Statistical physics of constrained and long-range interacting quantum systems: thermalization and critical properties

Defence of the Ph.D. thesis in Statistical Physics
Advisor: Marcello Dalmonte

SISSA

October 18, 2021

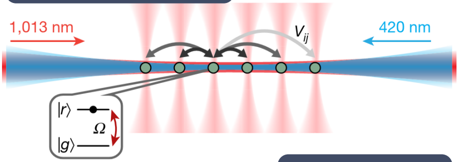
Eduardo Gonzalez Lazo

Introduction

Ultracold atoms and trapped ions experiments

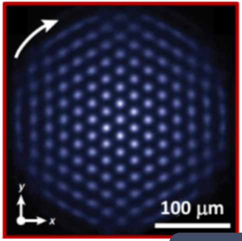
- ☐ With high degree of isolation
- ☐ Realize quantum Ising models
- ☐ With power-law-decaying interactions$(r^{-\alpha})$

Rb atoms in optical tweezers



[Bernien et al., 2017]

$\sim$ 200 Be ions stored in a Penning trap



[Monroe et al., 2021]

Introduction

$$H = \frac{\hbar\Omega}{2}\sum_i \sigma_x^i - \hbar\delta\sum_i n_i + \sum_{i<j}\frac{C_6}{R_{ij}^6} n_i n_j$$

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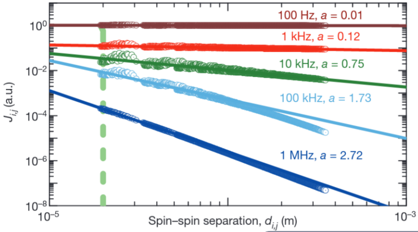

[Britton et al., 2012]

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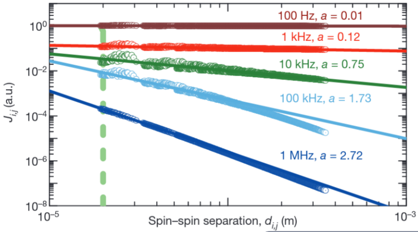

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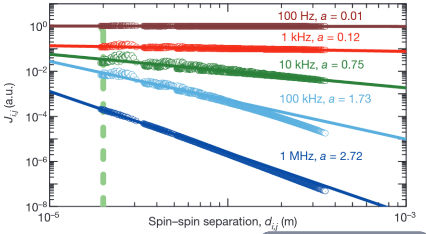

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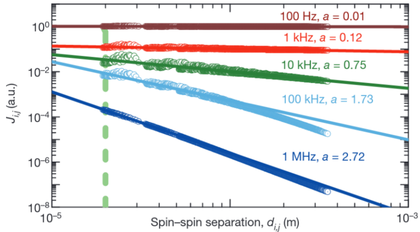

[Britton et al., 2012]

Contributes to the investigation of important theoretical problems

- Thermalization in isolated quantum systems
  - F.M. Surace, M. Votto, **EGL**, A. Silva, M. Dalmonte and G. Giudici, *Exact many-body scars and their stability in constrained quantum chains*, Phys. Rev. B **103** (2021)
  - P. Sierant, **EGL**, M. Dalmonte and A. Scardicchio and J. Zakrzewski, *Constraint-Induced Delocalization*, Phys. Rev. Lett. **127** (2021)
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Finite-temperature critical behavior of long-range quantum Ising models

How interaction range influences

- the critical behavior?
- thermalization?

1D LR Ising model in a transverse field

$$\hat{H} = -\sum_{ij} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z - \Gamma \sum_i \hat{\sigma}_i^x \qquad J_{ij} = \frac{1}{r_{ij}^{\alpha}}$$

[Campa et al., 2009]

Critical behavior

1D LR Ising model in a transverse field

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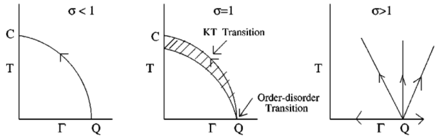

[Dutta and Bhattacharjee, 2001]

T=0

- $1 < \alpha \leq 5/3$
- $5/3 < \alpha < \alpha_1^*$
- $\alpha \geq \alpha_1^*$

T>0

- $1 < \alpha \leq 3/2$ — Mean-Field (MF)
- $3/2 < \alpha \leq \alpha_2^*$ — Nontrivial
- $\alpha > \alpha_2^*$ — Short Range (SR)

[Defenu et al., 2017][Defenu et al., 2015]

Critical behavior

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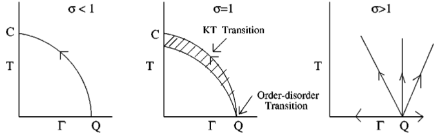

[Dutta and Bhattacharjee, 2001]

T=0

- $1 < \alpha \leq 5/3$
- $d_{uc} = 3(\alpha-1)/2$

T>0

- $1 < \alpha \leq 3/2$
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Mean-Field (MF)

[Defenu et al., 2017][Defenu et al., 2015]

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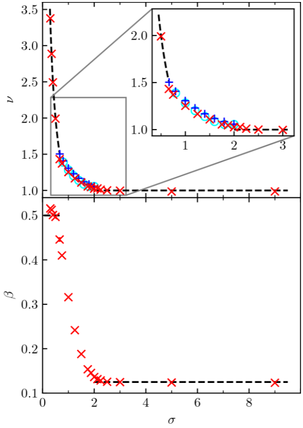


A Quantum Monte Carlo study

- Stochastic series expansion (SSE)
- Characterized the $T = 0$ transition

[Koziol et al., 2021]

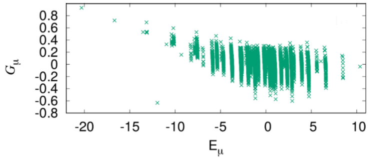
Thermalization

An analysis of the thermalization properties of the eigenstates is generally lacking

$$\hat{H} = -\frac{1}{K}\sum_{ij} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z - \Gamma\sum_i \hat{\sigma}_i^x \qquad J_{ij} = \frac{1}{r_{ij}^{\alpha}} \qquad \alpha \geq 0$$

Studied the relation between quantum chaos, ETH and ensemble equivalence

$$G_\mu = \langle\varphi_\mu|\,\frac{1}{N}\sum_{j=1}^{N}\hat{\sigma}_j^z\hat{\sigma}_{j+1}^z\,|\varphi_\mu\rangle$$



- For $0 < \alpha < 1$ eigenstates quantities do not show smooth dependence on energy

[Russomanno et al., 2021]

A thorough understanding of the thermal properties of the system is required

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$$\hat{H} = -\frac{1}{\boxed{K}} \sum_{ij} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z - \Gamma \sum_i \hat{\sigma}_i^x \qquad J_{ij} = \frac{1}{r_{ij}^{\alpha}} \qquad \alpha \geq 0$$

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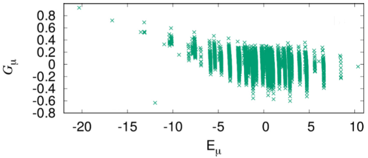

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[Russomanno et al., 2021]

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Our work aims to

- Study the 1D LR Ising model in a transverse field
- Answer whether quantum fluctuations change the nature of the thermal phase transition
- Determine universal and non-universal details
  - value of critical exponents
  - position of the critical points
- Use ab initio, non-perturbative solutions of the problem
- Study different α regimes
  - $\alpha = 0.05$, within the extremely long-range region $\alpha < 1$
  - $\alpha = 1.5$, at the boundary between MF and nontrivial behavior

The model

System Hamiltonian

$$\hat{H} = -\frac{V}{K}\sum_{i<j}\frac{\hat{S}_i^z \hat{S}_j^z}{r_{ij}^{\alpha}} - \sum_i \hat{S}_i^x$$

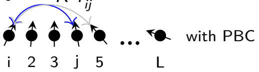
$$K \equiv (L-1)^{-1}\sum_{i\neq j} r_{ij}^{-\alpha}$$

$$\hat{S}_i^x = \frac{\hbar}{2}\sigma_i^x$$

The Kać renormalization factor

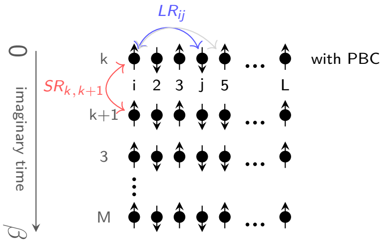
- ☐ Ensures the existence of a proper thermodynamic limit
- ☐ Do not affect the universal features of the model

$$J_{ij} = \frac{V}{K}\frac{1}{r_{ij}^{\alpha}}$$



Path Integral Monte Carlo (PIMC)

The model maps to a classical, anisotropic, 2D Ising model



The mapping is exact up to $O(\beta/M)$ corrections

β up to 1024
L up to 8192
M up to 65536

Properties of the quantum system are accessed via conventional Monte Carlo simulations

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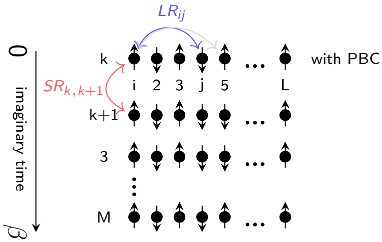

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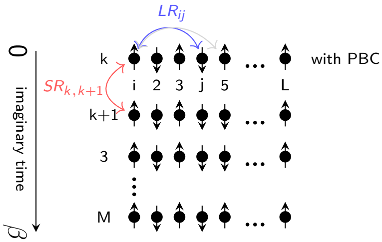

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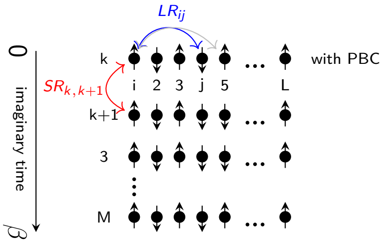

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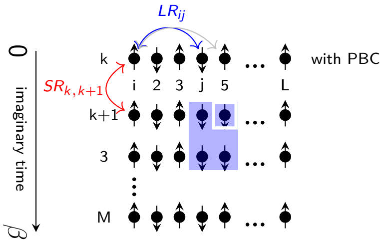


Critical slowing down problem

- Wolff cluster updates [Wolff, 1989] (short-range part)
- Long-range cluster updates [Luijten and Blöte, 1997] (long-range part)

Properties of the quantum system are accessed via conventional Monte Carlo simulations

Criticality and finite-size systems

Finite-size scaling hypothesis (FSS)

$$Q(t,L) = L^{\sigma} f\left(\xi/L\right)$$

$$Q(t,L) = L^{-k/\nu} g\left(tL^{1/\nu}\right)$$

For $d \geq d_{uc}$

Effective thermal exponent θ_t

$$Q(t,L) = L^{-k\theta_t} g\left(tL^{\theta_t}\right)$$

$$\frac{1}{\nu} = \frac{d_{uc}(\alpha)}{d}\theta_t$$

[Koziol et al., 2021]

PIMC gives direct access to observables

Binder cumulant

$$U = \frac{1}{2}\left[3 - \frac{\langle m_z^4\rangle}{\langle m_z^2\rangle^2}\right]$$

Susceptibility

$$\chi = \beta L(\langle m_z^2\rangle - \langle|m_z|\rangle^2)$$

Ground state phase transition

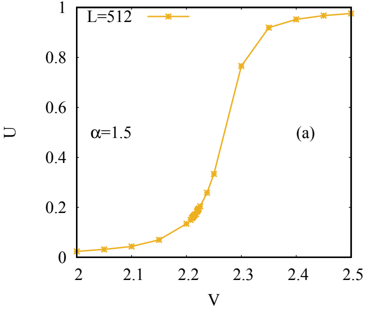
$$\hat{H} = -\frac{V}{K}\sum_{i<j}\frac{\hat{S}_i^z\hat{S}_j^z}{r_{ij}^{\alpha}} - \sum_i \hat{S}_i^x$$

$$U = \frac{1}{2}\left[3 - \frac{\langle m_z^4\rangle}{\langle m_z^2\rangle^2}\right] \qquad \alpha = 0.05, 1.5$$

FSS

$$V_U(L) = V_c\left(1 + aL^{-\omega-\theta_t}\right)$$
$$U(L, V_U(L)) = b + cL^{-\omega}$$

Curves $U(V, L)$ for system sizes L and $2L$ cross at size-dependent points $V = V_U(L)$



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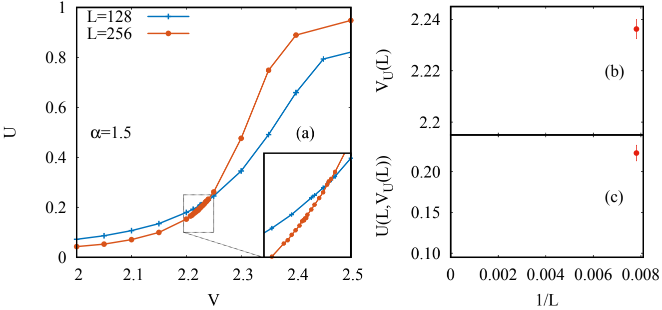

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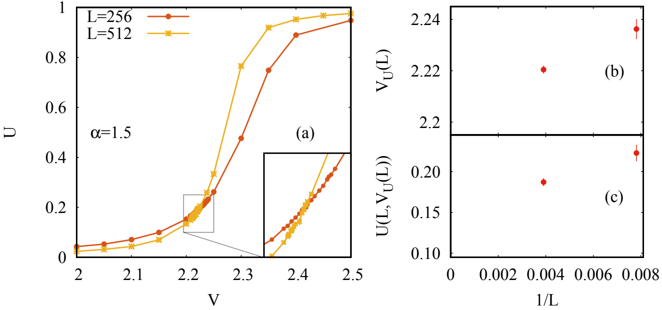

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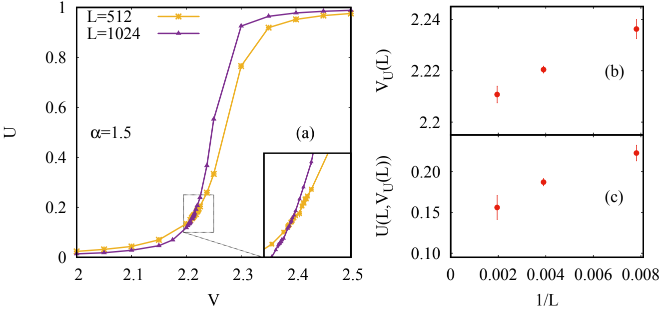

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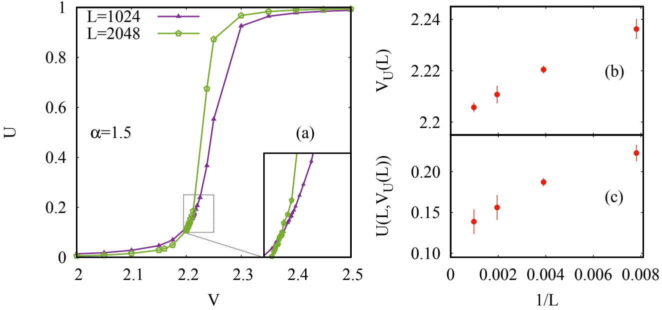

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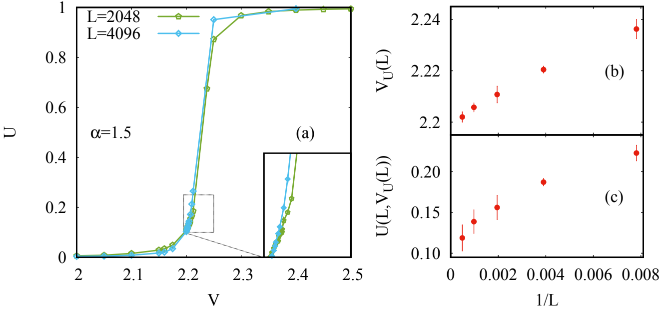

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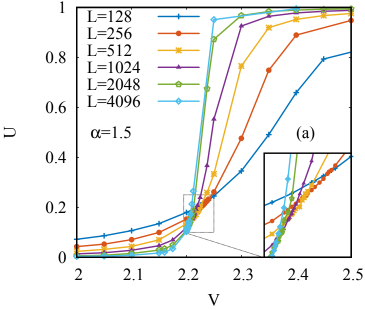

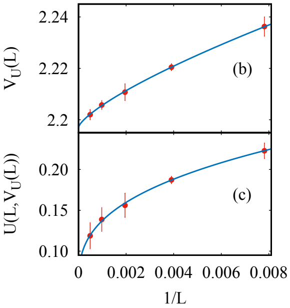

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$\alpha = 0.05, 1.5$

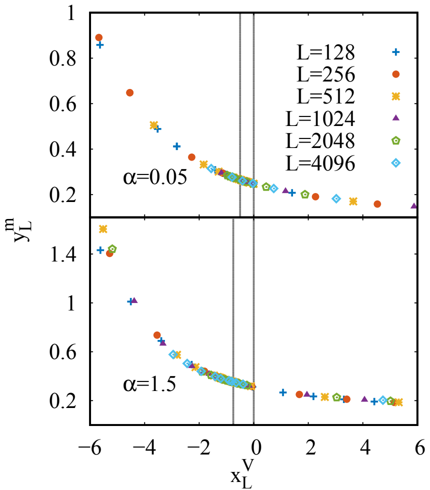
Data collapse

$$m_z^2 \sim L^{-2\beta_m\theta_t}\cdot f\left[L^{+\theta_t}\left(V_c - V\right)\right]$$

$$y_L^m \equiv m_z^2(L)L^{+2\beta_m\theta_t}$$

$$x_L^V \equiv \left(V_c - V\right)L^{\theta_t}$$

[Sandvik, 2010]



Ground state phase transition

α	V_c (BC)	V_c (DC)	θ_t (BC)	θ_t (DC)	$2\beta_m\theta_t$ (DC)
0.05	1.9997(4)	1.9999	0.50(7)	0.688	0.68
1.50	2.1972(7)	2.1981	0.39(6)	0.64	0.715

Comparison of the results

- SSE predictions in [Koziol et al., 2021]

α	θ_t	$2\beta_m\theta_t$
1.5	~ 0.667	~ 0.667

$\to$ MF

- MF predictions in [Botet and Jullien, 1983]

α	θ_t	$2\beta_m\theta_t$
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Finite temperature phase transition

$$\hat{H} = -\frac{V}{K}\sum_{i<j}\frac{\hat{S}_i^z\hat{S}_j^z}{r_{ij}^{\alpha}} - \sum_i \hat{S}_i^x$$

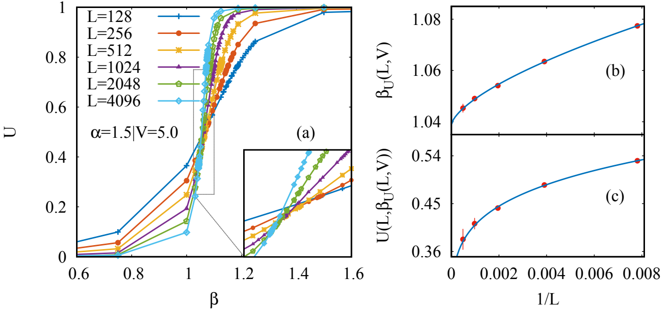
$$U = \frac{1}{2}\left[3 - \frac{\langle m_z^4\rangle}{\langle m_z^2\rangle^2}\right]$$

$\alpha = 0.05, 1.5 \quad | \quad V = 2.5, 3, 3.5, 5$

FSS

$$\beta_U(L,V) = \beta_c\left(1 + aL^{-\omega-\theta_t}\right)$$

$$U(L,\beta_U(L,V)) = b + cL^{-\omega}$$



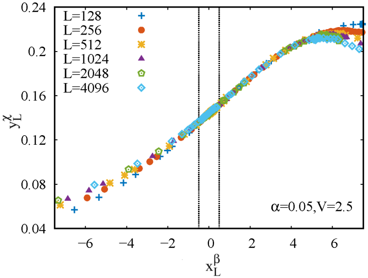
Finite temperature phase transition

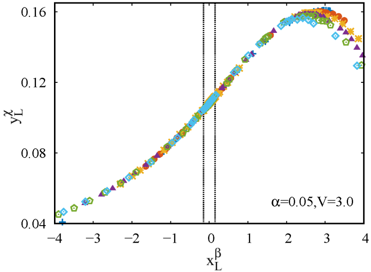
Data collapse

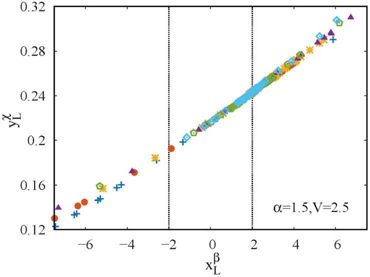
$$\chi \sim L^{\gamma\theta_t} \cdot f(L^{\theta_t}(\beta_c - \beta))$$

$$y_L^\chi \equiv \chi(L) L^{-\gamma\theta_t}$$

$$x_L^\beta \equiv (\beta_c - \beta) L^{\theta_t}$$







Finite temperature phase transition

		β_c		θ_t		$\gamma\theta_t$
	V	U	χ_{dc}	U	χ_{dc}	χ_{dc}
$\alpha = 0.05$	$V = 2.5$	2.2007(4)	2.20	/	0.51	0.505
	$V = 3.0$	1.6120(7)	1.612	/	0.485	0.515
	$V = 3.5$	1.299(1)	1.303	/	0.49	0.523
	$V = 5.0$	0.8474(2)*	0.8491	0.5(1)	0.50	0.524
$\alpha = 1.50$	$V = 2.5$	3.21(1)	3.229	0.49(7)	0.50	0.516
	$V = 3.0$	2.109(1)*	2.115	0.50(2)	0.52	0.538
	$V = 3.5$	1.647(6)	1.650	0.5(2)	0.52	0.545
	$V = 5.0$	1.039(1)	1.041	0.44(7)	0.530	0.550

Comparison of the results

- MC[1] predictions in [Luijten and Blöte, 1997]

α	V	θ_t	$\gamma\theta_t$
1.5	∞	~ 0.5	~ 0.5

$\rightarrow$ MF

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[1] Classical Monte Carlo

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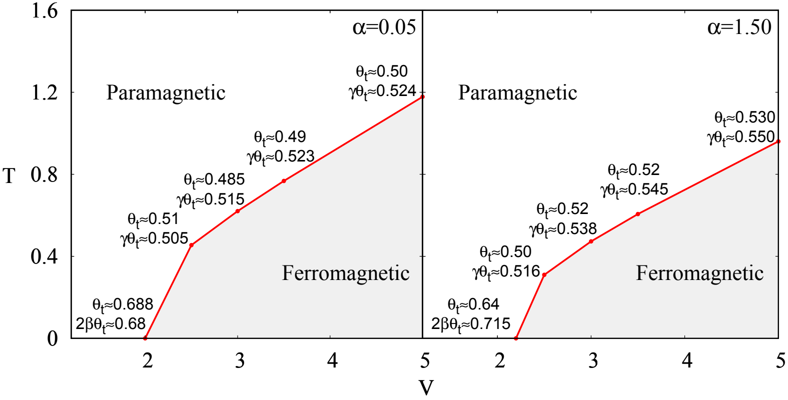
Criticality and phase diagram

$$\hat{H} = -\frac{V}{K}\sum_{i<j}\frac{\hat{S}_i^z\hat{S}_j^z}{r_{ij}^{\alpha}} - \sum_i \hat{S}_i^x$$



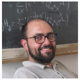
Conclusions

- We study the long-range quantum Ising chain
  - Characterising the phase diagram and critical behavior
- We find essential agreement with existing predictions when possible
  - We find compatibility of our $\alpha = 0.05$ results with the fully-connected universal properties
  - The non-zero T transition follows the classical prediction

Outlook

- Study the critical behaviour for $\alpha < 1$
- Study supersolidity and bilayer systems of dipolar bosons
  - by the use of PIMC methods in continuous space

Acknowledgements

Thank you for your attention

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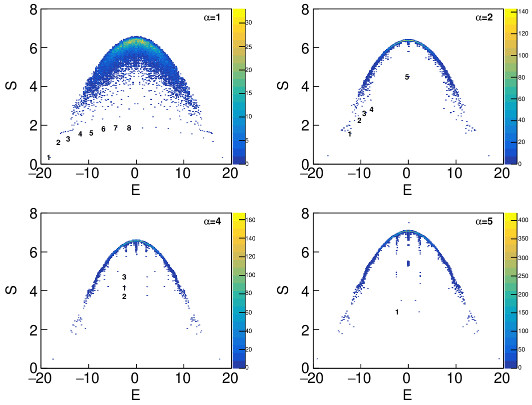
ETH characterization

$$H_0^\alpha = \sum_i P_{i-\alpha} \dots P_{i-1} X_i P_{i+1} \dots P_{i+\alpha},$$

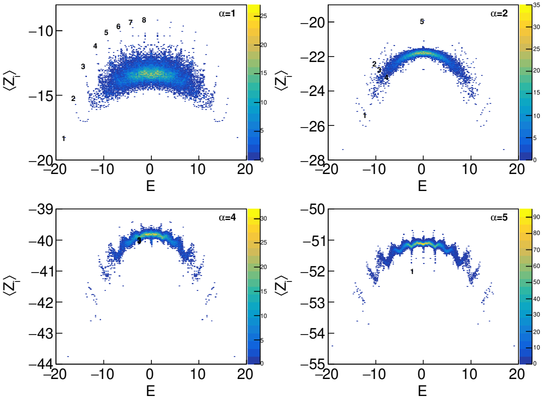
Half-chain bipartite entanglement entropy of eigenstates

$$S^{E_n} = -\,\mathrm{Tr}_A\left(\hat{\rho}_A^{E_n}\ln\hat{\rho}_A^{E_n}\right)$$



Local expectation values on the eigenstates

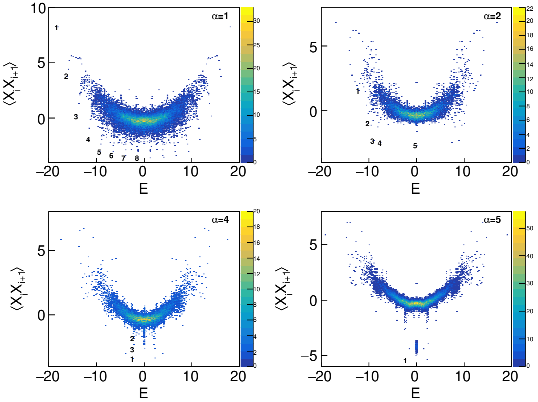
$$\langle Z_i \rangle = \langle E_n | \sum_i Z_i | E_n \rangle$$



ETH characterization

Local expectation values on the eigenstates

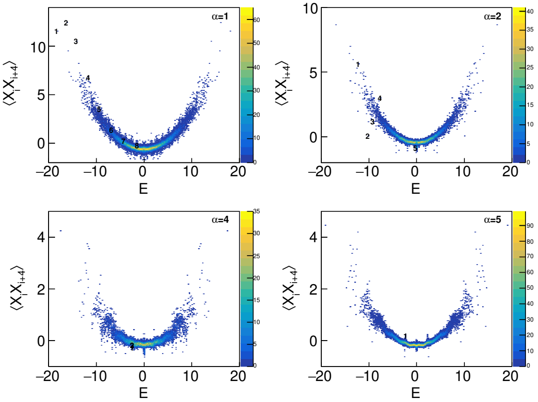
$$\langle X_i X_{i+1} \rangle = \langle E_n | X_i X_{i+1} | E_n \rangle$$



ETH characterization

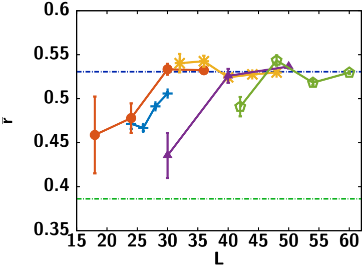
Local expectation values on the eigenstates

$$\langle X_i X_{i+4} \rangle = \langle E_n | \, X_i X_{i+4} \, | E_n \rangle$$



Spectral statistics

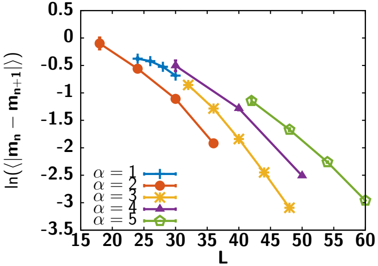
$$\bar{r} = \left\langle \frac{\mathrm{Min}\{\Delta E_n, \Delta E_{n+1}\}}{\mathrm{Max}\{\Delta E_n, \Delta E_{n+1}\}} \right\rangle$$



ETH characterization

Average difference of m_n between adjacent eigenstates

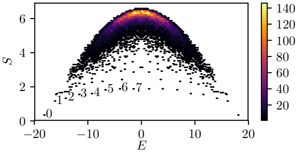
$$m_n = \langle E_n | \, \hat{\sigma}_i^z \, | E_n \rangle$$



Exact scars and their stability

$$H_0^\alpha = \sum_i P_{i-\alpha} \dots P_{i-1} X_i P_{i+1} \dots P_{i+\alpha},$$

Scars in the thermodynamic limit



- Numerical results reveal hybridization of these scars with thermal eigenstates

[Turner et al., 2018]

Exact scars in the form of MPS

$$OBC: \quad |\Gamma_{i,j}\rangle = \sum_{\{\sigma\}} v_i^T A_{\sigma_1\sigma_2} \dots A_{\sigma_{L-1}\sigma_L} v_j \, |\sigma_1\sigma_2 \dots \sigma_{L-1}\sigma_L\rangle \qquad i,j = 1,2$$

$$PBC: \quad |\Phi_1\rangle = \sum_{\{\sigma\}} \mathrm{Tr}[A_{\sigma_1\sigma_2} \dots A_{\sigma_{L-1}\sigma_L}] \, |\sigma_1\sigma_2 \dots \sigma_{L-1}\sigma_L\rangle \qquad |\Phi_2\rangle = T_x \, |\Phi_1\rangle$$

$$|\Gamma_{11}\rangle, |\Gamma_{22}\rangle, |\Phi_i\rangle \to E = 0 \qquad |\Gamma_{12}\rangle \to E = \sqrt{2} \qquad |\Gamma_{21}\rangle \to E = -\sqrt{2}$$

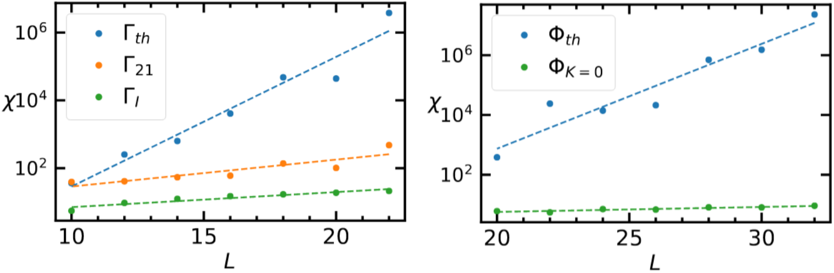
[Lin and Motrunich, 2019]

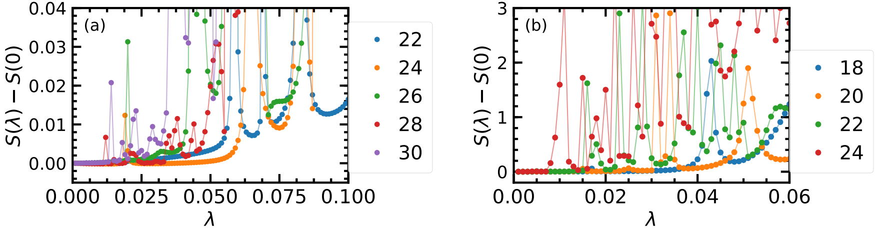
Stability

An eigenstate of H_0 is stable if it can be deformed to an eigenstate of $H_0 + \lambda V$ with a local unitary transformation in the thermodynamic limit

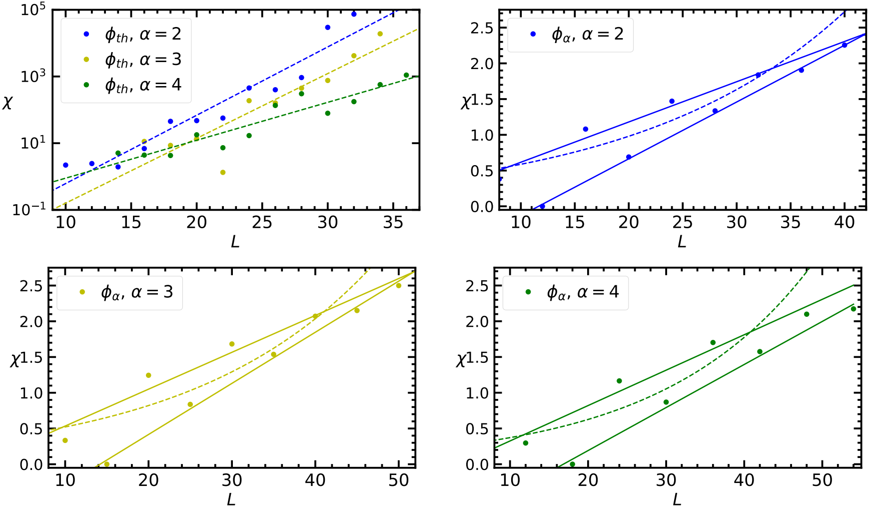
Fidelity susceptibility

$$\chi_F\left[|n^0\rangle\right] = \lim_{\lambda\to 0} \frac{-2\ln|\langle n^0|n^\lambda\rangle|}{\lambda^2} = \sum_{m\neq n}\left|\frac{\langle m^0|V|n^0\rangle}{E_n^0 - E_m^0}\right|^2$$





Bipartite entanglement entropy of the states (a) $|\Phi^{\lambda}_{K=0}\rangle$ and (b) $|\Gamma^{\lambda}_{l}\rangle$ as a function of λ. Peaks in this quantity signal hybridization of the perturbed state with thermal eigenstates. By increasing the system size, we find peaks closer and closer to $\lambda = 0$, suggesting that the scar eigenstates are not stable in the thermodynamic limit.

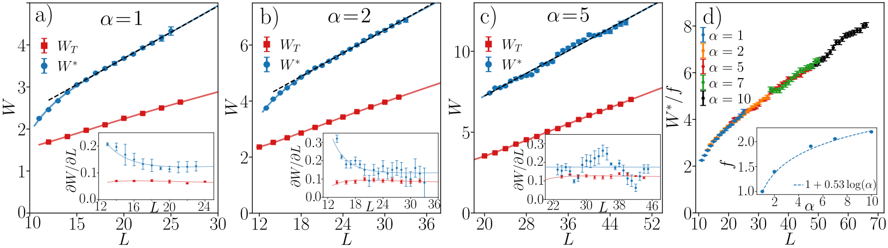


Scaling of the fidelity susceptibility with system size. The results shown refer to the generic states ϕ_{th} (upper left panel) and the scarred eigenstates ϕ_α (upper right panel and lower panels). Dashed lines are obtained from fits with an exponential scaling, solid lines with linear scaling. The result points at the same behavior occuring in the PXP model.

Constraint-induced delocalization

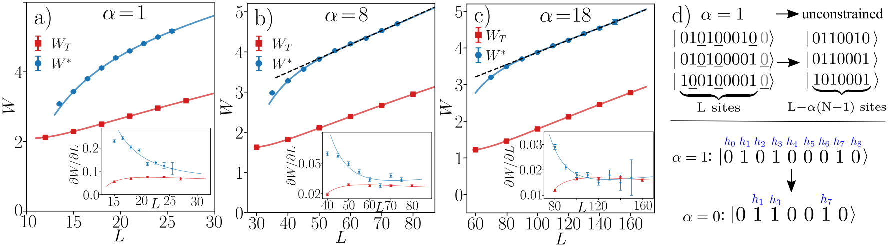
$$\hat{H} = \sum_{i=1}^{L} P_i^\alpha S_i^x P_{i+1+\alpha}^\alpha + \sum_{i=1}^{L} h_i S_i^z$$

$$P_i^\alpha = \prod_{j=i-\alpha}^{i-1} (1/2 - S_j^z) \qquad h_i \in [-W/2, W/2]$$



a)
$\alpha=1$
W_T
W^*
b)
$\alpha=2$
c)
$\alpha=5$
d)
$\alpha=1$
$\alpha=2$
$\alpha=5$
$\alpha=7$
$\alpha=10$
$1+0.53\log(\alpha)$
W
L
$\partial W/\partial L$
W^*/f
f
α

SISSA



a) $\alpha = 1$
W_T
W^*
W
L
$\partial W/\partial L$
b) $\alpha = 8$
c) $\alpha = 18$
d) $\alpha = 1$ → unconstrained
$|0101000100\rangle$ $|0110010\rangle$
$|0101000010\rangle$ → $|0110001\rangle$
$|1001000010\rangle$ $|1010001\rangle$
L sites
L−α(N−1) sites
h_0 h_1 h_2 h_3 h_4 h_5 h_6 h_7 h_8
$\alpha = 1$: $|0\ 1\ 0\ 1\ 0\ 0\ 0\ 1\ 0\rangle$
h_1 h_3 h_7
$\alpha = 0$: $|0\ 1\ 1\ 0\ 0\ 1\ 0\rangle$

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