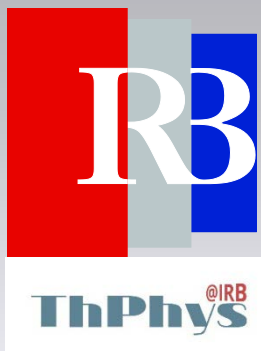


The Frustration of being Odd

Fabio Franchini

Rudjer Boskovic Institute, Zagreb, Croatia

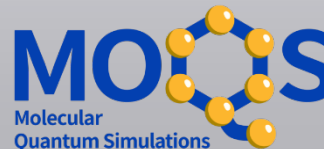


with: Salvatore Marco Giampaolo,
Gianpaolo Torre,
Jovan Odavić
Riccarda Bonsignori
Rudjer Boskovic Institute
Alberto Catalano
UniStra/Rudjer Boskovic Institute
Vanja Marić (former student)
Paris Saclay (SISSA/RBI)
and others...

Based on:

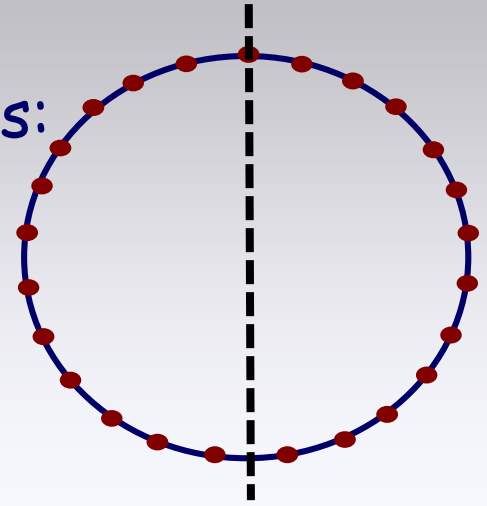
- *J. Phys. Commun.* 3, 081001 (2019);
- *New J. Phys.* 22 083024 (2020);
- *Nature's Comm. Phys.* 3, 220 (2020);
- *J. Phys. A* 54 025201 (2020);
- *Sci Rep* 11, 6508 (2021);
- *Phys. Rev. B* 103, 014429 (2021);
- *Phys. Rev. B* 105, 064408 (2022);
- *SciPost Phys.* 12, 075 (2022);
- *Phys. Rev. B* 105, 184424 (2022);
- *Phys. Rev. B* 106, 125145 (2022);
- arXiv:2209.10541; arXiv:2210.13495;
arXiv:2307.02529 & work in progress

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European Regional Development Fund - the Competitiveness and
Cohesion Operational Programme (KK.01.1.1.01.0004)
Horizon 2020 Marie Skłodowska-Curie MoQS ITN (GA #955479).



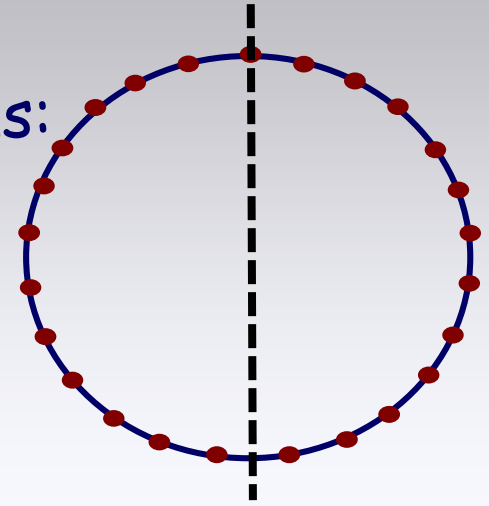
Frustrated Boundary Conditions

- We revisited an old problem for spin chains:
the effect of **periodic b.c.** with
an **ODD** number of sites
- Referred as: **Frustrated Boundary Conditions (FBC)**



Frustrated Boundary Conditions

- We revisited an old problem for spin chains:
the effect of **periodic b.c.** with
an **ODD** number of sites
- Referred as: **Frustrated Boundary Conditions (FBC)**
- Why such interest?
- From one side: b.c. can only matter in finite systems
(are we sure?)
- From another side: **FBC are special**



1D Classical Ising

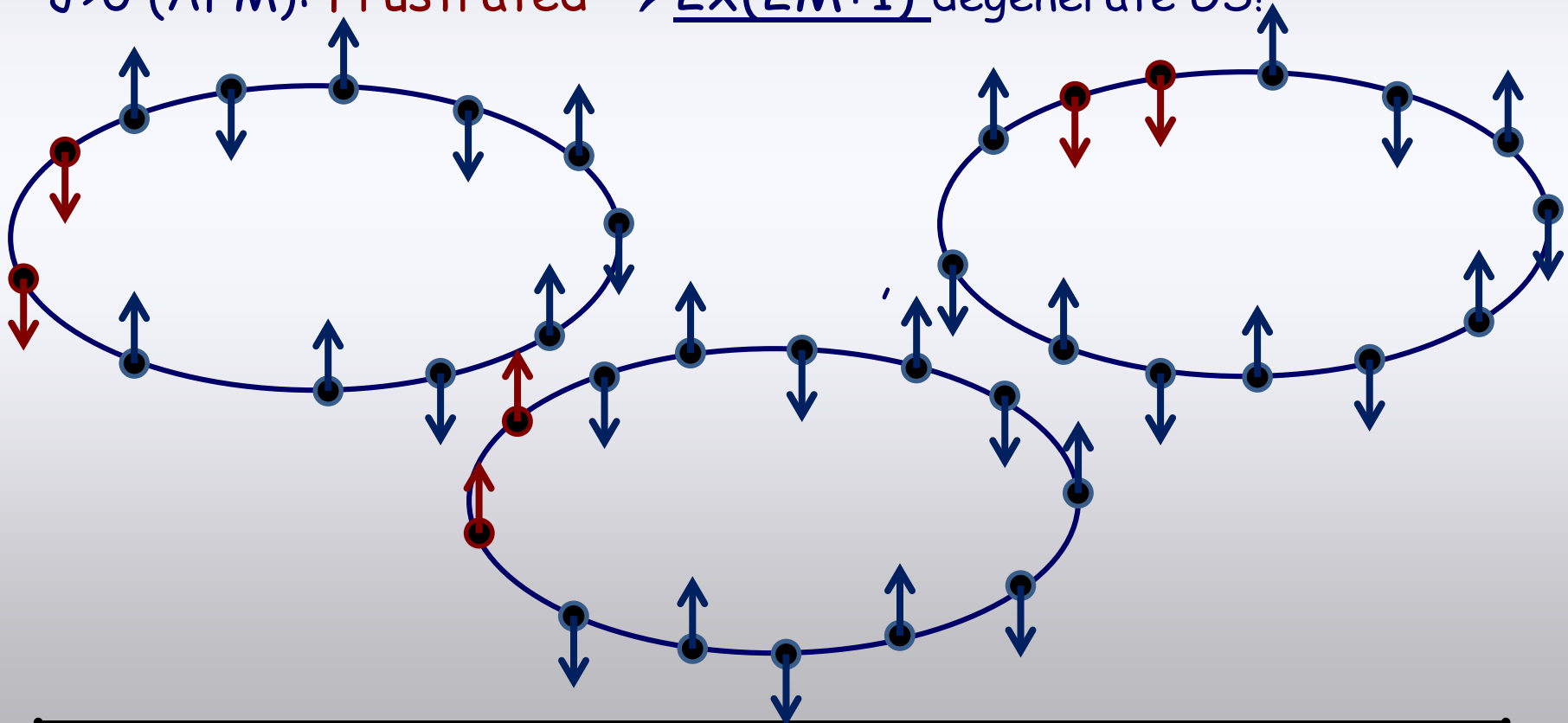
$$H_{\text{Ising}} = J \sum_{l=1}^{2M+1} \sigma_l^x \sigma_{l+1}^x$$

- $J < 0$ (Ferromagnetic): 2 deg ground states

1D Classical Ising

$$H_{\text{Ising}} = J \sum_{l=1}^{2M+1} \sigma_l^x \sigma_{l+1}^x$$

- $J < 0$ (Ferromagnetic): 2 deg ground states
- $J > 0$ (AFM): **Frustrated** → $2 \times (2M+1)$ degenerate GS!



Perturbative picture

$$H = \frac{1}{2} \sum_{l=1}^{2M+1} (\sigma_l^x \sigma_{l+1}^x + \lambda h_l)$$

- At $\lambda=0$: **2N-degenerate GS** (2 x Neel with 1 domain wall)
(compare to 2-degenerate for N even, i.e not frustrated)
- Turn on $\lambda \neq 0$: degeneracy lifted, GS part of a band
- Perturbative picture: low-energy eigenstates as a **traveling domain wall** with different momenta

Laumann et al, PRL (2012)

Order parameter

$$H_{\text{Ising}} = \frac{1}{2} \sum_{l=1}^{2M+1} (\sigma_l^x \sigma_{l+1}^x + \lambda \sigma_l^y \sigma_{l+1}^y)$$

- Without frustration, Z_2 broken phase: $\langle \sigma_j^x \rangle = \pm (-1)^j m_x$
- Staggered order **not compatible** with pbc and odd # sites

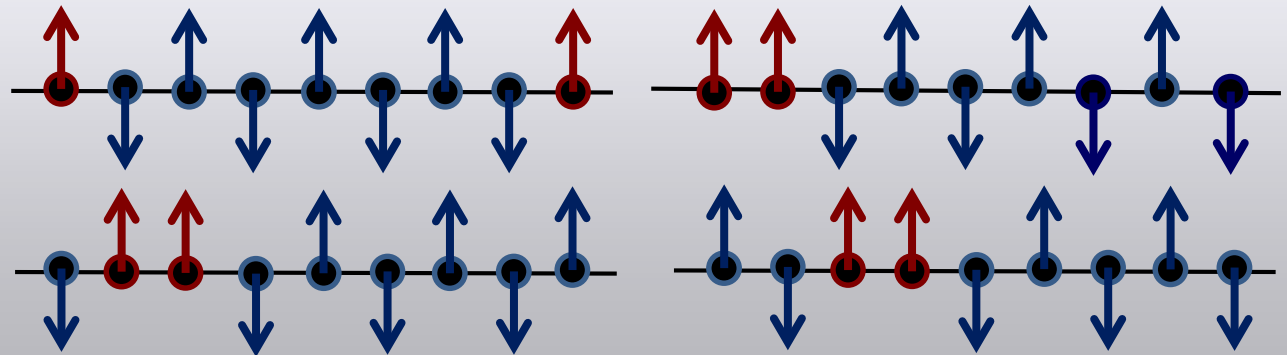
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order \rightarrow **vanishing magnetization**

$$\langle \sigma_j^x \rangle = \pm \frac{\tilde{m}_x}{2M+1} \rightarrow 0$$



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order \rightarrow **vanishing magnetization** $\langle \sigma_j^x \rangle = \pm \frac{\tilde{m}_x}{2M+1} \rightarrow 0$

- Alternatively: 2 counterpropagating waves

\Rightarrow **non perfect staggerization (& beats)**

$$\langle \sigma_j^x \rangle = (-1)^j \cos \left(\pi \frac{j}{N} + \theta \right) m_x$$

Paradoxical conclusion?

$$H_{\text{Ising}} = \frac{1}{2} \sum_{l=1}^{2M+1} (\sigma_l^x \sigma_{l+1}^x + \lambda \sigma_l^y \sigma_{l+1}^y)$$

- XY chain posterchild for SSB \Rightarrow order parameter
- Perturbative calculation show fragility against FBC

Can boundary conditions affect bulk order?

Paradoxical conclusion?

$$H_{\text{Ising}} = \frac{1}{2} \sum_{l=1}^{2M+1} (\sigma_l^x \sigma_{l+1}^x + \lambda \sigma_l^y \sigma_{l+1}^y)$$

- XY chain posterchild for SSB \Rightarrow order parameter
- Perturbative calculation show fragility against FBC

Can boundary conditions affect bulk order?

We perform non-perturbative analytically exact and numerical analysis to analyze the subtle effects of FBC

- Non perturbative calculations confirm perturbative picture!

Frustrated Systems

- Certain degree of frustration is very common
- In any dimension, due to closed AFM loops
- Typically: **extensive frustration**
(# loops scale with system size)
 - **Ordered** (ANNNI model, spin-ice...)
 - **Disordered** (Sherrington-Kirkpatrick model, spin glasses...)
- Peculiar physics: residual entropy, local zero-modes, algebraic decay, artificial EM, monopoles, Dirac strings...
- Hard problem

Frustrated Boundary Conditions

- We pursue a **bottom-up** approach
- We consider a simple setting:

spin chains with **frustration only from b.c. (FBC)**
- We find emergent phenomenologies **reminiscent** of extensive frustration case!

Chain in zero field

$$H = \sum_{j=1}^{2M+1} \left[\cos \delta \left(\cos \phi \sigma_j^x \sigma_{j+1}^x + \sin \phi \sigma_j^y \sigma_{j+1}^y \right) - \sin \delta \sigma_j^z \sigma_{j+1}^z \right]$$

- In absence of external fields, H is **T-Symmetric**
 \Rightarrow **Kramer's degeneracy**
- **GS is at least 2-fold degenerate even at finite size**

Chain in zero field

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- In absence of external fields, H is **T-Symmetric**

⇒ **Kramer's degeneracy**

- GS is at least **2-fold degenerate** even at finite size

- Any GS choice breaks a parity symmetry: $\Pi^\alpha \equiv \prod_{j=1}^N \sigma_j^\alpha$, $\alpha = x, y, z$
⇒ we can **SSB** at finite N !

- Avoid usual tricky order of limits with external field

XYZ Chain in zero field

$$H = \sum_{j=1}^{2M+1} \left[\cos \delta \left(\cos \phi \sigma_j^x \sigma_{j+1}^x + \sin \phi \sigma_j^y \sigma_{j+1}^y \right) - \sin \delta \sigma_j^z \sigma_{j+1}^z \right]$$

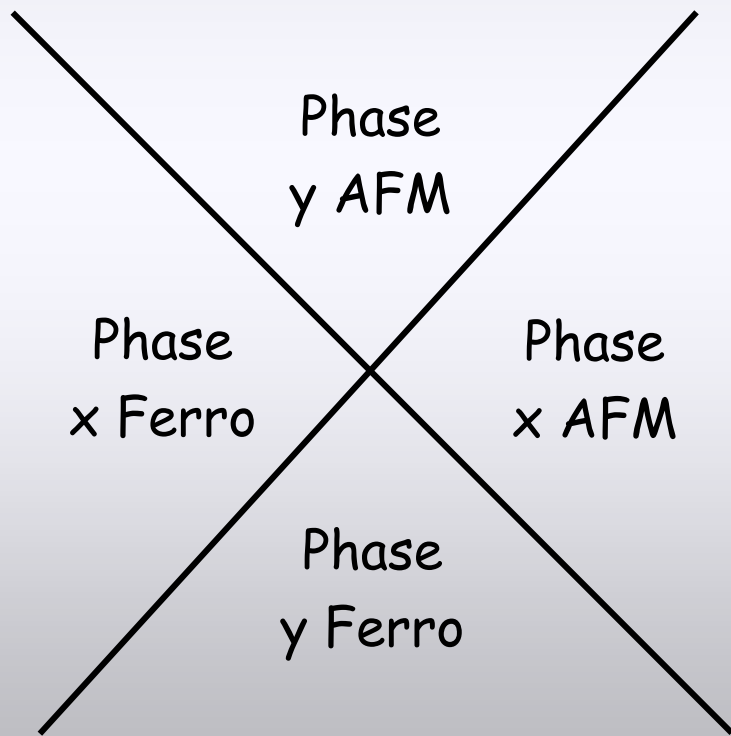
- Exact finite size degeneracy allow "SSB at finite N"
- We also found a way to compute 1-point fct. directly
⇒ Exact finite size expressions for observables (magnetization)
and follow them to the thermodynamic limit

XYZ Chain in zero field

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Duality
 $\sigma_j^x \leftrightarrow \sigma_j^y$

$N=2M$: not frustrated



XYZ Chain in zero field

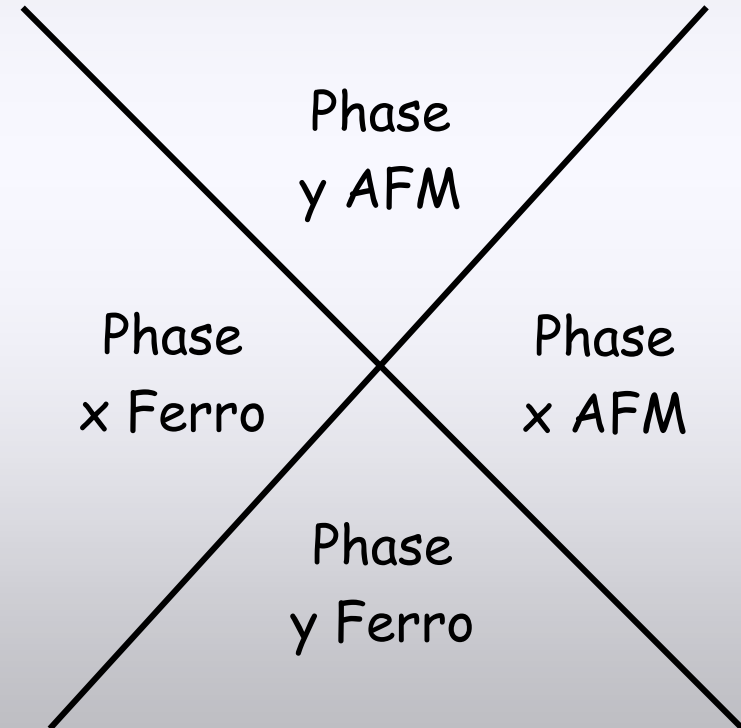
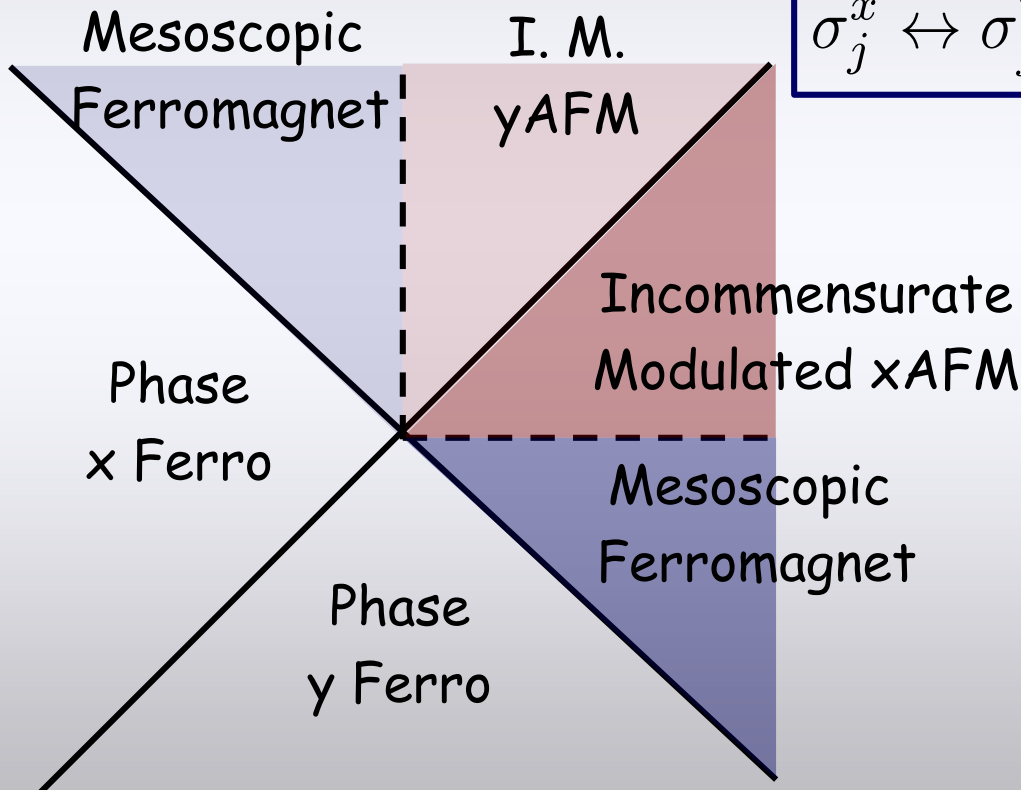
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$N=2M+1$

Duality

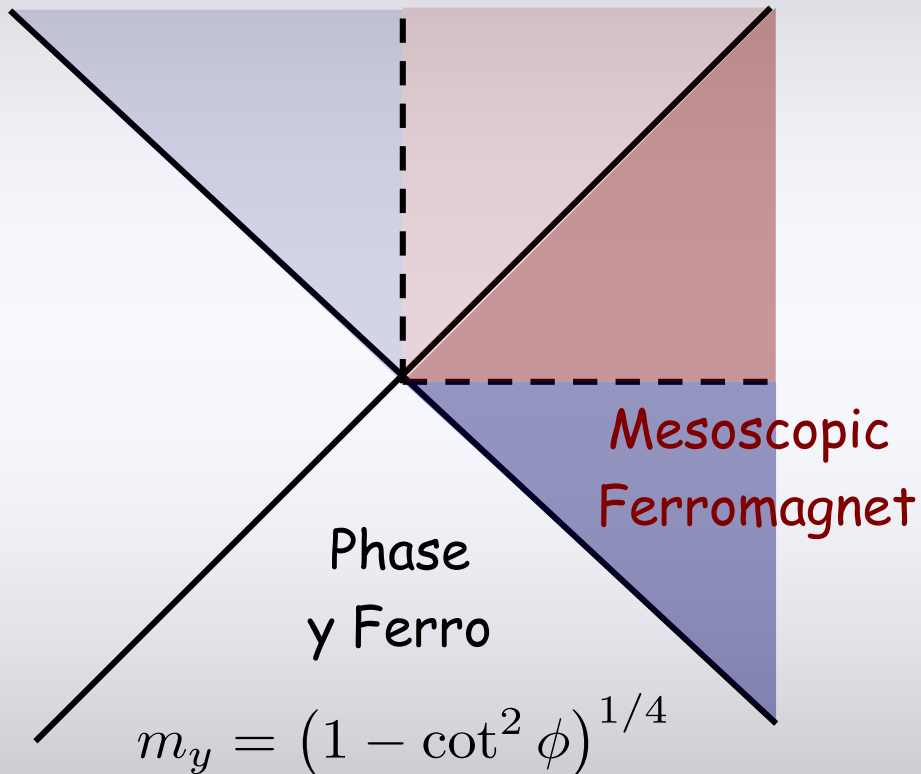
$$\sigma_j^x \leftrightarrow \sigma_j^y$$

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$$m_\alpha \simeq \frac{\tilde{m}_\alpha}{N^\gamma} \xrightarrow{N \rightarrow \infty} 0$$

All magnetizations decay algebraically to zero and are not staggered!

Consistency check
on methodology!

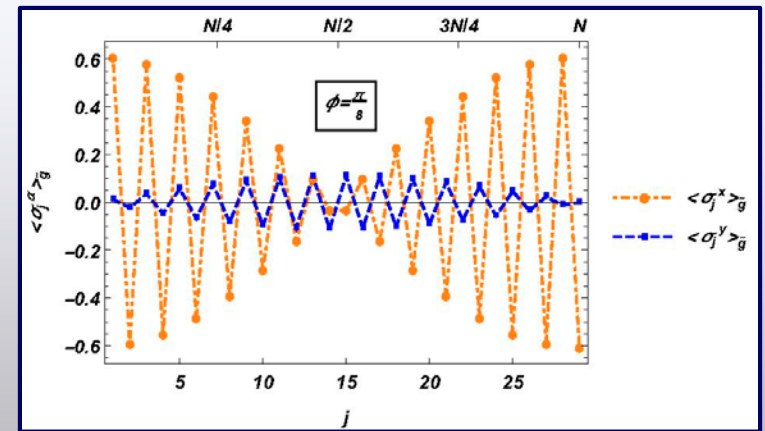
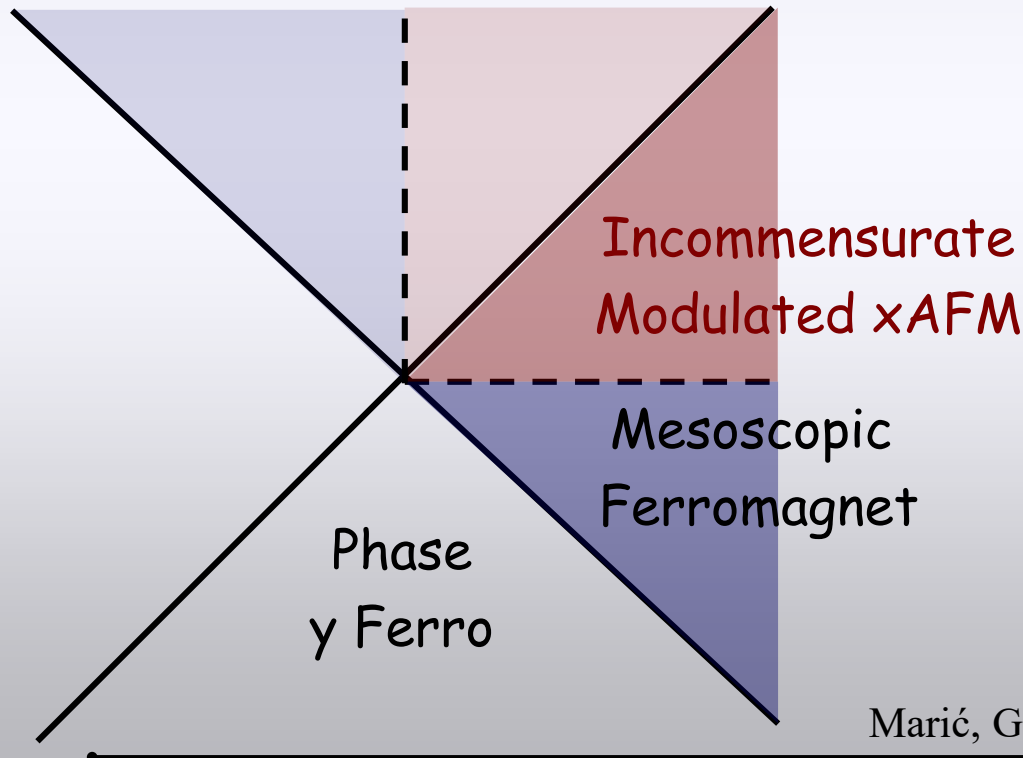
Marić, Giampaolo, Kulić, Franchini, New J. Phys. 22 083024 (2020)

Incommensurate Modulated AFM

$$H = \sum_{j=1}^{2M+1} \left[\cos \phi \sigma_j^x \sigma_{j+1}^x + \sin \phi \sigma_j^y \sigma_{j+1}^y \right]$$

- **IMAFM:** $\phi \in (0, \pi/4)$

- 2 frustrated) AFM int.
- Lowest energy states have finite momentum $\pm\pi/2$
- GS can break transl. Inv.



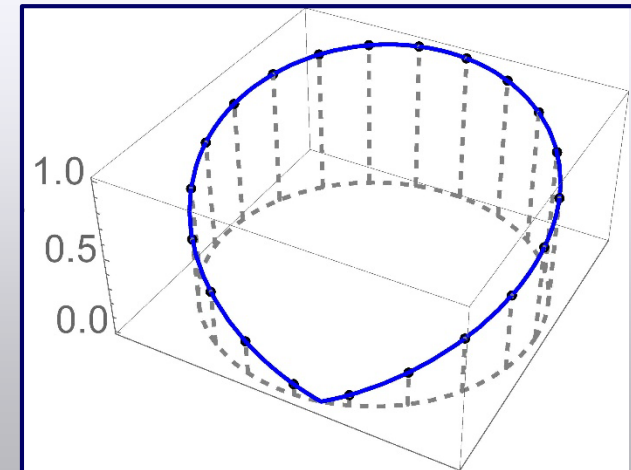
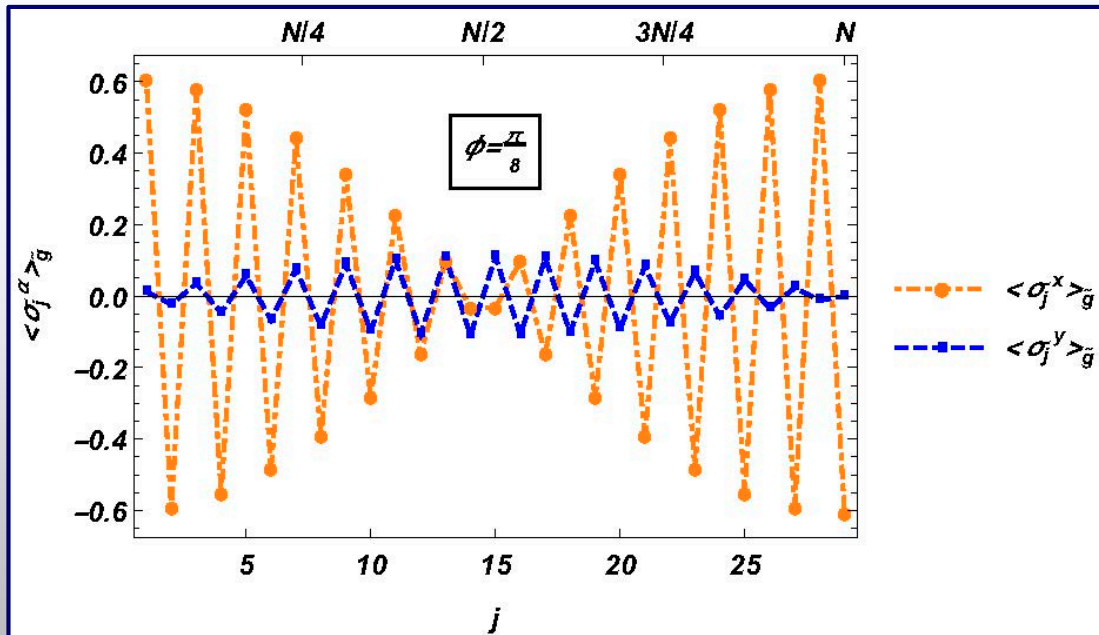
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$$\langle \tilde{g} | \sigma_j^\alpha | \tilde{g} \rangle = (-1)^j \cos \left(\pi \frac{j}{N} + \tilde{\theta}_\alpha \right) f_\alpha$$



Incommensurate Modulated AFM

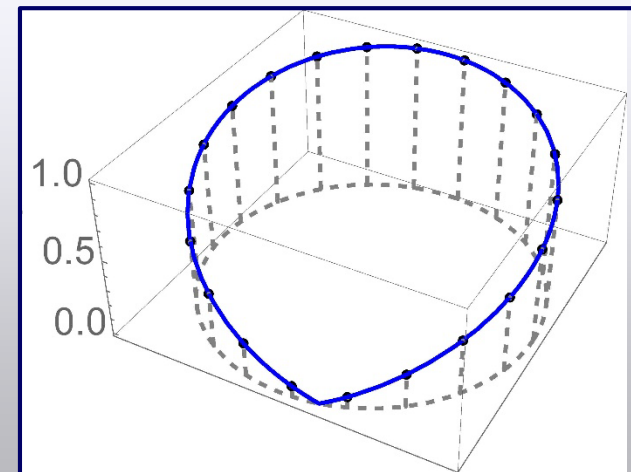
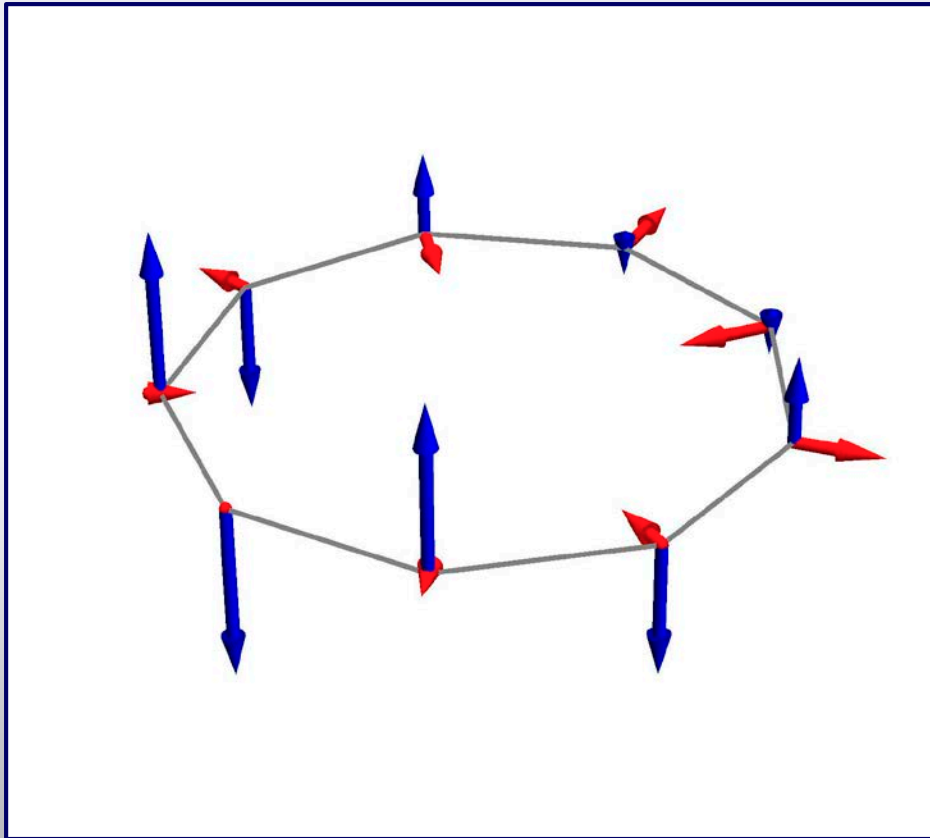
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- **IMAFM:** $\phi \in (0, \pi/4)$

$$p \equiv \frac{\pi}{2} \left(1 + \frac{1}{N} \right)$$

$$|\tilde{g}\rangle \equiv \frac{1}{\sqrt{2}} \left[|\pm p, +\rangle + e^{i\theta} |\mp p, -\rangle \right]$$

$$\langle \tilde{g} | \sigma_j^\alpha | \tilde{g} \rangle = (-1)^j \cos \left(\pi \frac{j}{N} + \tilde{\theta}_\alpha \right) f_\alpha$$

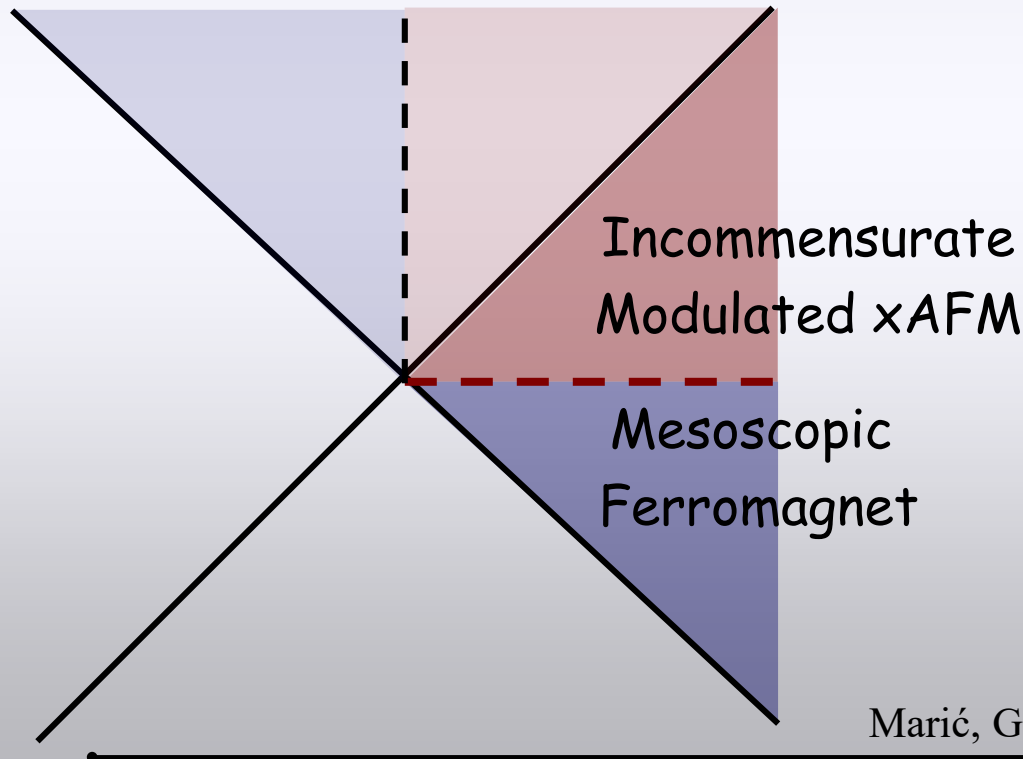


Quantum phase transition?

$$H = \sum_{j=1}^{2M+1} [\cos \phi \sigma_j^x \sigma_{j+1}^x + \sin \phi \sigma_j^y \sigma_{j+1}^y]$$

$$\left. \frac{dE_g}{d\phi} \right|_{\phi \rightarrow 0^-} - \left. \frac{dE_g}{d\phi} \right|_{\phi \rightarrow 0^+} = 2 \left(1 + \cos \frac{\pi}{N} \right)$$

- $\phi=0$ (classical Ising)
 - **Level crossing** (change in GS degeneracy: $2 \leftrightarrow 4$)
 - **Finite discontinuity** in 1^o derivative of GS energy
 - Akin to a 1^o order b-QPT
- \Rightarrow **Boundary-less b-QPT**



Marić, Giampaolo, Franchini, Comm. Phys. 3, 220 (2020)

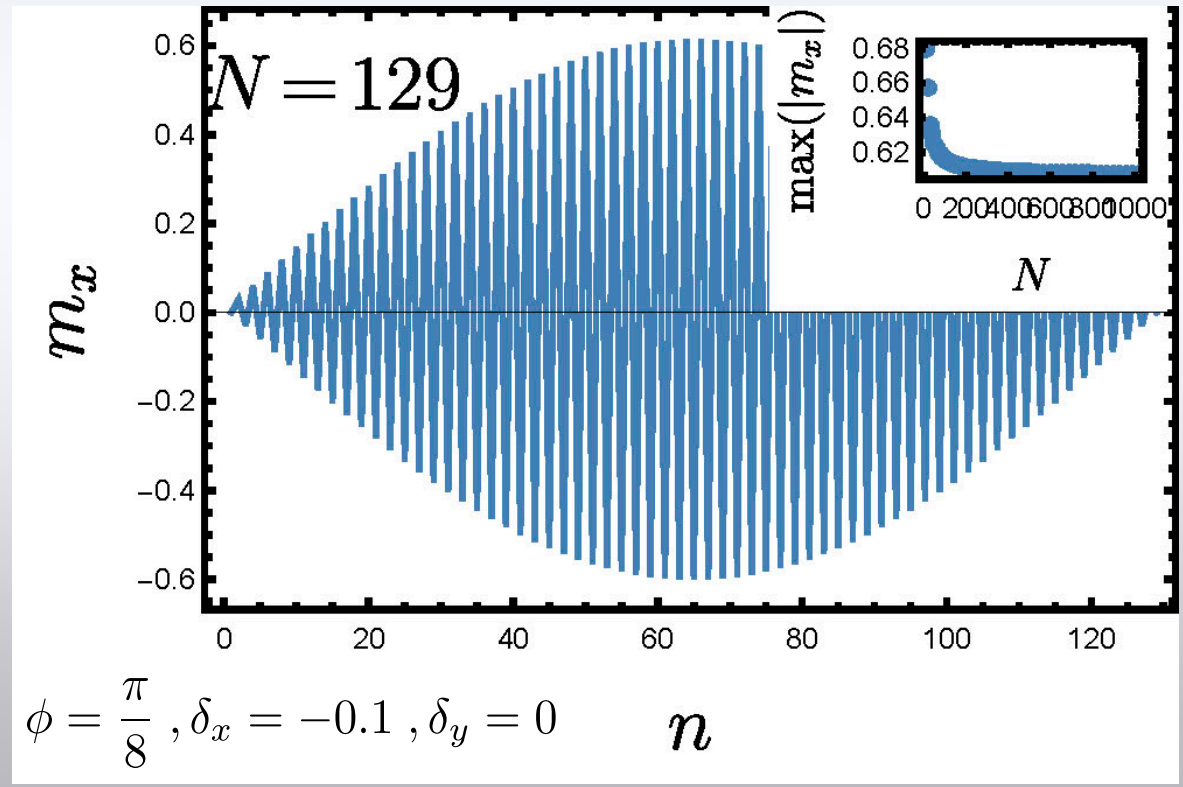
Defects

$$H = \sum_{j=1}^{2M} [\cos \phi \sigma_j^x \sigma_{j+1}^x + \sin \phi \sigma_j^y \sigma_{j+1}^y] + \cos(\phi + \delta_x) \sigma_{2M+1}^x \sigma_1^x + \sin(\phi + \delta_y) \sigma_{2M+1}^y \sigma_1^y$$

- Physics discussed so far often dismissed as fragile
- A single AFM defect **stabilizes** the incommensurate AFM order!
- No defect as QPT between Ising and kink phases

Camprostrini et al, PRE 91 (2015)

Torre, Marić, FF, Giampaolo, PRB 103 (2021)



Loschmidt Echo

- FBC: massive to gapless, but deemed unobservable
- Detect difference in spectrum through a Quantum Quench

$$H_0 = \sum_{l=1}^N (\sigma_l^x \sigma_{l+1}^x + h \sigma_l^z) \longrightarrow H_1 = H_0 + \lambda \sigma_N^z$$

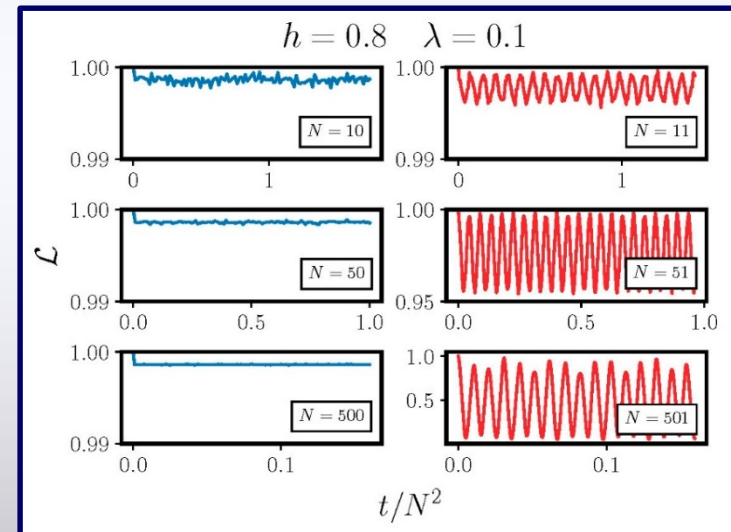
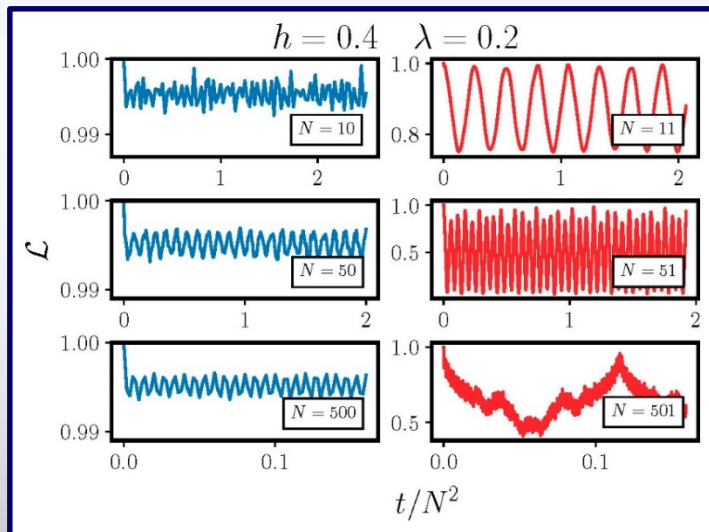
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LE distinguishes between the parity of the chain length!

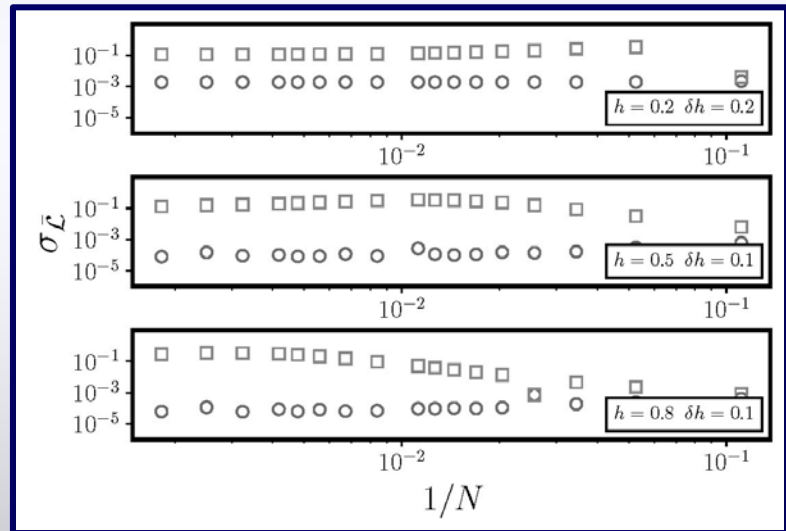
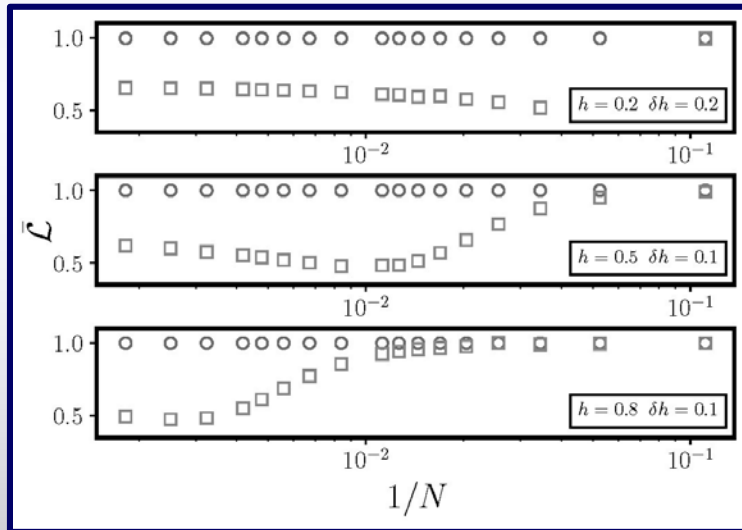
Torre, Marić, Kuić, F. F. S.M. Giampaolo, PRB (2022)

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Torre, Marić, Kuić, F. F. S.M. Giampaolo, PRB (2022)

Loschmidt Echo

- Detect difference in spectrum through a **Quantum Quench**

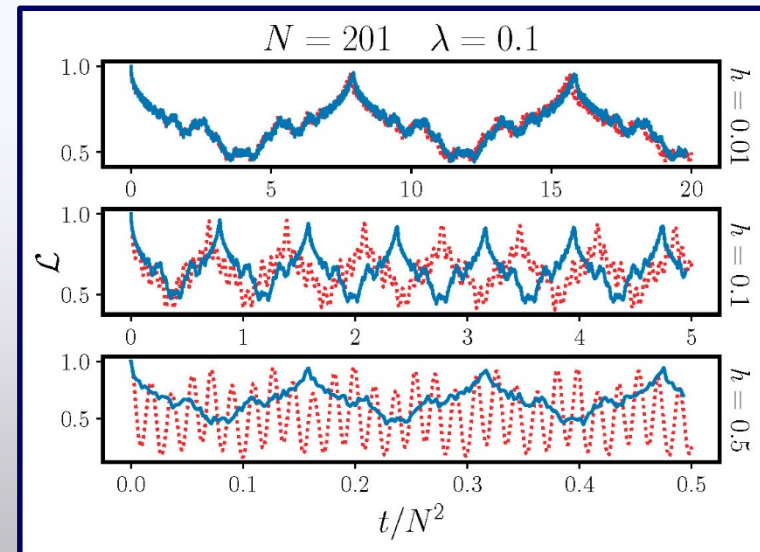
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- Loschmidt Echo: $\mathcal{L}(t) = |\langle 0 | e^{-iH_1 t} | 0 \rangle|^2$, $|0\rangle$ GS of H_0
- Perturbative calculation (domain wall basis):

$$\mathcal{L}(t) \simeq \mathcal{F} \left(\frac{2ht}{N^2} \right)$$

$$\mathcal{F}(x) = \lim_{M \rightarrow \infty} \left| \frac{1}{2M^2} \sum_{k=1}^M \tan^2 \left[\frac{(2k-1)\pi}{4M} \right] \times \exp \left\{ -ix(2M+1)^2 \cos \left[\frac{(2k-1)\pi}{2M} \right] \right\} \right|^2$$

- LE continuous, but **nowhere differentiable**



Torre, Marić, Kuić, F. F. S.M. Giampaolo, PRB (2022)

Complexity

- Loschmidt echo's features point for **greater complexity**
- We measure it as **Stabilizer Renyi Entropy (SRE or magic)**

$$\mathcal{M}_2(|\psi\rangle) = -\log_2 \left(\frac{1}{2^L} \sum_P \langle \psi | P | \psi \rangle^4 \right)$$

$$P = \bigotimes_{j=1}^L P_j, \quad P_j \in \{\sigma_j^0, \sigma_k^x, \sigma_j^y, \sigma_j^z\}$$

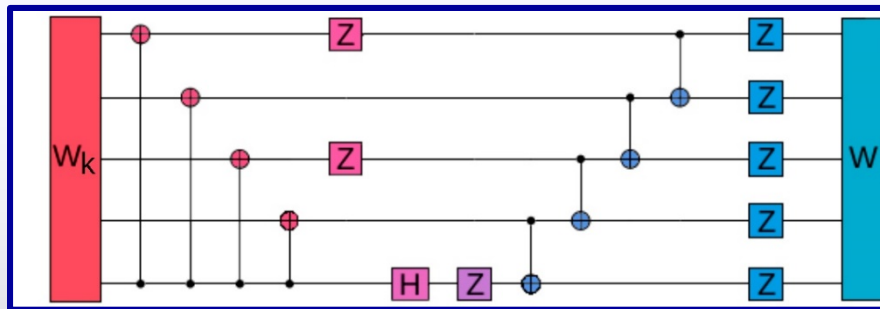
- Distance from Clifford states that can **be efficiently** classically simulated

W-States

- W-states: entangled & not separable after measurement:

$$|W\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^N \sigma_j^+ |0\rangle^{\otimes N}$$

- Near classical point, topologically frustrated gs as superposition of **kink states realizes** a W-state



(exact, SRE preserving, map between kink and W-state)

$$\mathcal{M}_2^W(L) = 3 \log_2(L) - \log_2(7L - 6)$$

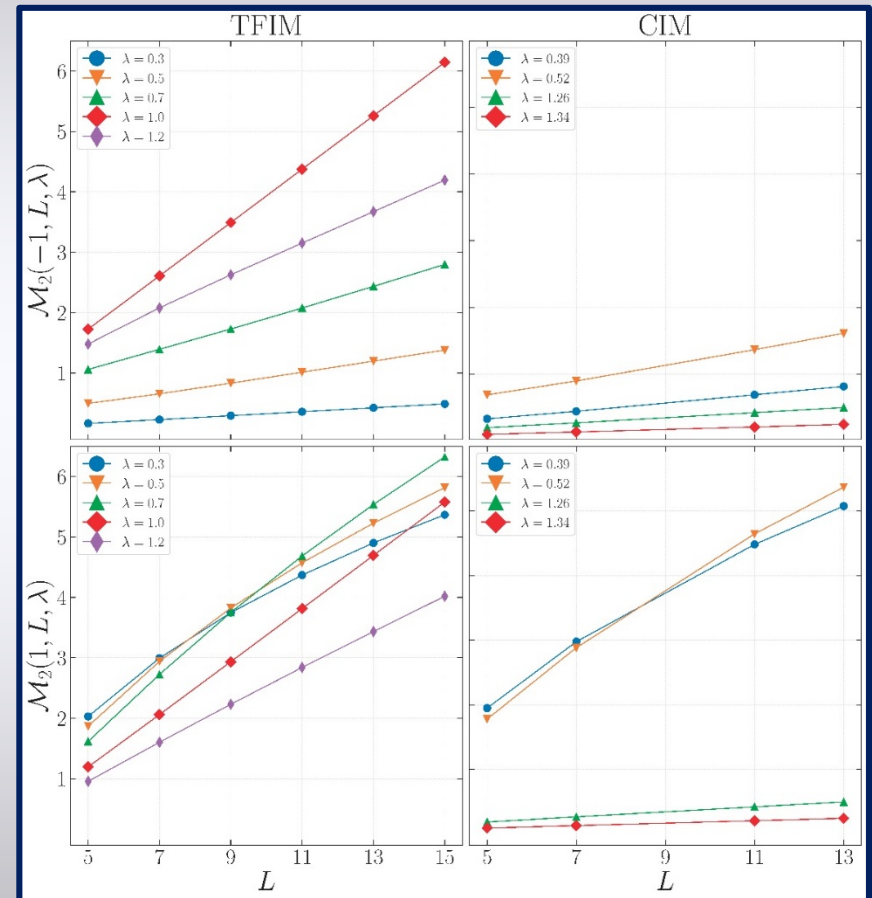
- SRE of W-state growth **logarithmically!**

SRE in topologically frustrated chains

- SRE can be decomposed as non-frustrated volume contribution and W -state logarithmic one

$$\mathcal{M}_2(J = 1, L, \lambda) = \mathcal{M}_2(J = -1, L, \lambda) + \mathcal{M}_2^W(L)$$

- FBC add non-local complexity of W -state nature

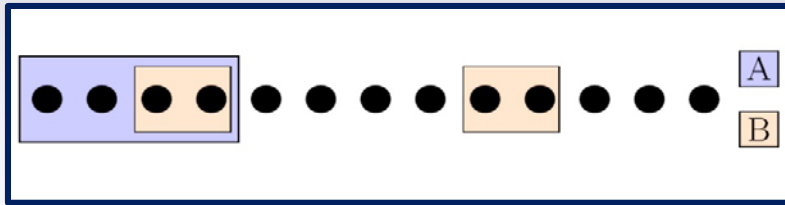


Odavić, Torre, Mijić, Davidović, F. F., Giampaolo, arXiv:2210.13495

Disconnected Topological Entropy

- Consider tripartition of chain: A , B and their complement $\overline{A \cup B}$:

$$S_{\alpha}^D = S_{A,\alpha} + S_{B,\alpha} - S_{A \cup B,\alpha} - S_{A \cap B,\alpha} \quad S_{A,\alpha} = \frac{1}{1-\alpha} \log \text{Tr}_A \rho_A^{\alpha}$$



$$\rho_A = \text{Tr}_{\overline{A}} |0\rangle\langle 0|$$

- It is called “**disconnected entropy**” and was shown to be non-zero for Symmetry Protected Topological phases.

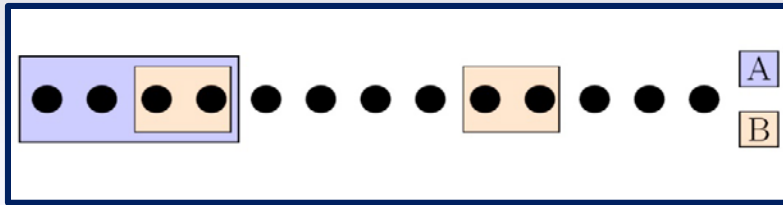
Micallo et Al. SciPost Phys. Core 3, 012 (2020)

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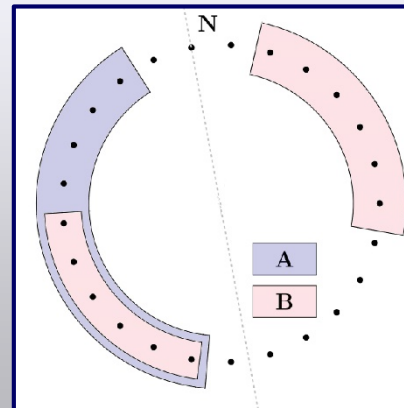
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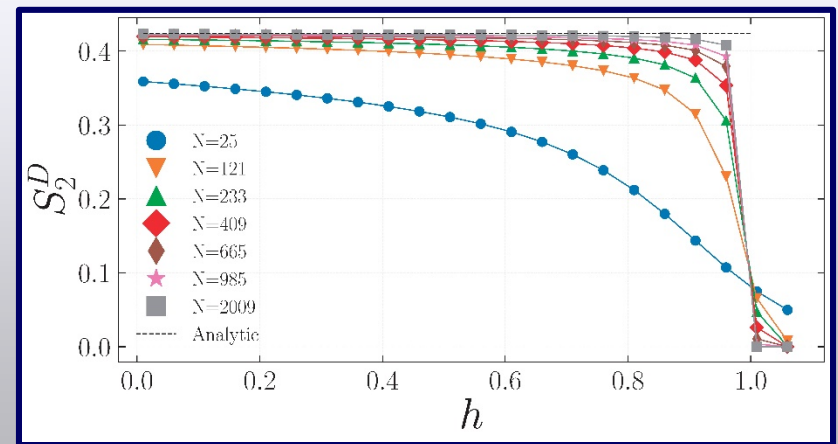
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- Topologically frustrated Ising chain:

$$H = \sum_{j=1}^{2M+1} \sigma_j^x \sigma_{j+1}^x - h \sigma_j^z$$

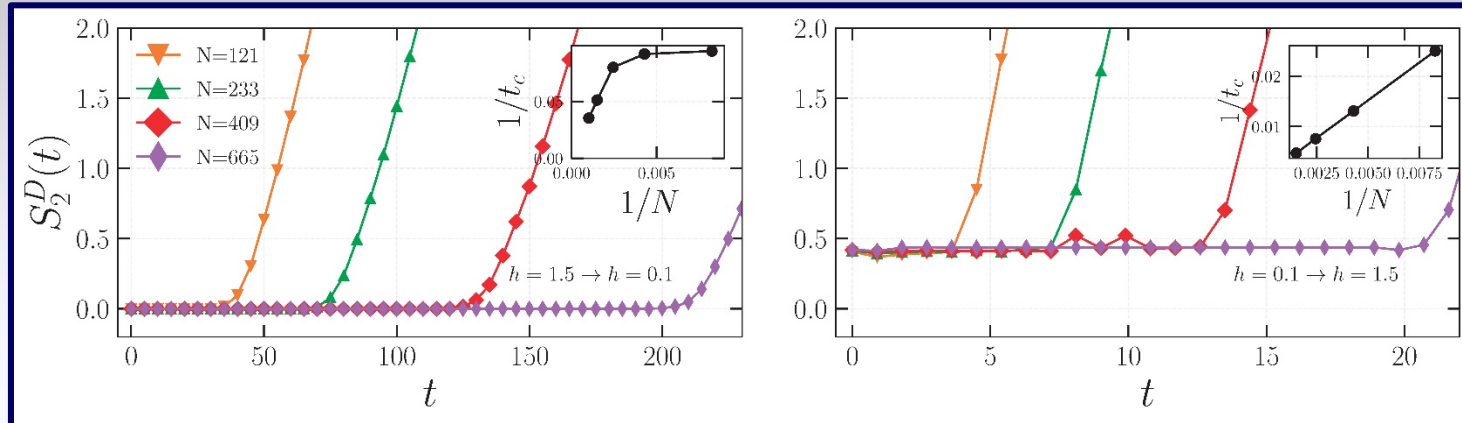


Micallo et Al. SciPost Phys. Core 3, 012 (2020)

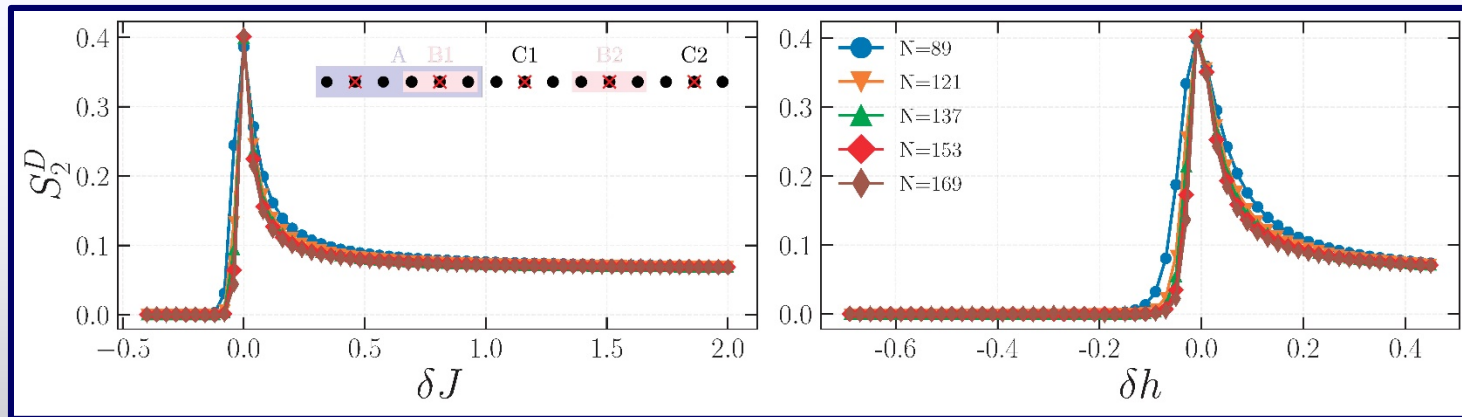


Disconnected Topological Entropy

- It is finite and resilient:



with
global
quench



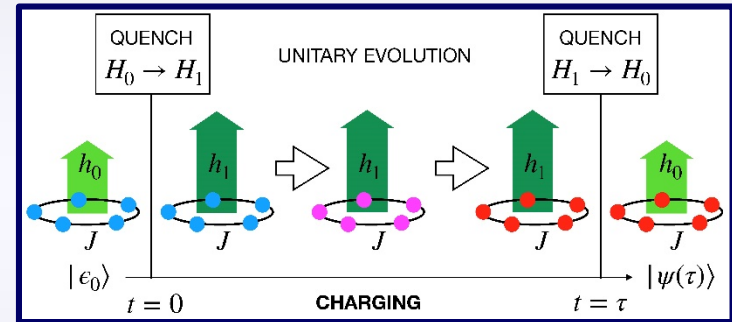
with
AFM
defects

S^D detects long-range entanglement due to fractional nature of single excitation in ground state

Technological applications

- **Quantum Battery**: quantum mechanical system that can store and transfer energy coherently
- Our charging protocol: global **quantum quench** on Ising chain

$$H_0 = \sum_{l=1}^N (\sigma_l^x \sigma_{l+1}^x + h \sigma_l^z)$$

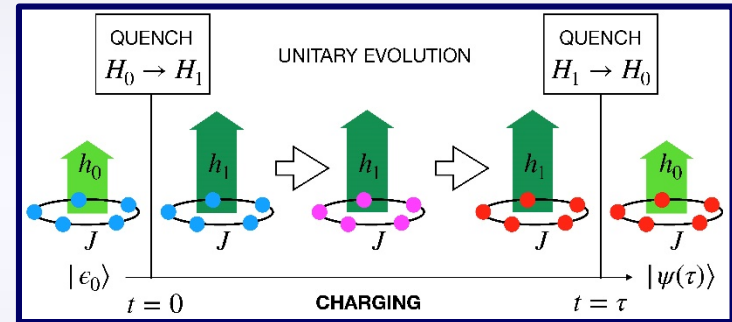


Catalano, Giampaolo, Morsch,
Giovannetti, F. F., arXiv:2307.02529

Technological applications

- **Quantum Battery**: quantum mechanical system that can store and transfer energy coherently
- Our charging protocol: global **quantum quench** on Ising chain

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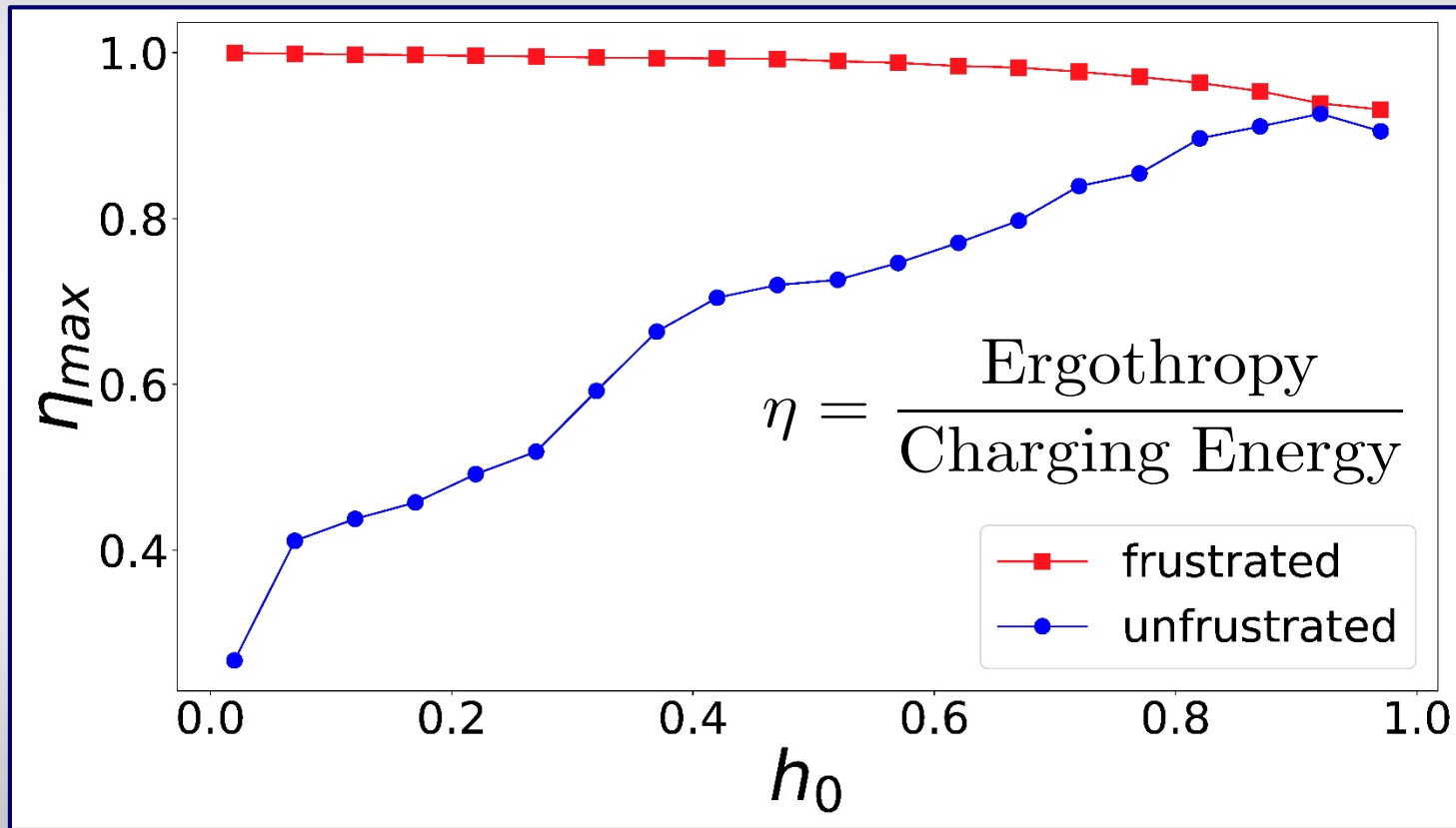


- We model **intrinsic decoherence** after quench as emergence of **diagonal ensemble** (pure \rightarrow mixed state)
- We use **ergotropy** as figure of merit: energy extractable through unitary transformation

Catalano, Giampaolo, Morsch,
Giovannetti, F. F., arXiv:2307.02529

Robustness against decoherence

- Frustrated chain more resilient against decoherence than non-frustrated counterpart



$N = 25$

$\Delta h = 0.01$

$$\eta = \frac{\text{Ergoentropy}}{\text{Charging Energy}}$$

—■— frustrated
—●— unfrustrated

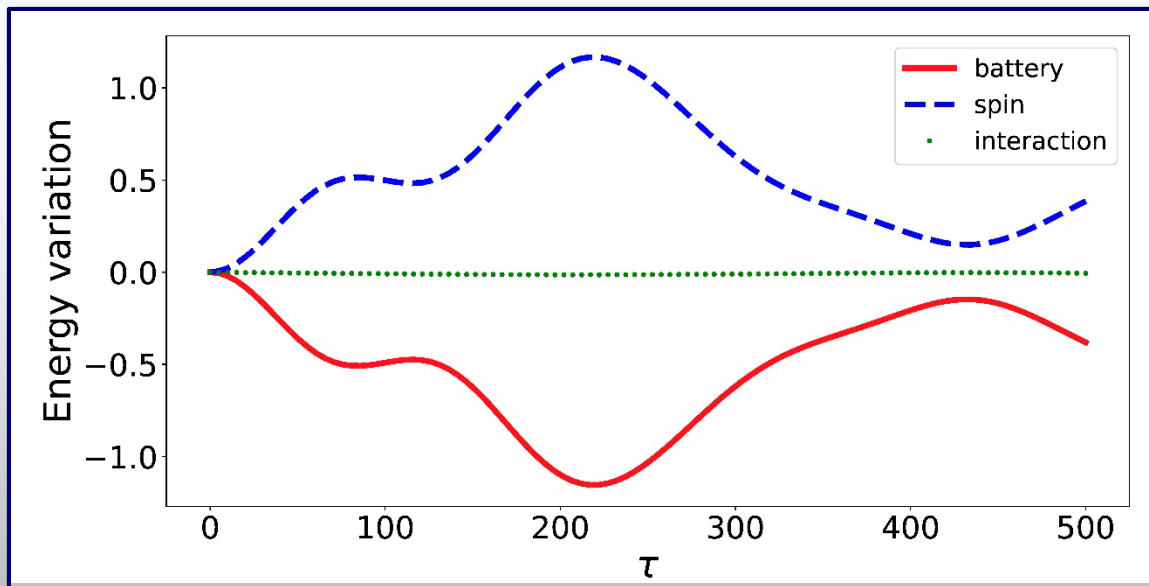
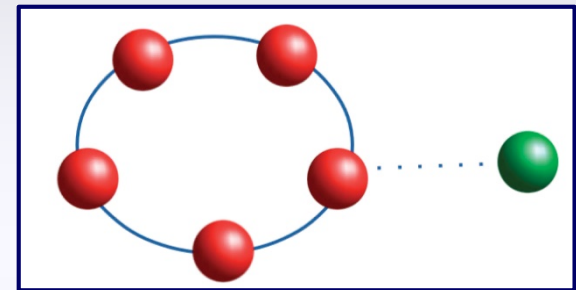
Catalano, Giampaolo, Morsch,
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Discharging

- Test: energy extraction to additional, isolated spin

$$H = \sum_{j=1}^N \sigma_j^x \sigma_{j+1}^x - h \sum_{j=1}^N \sigma_j^z + \lambda H_{int} + \omega \sigma_S^z$$

$$H_{int} = \sigma_1^+ \sigma_S^- + \sigma_1^- \sigma_S^+$$



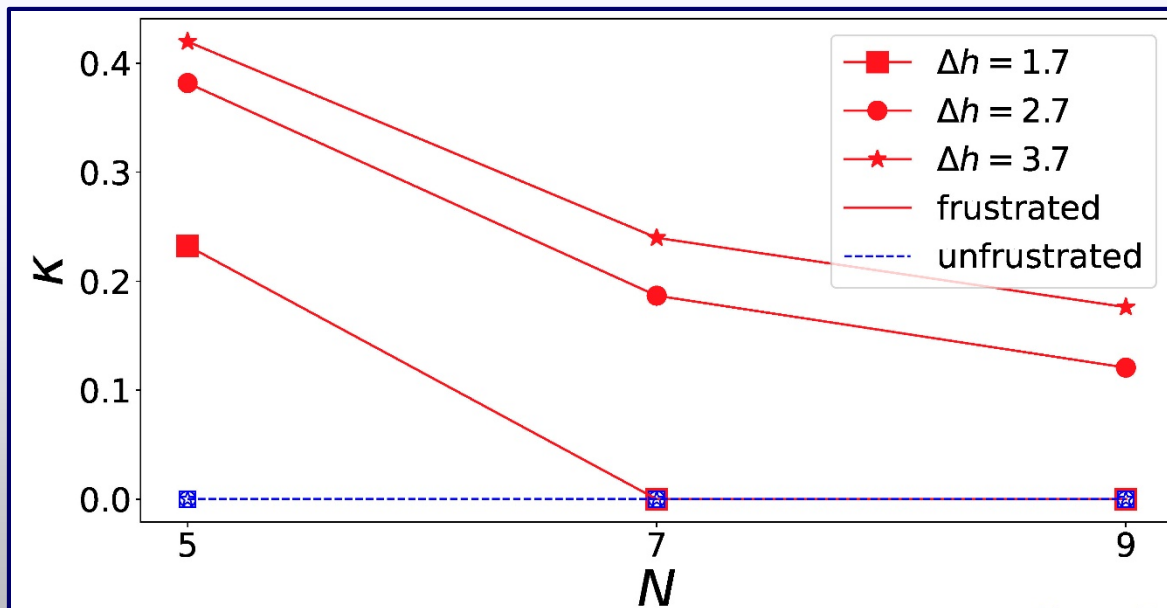
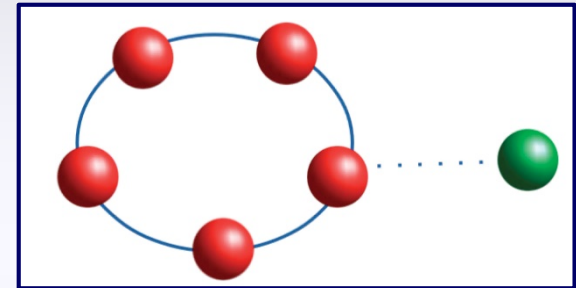
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Frustrated chain transfers **work**, not just heat as non-frustrated chain

Catalano, Giampaolo, Morsch, Giovannetti, F. F., arXiv:2307.02529

FBC and beyond

- Frustrated boundary conditions can **change** the local, bulk **order** (mesoscopic, modulated) and the **quantum phase transitions** (new b-QPT and replacing 2^o order QPT)
- More **complex** ground state, **non-local** correlations
- Frustration known to give **new physics** in quantum systems

Outlook:

- Add more frustration and follow its effects
- Add disorder (spin glass, many body localization)
- Technological exploitation:
 - ❑ Quantum batteries
 - ❑ New platform for quantum computation (new q-bit encoding)

Thank you!