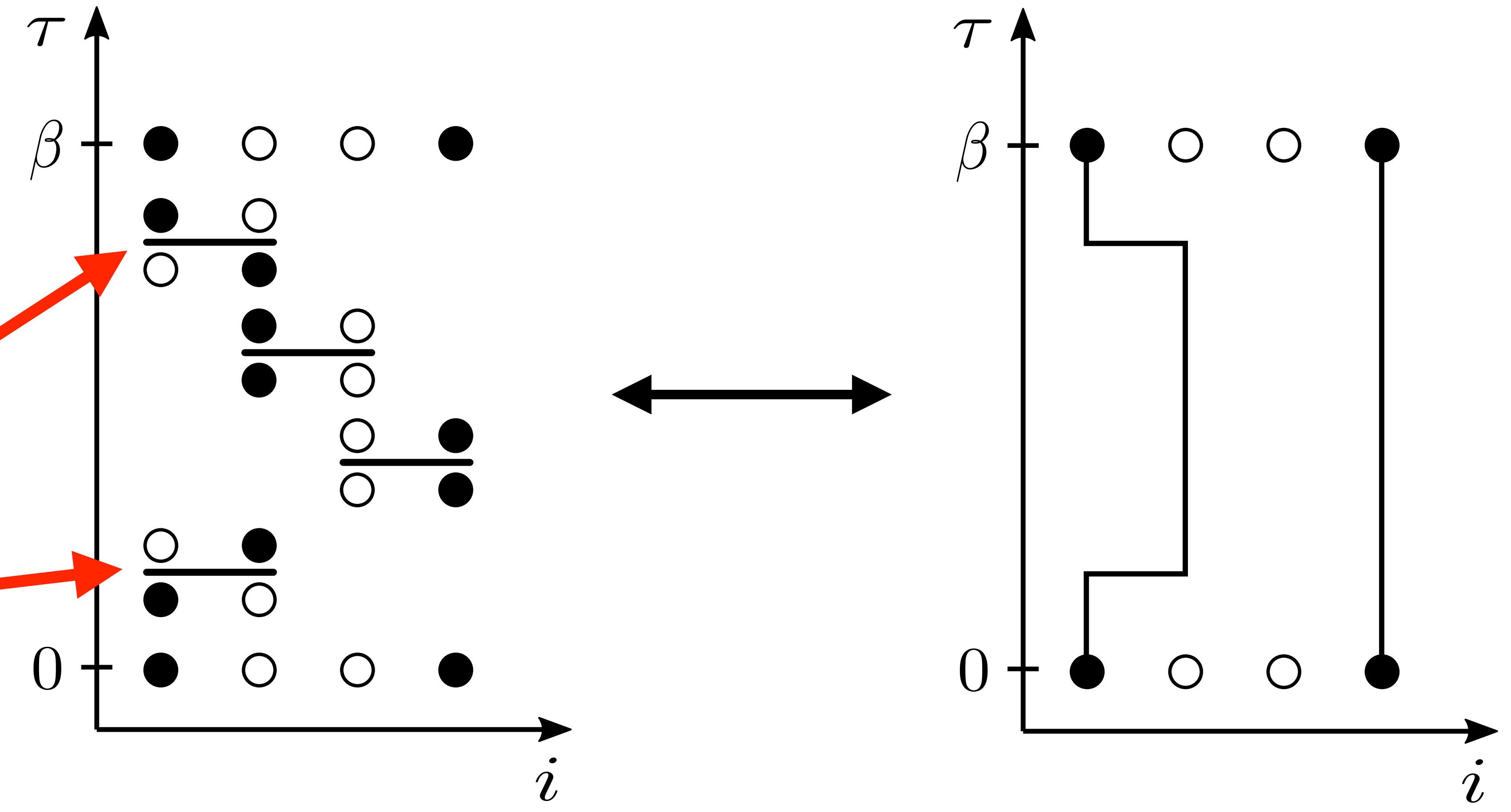
$$\hat{H}_{1,b} = -\frac{J}{2} \left[\hat{S}^+_{i(b)} \hat{S}^-_{j(b)} + \hat{S}^-_{i(b)} \hat{S}^+_{j(b)} \right] \quad \longrightarrow$$



vertices

World-line representation of imaginary-time evolution:

defined by off-diagonal vertices

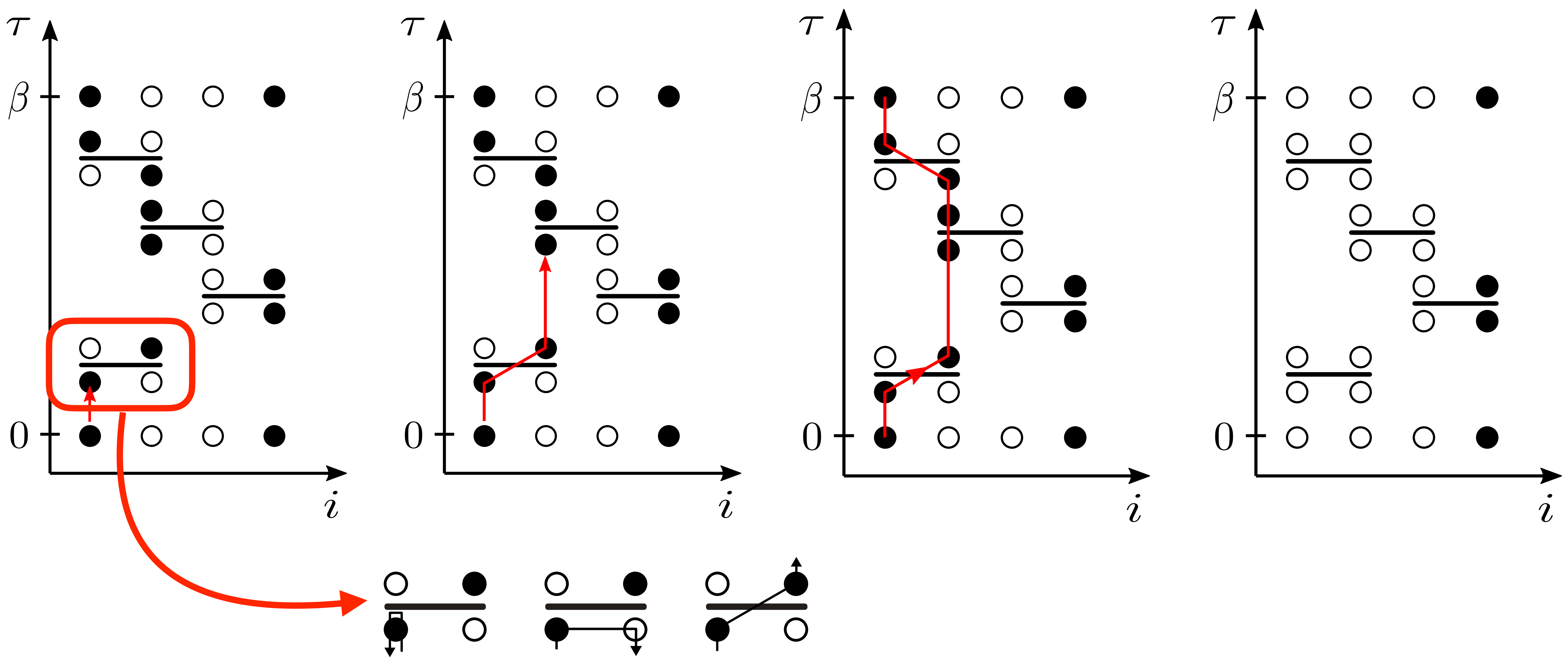


Stochastic series expansion

Syljuåsen, Sandvik, PRB (2002)

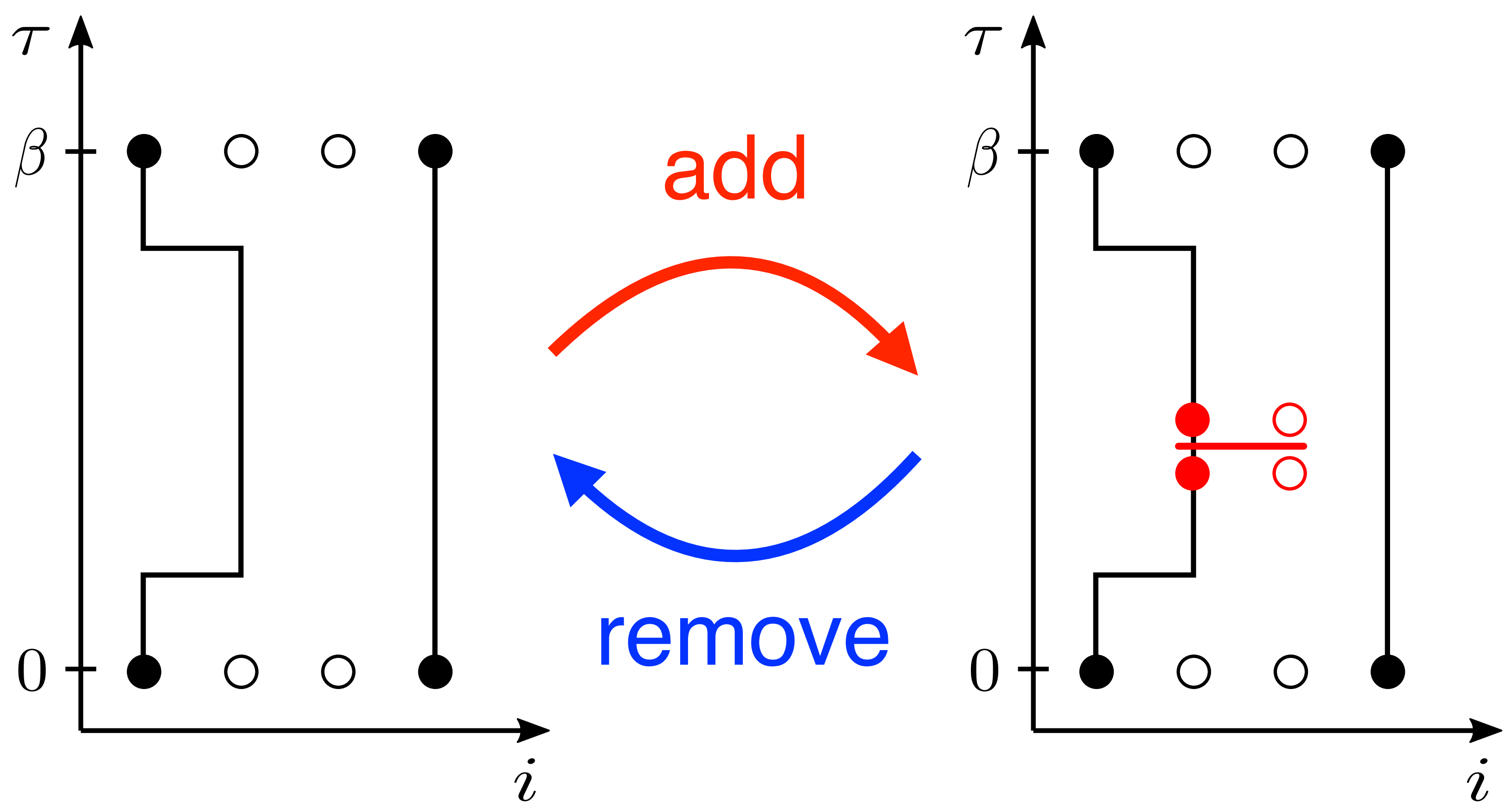
Directed-loop updates:

- Global updates with acceptance 1
  $\longrightarrow$ computational effort $\mathcal{O}(\beta L)$
- Detailed balance is satisfied on the vertex level (directed-loop equations)
- Sample the index sequence S_n and the initial state $|\alpha\rangle$



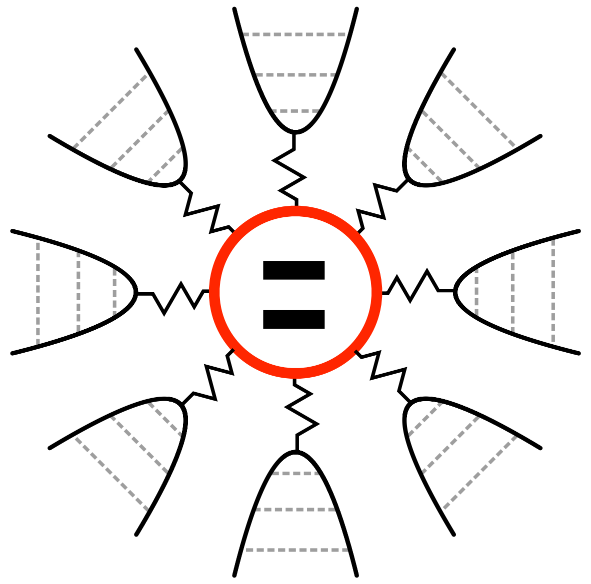
Diagonal updates:

- Sample the expansion order n for a fixed world-line configuration



Numerical simulation of spin-boson models

$$\hat{H} = -\sum_{\ell} h_\ell \hat{S}_\ell + \sum_{q\ell} \omega_q \hat{a}^\dagger_{q\ell} \hat{a}_{q\ell} + \sum_{q\ell} \gamma_{q\ell} \left(\hat{a}^\dagger_{q\ell} + \hat{a}_{q\ell} \right) \hat{S}_\ell$$

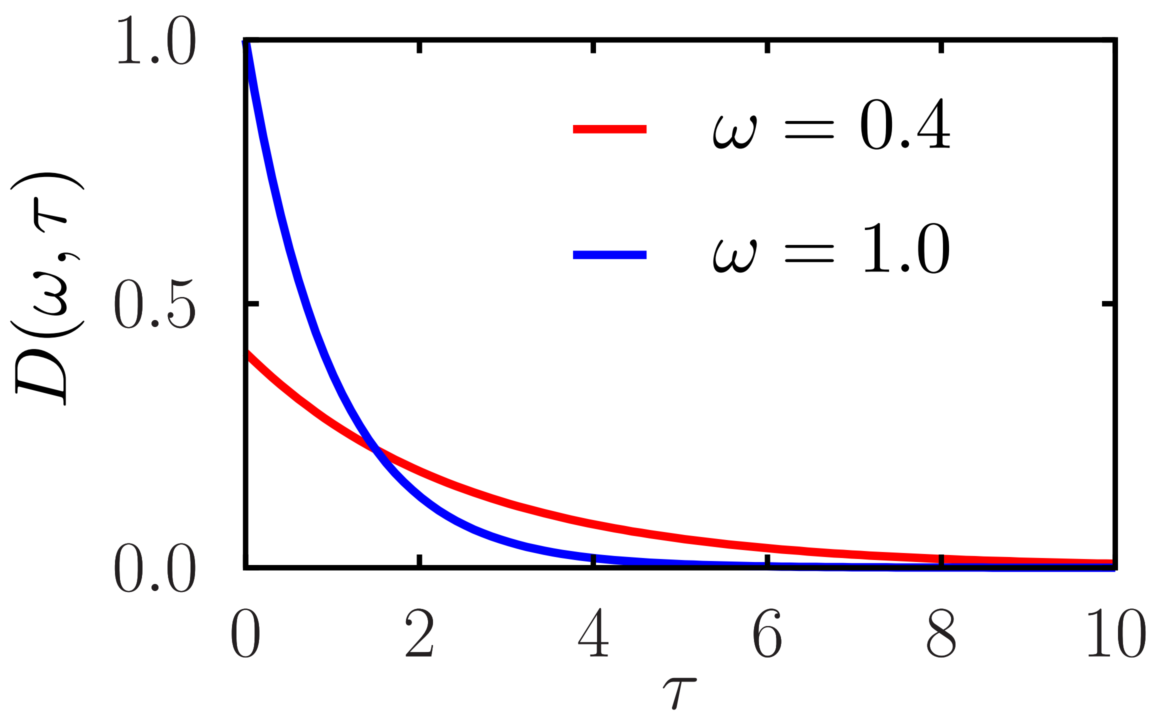


Numerical study is challenging because

- **DMRG**: for every bosonic mode, we have an **infinite bosonic Hilbert space**
  ⟶ Wilson chain (logarithmic discretization of the bath spectrum) Guo, Weichselbaum, von Delft, Vojta, PRL (2012)
- **QMC**: already for one bosonic mode, local updates lead to **long autocorrelation times**

Path integral: bosons can be integrated out exactly: Feynman, PR (1955)

$$\mathcal{S} = \mathcal{S}_{\text{Berry}} - \iint_0^\beta d\tau d\tau' \sum_{q\ell} \gamma^2_{q\ell} \, S_\ell(\tau) \, D(\omega_q, \tau - \tau') \, S_\ell(\tau')$$



- nonlocal interaction in imaginary time mediated by free boson propagator
  ⟶ for a single mode: $D(\omega, \tau) \sim e^{-\omega\tau}$
  ⟶ for continuous spectrum $J_\ell(\omega) \propto w^s$: $K_\ell(\tau) = \frac{1}{\pi} \int d\omega \, J_\ell(\omega) \, D(\omega, \tau) \sim 1/\tau^{1+s}$
- retarded spin-boson models have been studied using various QMC methods
  Winter, Rieger, Vojta, Bulla, PRL (2009); Otsuki, PRB (2013); Cai, Schollwöck, Pollet, PRL (2014); …
- also: continuous-time QMC impurity solvers Gull et al., Rev. Mod. Phys. (2011)

Directed-loop quantum Monte Carlo with wormhole updates

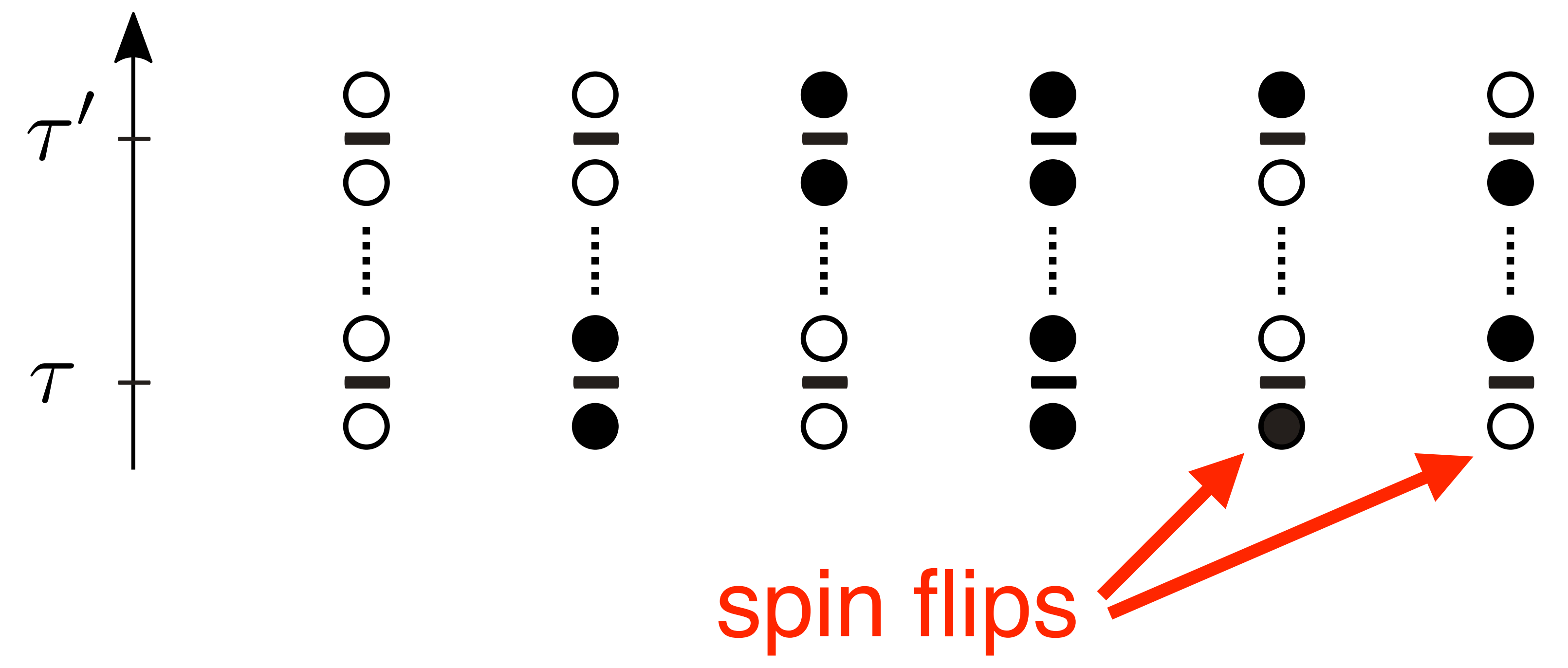
Diagrammatic expansion of the partition function in $\hat{\mathcal{H}}$:

MW, PRB (2022)

$$Z = Z_\mathrm{b}\,\mathrm{Tr_s}\,\hat{\mathcal{T}}_\tau\, e^{-\hat{\mathcal{H}}}$$ ⟵ using interaction representation

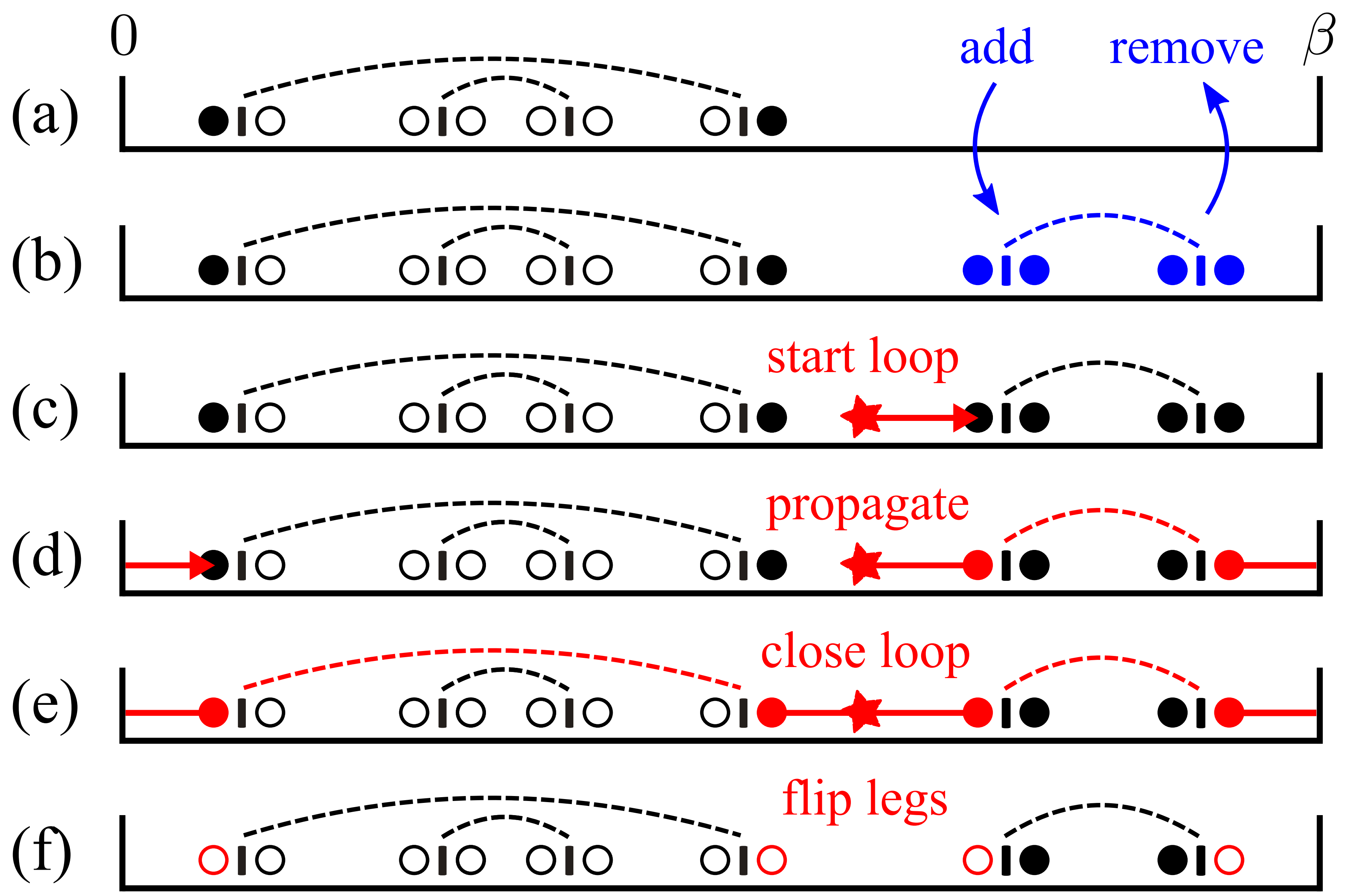
$$\hat{\mathcal{H}} = -\frac{1}{\pi}\int_0^\infty d\omega\, J(\omega) \iint_0^\beta d\tau d\tau' D_+(\omega, \tau-\tau')\, \hat{\mathbf{S}}(\tau)\cdot\hat{\mathbf{S}}(\tau')$$

⟶ world-line representation as in stochastic series expansion



Diagonal updates:

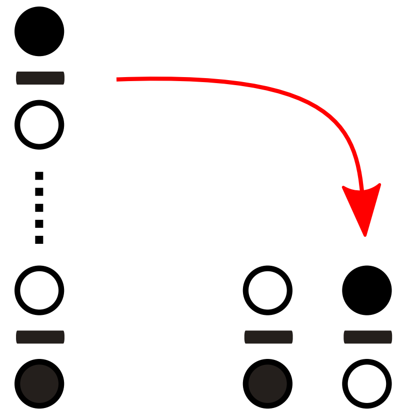
⟶ sample distance w.r.t. boson propagator



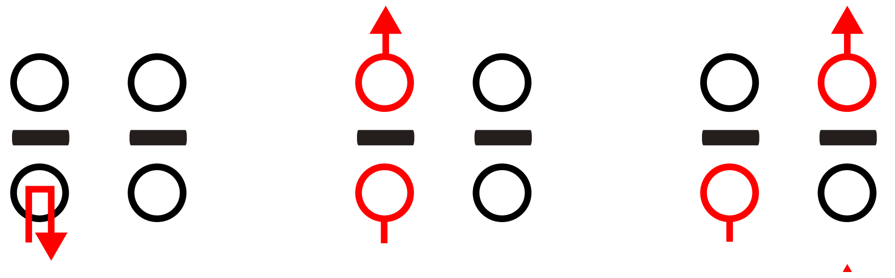
Directed-loop updates:

⟶ interaction vertex is equivalent to Heisenberg model via mapping

$$\hat{\mathbf{S}}(\tau)\cdot\hat{\mathbf{S}}(\tau') \leftrightarrow \hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j$$



⟶ choose exit legs as usual

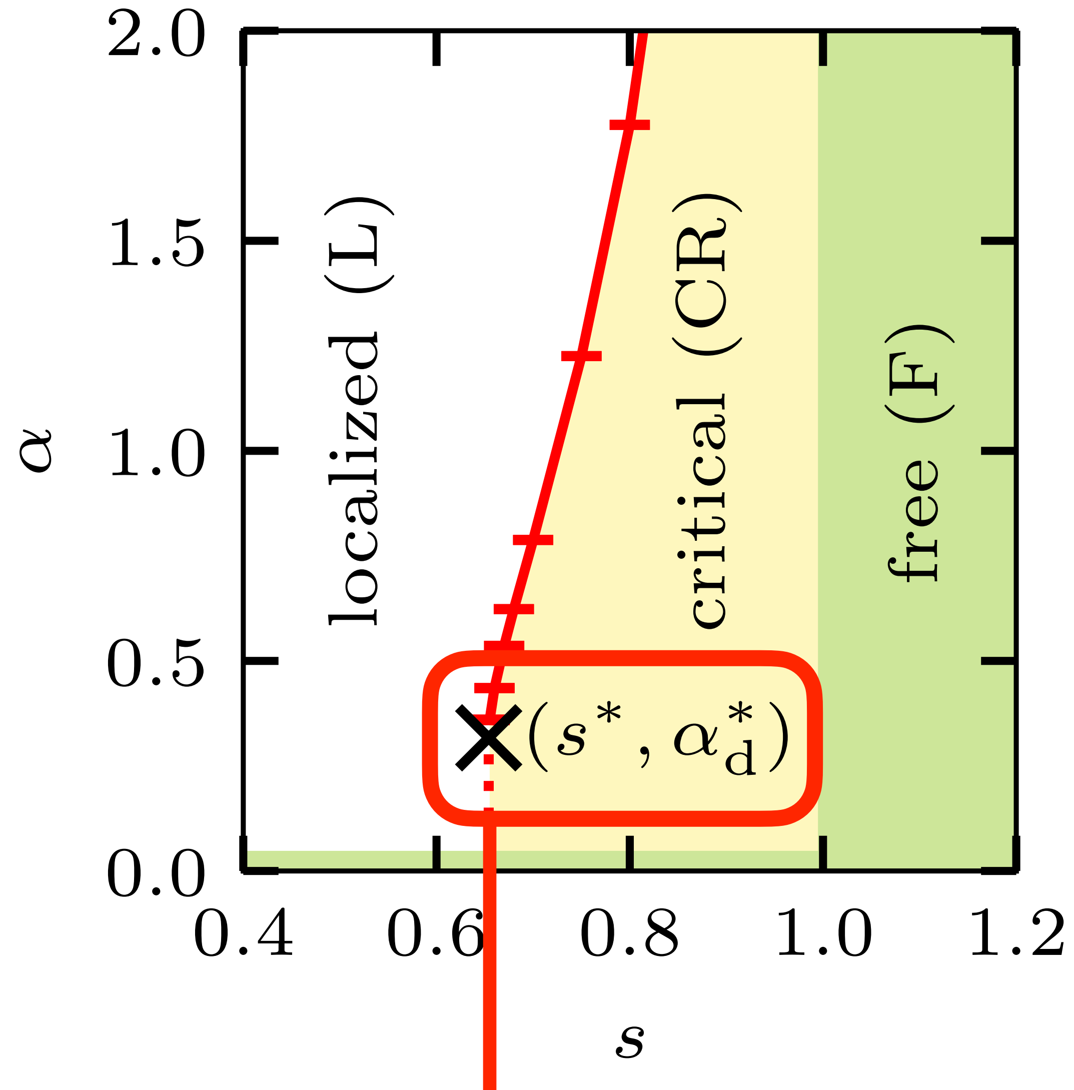


⟶ **wormhole updates** with nonlocal tunneling

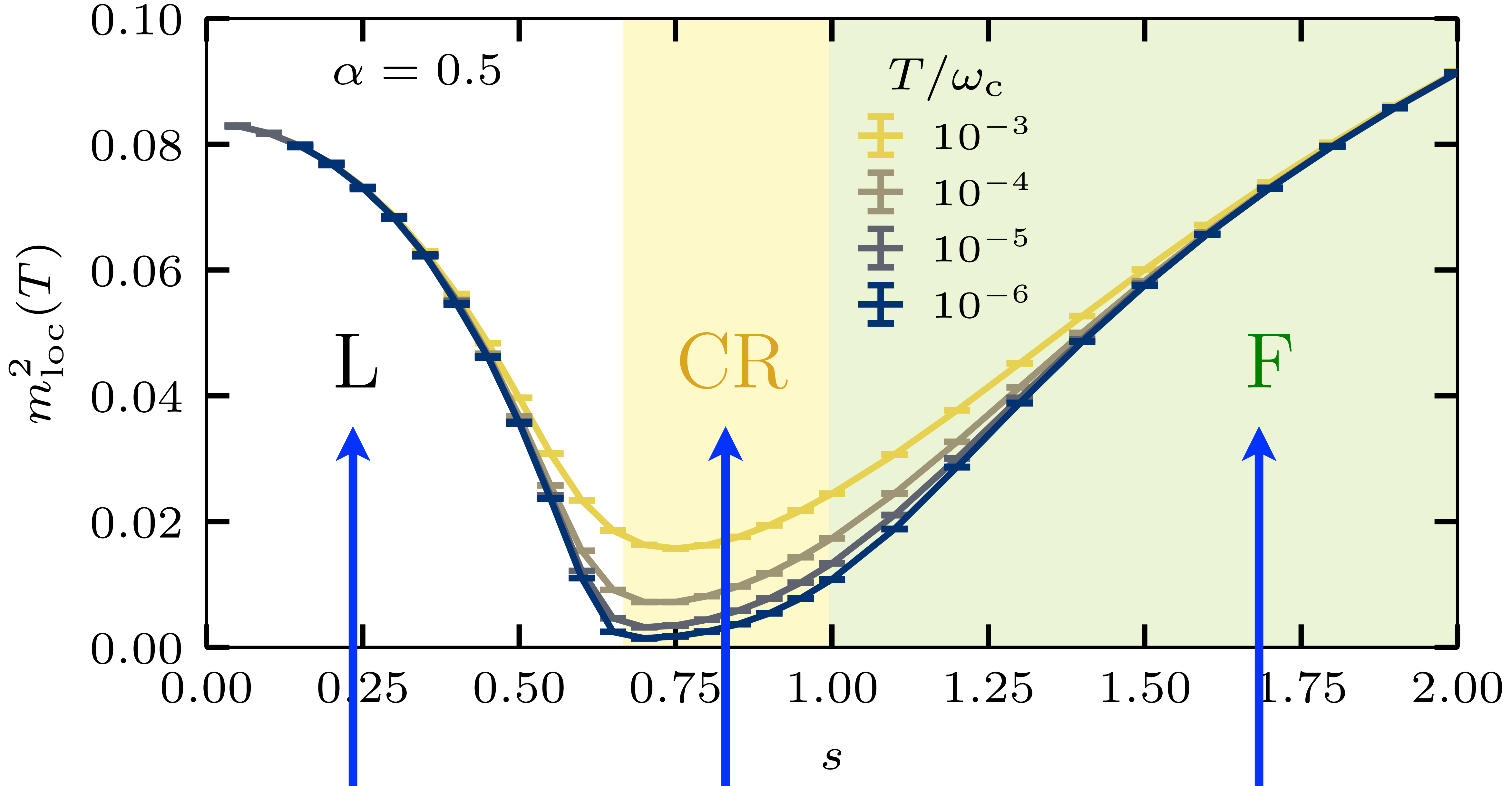
Fixed-point annihilation in the SU(2)-symmetric spin-boson model

MW, Vojta, Phys. Rev. Lett. **130**, 186701 (2023)

Phase diagram & local-moment formation



→ phases can be detected via local moment: $m_{\mathrm{loc}}^2(T) = \langle \hat{S}_x(\tau = \beta/2)\hat{S}_x(0) \rangle$



Why does the phase boundary disappear?

$\chi_x(T) = m_{\mathrm{loc}}^2/T + cT^{-s}$

localized (L)

$\chi_x(T) \propto T^{-s}$

critical (CR)

$\chi_x(T) = m_{\mathrm{loc}}^2/T$

free (F)

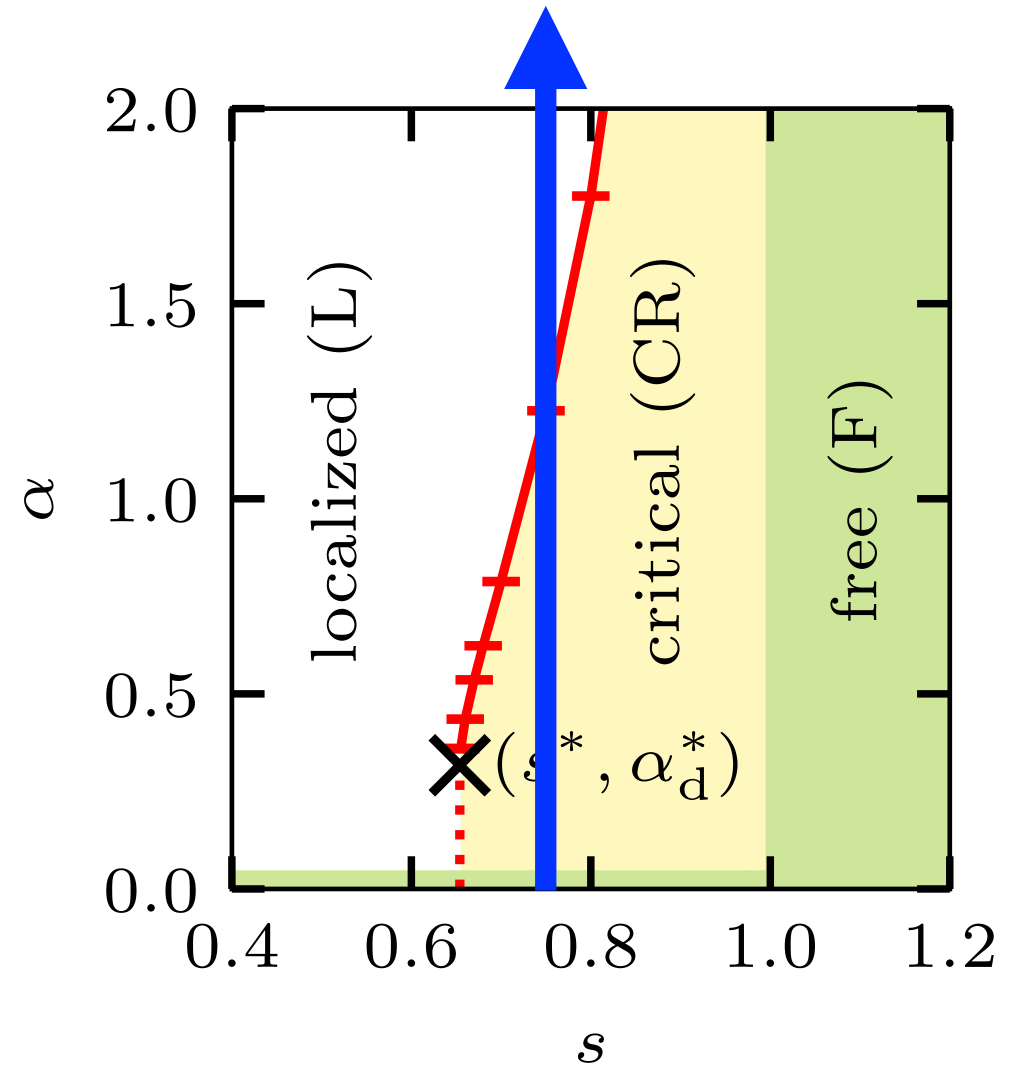
frustration of decoherence

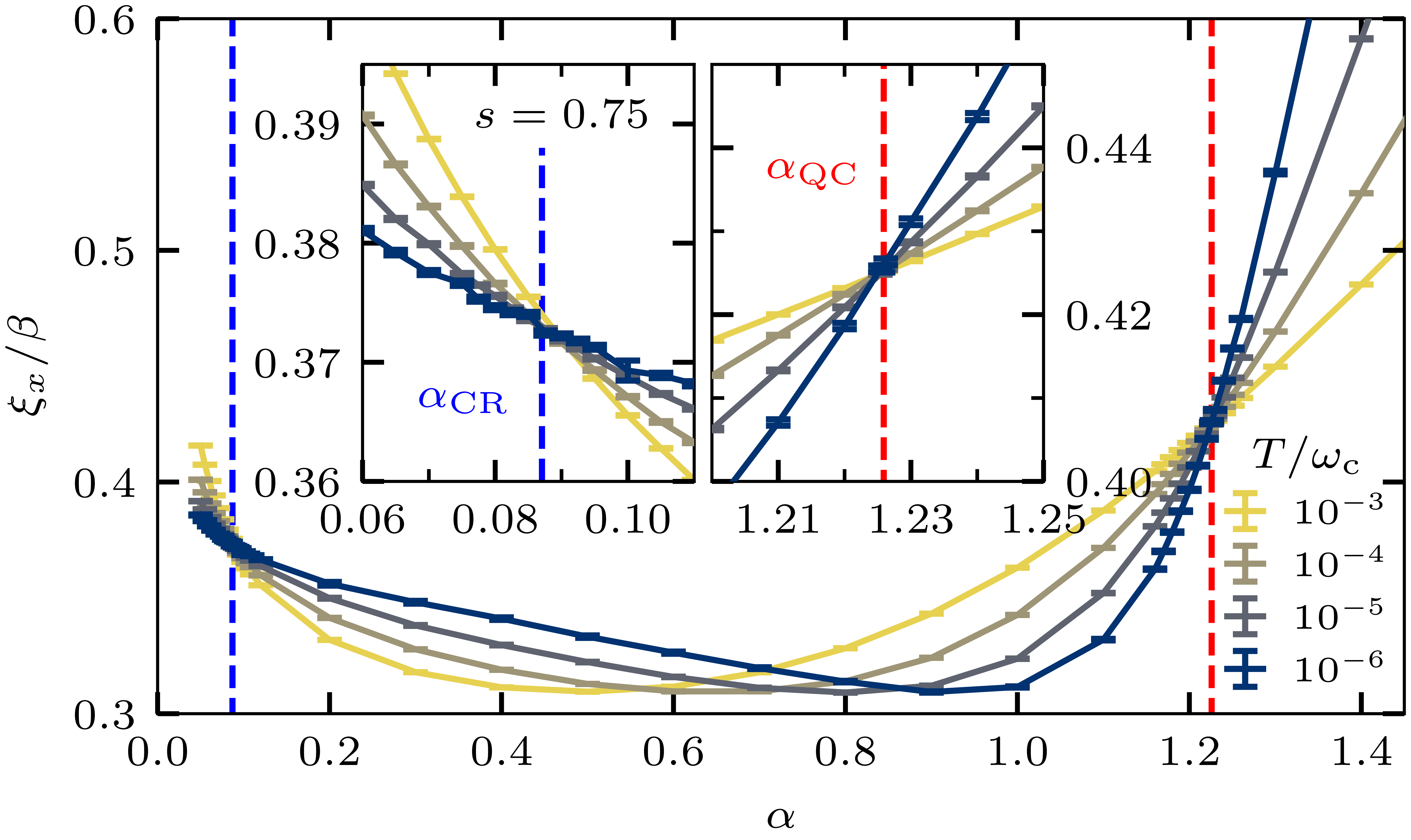
Castro Neto et al., PRL (2003)

Estimation of the fixed-point couplings via finite-size scaling

Spin susceptibility: $\chi_x(\mathrm{i}\Omega_n) = \int_0^\beta d\tau\, e^{\mathrm{i}\Omega_n \tau} \langle \hat{S}_x(\tau)\hat{S}_x(0)\rangle$

Correlation length in imaginary time: $\xi_x = \frac{1}{\Omega_1}\sqrt{\frac{\chi_x(\mathrm{i}\Omega_0)}{\chi_x(\mathrm{i}\Omega_1)} - 1}$





→ L phase: χ_x/β diverges

→ CR phase: χ_x/β is finite

We find **two fixed points** at intermediate couplings!

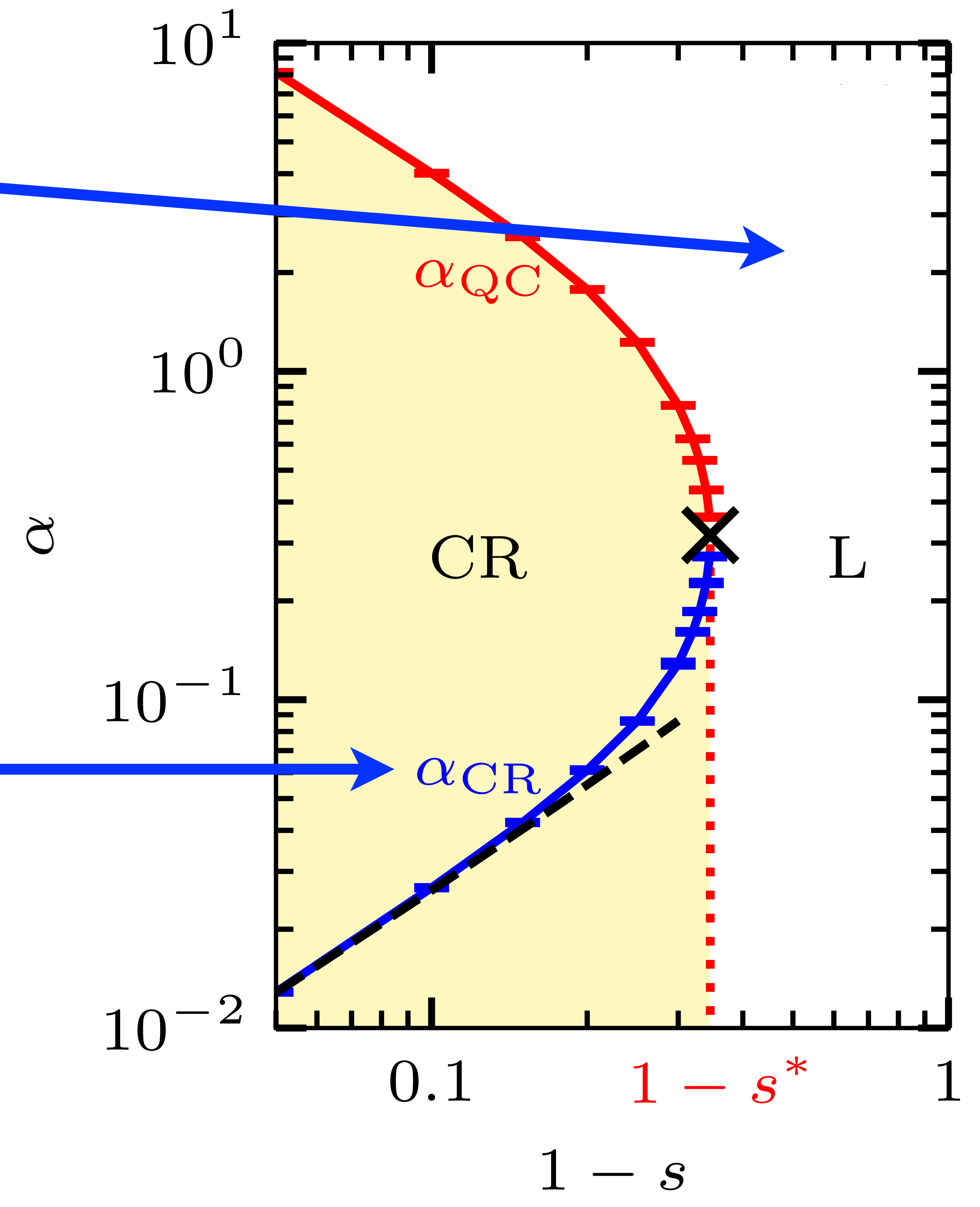
Renormalization-group structure & fixed-point annihilation

localized (L) phase
verified by **QMC**

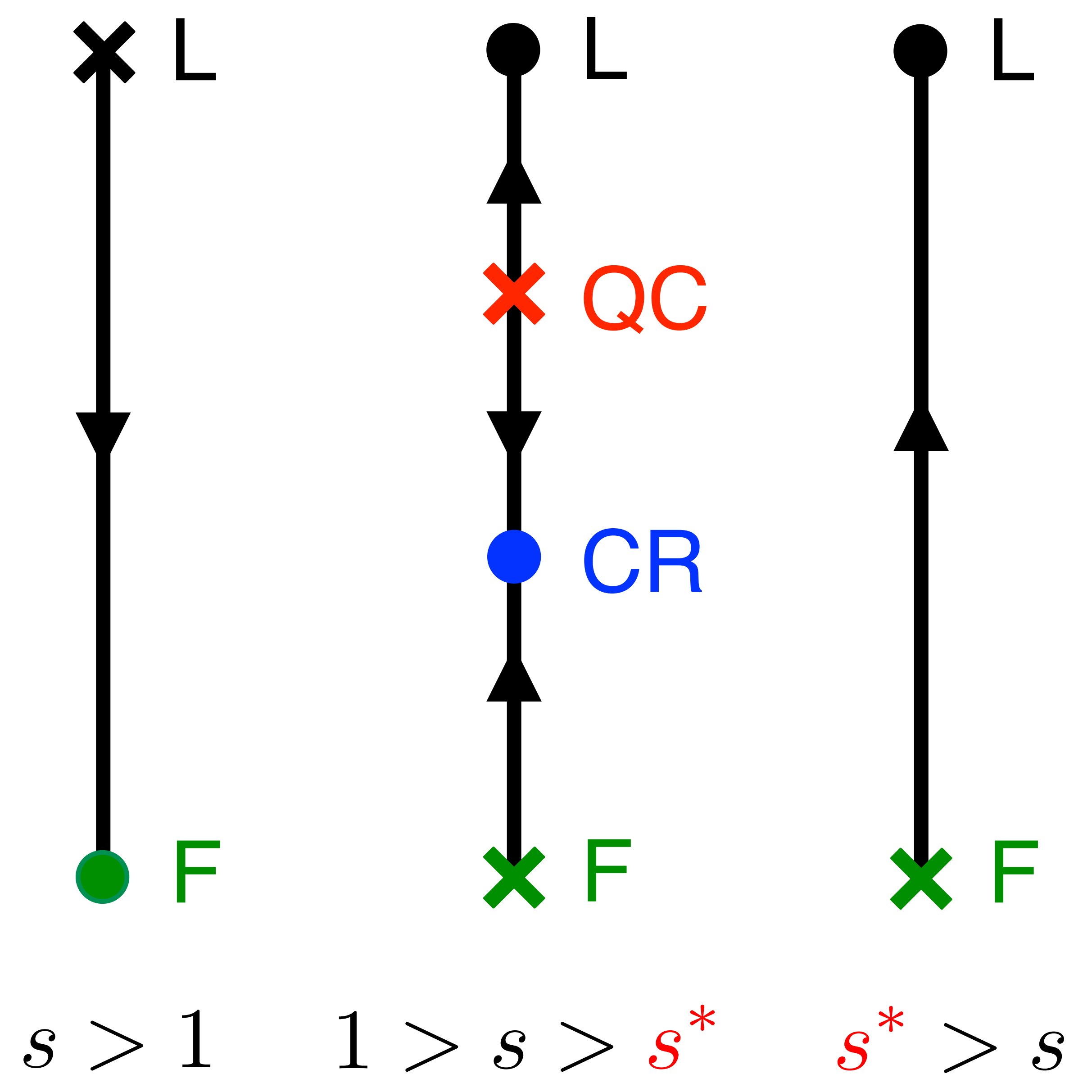
Otsuki, PRB (2013)
Cai, Si, PRB (2019)

stable fixed point (CR)
predicted by **perturbative RG**

Vojta, Buragohain, Sachdev, PRB (2000)
Zhu, Si, PRB (2002)
Zarand, Demler, PRB (2002)



Schematic RG flow:



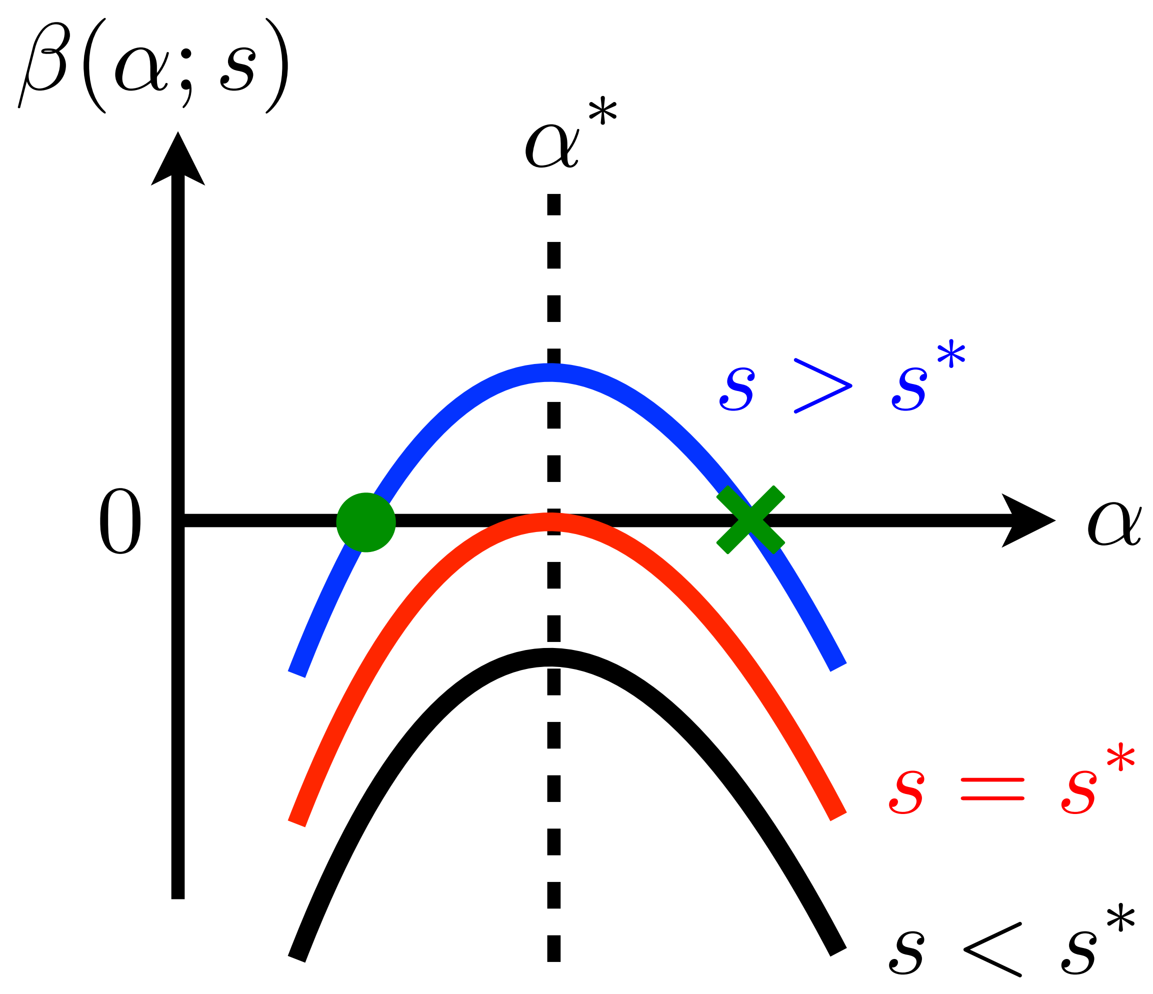
What is new about our work?

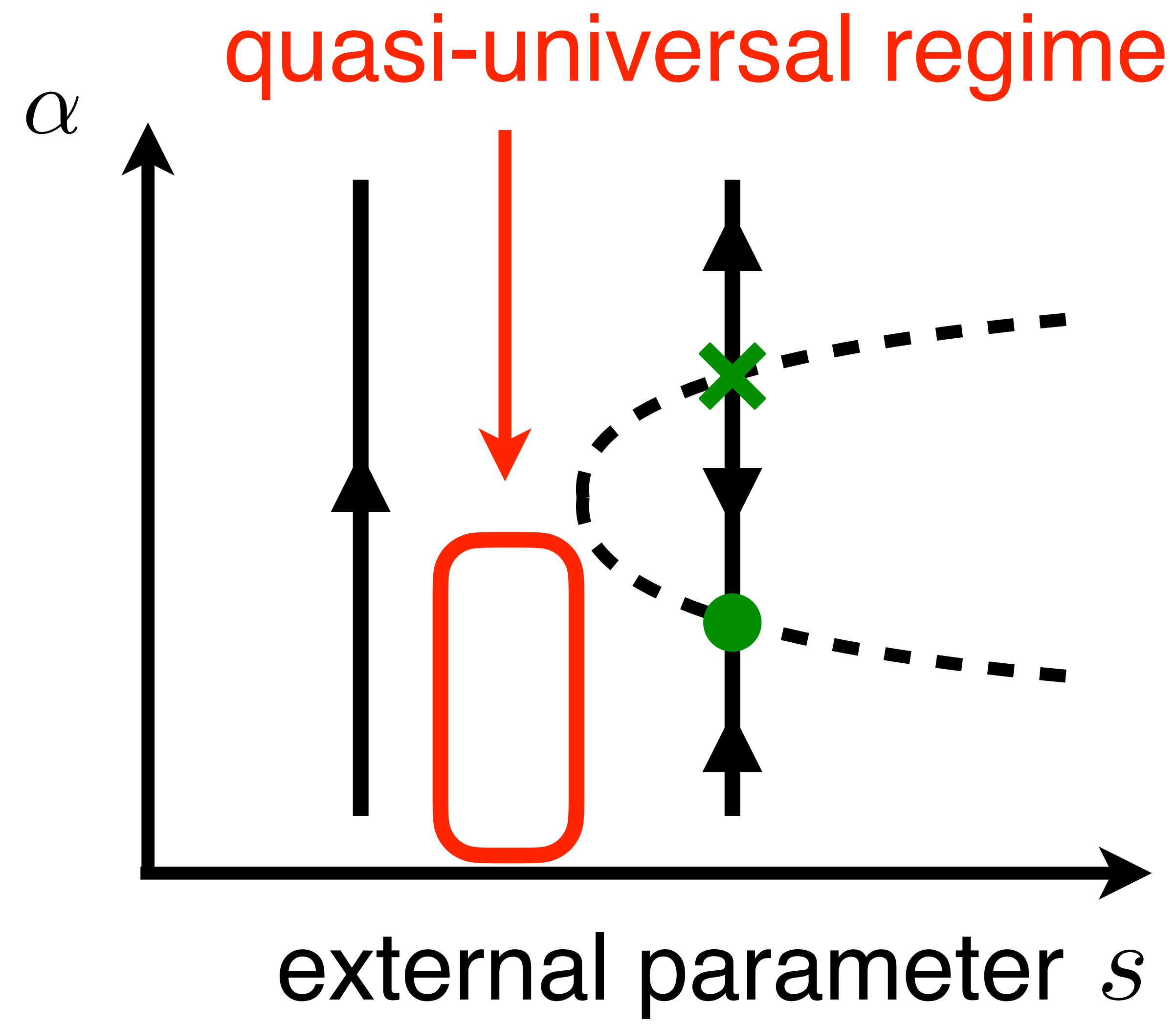
⟶ for the first time, we directly monitor fixed-point annihilation

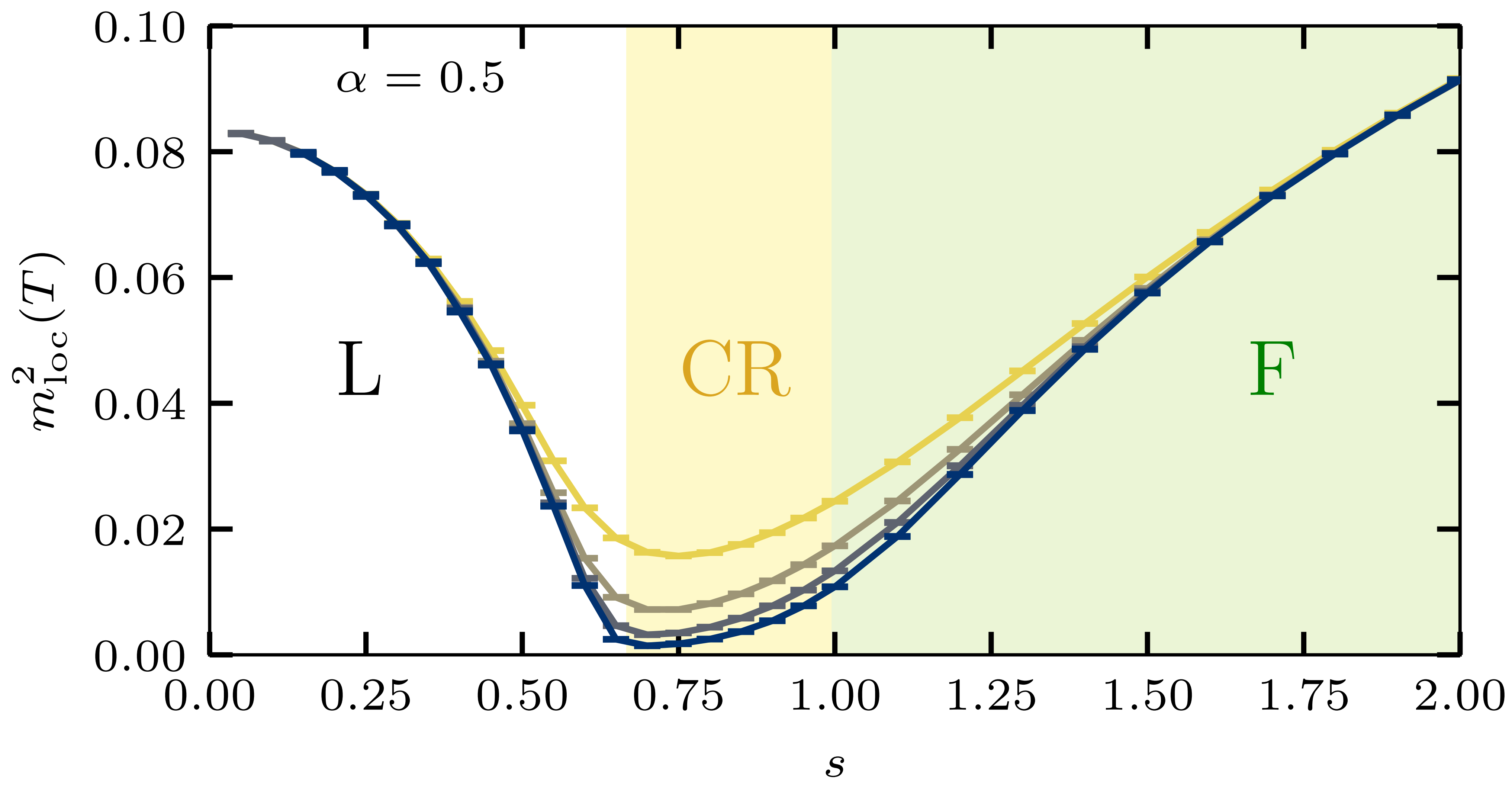
⟶ approximate fixed-point duality

⟶ determine critical exponents at $\alpha_{\rm QC}$ ⟶ further information: **MW**, Vojta, PRL (2023)

Why is the annihilation of two fixed points interesting?







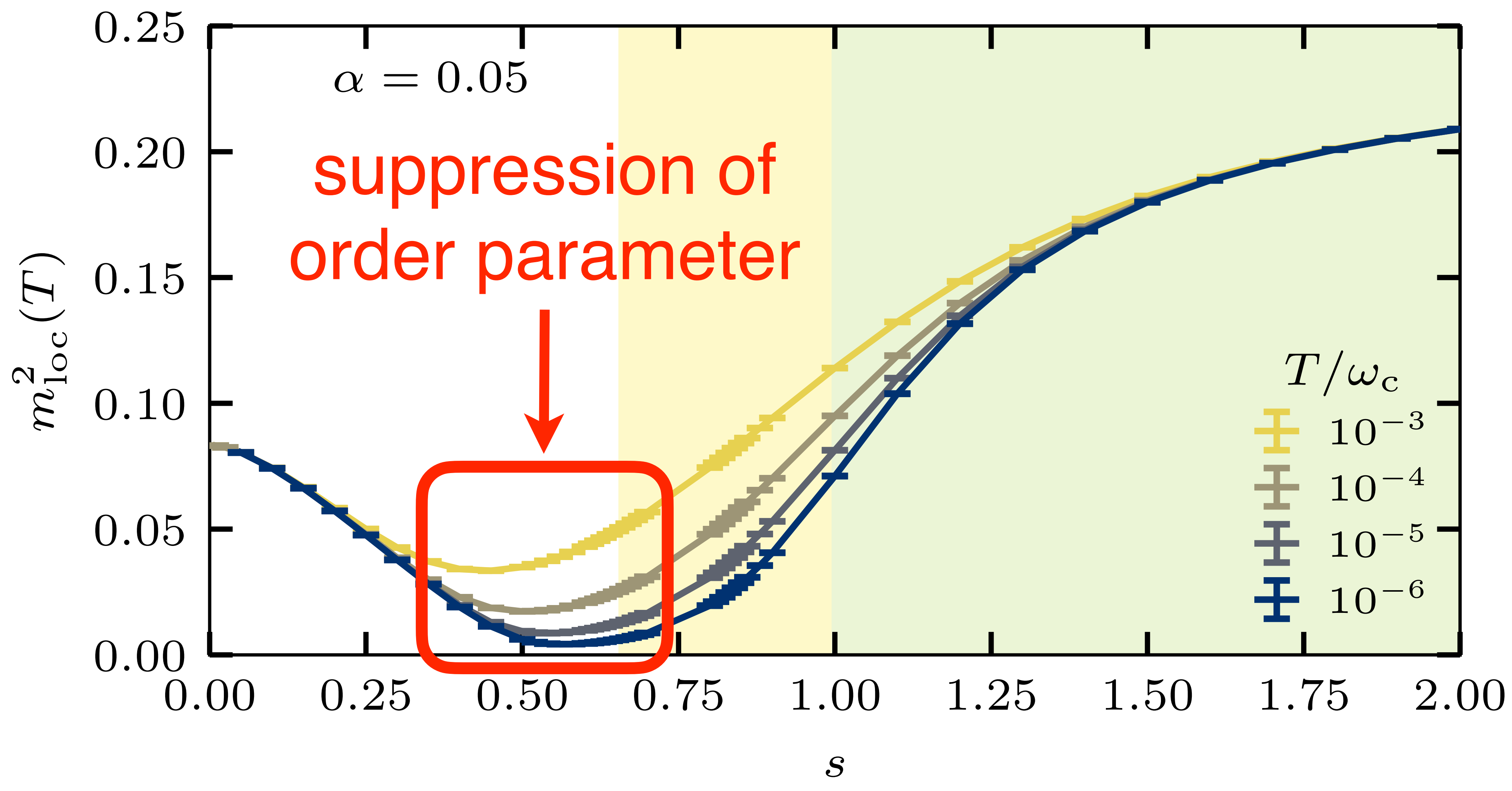
Consider the RG **beta function**:

$$\beta(\alpha; s) = \frac{d\alpha}{d\ln\mu} = (s - s^*) - (\alpha - \alpha^*)^2$$

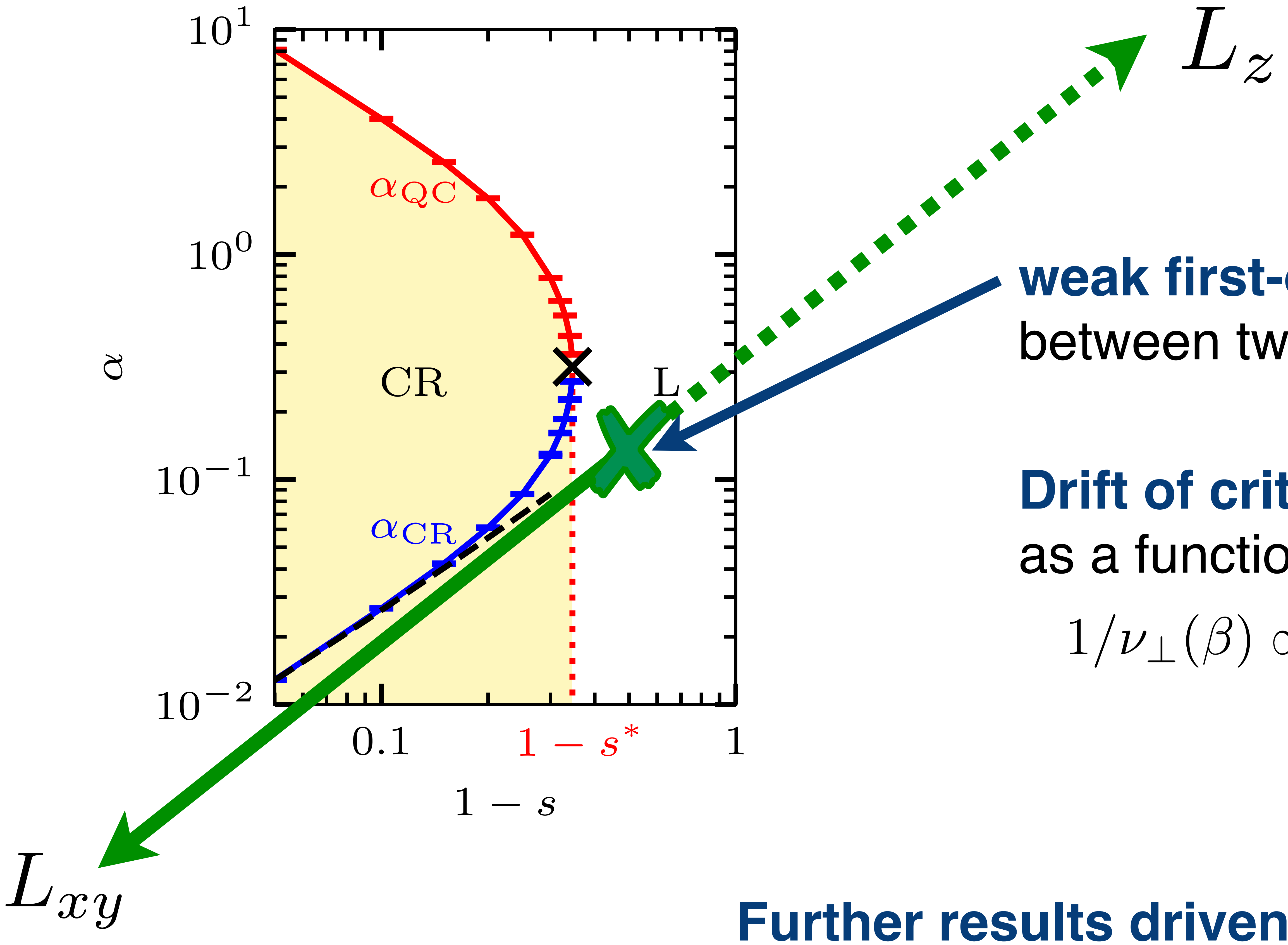
→ order parameter in quasi-universal regime:

$$m \sim \theta(s^* - s)\ \exp\left[-\frac{c}{\sqrt{s^* - s}}\right]$$

→ further information: Kaplan, Lee, Son, Stephanov, PRD (2009)



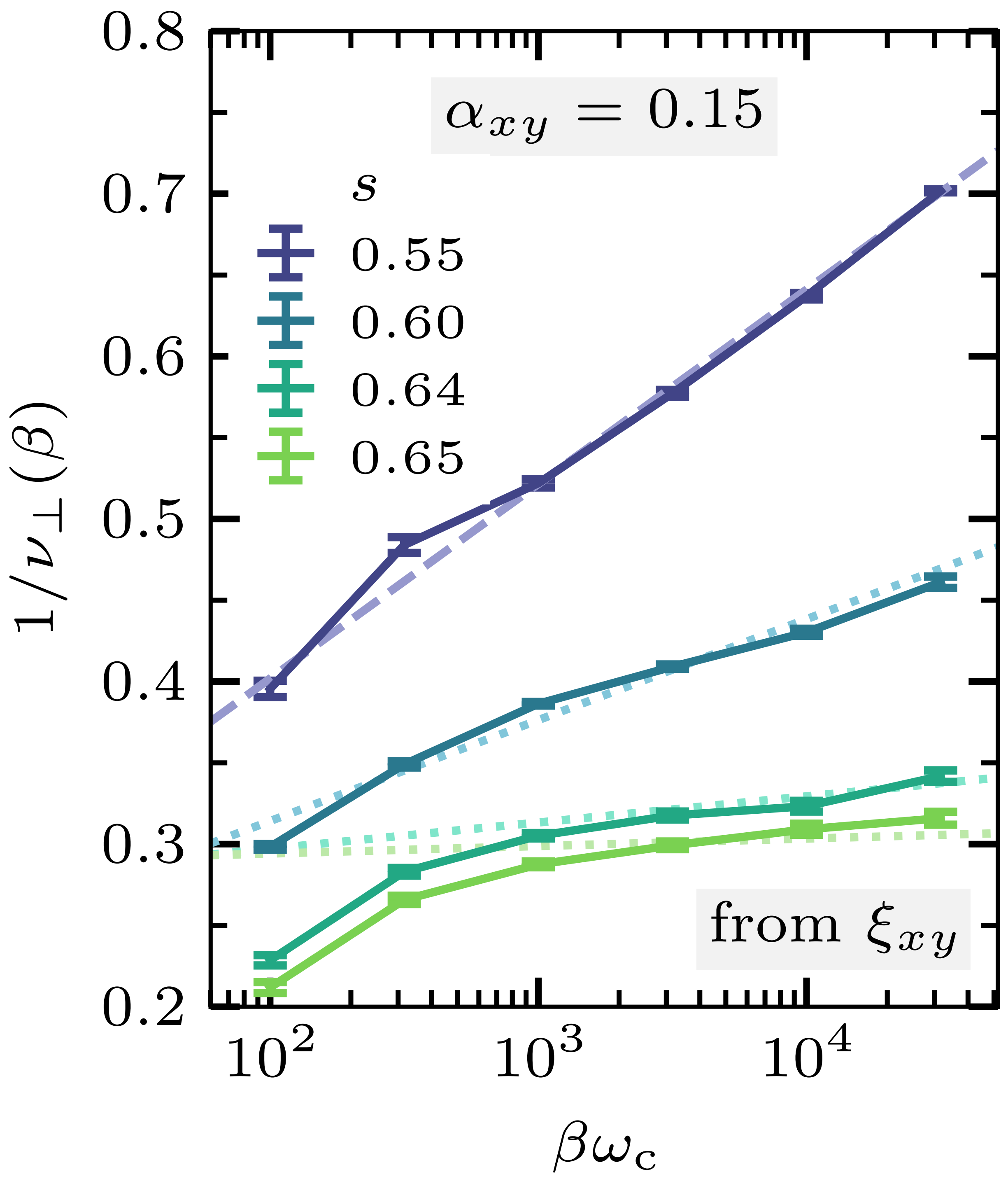
Pseudo-critical scaling near the fixed-point collision



weak first-order transition
between two ordered states

Drift of critical exponents
as a function of temperature

$$1/\nu_\perp(\beta) \propto |s - s^*| \log \beta$$



Further results driven by anisotropy:

- scaling at symmetry-enhanced first-order transition
- transition can be tuned from first- to second-order

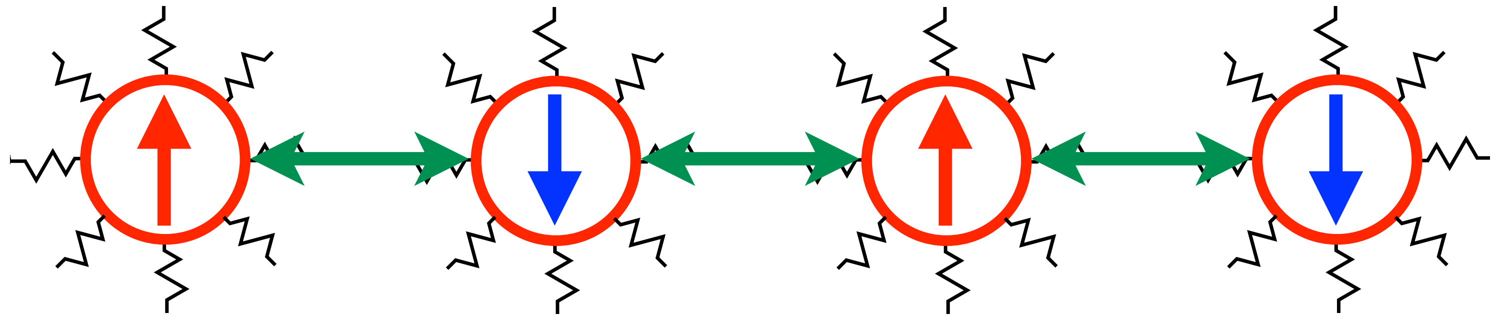
⟶ for details see: **MW**, arXiv (2024)

Dissipation-induced order in the S = 1/2 quantum spin chain

MW, Luitz, Assaad, Phys. Rev. Lett. **129**, 056402 (2022)

1D Heisenberg model coupled to an ohmic bath

$$\hat{H} = J\sum_i \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} + \sum_{iq} \omega_q\, \hat{\mathbf{a}}^\dagger_{iq} \cdot \hat{\mathbf{a}}_{iq} + \sum_{iq} \lambda_q \left(\hat{\mathbf{a}}^\dagger_{iq} + \hat{\mathbf{a}}_{iq}\right) \cdot \hat{\mathbf{S}}_i$$



Physical relevance:

- weakly-coupled spin chains in bulk system Lake, Tennant, Frost, Nagler, Nat. Mater. (2005)
- magnetic adatoms on a surface Toskovic et al., Nat. Phys. (2016)

⟶ Heisenberg chain Kondo-coupled to 2D Fermi liquid Danu, Vojta, Grover, Assaad, PRB (2022)

⟶ Hertz-Millis theory leads to spin-spin interaction mediated by $\chi_0(i-j,\tau-\tau') \sim 1/[(\tau-\tau')^2 + |i-j|^4]$

Bosonic bath can be traced out exactly, i.e, $Z = Z_\mathrm{b}\, \mathrm{Tr_s}\, \hat{\mathcal{T}}_\tau\, e^{-\hat{\mathcal{H}}_\mathrm{s} - \hat{\mathcal{H}}_\mathrm{ret}}$, to obtain a **retarded spin interaction:**

$$\mathcal{H}_\mathrm{ret} = -\iint_0^\beta d\tau d\tau' \sum_i K(\tau-\tau')\, \hat{\mathbf{S}}_i(\tau) \cdot \hat{\mathbf{S}}_i(\tau')$$

bath propagator: $K(\tau) \sim 1/\tau^{1+s}$

- global SO(3) symmetry of system + bath preserved $\hat{\mathbf{J}}_\mathrm{tot} = \sum_i \hat{\mathbf{S}}_i + \sum_{iq} \hat{\mathbf{Q}}_{iq} \times \hat{\mathbf{P}}_{iq}$
- long-range interaction in imaginary time can invalidate **Mermin-Wagner theorem**
- at Heisenberg critical point, the scaling dimension is $\Delta = 1 - s$ ⟶ ohmic bath is marginal perturbation

Detecting long-range antiferromagnetic order

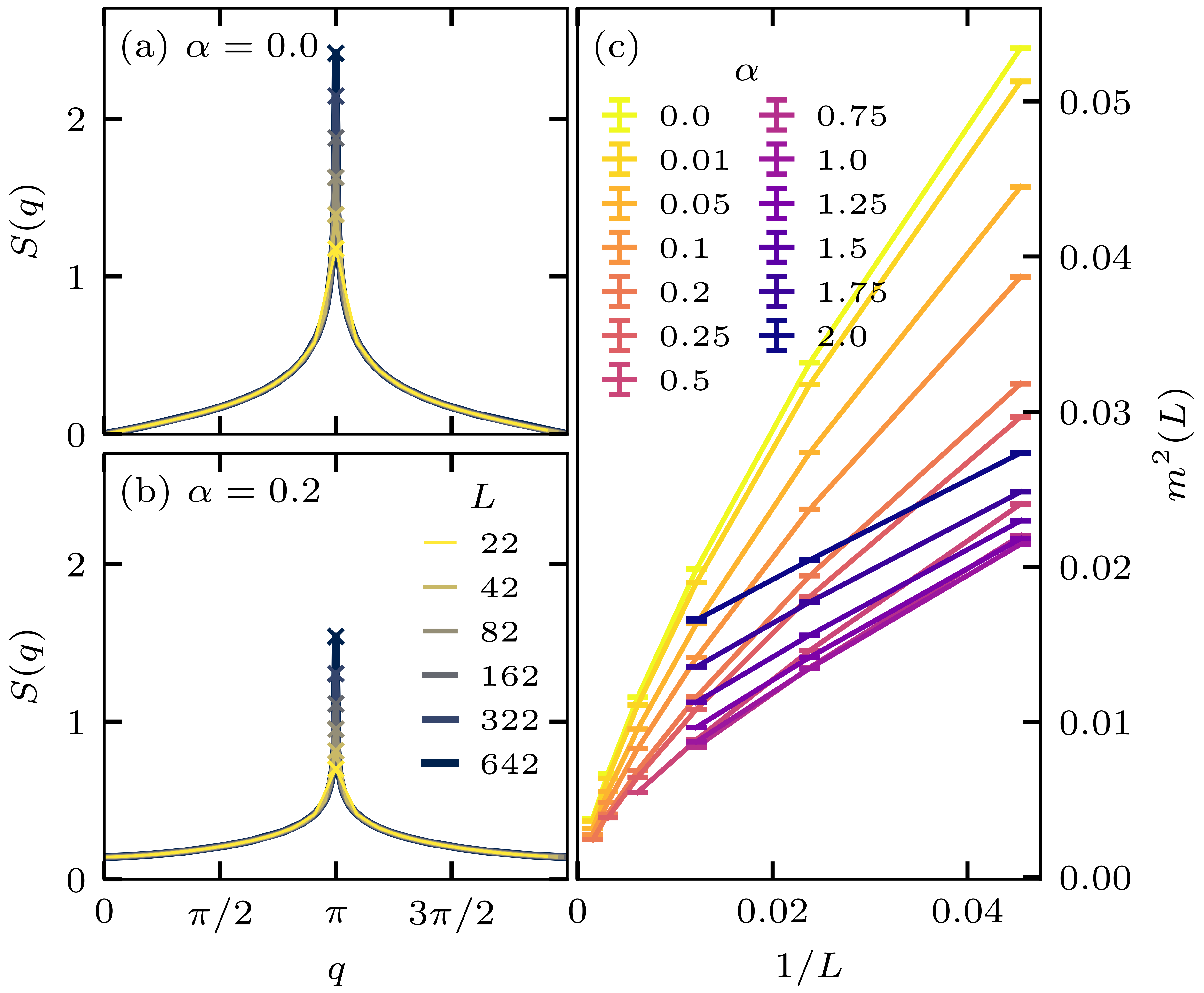
We consider the **spin structure factor**

$$S(q) = \frac{1}{L}\sum_{ij} e^{\mathrm{i}q(i-j)}\langle \hat{S}_i^z \hat{S}_j^z\rangle$$

and the **AFM order parameter**

$$m^2(L) = S(q=\pi)/L$$

- Heisenberg limit $(\alpha = 0)$: $S(q=\pi) \propto \log(L)$, $m^2(L\to\infty) = 0$
- The **coupling to the bath** leads to:
  - ⟶ breaking of the total spin symmetry, i.e., $$S(q=0) = \langle \hat{\mathbf{S}}^2_{\mathrm{tot}}\rangle/L > 0$$
  - ⟶ apparent reduction of order for small α
  - ⟶ clear signature of AFM order for large α



Detecting long-range antiferromagnetic order

Finite-size scaling via RG-invariant **correlation ratio**

$$R = 1 - \frac{S(Q+\delta q)}{S(Q)} \qquad Q = \pi \qquad \delta q = 2\pi/L$$

- Crossing analysis for system sizes $(L, 2L-2)$: pseudocritical coupling goes to zero as $\alpha_c(L) \simeq 1/\ln(L)$

<u>**Conclusion 1:**</u>

True long-range antiferromagnetic order for any $\alpha > 0$

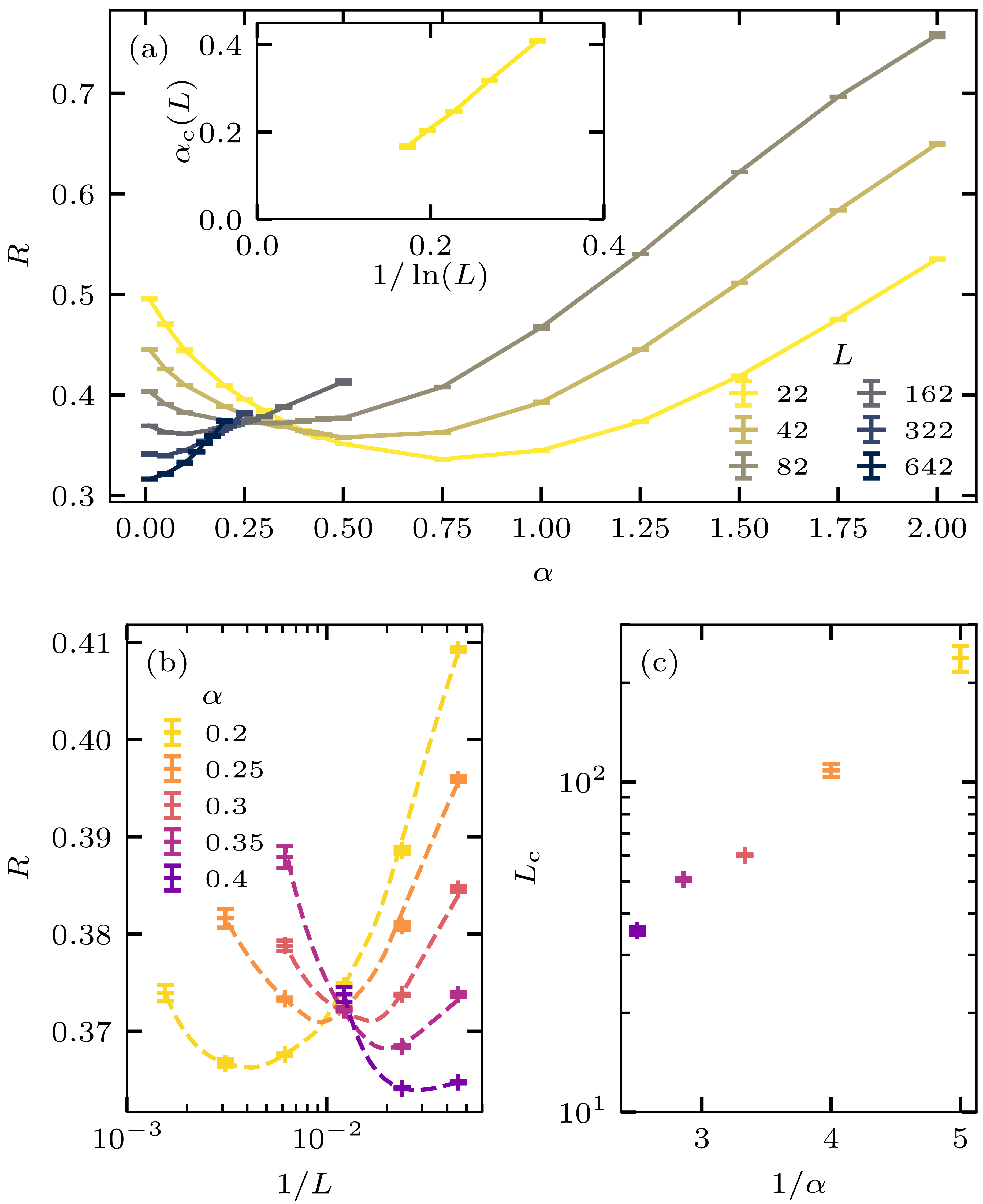
$\Longleftrightarrow$ Spontaneous breaking of the global SO(3) symmetry of system + bath (beyond Mermin-Wagner theorem)

- $R(L)$ only increases beyond length scale $L_c(\alpha) \propto e^{\xi/\alpha}$

<u>**Conclusion 2:**</u>

Coupling to the ohmic bath is marginally relevant

$\Longleftrightarrow$ Exponentially large lattices are required to observe ordering for small α



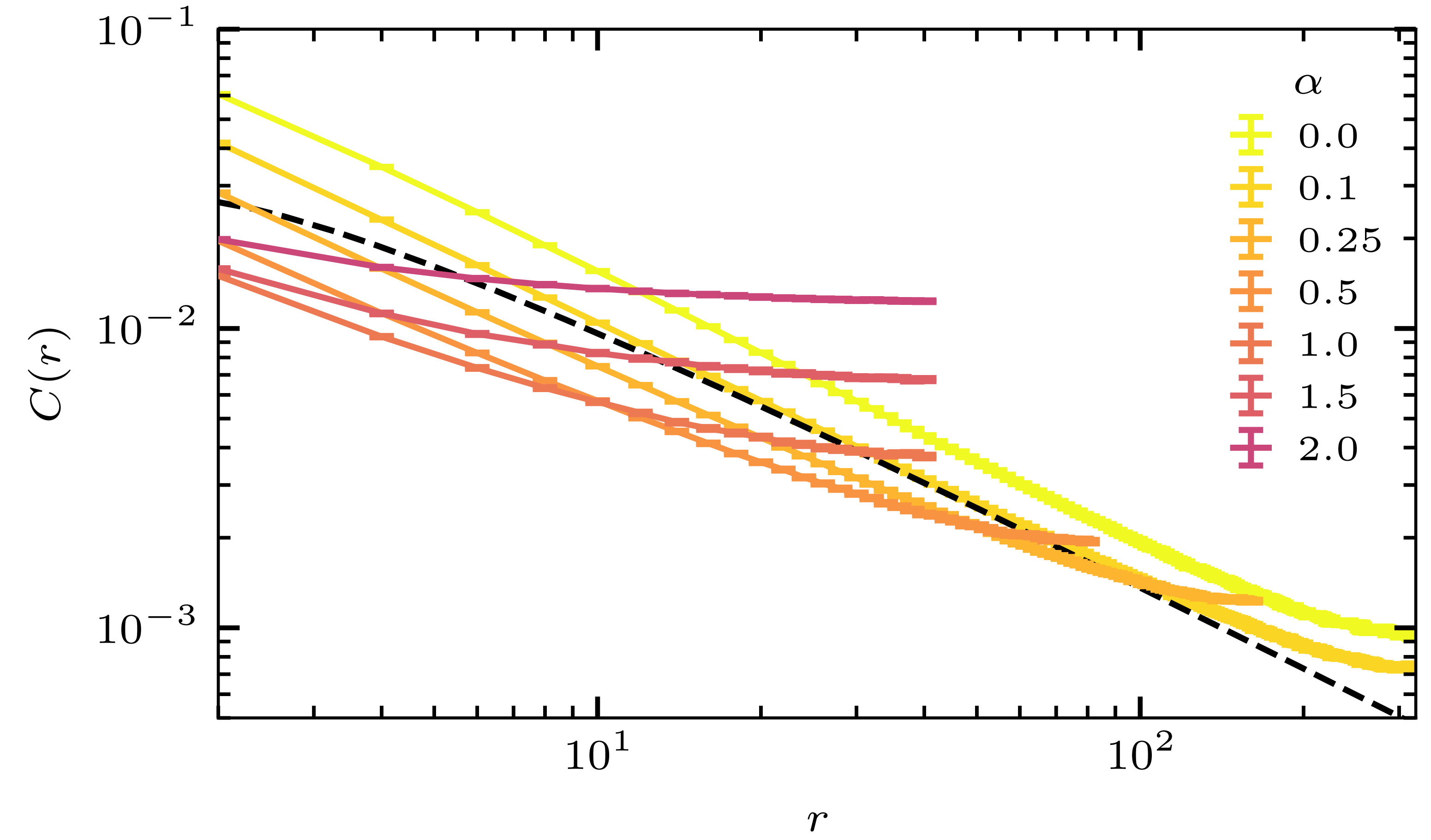
Properties of the long-range-ordered phase

Linear spin-wave theory:

- inverse propagator $\omega^2 + (v_\mathrm{s} k)^2 + c\,\alpha\,|\omega|^s$ $\quad s = 1$

  $\longrightarrow$ quantum fluctuations do not destroy antiferromagnetic order anymore

  $\longrightarrow$ conformal invariance is broken $\longrightarrow$ $z = 2$



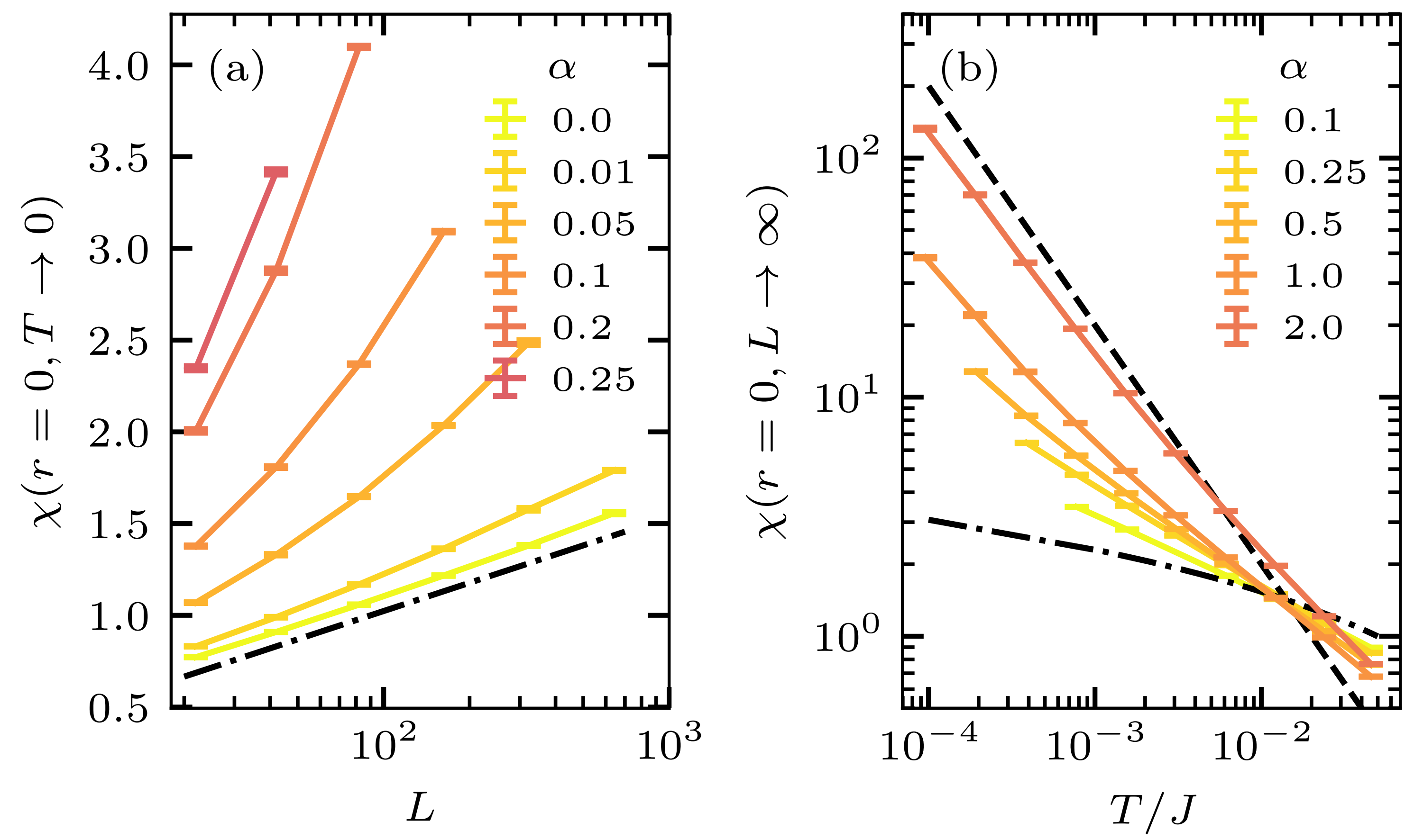
Real-space correlations:

- $r < L_\mathrm{c}(\alpha)$: characteristic decay of Heisenberg limit
- $r > L_\mathrm{c}(\alpha)$: long-range order is approached as $m^2 \propto e^{-\xi/\alpha}$

Dynamical correlations

$$\chi(r=0, L, \beta) = \frac{1}{L} \sum_{i=1}^{L} \int_0^\beta d\tau\, \langle \hat{S}_i^z(\tau) \hat{S}_i^z(0) \rangle$$

- $r < L_\mathrm{c}(\alpha)$: temporal correlations deviate strongly from Heisenberg limit
- $r > L_\mathrm{c}(\alpha)$: long-range order: $\chi(r=0, L \to \infty, \beta) \propto \beta$



Conclusions

Honorable mention

Dissipation-induced order in the 1D Bose-Hubbard model

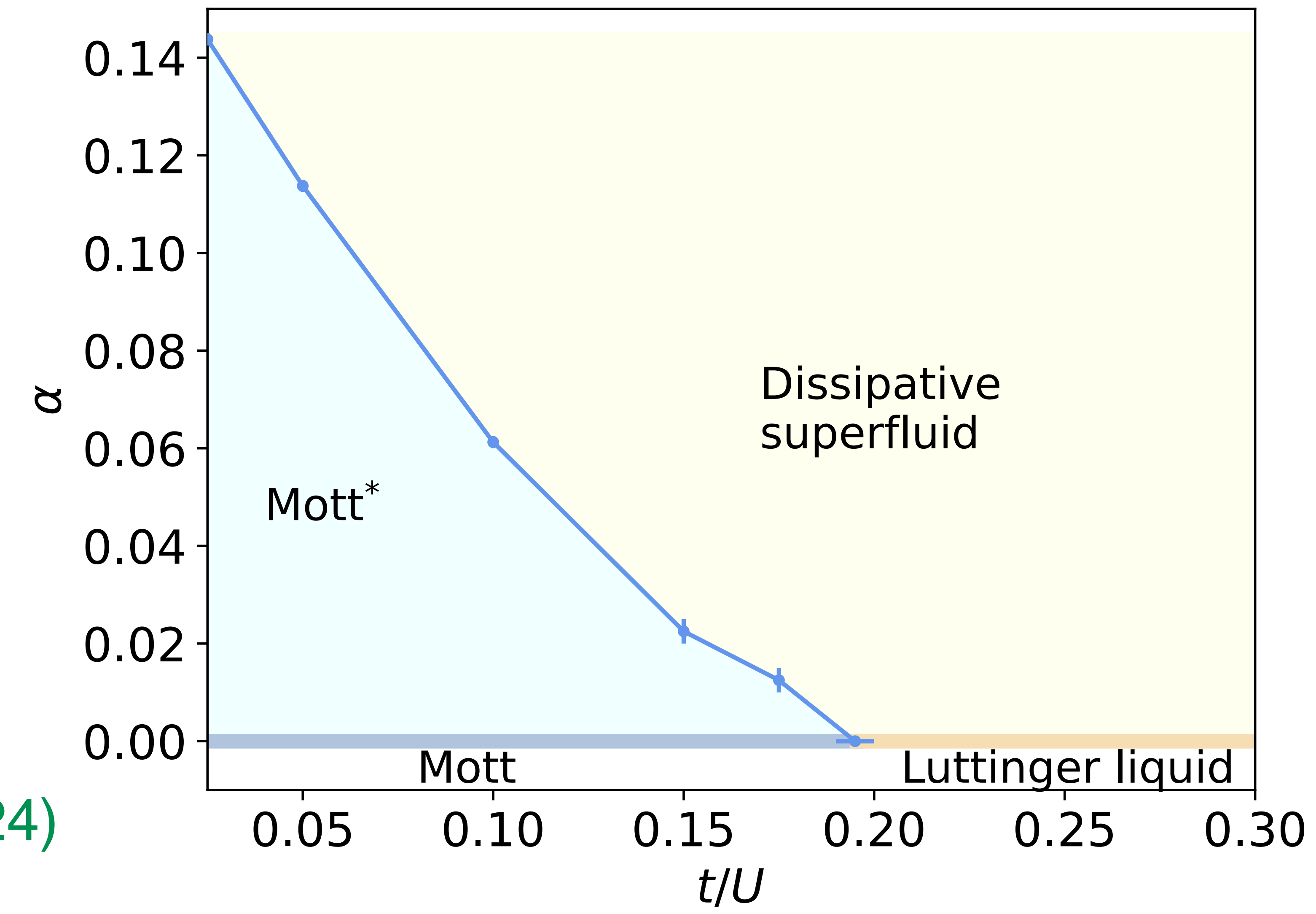
$$\hat{H}_\mathrm{s} = -t\sum_i (\hat{b}_i^\dagger \hat{b}_{i+1} + \mathrm{H.c.}) + \frac{U}{2}\sum_i \hat{b}_i^\dagger \hat{b}_i^\dagger \hat{b}_i \hat{b}_i - \mu \sum_i \hat{b}_i^\dagger \hat{b}_i$$

⟶ bath: $\hat{H}_\mathrm{b} = \sum_{iq} \omega_q \hat{a}_{iq}^\dagger \hat{a}_{iq}$ $\quad \hat{H}_\mathrm{sb} = \sum_{iq} \lambda_q (b_i^\dagger a_{iq} + \mathrm{H.c.})$

⟶ implementation within worm algorithm

⟶ long-range superfluid order in 1D

Ribeiro, McClarty, Ribeiro, **MW**, PRB (2024)



Light-matter interactions

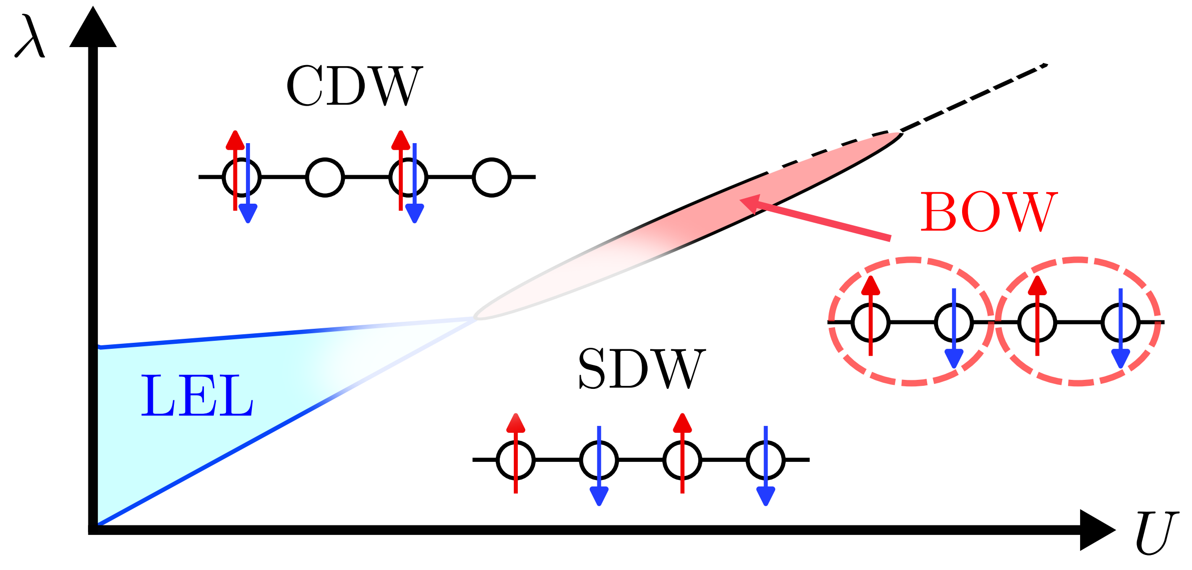
⟶ e.g., Dicke-type models: $\hat{H} = \hat{H}_\mathrm{s} + \omega_0\, \hat{a}^\dagger \hat{a} + \frac{\lambda}{\sqrt{L}} (\hat{a}^\dagger + \hat{a}) \sum_i \hat{S}_i^x$

Electron-phonon interactions

⟶ directed-loop algorithm for ret. interactions **MW**, Assaad, Hohenadler, PRL (2017)

⟶ e.g., 1D Hubbard-Holstein model

$$\hat{H} = -t\sum_{i\sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{i+1,\sigma}^\dagger + \mathrm{H.c.}) + U\sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} + \omega_0 \sum_i \hat{a}_i^\dagger \hat{a}_i + \gamma \sum_i (\hat{a}_i^\dagger + \hat{a}_i)\, \hat{n}_i$$



MW, arXiv (2024)

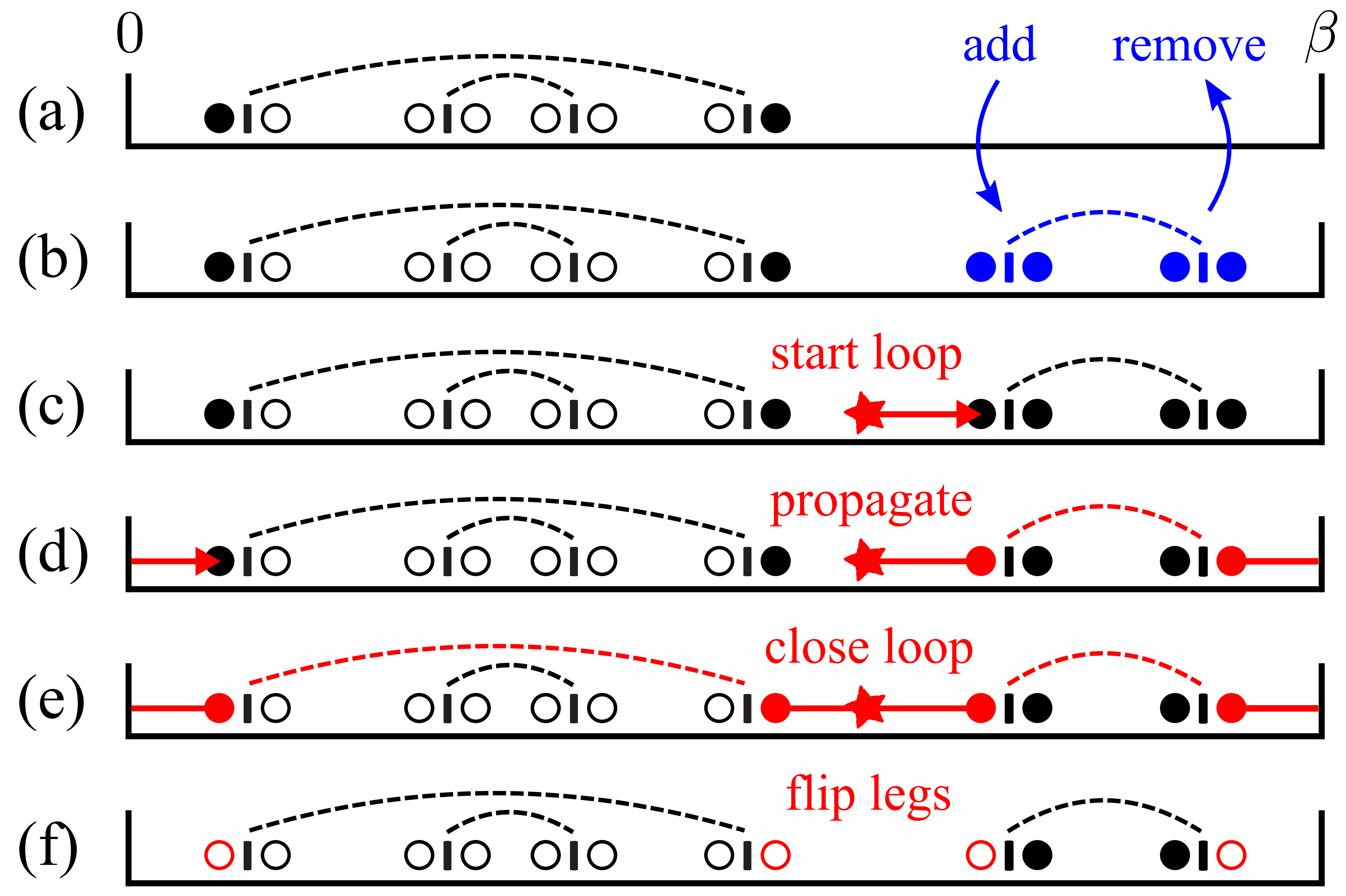
Conclusions

Main results:

(i) generalization of directed-loop algorithm to retarded spin-flip interactions using the novel wormhole updates

(ii) spin-boson model: fixed-point annihilation & pseudo-criticality

(iii) Heisenberg chain: dissipation-induced AFM order beyond the Mermin-Wagner theorem



Applicability of the method:

(i) retarded spin-flip interactions: quantum dissipation, light-matter interactions, …

(ii) spin-phonon & 1D electron-phonon interactions ⟶ **MW**, Assaad, Hohenadler, PRL (2017)

Thanks to:

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