Participation Entropies and Spectroscopy for Quantum Spin Models

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This Talk

* Shannon-Rényi (participation) entropies for quantum many-body systems

* Participation spectra
  An alternative route for entanglement Hamiltonian and spectra

* References

D.J Luitz, F. Alet, NL, Phys. Rev. Lett. 112, 057203 (2014)
D.J Luitz, F. Alet, NL, Phys. Rev. B. 89, 165106 (2014)
D.J Luitz, NL, F. Alet, JSTAT P08007 (2014)

Shannon-Rényi (Participation) entropies

Expand a given state in a computational local basis

$$|\mathrm{GS}\rangle = \sum_{i=1}^{\mathcal{N}} a_i |i\rangle \quad \text{Define} \quad p_i = |a_i|^2, \quad \sum_i p_i = 1$$

$$S_q = \frac{1}{1-q} \ln \sum_i p_i^q \qquad S_1 = -\sum_i p_i \ln p_i$$

Simple expectations

$$p_i \propto \exp(-i/\xi) \Rightarrow S_q \approx \ln \xi \qquad \textbf{localized}$$

$$p_i \propto 1/\mathcal{N} \Rightarrow S_q \approx \ln \mathcal{N} \qquad \textbf{delocalized}$$

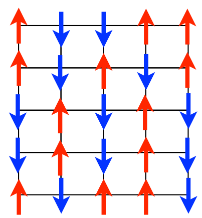
Multifractality

$$S_q = D_q \ln \mathcal{N} \quad \text{with} \quad D_q < 1$$

Quantum Monte Carlo sampling

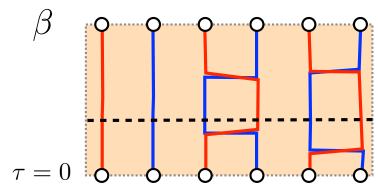
- Importance sampling actually does the exact job !
- Probability of seeing configuration $|i\rangle$ in Monte Carlo

Classical MC



$$p_i^{\rm MC} \propto e^{-\beta E_i}$$

Quantum MC



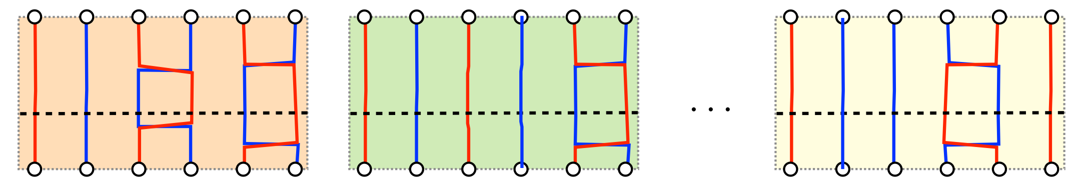
$|i\rangle = |\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\rangle$

$$p_i^{\rm MC} \propto \langle i|e^{-\beta H}|i\rangle \overset{\beta\to\infty}{=} a_i^2 = p_i$$

$$p_i = \langle |i\rangle\langle i|\rangle$$

- Measure Histogram $H(|i\rangle)$ and normalize to obtain all p_i and therefore all S_q

- Replica trick for integer $q \geq 2$: Simulate q independent copies



$|i_1\rangle = |\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\rangle$ $\quad |i_2\rangle = |\uparrow\downarrow\uparrow\downarrow\downarrow\uparrow\rangle$ $\quad \cdots \quad |i_q\rangle = |\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\rangle$

Estimator for $\sum_i p_i^q = \langle \delta_{|i_1\rangle,|i_2\rangle,\cdots,|i_q\rangle}\rangle$

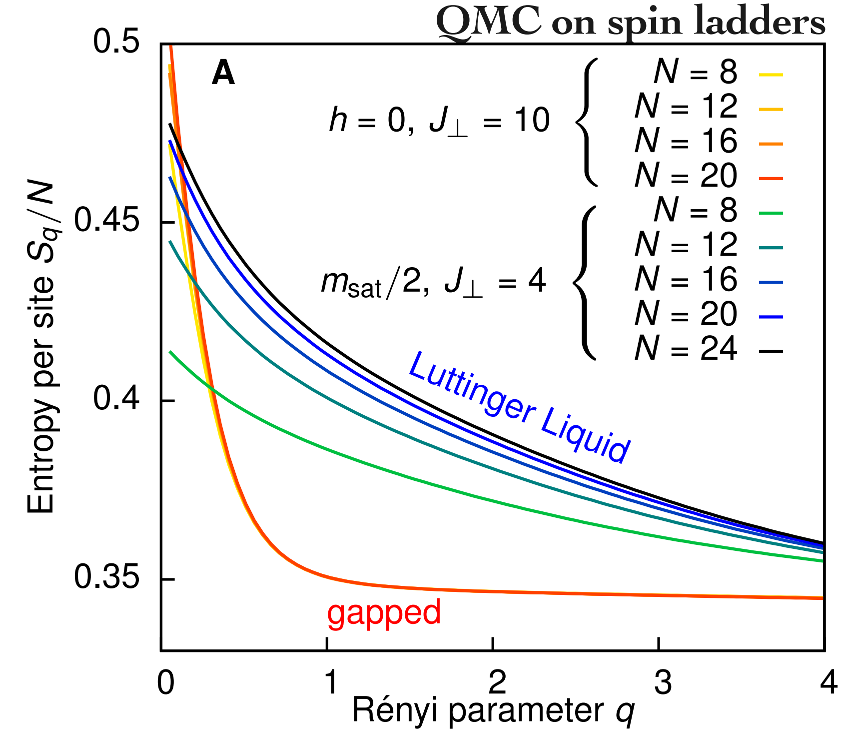
- S_∞ is easily measured as $S_\infty = -\ln(p_{\max})$

Generic multifractal behavior for quantum many-body systems, independent of the physical state

mutifractal dimension

$$S_q = D_q \ln \mathcal{N}$$

QMC on spin ladders



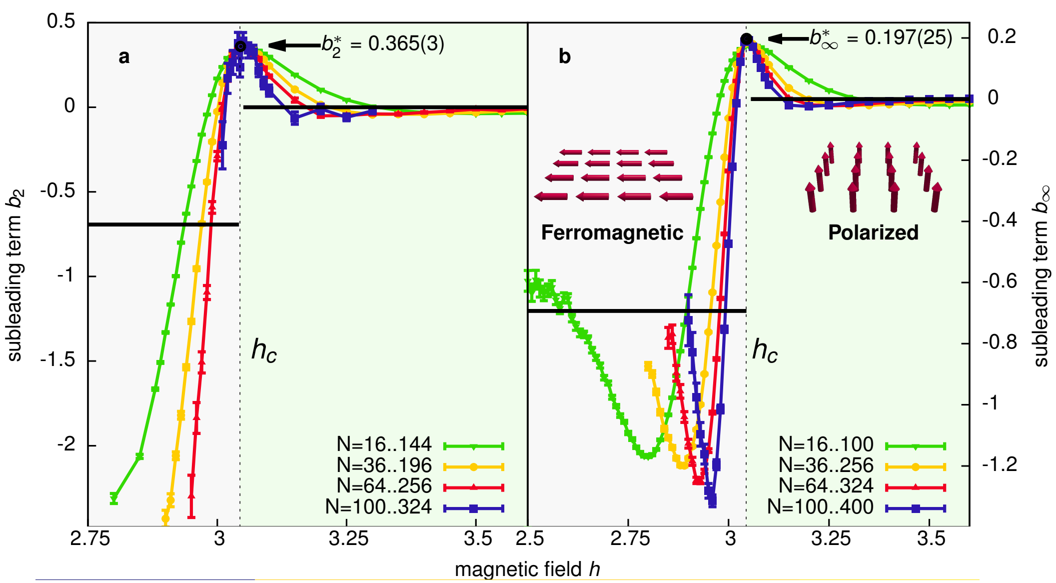
Y. Atas and E. Bogomolny, Phys. Rev. E 86, 021104 (2012)

J. Rodríguez-Laguna, P. Migdal, M. Ibáñez Berganza, M. Lewenstein, G. Sierra, New J. Phys. 14, 053028 (2012)

Universality encoded in subleading terms

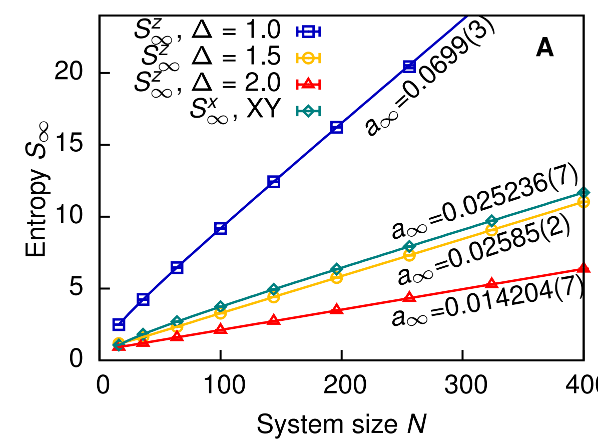
$$S_q = D_q \ln \mathcal{N} \quad + \quad \cdots$$

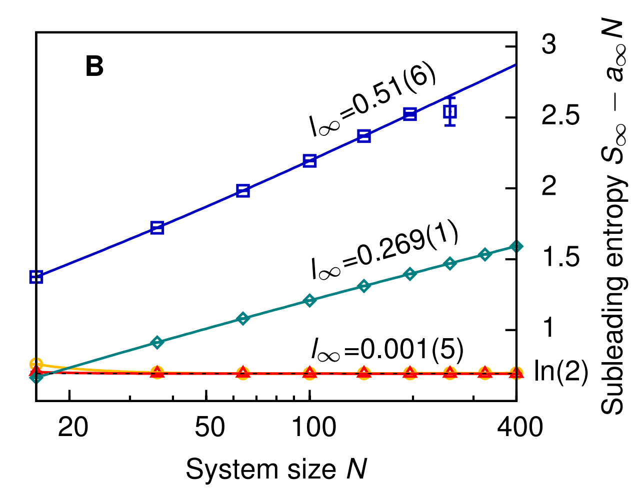
$S_q = a_q N + b + o(1)$ **Gapped states**



Continuous symmetry broken phases

$$S_q = a_q N + \boldsymbol{l_q \ln N} + b_q + \mathcal{O}\left(\frac{1}{N}\right)$$





Luttinger liquids

$$b_q = -\frac{1}{2}\left(\ln K + \frac{\ln q}{q-1}\right) \qquad \text{for} \quad q \leq q_c = K d^2$$

$$b_q = \frac{1}{1-q}\left(q \ln \sqrt{K} + \ln \mathcal{D}\right) \qquad \text{for} \quad q \geq q_c$$

Critical points

$$S_q = a_q N + \boldsymbol{b_q} + \mathcal{O}\left(\frac{1}{N}\right)$$

J.M Stephan, S. Furukawa, G. Misguich, V. Pasquier, Phys. Rev. B 80, 184421 (2009)

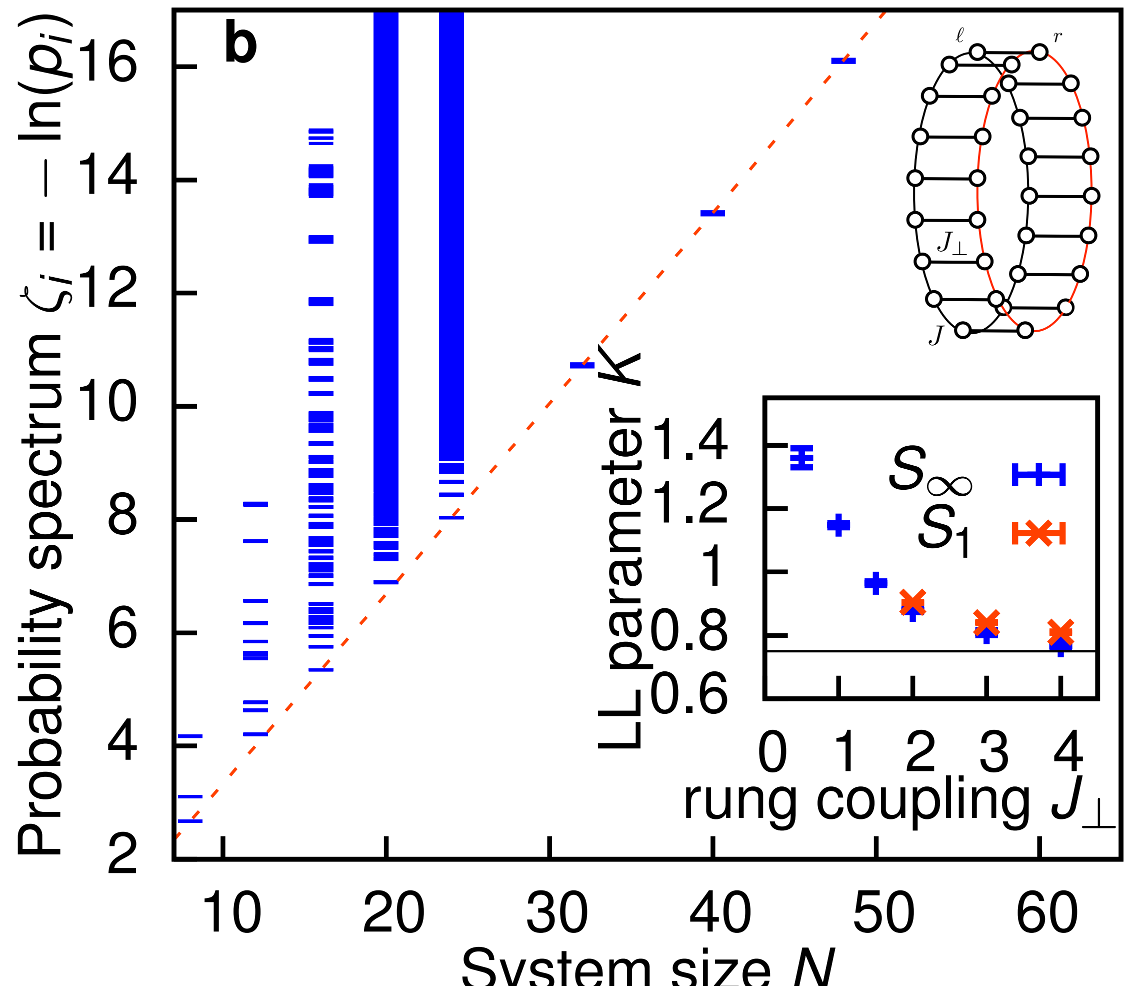
Universality in a single coefficient of the wave function

* Quantum antiferromagnet

$$|\mathrm{GS}\rangle = a_{\max}\Big(|\uparrow\downarrow\uparrow\cdots\downarrow\rangle + e^{i\theta}|\downarrow\uparrow\downarrow\cdots\uparrow\rangle\Big)$$
$$+a'_{\max}\Big(|\uparrow{\color{red}\downarrow\downarrow}{\color{green}\uparrow\uparrow}\downarrow\uparrow\cdots\downarrow\rangle+\cdots\Big)$$
$$+\cdots$$

$$S_\infty = -\ln p_{\max}$$

$$b_\infty = -\frac{1}{2}\ln K_{\mathrm{LL}}$$



A quite new field

Editors' Suggestion

Shannon and entanglement entropies of one- and two-dimensional critical wave functions
Phys. Rev. B **80**, 184421 – Published 20 November 2009
Jean-Marie Stéphan, Shunsuke Furukawa, Grégoire Misguich, and Vincent Pasquier

Phase transition in the Rényi-Shannon entropy of Luttinger liquids
Phys. Rev. B **84**, 195128 – Published 28 November 2011
Jean-Marie Stéphan, Grégoire Misguich, and Vincent Pasquier

Logarithmic Terms in Entanglement Entropies of 2D Quantum Critical Points and Shannon Entropies of Spin Chains
Phys. Rev. Lett. **107**, 020402 – Published 5 July 2011
Michael P. Zaletel, Jens H. Bardarson, and Joel E. Moore

Multifractality of eigenfunctions in spin chains
Phys. Rev. E **86**, 021104 – Published 3 August 2012
Y. Y. Atas and E. Bogomolny

Universal Behavior of the Shannon Mutual Information of Critical Quantum Chains
Phys. Rev. Lett. **111**, 017201 – Published 2 July 2013
F. C. Alcaraz and M. A. Rajabpour

Universal Behavior beyond Multifractality in Quantum Many-Body Systems
Phys. Rev. Lett. **112**, 057203 – Published 6 February 2014
David J. Luitz, Fabien Alet, and Nicolas Laflorencie

Shannon-Rényi entropies and participation spectra across three-dimensional $O(3)$ criticality
Phys. Rev. B **89**, 165106 – Published 7 April 2014
David J. Luitz, Fabien Alet, and Nicolas Laflorencie

Editors' Suggestion

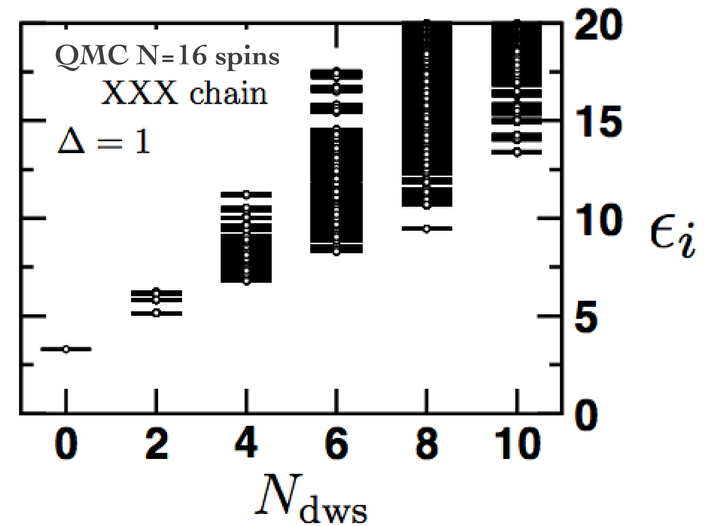
Shannon and Rényi mutual information in quantum critical spin chains
Phys. Rev. B **90**, 045424 – Published 25 July 2014
Jean-Marie Stéphan

Universal behavior of the Shannon and Rényi mutual information of quantum critical chains
Phys. Rev. B **90**, 075132 – Published 19 August 2014
F. C. Alcaraz and M. A. Rajabpour

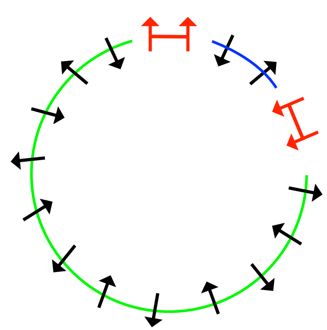
Full Participation Spectrum

✱ **XXZ chain** $\mathcal{H} = \sum_{i=1}^{L} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right)$

$$|\mathrm{GS}\rangle = \sum_{i=1}^{\mathcal{N}} a_i |i\rangle \qquad \epsilon_i = -\ln p_i$$



✱ **Spectrum is resolved in term of domain walls**



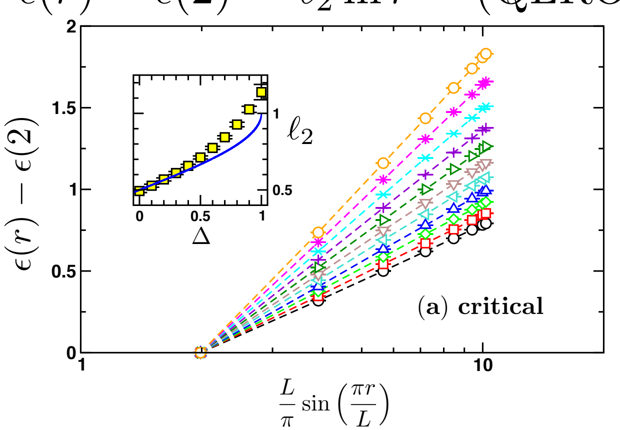
✱ **Spectral gap finite**

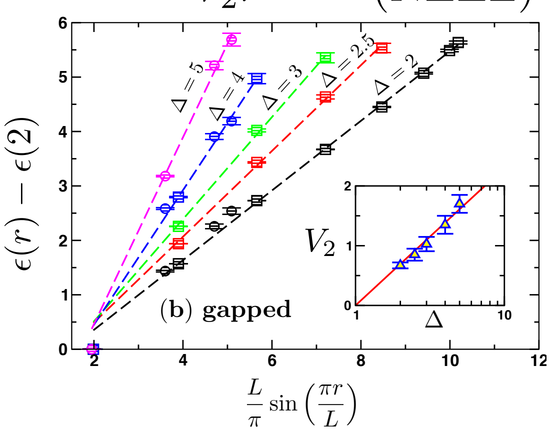
$$\mathcal{G} = -\ln\left(\left[\frac{2E_{\mathrm{gs}}}{N_{\mathrm{bonds}}} + \frac{\Delta}{2}\right]^2\right)$$

$$= -\ln\left(\left[\frac{2(E_{\mathrm{gs}} - E_{\mathrm{classical}})}{N_{\mathrm{bonds}}}\right]^2\right)$$

✱ **Confining potential for the domain walls**

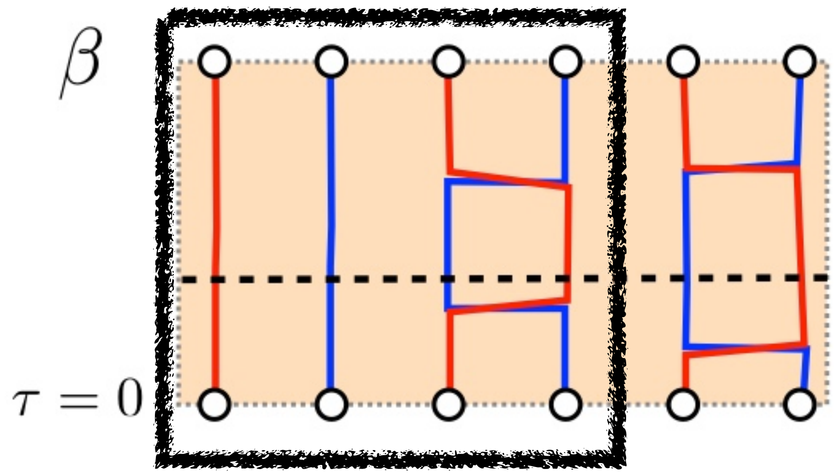
$\epsilon(r) - \epsilon(2) \sim \ell_2 \ln \tilde{r}$ (QLRO) $\qquad \sim V_2 \tilde{r}$ (NEEL)





Subsystems

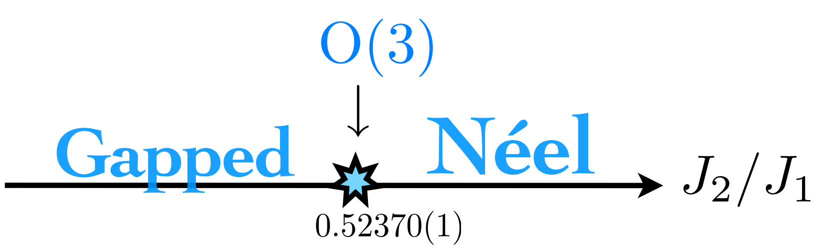
* Diagonal component of the reduced density matrix accessible using QMC



$$|i\rangle_{\rm B} = |\uparrow\downarrow\downarrow\uparrow\rangle$$

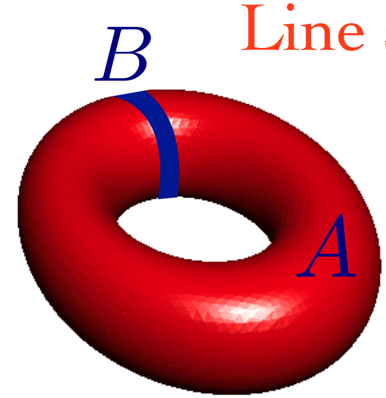
* 1D subsystem in 2D dimerized S=1/2 Heisenberg model

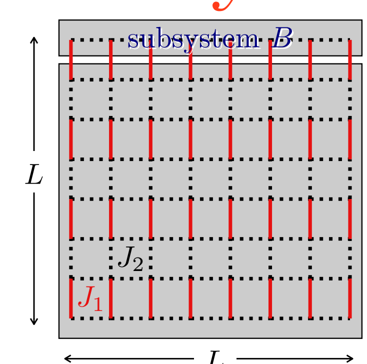
$$H_{\rm dimer} = J_1 \sum_{\rm dimers} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\rm links} \vec{S}_i \cdot \vec{S}_j$$



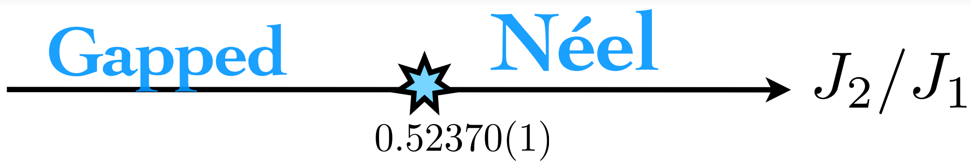
A.W. Sandvik (2010)

Line shaped subsystem



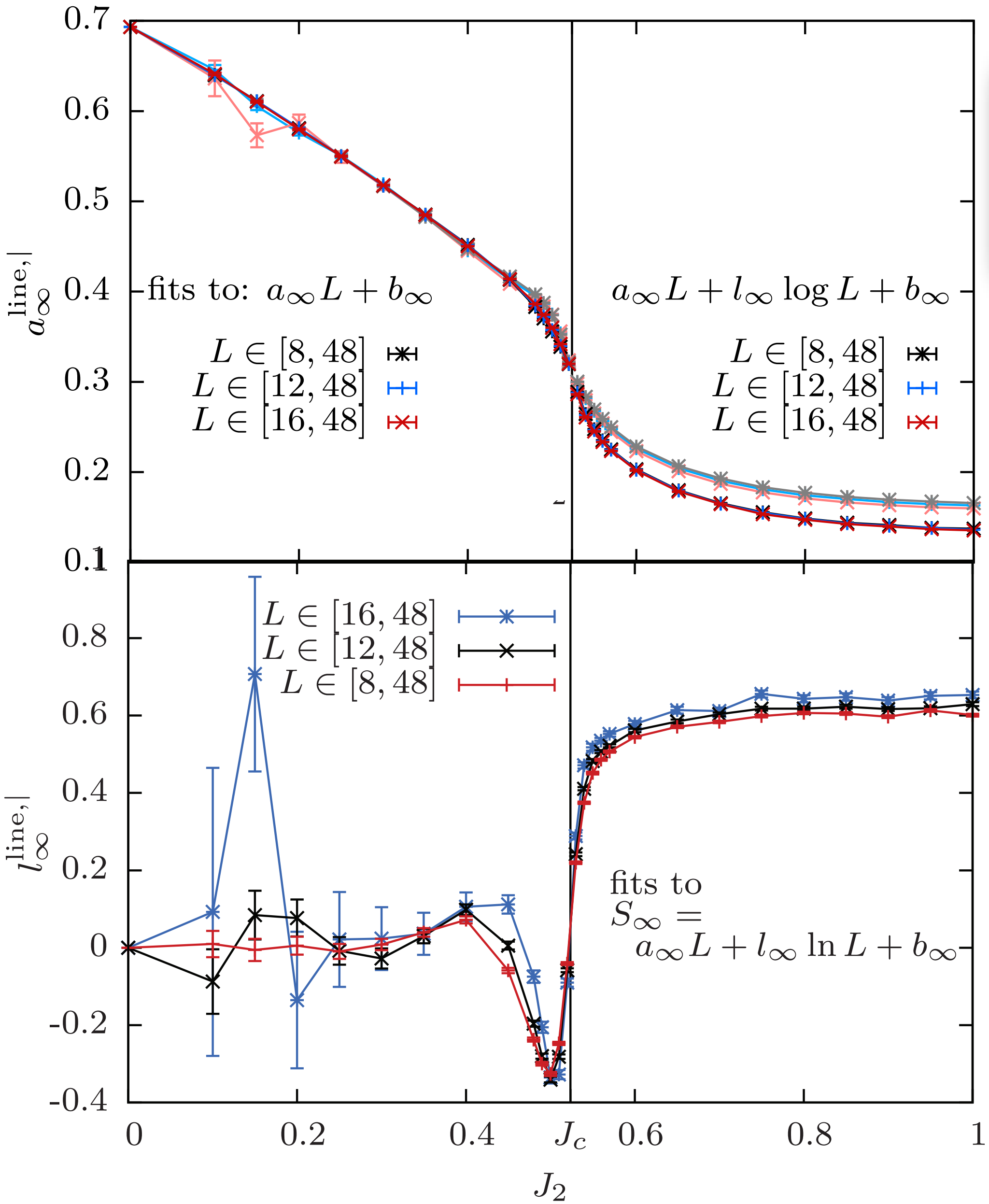


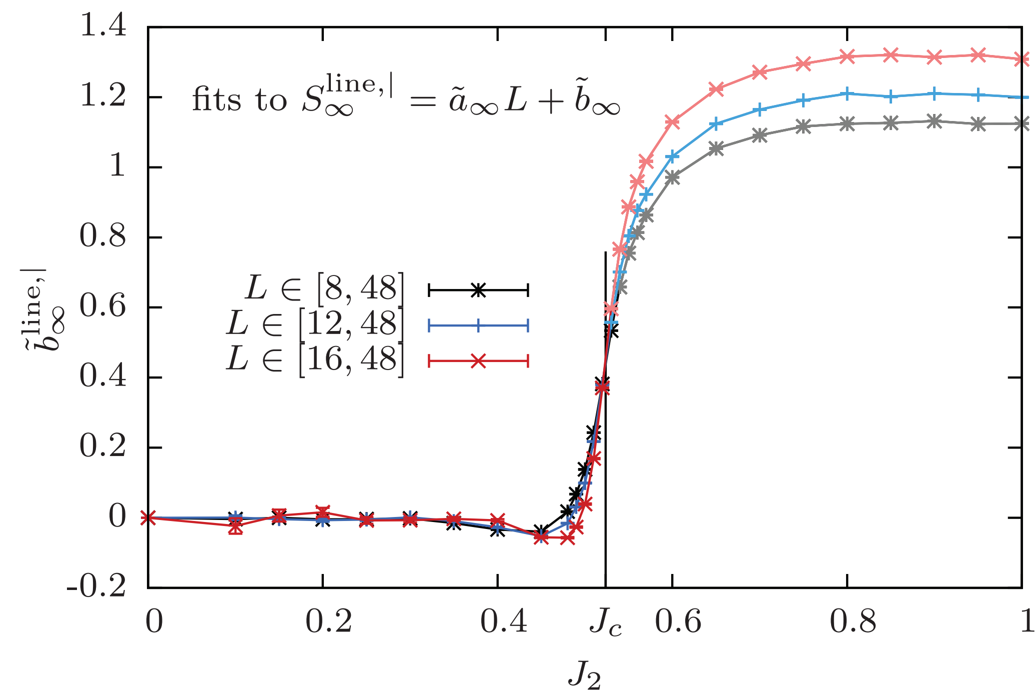
Participation entropy of a line subsystem across O(3)



$$S_\infty^{\mathrm{line}} = -\ln p_{\mathrm{Neel}}^{\mathrm{line}}$$

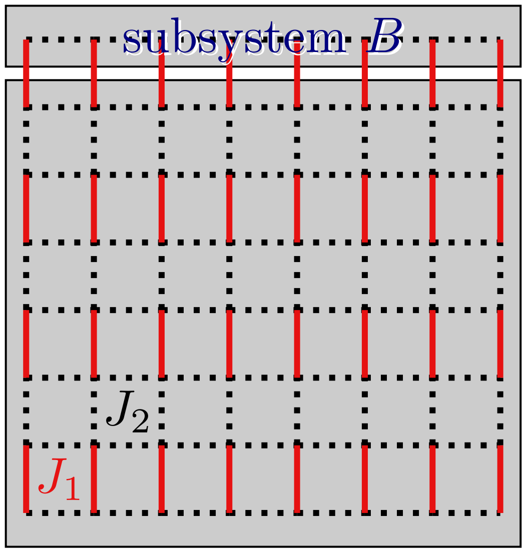
$$S_\infty^{\mathrm{line}}(L) = a_\infty^{\mathrm{line}} L + l_\infty^{\mathrm{line}} \ln L + b_\infty^{\mathrm{line}}$$

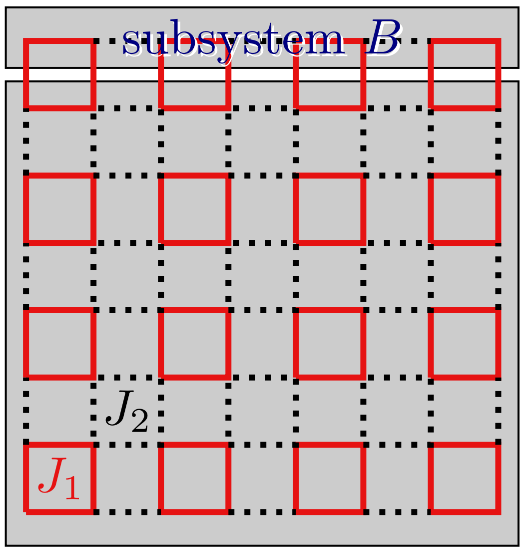




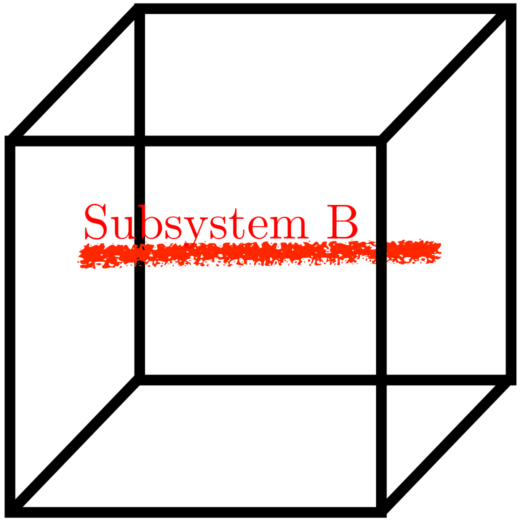
Universal constant at the O(3) critical point

✱ 2D Quantum critical point





✱ 3D Classical transition at finite T



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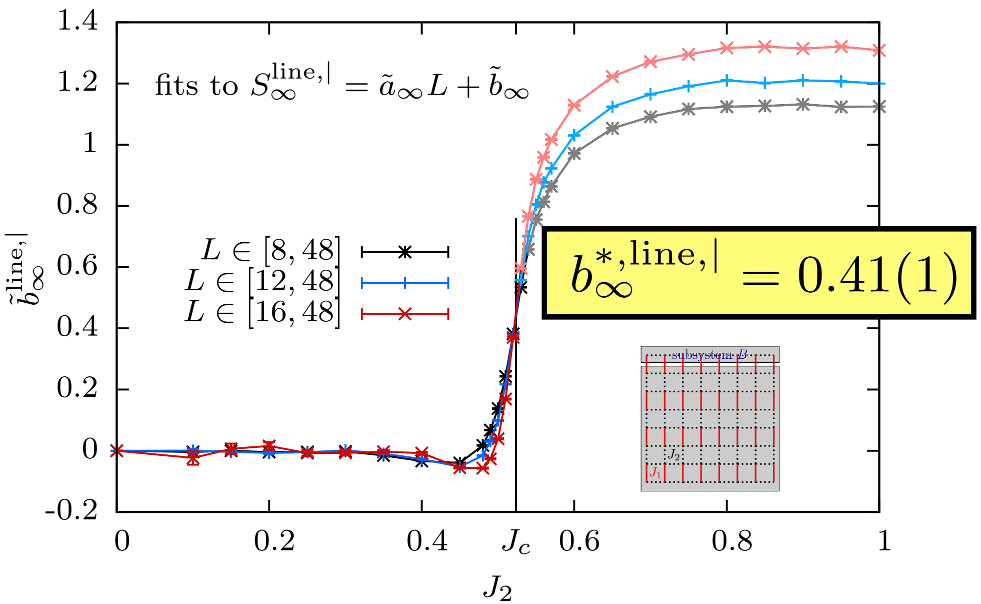
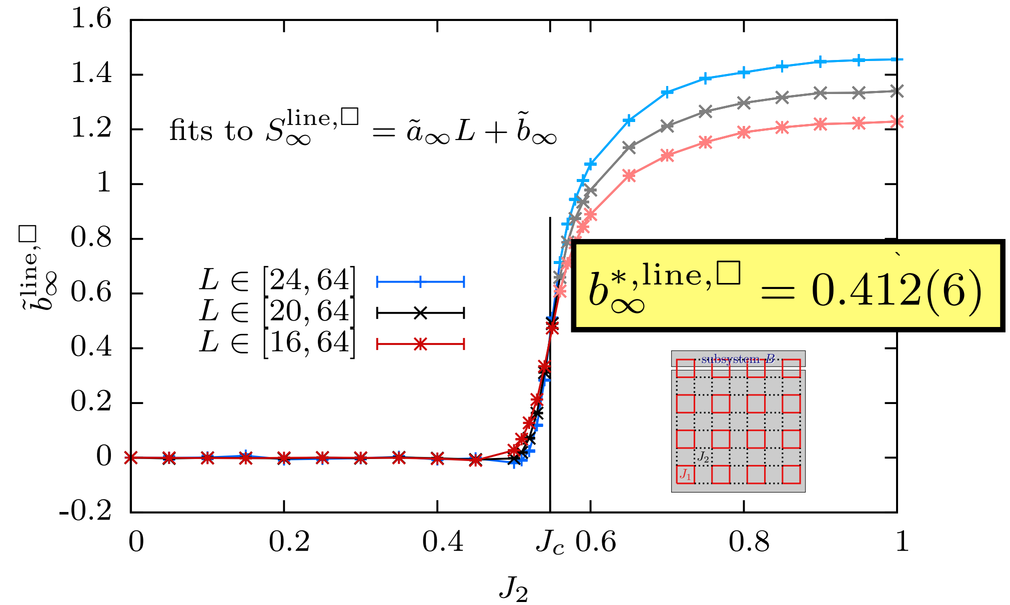
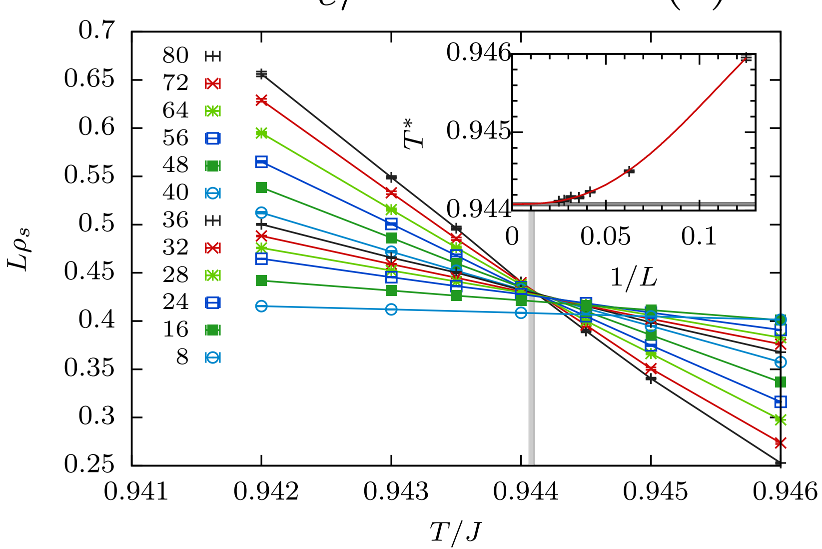
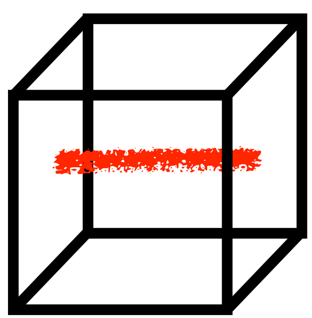


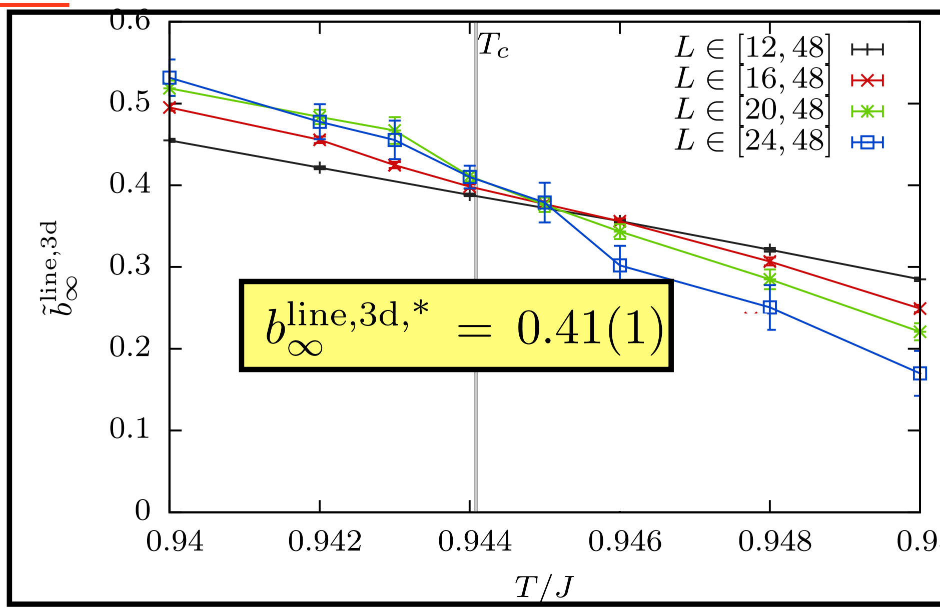


✱ 3D Classical transition at finite T

$T_c/J = 0.94408(2)$

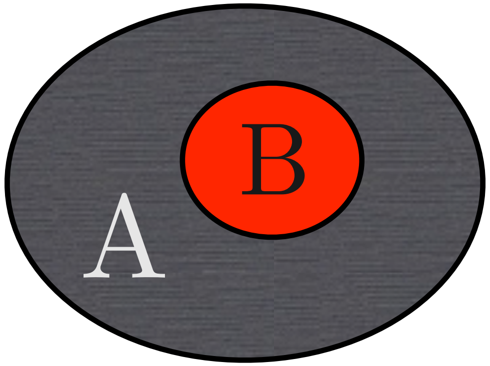






Participation Spectra of subsystems

Reduced density matrix



$$\hat{\rho}_{\mathrm{B}} = \mathrm{Tr}_{\mathrm{A}} |\mathrm{GS}\rangle\langle\mathrm{GS}| = \exp(-\beta_{\mathrm{eff}}\mathcal{H}_E)$$

$$(-\ln \hat{\rho}_{\mathrm{B}}) \quad \longrightarrow \quad \text{Entanglement Spectrum}$$

$$\hat{\mathcal{H}}_E = \text{ Entanglement Hamiltonian}$$

Very hard to compute in general cases

Participation spectrum = diagonal of the RDM

$$\epsilon_i^B = -\ln\left(\langle i|\hat{\rho}_B|i\rangle\right)$$

Accessible using QMC in a given computational basis (e.g. {Sz})

If $\mathcal{H}_E$ is the correct Entanglement Hamiltonian and β_{eff} the correct effective temperature, then

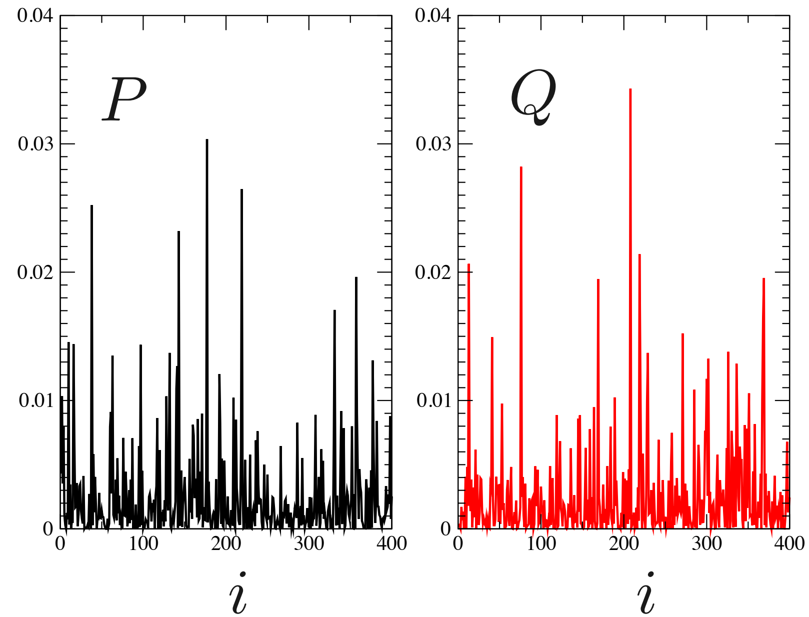
$$\epsilon_i^E = -\ln\left(\langle i|\exp(-\beta_{\mathrm{eff}}\hat{\mathcal{H}}_E)|i\rangle\right) = \epsilon_i^B \quad \forall i, \ (i.e.\ 2^N numbers!)$$

How much two spectra are close ?

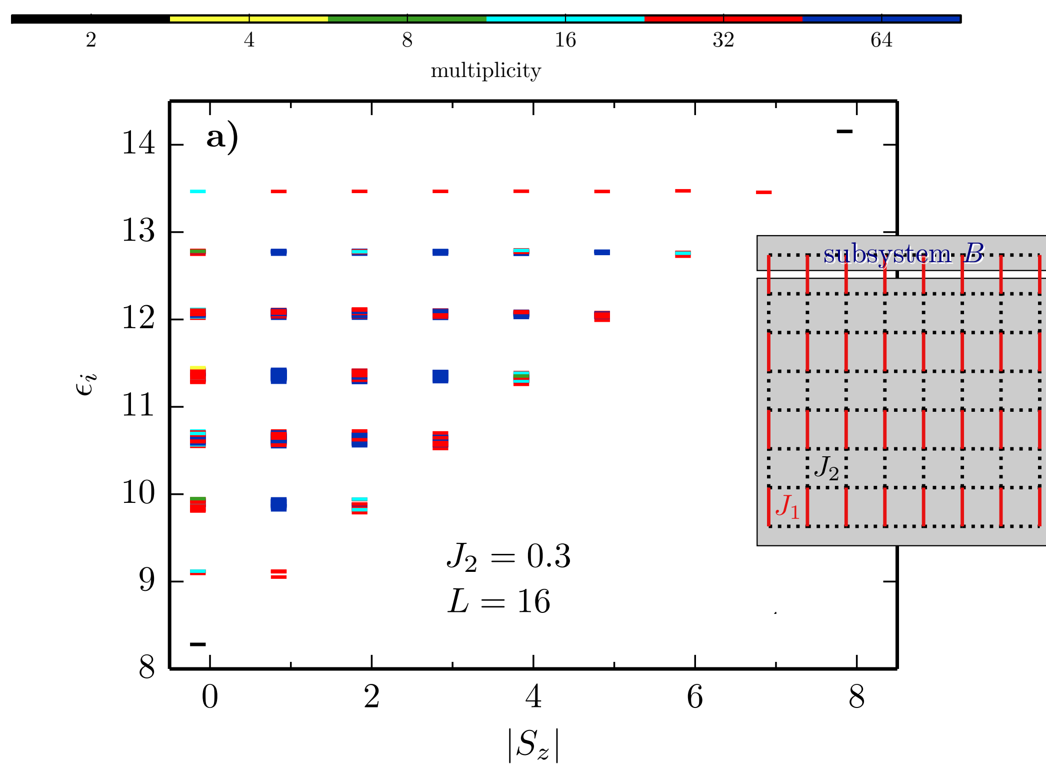
✱ Kulback-Leibler and Rényi divergences

$$I_1(Q|P) = \sum_i Q_i \ln \frac{Q_i}{P_i}$$

$$I_q(Q|P) = \frac{1}{1-q} \ln \left(\sum_i \frac{Q_i^q}{P_i^{q-1}} \right)$$



✱ Example for a gapped phase



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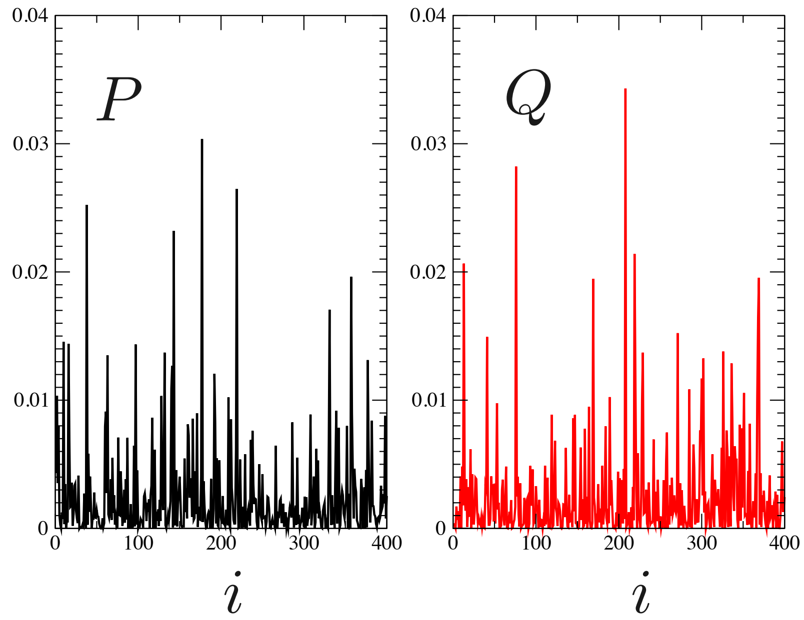


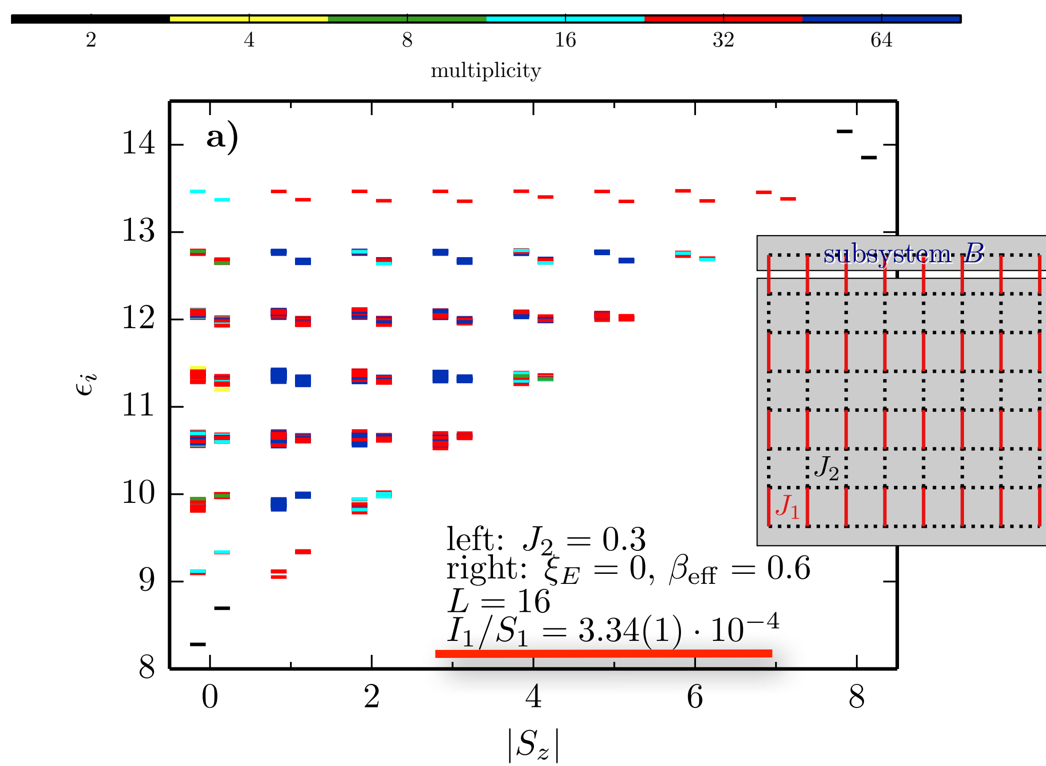
✱ Example for a gapped phase

$$\mathcal{H}_E = \sum_{i \in B} \vec{S}_i \cdot \vec{S}_{i+1}, \qquad \text{and} \qquad T_{\text{eff}} = \frac{1}{2J_2}$$

Short range

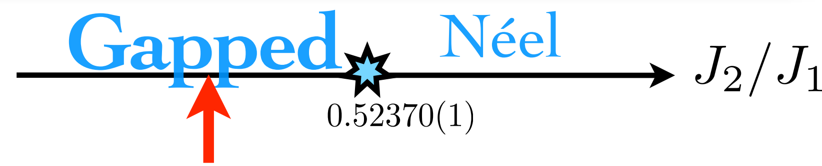
Entanglement Hamiltonian

LADDERS: Poilblanc et al. 2012-2012, Lauchli and Schliemann (2012), Chen and Fradkin (2013)...



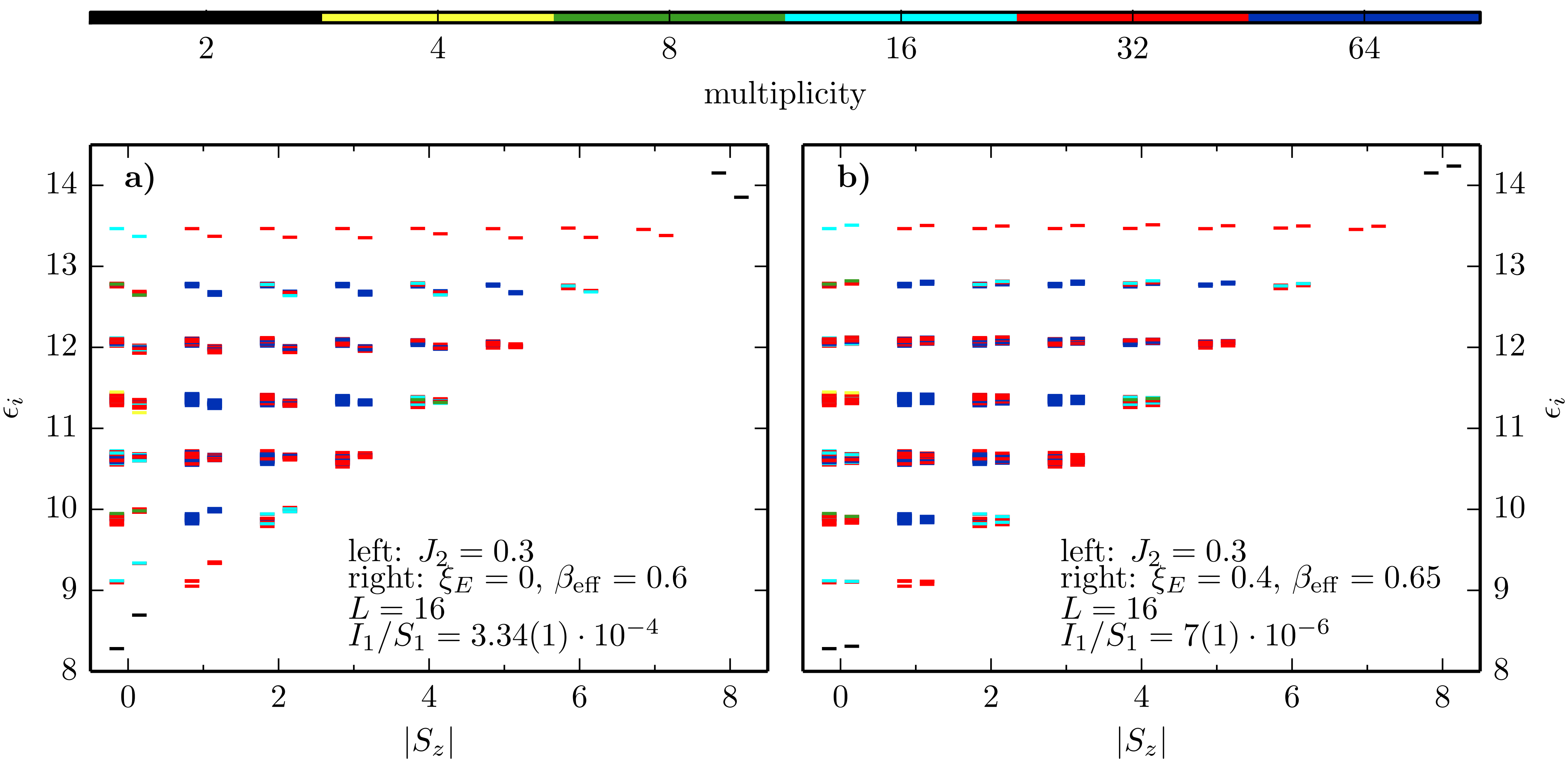
Good agreement but can be improved

Best entanglement Hamiltonian in the gapped regime?

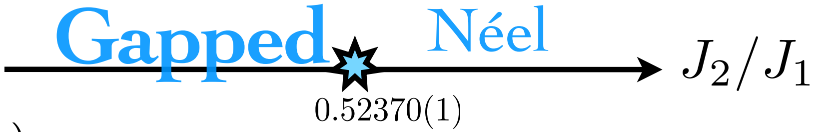


$$\mathcal{H}_E(\xi) = -\sum_{i,j\in B} (-1)^{r_{ij}} \mathrm{e}^{-\frac{(r_{ij}-1)}{\xi_E}} \vec{S}_i \cdot \vec{S}_j$$

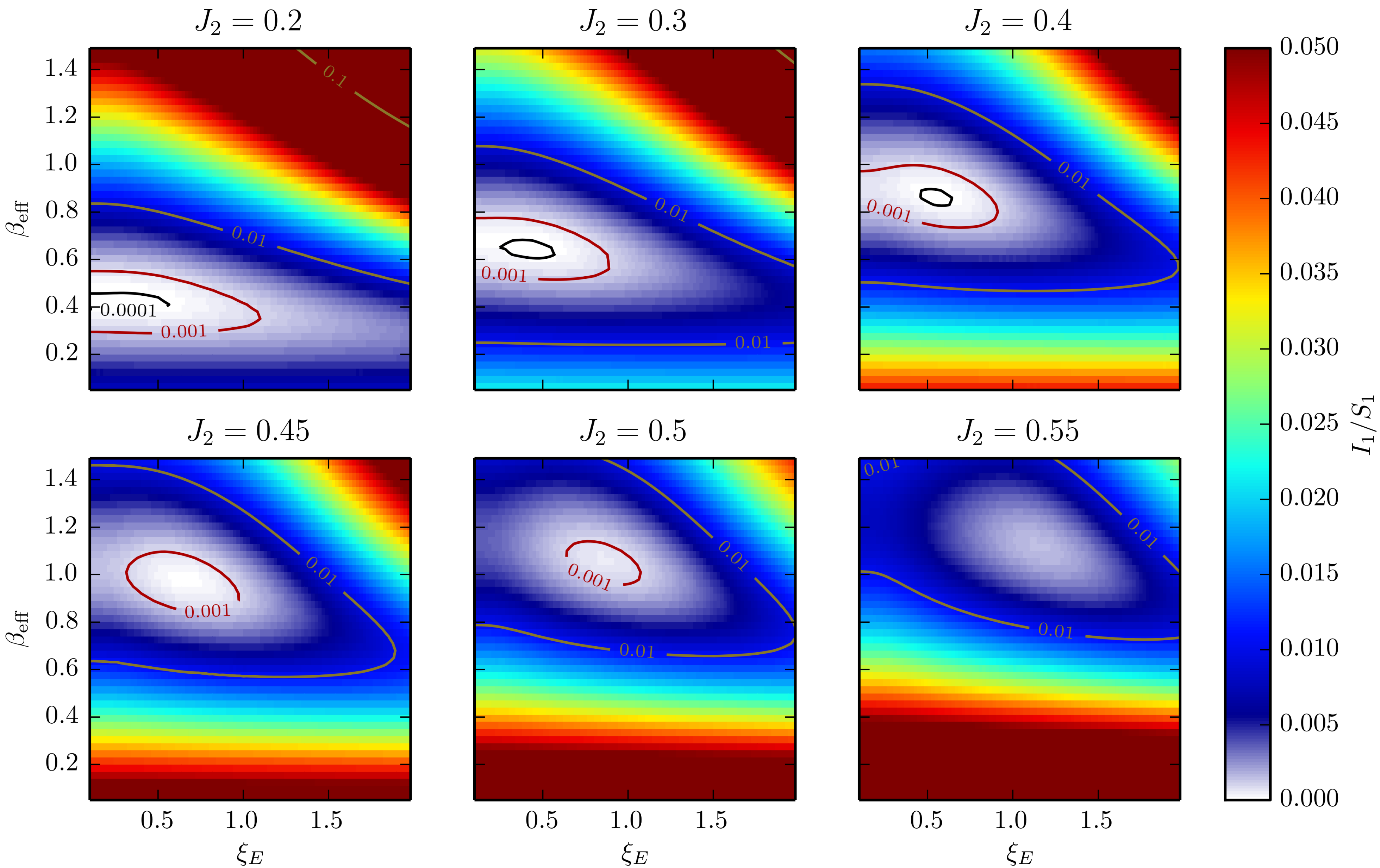
for spin ladders, see: J. I. Cirac, D. Poilblanc, N. Schuch, and F. Verstraete, PBR 2012



Across the gapped regime



$$\mathcal{H}_E(\xi) = -\sum_{i,j\in B} (-1)^{r_{ij}} \mathrm{e}^{-\frac{(r_{ij}-1)}{\xi_E}} \vec{S}_i \cdot \vec{S}_j$$



Effective parameters in the gapped regime

Perturbative expansion J2<<1 [Lauchli-Schlieman 2012]

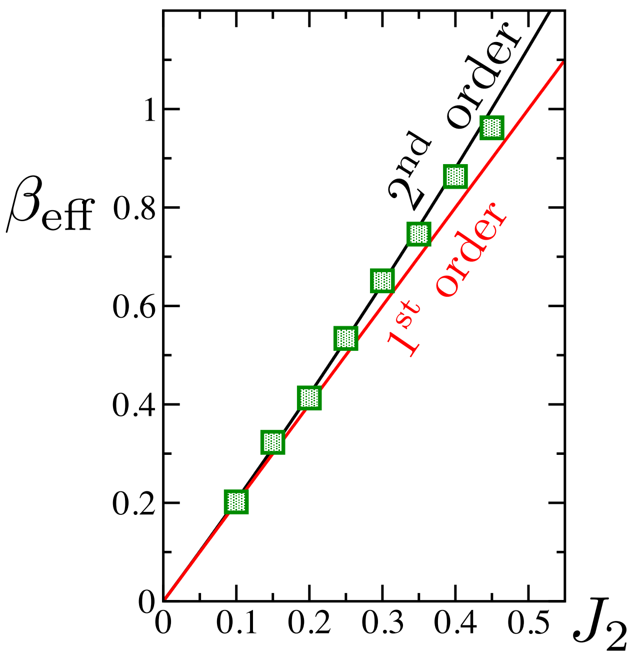
$$\mathcal{H}_E = \vec{S}_i \cdot \vec{S}_{i+1} + \propto (-1)^r (J_2)^r \vec{S}_i \cdot \vec{S}_{i+1+r} + \text{multi} - \text{spin terms}$$

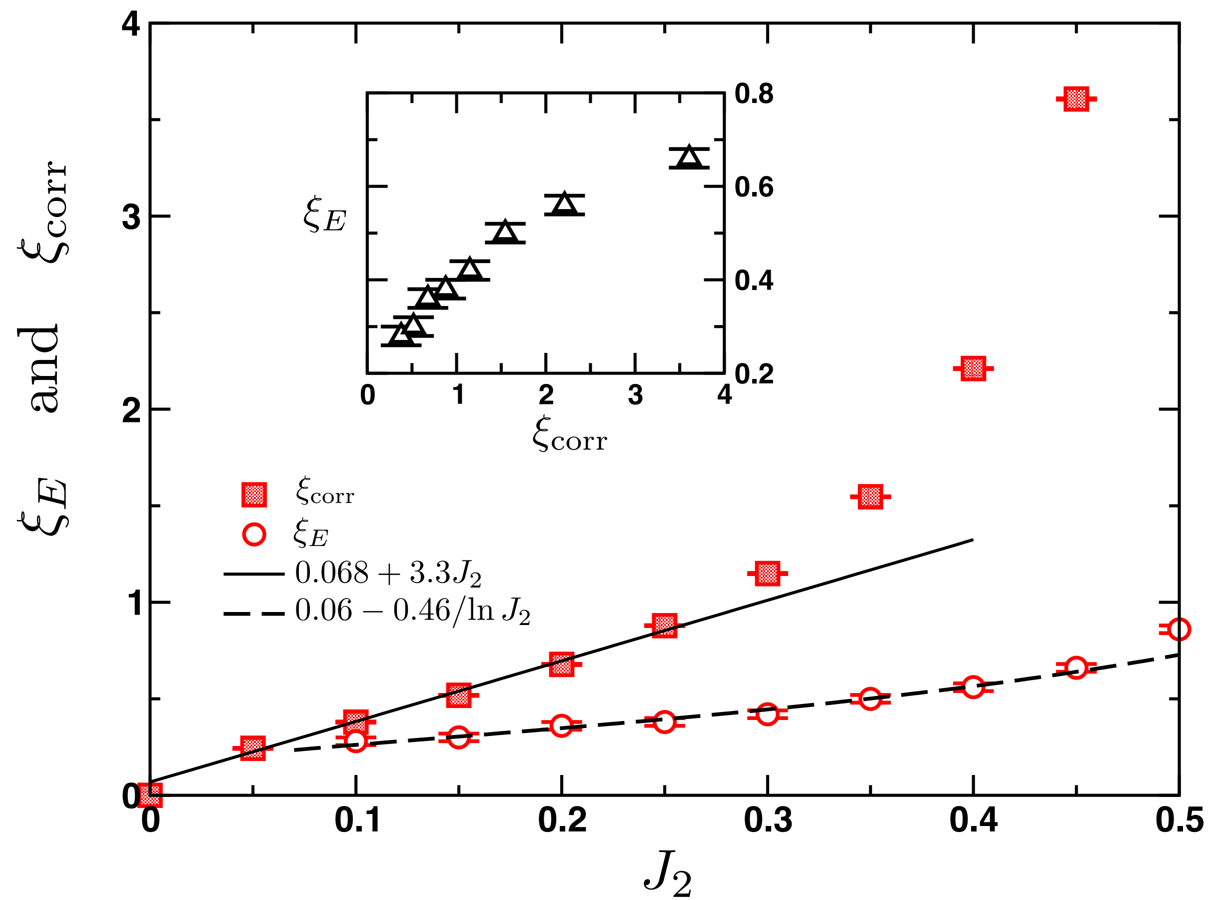
restricting to $\mathcal{H}_E(\xi) = -\sum_{i,j \in B} (-1)^{r_{ij}} e^{-\frac{(r_{ij}-1)}{\xi_E}} \vec{S}_i \cdot \vec{S}_j$

$$\boxed{\xi_E \propto -\frac{1}{\ln J_2} \ll \xi_{\text{corr}}}$$

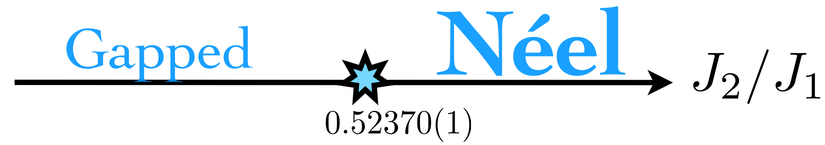
Effective temperature

$$\beta_{\text{eff}} = 2J_2 + \frac{1}{2} J_2^2 + \cdots$$





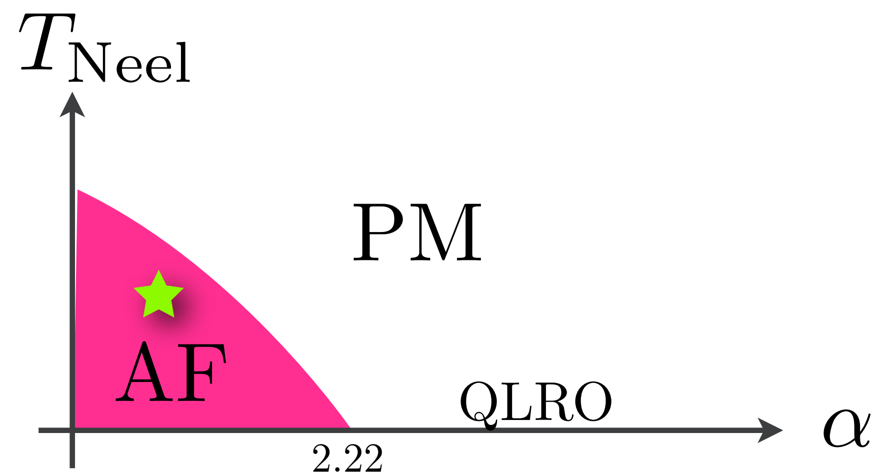
Ordered side

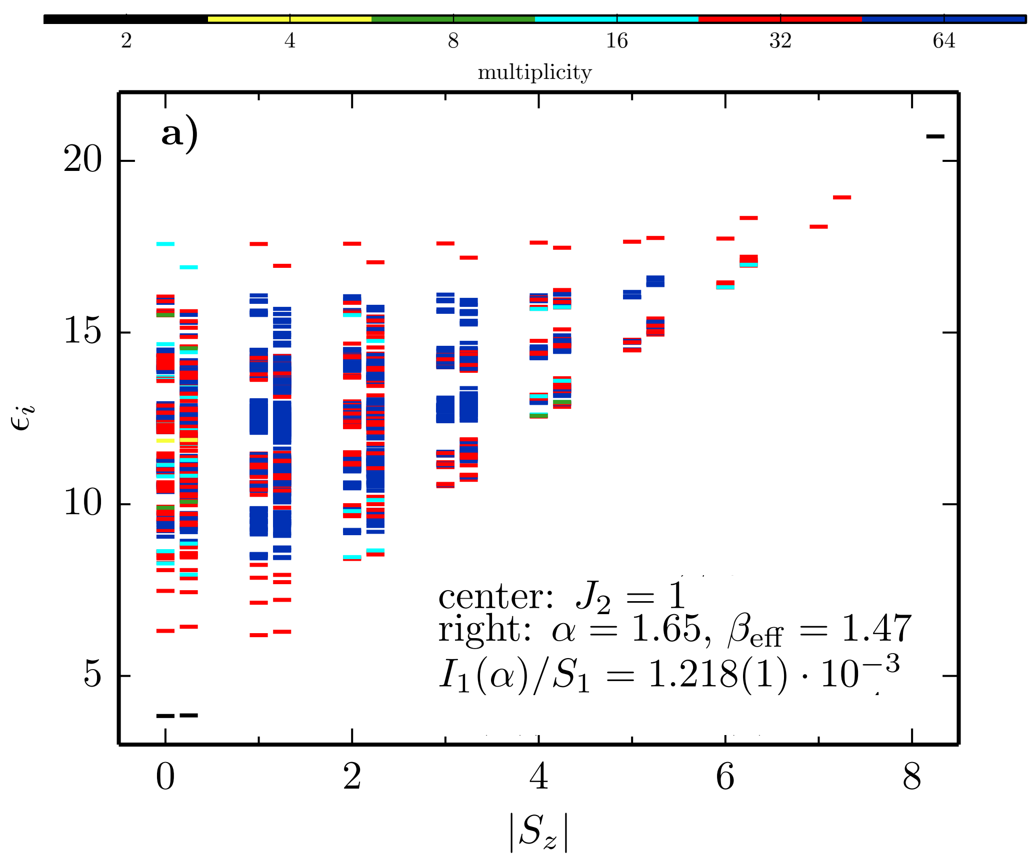


✱ **For our 1D subsystem, H_E is 1D and must display LRO at finite T because the entanglement entropy has a volume law**

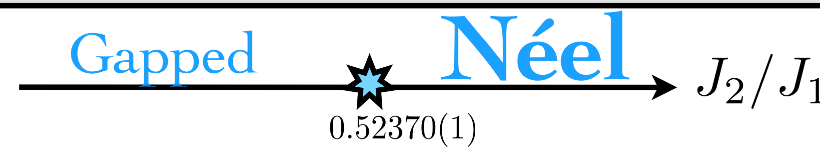
$$\mathcal{H}_E(\alpha) = -\sum_{i\in B}\sum_{j\in B}\frac{(-1)^{r_{ij}}}{r_{ij}^{\alpha}}\vec{S}_i\cdot\vec{S}_j$$

E. Yusuf, A. Joshi and K. Yang, Phys. Rev. B 69, 144412 (2004)
NL, I. Affleck and M. Berciu, J. Stat. Mech. (2005) P12001

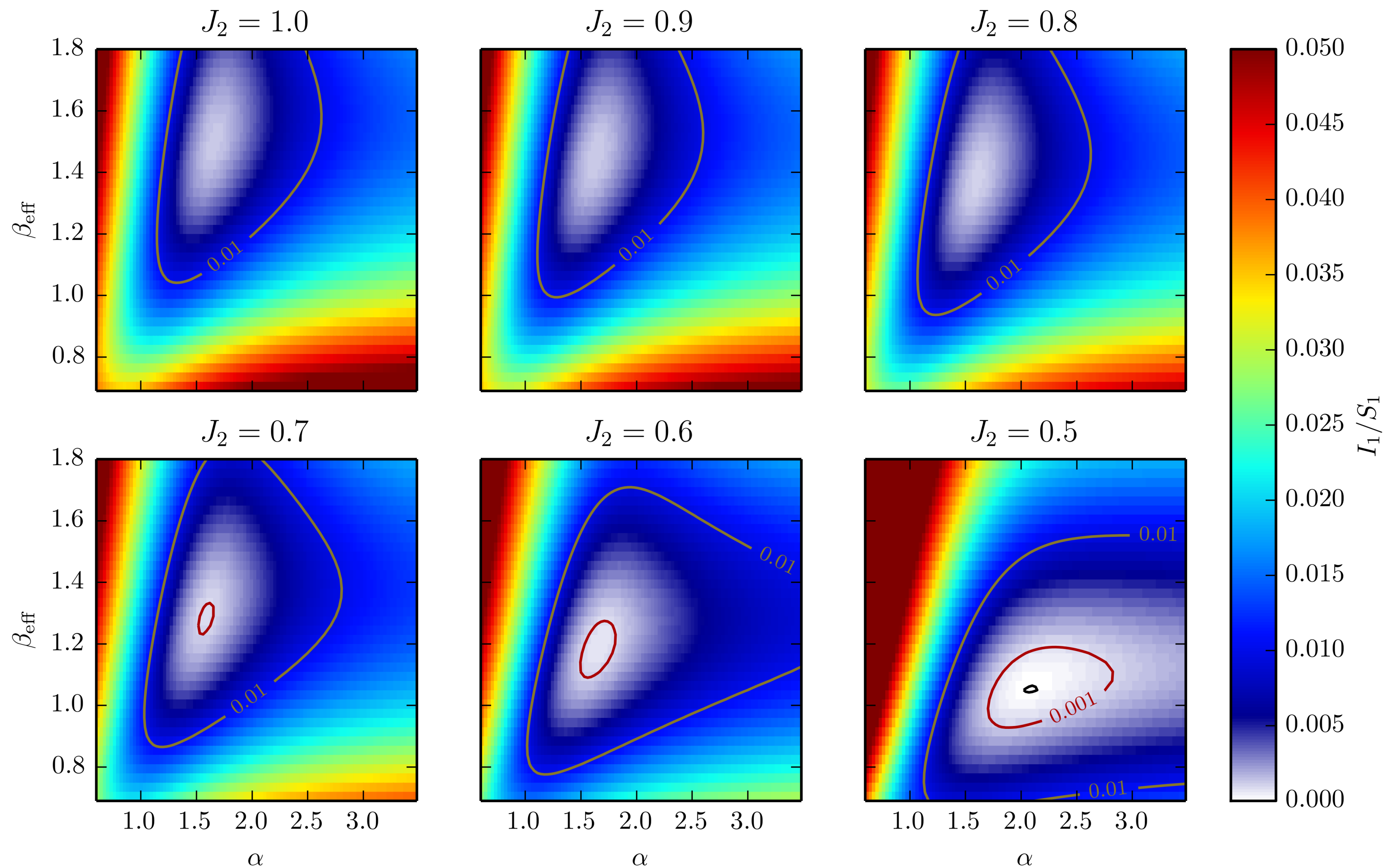




Accross the Néel phase



$$\mathcal{H}_E(\alpha) = -\sum_{i\in B}\sum_{j\in B}\frac{(-1)^{r_{ij}}}{r_{ij}^{\alpha}}\vec{S}_i\cdot\vec{S}_j$$



Very Good agreement but can be improved

Entanglement Spectrum of the Two-Dimensional Bose-Hubbard Model

Phys. Rev. Lett. **110**, 260403 – Published 26 June 2013

Vincenzo Alba, Masudul Haque, and Andreas M. Läuchli

Entanglement spectroscopy of SU(2)-broken phases in two dimensions

Phys. Rev. B **88**, 144426 – Published 30 October 2013

F. Kolley, S. Depenbrock, I. P. McCulloch, U. Schollwöck, and V. Alba

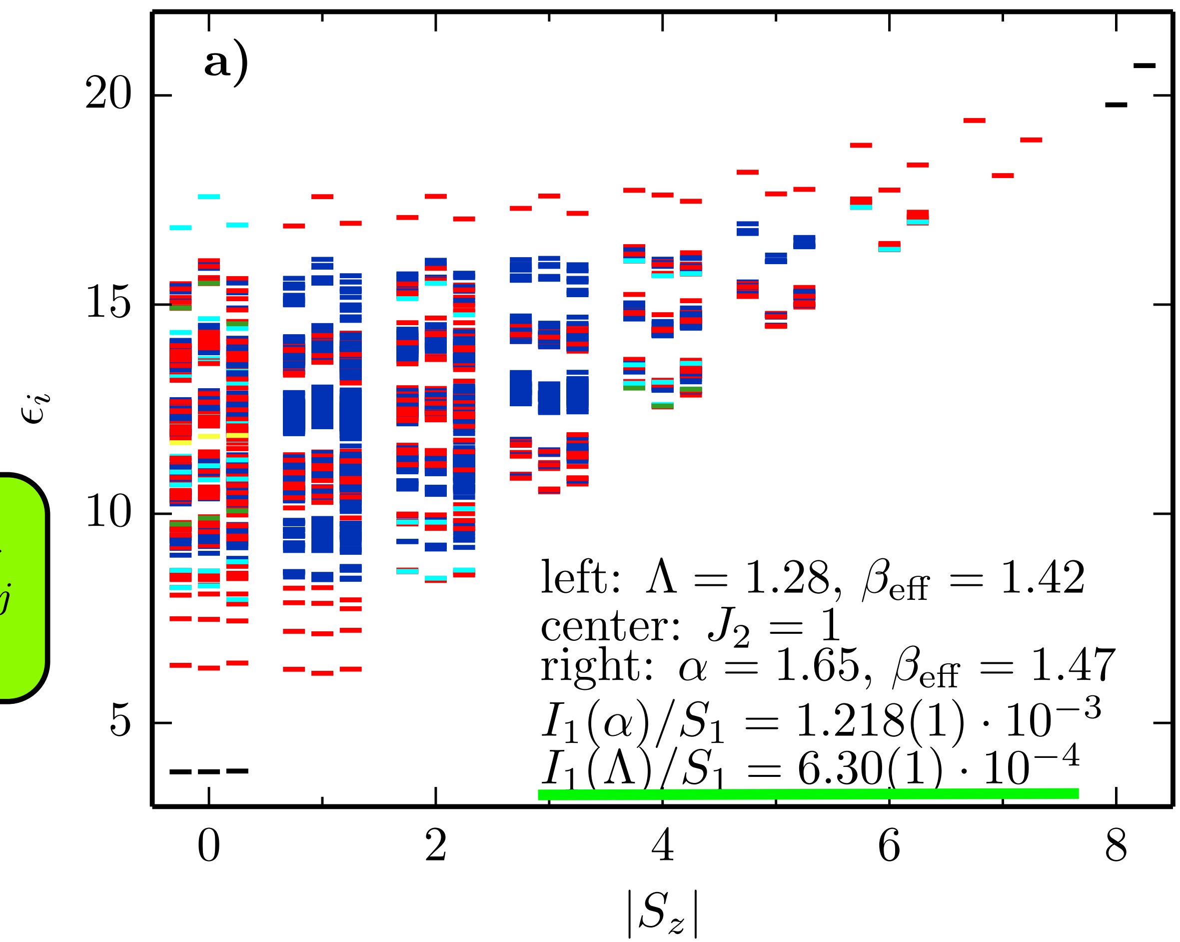
$$\mathcal{H}_E \sim [\mathcal{H}_T + \mathcal{H}_{sw}]$$

Entanglement spectrum displays «tower of states» structure + spin-wave like spectrum E(k) ~ k

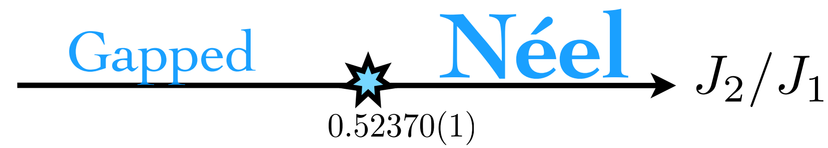
$$\mathcal{H}_E(\alpha) = -\sum_{i\in B}\sum_{j\in B}\frac{(-1)^{r_{ij}}}{r_{ij}^{\alpha}}\vec{S}_i\cdot\vec{S}_j$$

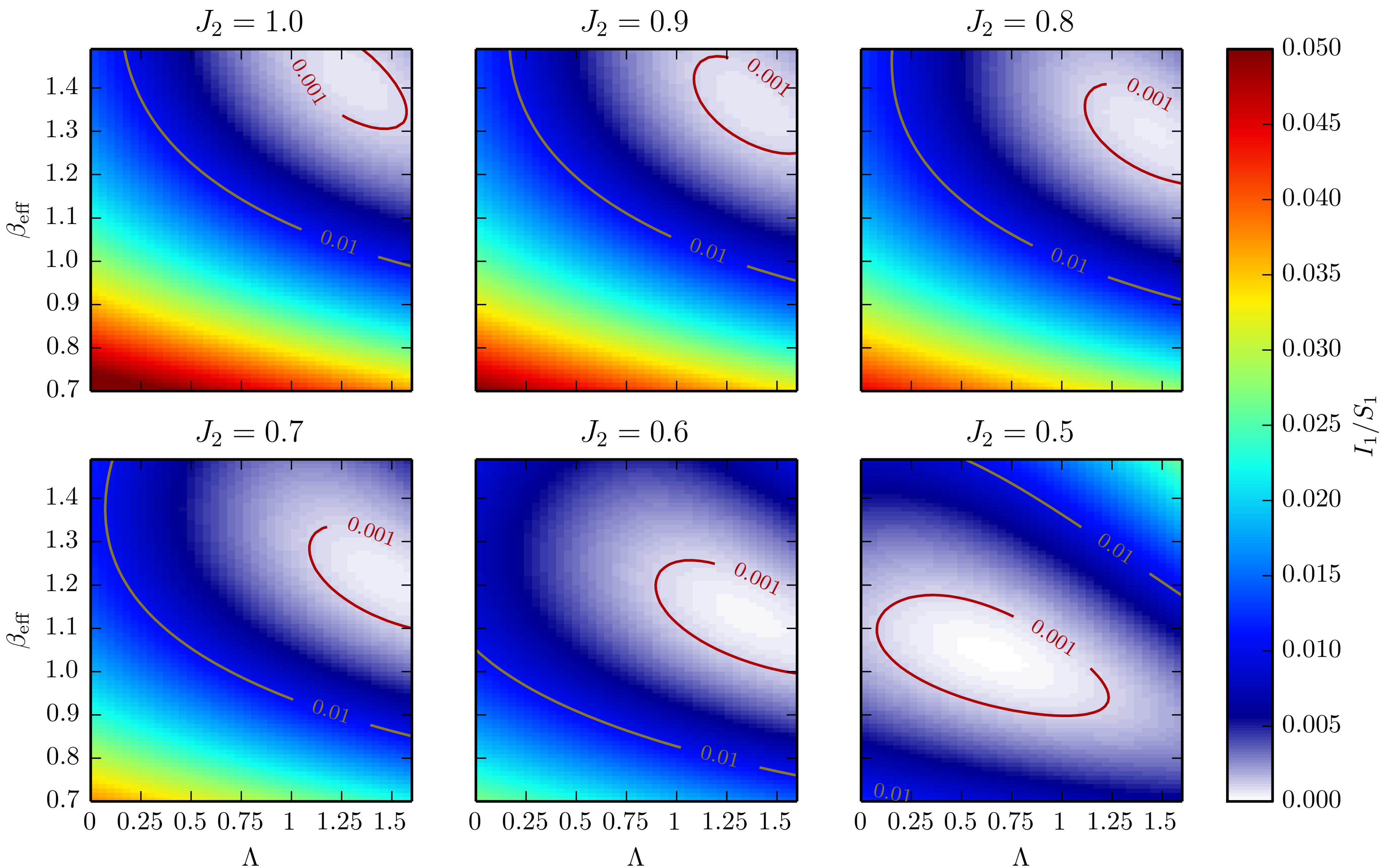
$$\omega(k) \propto |k|^{(\alpha-1)/2}$$

$$\boxed{\mathcal{H}_E(\Lambda) = \sum_{\substack{i,j\in B\\ i>j}}(-1)^{r_{ij}}\left(\frac{\Lambda}{L}+\frac{1}{r_{ij}^3}\right)\vec{S}_i\cdot\vec{S}_j}$$



$$\mathcal{H}_E(\Lambda) = \sum_{\substack{i,j\in B \\ i>j}} (-1)^{r_{ij}} \left(\frac{\Lambda}{L} + \frac{1}{r_{ij}^3} \right) \vec{S}_i \cdot \vec{S}_j$$

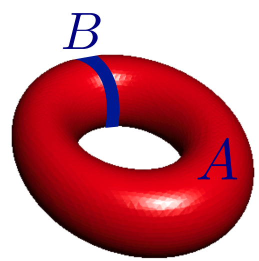


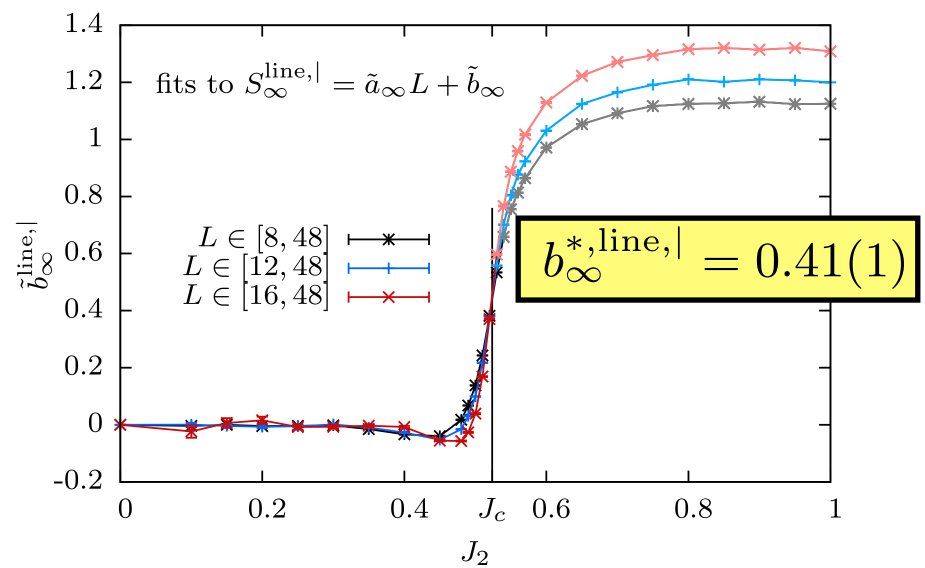


Conclusions

* Shannon-Rény entropies and participation spectra can be efficiently computed using Quantum Monte Carlo simulations

* Shannon-Rényi (participation) entropies for quantum many-body systems encodes universality in subleading terms, for both full- and sub-systems





* Participation spectra of subsystems can be quantitatively compared to spectra of trial Entanglement Hamiltonian at finite T

Gapped

Néel

J_2/J_1

0.52370(1)

?

$$\mathcal{H}_E(\xi) = -\sum_{i,j\in B} (-1)^{r_{ij}} \mathrm{e}^{-\frac{(r_{ij}-1)}{\xi_E}} \vec{S}_i \cdot \vec{S}_j$$

$$\mathcal{H}_E(\Lambda) = \sum_{i,j\in B} (-1)^{r_{ij}} \left(\frac{\Lambda}{L} + \frac{1}{r_{ij}^3}\right) \vec{S}_i \cdot \vec{S}_j$$