Complexity in frustrated systems

Excitation Energy Transport in Physical, Chemical, and Biological Systems
The Summit Meeting 2023

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HrZZ Croatian Science Foundation

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Hybrid Scale

Frustrated chemistry

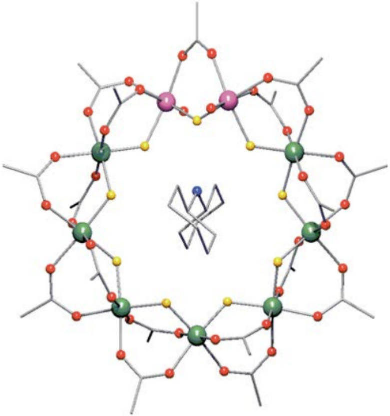

Figure 1. The structure of **4** in the crystal. The hydrogen atoms have been omitted for clarity. Bond length ranges [Å]: Cr–F 1.9098–1.9338, Cr–O 1.915–1.968, V–F 1.9494–2.0114, V–O(oxide) 1.580, V–O(pivalate) 1.989–2.185 (av esd 0.002). Cr dark green; V purple; F yellow; O red; N blue; C grey.

Angewandte Chemie
GDCh Eine Zeitschrift der Gesellschaft Deutscher Chemiker

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The Magnetic Möbius Strip: Synthesis, Structure, and Magnetic Studies of Odd-Numbered Antiferromagnetically Coupled Wheels†

Olivier Cador Dr., Dante Gatteschi Prof., Roberta Sessoli Prof., Finn K. Larsen Prof., Jacob Overgaard Dr., Anne-Laure Barra Dr., Simon J. Teat Dr., Grigore A. Timco Dr., Richard E. P. Winpenny Prof. ... See fewer authors

First published: 29 September 2004 | https://doi.org/10.1002/ange.200460211 | Citations: 33

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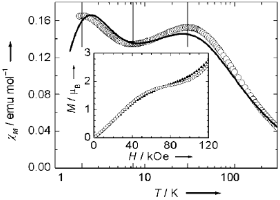
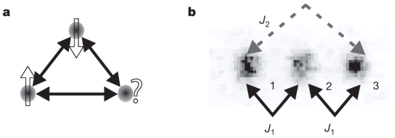


Figure 2. Variation of χ_M with temperature for **2**. The solid line corresponds to the calculated values with $J = 16$ K, $J' = 70$ K, and $\langle g \rangle = 2$. In the inset the magnetization versus field measured at 1.6 K (○) and 2.0 K (▲) is shown.

Frustrated physics



- Trapped ions (Yb) experiment
- Quantum simulator of antiferromagnetic Ising spins
- Connections between ground-state degeneracy and entanglement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Published: 03 June 2010

Quantum simulation of frustrated Ising spins with trapped ions

K. Kim, M.-S. Chang, S. Korenblit, R. Islam, E. E. Edwards, J. K. Freericks, G.-D. Lin, L.-M. Duan & C. Monroe

Nature **465**, 590–593 (2010) | Cite this article

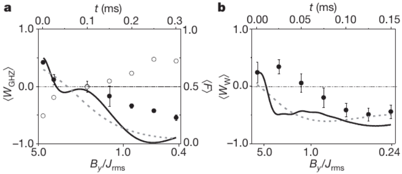

Figure 3 | Entanglement generation through the quantum simulation.

Overview of the talk

1. Experimental evidence of the effects of topological frustration
2. Minimal model
3. Excess of entanglement
4. Long-range nature of entanglement
5. Robustness to local disentangling gates
6. Complexity of entanglement spectrum
7. Conclusions and outlook

arXiv > quant-ph > arXiv:2209.10541

Quantum Physics

[Submitted on 21 Sep 2022]

Complexity of frustration: a new source of non-local non-stabilizerness

J. Odavić, T. Haug, G. Torre, A. Hamma, F. Franchini, S. M. Giampaolo

arXiv > quant-ph > arXiv:2210.13495

Quantum Physics

[Submitted on 24 Oct 2022]

Random unitaries, Robustness, and Complexity of Entanglement

J. Odavić, G. Torre, N. Mijić, D. Davidović, F. Franchini, S. M. Giampaolo

RBI-ThPhys-2023-xx

Long-range entanglement and topological excitations

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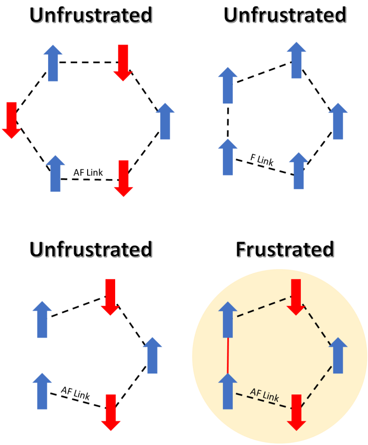
(Dated: July 26, 2023)

Topological (geometrical) frustration... in Ising spins

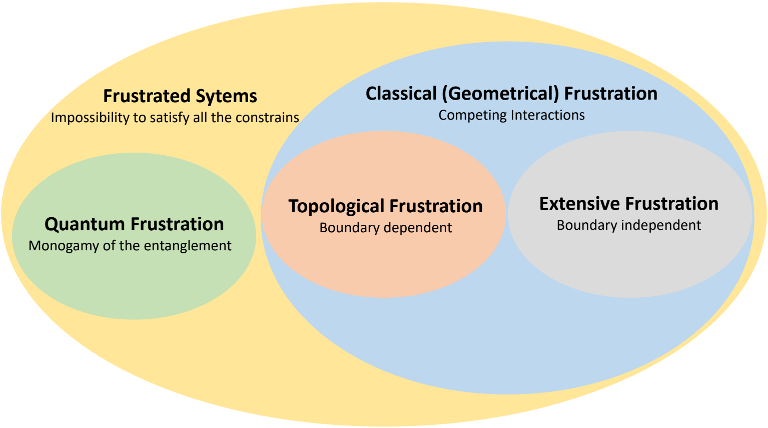


Our focus

- Spatially invariant one-dimensional systems with
  1. Periodic boundary conditions
  2. Odd number of spins
  3. Antiferromagnetic coupling

  we denote as frustrated boundary conditions (FBC)

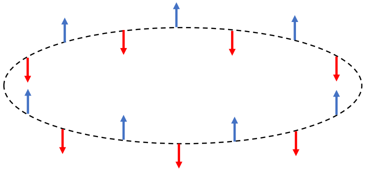
In the swamplands of frustration



Topological Frustration: a simple classical case

$$H = \sum_{i=1}^{L} \sigma_i^z \sigma_{i+1}^z$$

Even L

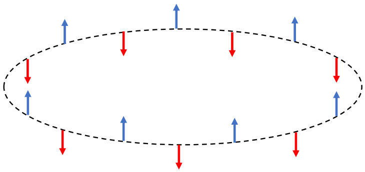


- twofold degenerate ground state manifold
- finite energy gap

Topological Frustration: a simple classical case

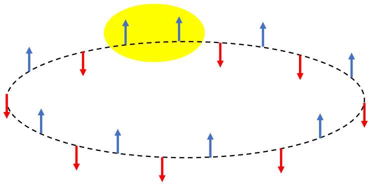
$$H = \sum_{i=1}^{L} \sigma_i^z \sigma_{i+1}^z$$

Even L



- twofold degenerate ground state manifold
- finite energy gap

Odd L

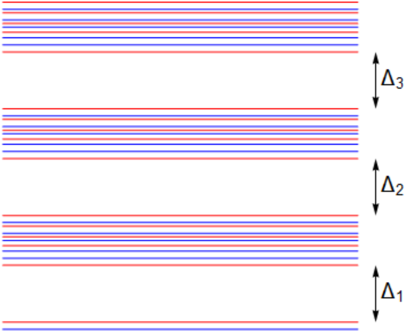


- $2L$-fold degenerate ground state manifold
- finite energy gap

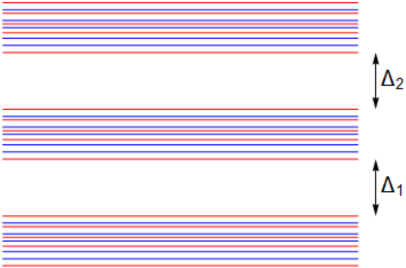
Entering the quantum regime. The energy spectrum

$$H = \sum_{i=1}^{L} \sigma_i^z \sigma_{i+1}^z - \lambda \sum_{i=1}^{L} \sigma_i^x$$

Unfrustrated



Frustrated



Minimal topologically frustrated quantum model

One-dimensional transverse field Ising model (TFIM) spin-1/2 quantum chain

$$H = J \sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - h \sum_{i=1}^{N} \sigma_i^x .$$

- Hamiltonian as tensor product of Pauli matrices Hilbert space $\mathcal{H}^{(N)} = \mathbb{C}^{2^N}$ of dimension 2^N.
- J coupling between the spins, and h the magnetic field
- Mappable via Jordan-Wigner transformation to free fermions, even in presence of frustration.

Entanglement measures

- Rényi-α entanglement entropy

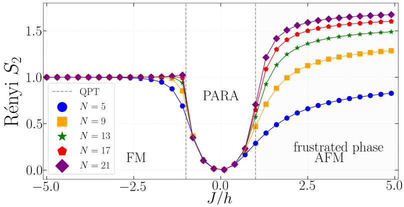
$$S_\alpha(\rho_A) = \frac{1}{1-\alpha} \log_2 \mathrm{Tr}\,[\rho_A^\alpha], \quad \text{with} \quad \alpha \in [0,1) \cup (1,\infty]$$

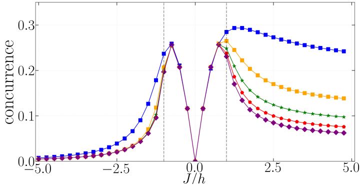
where the reduced density matrix is defined as a partial trace over the full density matrix

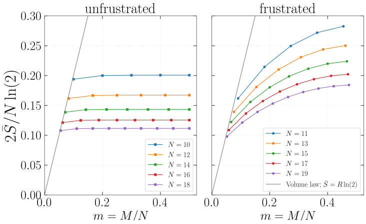
$$\rho_A^\alpha = \mathrm{Tr}_B |\Psi\rangle\langle\Psi| \tag{1}$$

- Von Neumann entanglement entropy (Rényi $\alpha \to 1$)
- Nearest-neighbor concurrence (short-range entanglement)

Entanglement properties







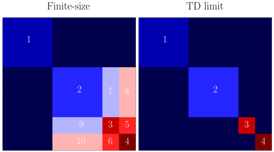
Beyond area-law (local) contribution in entanglement in topologically frustrated chains.

Explanation - Reduced density matrix

1. The ground state at $h \to 0^+$ can be represented as a linear superposition of kink states

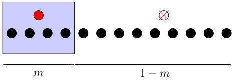
$$|W_k\rangle = \frac{1}{\sqrt{N}} \left(|{+}{+} - + - \ldots\rangle + |- {+}{+} - +\ldots\rangle + |+ - {+}{+} - \ldots\rangle + \ldots \right),$$

with exact half-chain reduced density matrix $\rho^{\text{frus}}_{[m=N/2]}$



* 1 and 2: Néel orders, 3: kink even site, 4: kink odd site, dark blue → zeroes

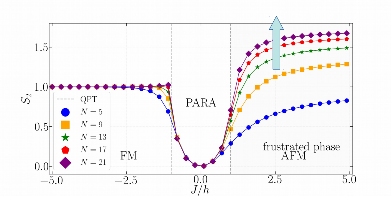
2. Semi-classical picture of a quasiparticle[1]



$$\rho^{\text{frus}}_{[m]} = \rho^{\text{unfrus}}_{[m]} \otimes \rho^{\text{semi}}_{[m]}, \qquad \text{where} \qquad \rho^{\text{semi}}_{[m]} = m|0\rangle\langle 0| + (1-m)|1\rangle\langle 1|.$$

[1] Giampaolo, Ramos, and Franchini; J. Phys. Comm. **3**, 081001 (2019)

Exact results in the thermodynamic limit

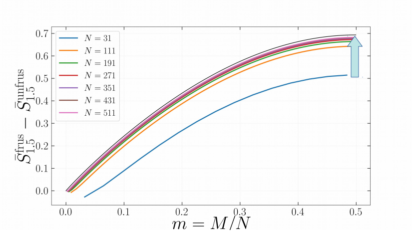


We obtain for the Rényi-α entanglement[2,3]

$$S_\alpha(\rho^{\text{frus}}_{[m]}) = \frac{1}{1-\alpha} \log\left(m^\alpha + (1-m)^\alpha\right) + \log 2,$$

and in the limit $\alpha \to 1$ the von Neumann

$$S_1(\rho^{\text{frus}}_{[m]}) = -m\log(m) - (1-m)\log(1-m) + \log 2.$$



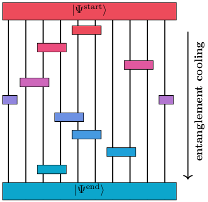
- quasiparticle in the ground state!
- excess of long-range entanglement (beyond area-law)!
- entanglement immune to the introducing integrability breaking terms!

[2] Castro-Alvaredo, De Fazio, Doyon, and Szécsényi; Phys. Rev. Lett. **121**, 170602 (2018); JHEP **39** (2018);JHEP **58** (2019).

[3] You, Wybo, Pollmann, and Sondhi; Phys. Rev. B **106**, L161104 (2022).

How robust (stochastically irreversible) is this?

- We attempt to disentangle the frustrated ground state using the entanglement cooling



- Simulated annealing Metropolis Monte-Carlo quantum circuit[4]

Set 1	Set 2
$h_j^{(1)} = \sigma_j^z \otimes \mathbb{I}_{j+1} + \mathbb{I}_j \otimes \sigma_{j+1}^z$	$h_j^{(4)} = \sigma_j^x \otimes \mathbb{I}_{j+1} + \mathbb{I}_j \otimes \sigma_{j+1}^x$
$h_j^{(2)} = \sigma_j^x \otimes \sigma_{j+1}^x$	$h_j^{(5)} = \sigma_j^y \otimes \mathbb{I}_{j+1} + \mathbb{I}_j \otimes \sigma_{j+1}^y$
$h_j^{(3)} = \sigma_j^y \otimes \sigma_{j+1}^y$	$h_j^{(6)} = \sigma_j^z \otimes \sigma_{j+1}^z$

- Set 1 is parity preserving
- Sets 1 & 2 are taken together from the universal set[5]

- focus on Rényi-2 due to less computational demand
- use GPU parallel code[6]

[4] Yang, Hamma, Giampaolo, Mucciolo, and Chamon, Phys. Rev. B **96**, 020408 (2017)

[5] Barenco, Bennett, Cleve, DiVincenzo, Margolus, Shor, Sleator, Smolin, and Weinfurter, Physical Review A **52**, 3457 (1995).

[6] N. Mijić, and D. Davidović; arXiv:2203.09353 (2022).

Entanglement cooling results - arXiv.2210.13495

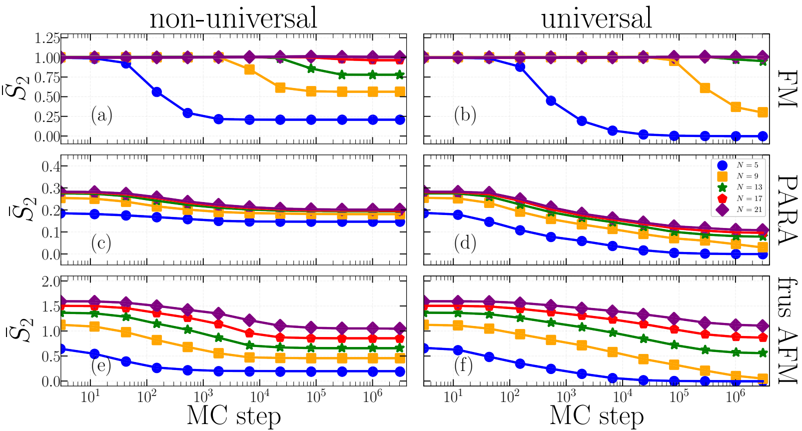
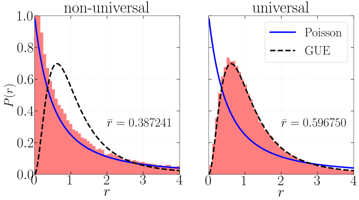
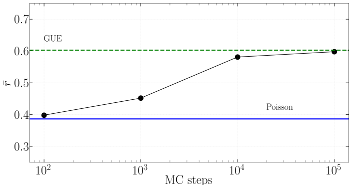


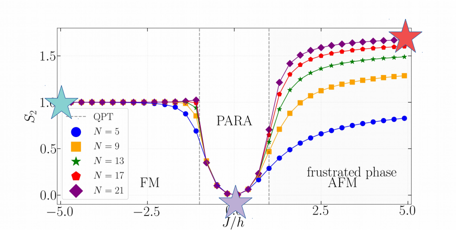
Figure: Averaged half-chain Rényi-2 entanglement entropy during the entanglement cooling over $M = 96$ Metropolis MC trajectories for ground states of the TFIM Hamiltonian different macroscopic phases.





- Consecutive entanglement spectrum spacing ratio histogram and average at the end of the cooling algorithm.
- Frustrated ground state starting point.

Set 1	Set 2
$h_j^{(1)} = \sigma_j^z \otimes \mathbb{I}_{j+1} + \mathbb{I}_j \otimes \sigma_{j+1}^z$	$h_j^{(4)} = \sigma_j^x \otimes \mathbb{I}_{j+1} + \mathbb{I}_j \otimes \sigma_{j+1}^x$
$h_j^{(2)} = \sigma_j^x \otimes \sigma_{j+1}^x$	$h_j^{(5)} = \sigma_j^y \otimes \mathbb{I}_{j+1} + \mathbb{I}_j \otimes \sigma_{j+1}^y$
$h_j^{(3)} = \sigma_j^y \otimes \sigma_{j+1}^y$	$h_j^{(6)} = \sigma_j^z \otimes \sigma_{j+1}^z$



Limits

- FM Greenberger–Horne–Zeilinger state

$$|GHZ\rangle = \frac{1}{\sqrt{2N}} \left(|+\rangle^{\otimes N} + |-\rangle^{\otimes N} \right)$$

- PARA

$$|\psi\rangle = |+ \text{ or } -\rangle^{\otimes N}$$

- frustrated AFM W-state

$$|W\rangle = \frac{1}{\sqrt{N}} \left(|100...0\rangle + |010...0\rangle + ... + |000...1\rangle \right)$$

Wait, but HOW?!

Transforming $|W_k\rangle$ in a $|W\rangle$ state - arXiv:2209.10541

$$|W_k\rangle = \hat{\mathcal{S}}\,|W\rangle$$

$$|W\rangle = \frac{1}{\sqrt{N}}\left(|100...0\rangle + |010...0\rangle + ... + |000...1\rangle\right)$$

$$|W_k\rangle = \frac{1}{\sqrt{N}}\left(|++-+-...\rangle + |-++-+...\rangle + |+-++-...\rangle + ...\right),$$

$|W\rangle$ retain the maximum amount of b. entanglement after local measurement on one of its part.

$$\hat{\mathcal{S}} = \prod_{i=1}^{N-1} \mathsf{C}(N, N-i)\left(\prod_{i=1}^{M} \sigma^z_{2i-1}\right)\mathsf{H}(N)\sigma^z_N \prod_{i=1}^{N-1} \mathsf{C}(i, i+1)\Pi^z$$

Clifford gates (Clifford circuits)

- $\mathsf{H}(i)$ – Hadamard Gate
- $\mathsf{C}(i, j)$ – C-Not Gate
- $\Pi^z = \bigotimes_{i=1}^N \sigma^z_i$

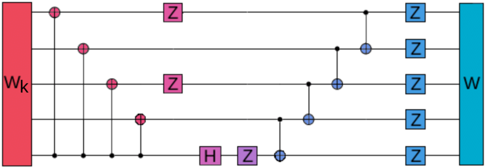


Figure: Clifford circuit $\hat{\mathcal{S}}$ for $N = 5$.

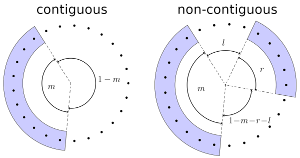
- **These two states are of equal complexity!**

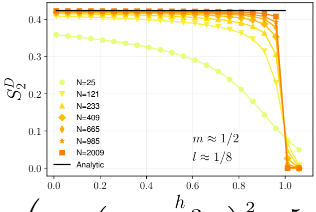
Topological ground states? - unpublished

- Topological Entanglement Entropy - universal constant capturing global entanglement in the ground-state[7]
- Inspired by one-dimensional Su-Schrieffer-Heeger (SSH) example we use

$$S_\alpha^{\mathrm{D}} = S_{\mathrm{A},\alpha} + S_{\mathrm{B},\alpha} - S_{\mathrm{A}\cup\mathrm{B},\alpha} - S_{\mathrm{A}\cap\mathrm{B},\alpha} \quad \text{either} \quad 0, 1$$

- Either **zero** (non-topological) or **one** (topological)





$$S_2^{\mathrm{D}}(m,l) = -\log\left(l^2 + (1-l-m)^2 + \frac{m^2}{2}\right) + \log\left(l^2 + \left(1 - l - \frac{3m}{2}\right)^2 + \frac{5m^2}{4}\right)$$

$$+ \log\left(\frac{m^2}{4} + \left(1 - \frac{m}{2}\right)^2\right) - \log\left(m^2 + (1-m)^2\right).$$

[7] Kitaev and Preskill, PRL **96**, 110404 (2006); Levin and Wen, PRL **96**, 110405 (2006)

The end!

Thank you for your attention!

Key points!

- Boundary conditions matter! Beyond Landau paradigm?
- Effects of frustration on entanglement
- Entanglement robustness
- Quantum information perspective
- Link between W and kink W state
- Long-range entanglement and topology?