FRUSTRATION OF BEING ODD

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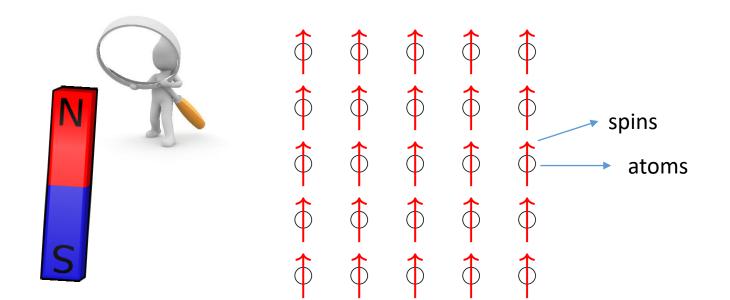


Outline

- Magnetic systems, Landau theory
- Frustration
- Research problem: Frustration + Quantum Mechanics, exact results
- Examination of particular models
- Incompletness of the Landau Theory (boundaries affect local order)
- Conclusions

FERROMAGNETS

- spins like to point in the SAME direction
- Order parameter: $\langle \vec{S}_j \rangle$



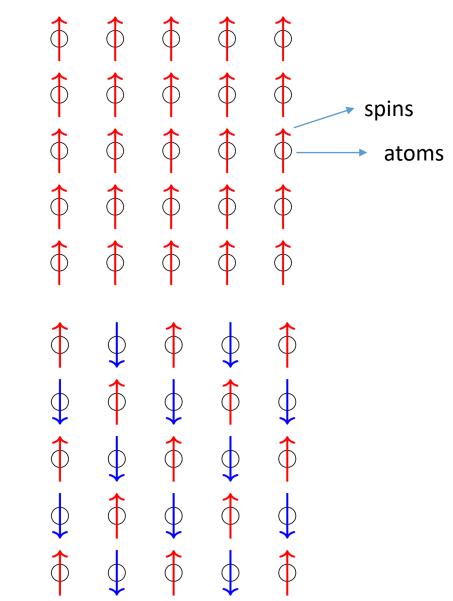
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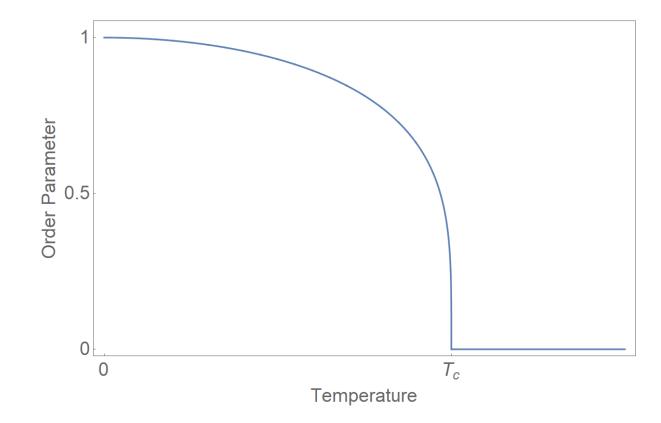
ANTIFERROMAGNETS

- spins like to point in the OPPOSITE directions
- Order parameter: $\langle (-1)^j \vec{S}_j \rangle$



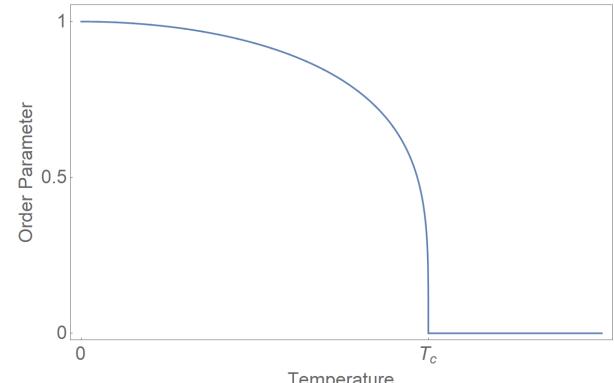
Phases and phase transitions

• Order parameter vanishes above the critical temperature



Phases and phase transitions

Order parameter ${\bullet}$ vanishes above the critical temperature



Phase transitions:

Temperature

- Classical: Changing the temperature.
- Quantum: Changing a parameter of the Hamiltonian at zero • temperature.

- Phase transitions Spontaneous Symmetry Breaking
 - Exceptions: BKT transition,
- Order parameter Zero in one phase, non-zero in the other.

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 In antiferromagnets critical behavior depends on the shape of the lattice (related to Frustration)

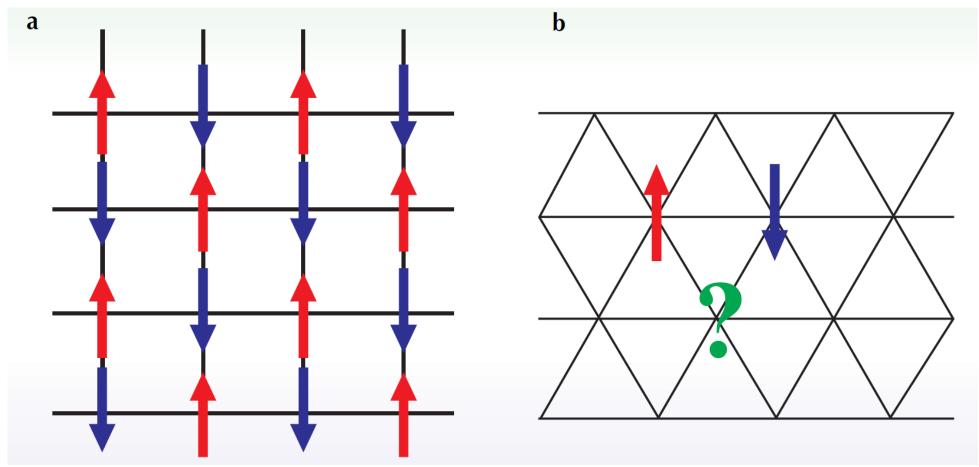
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- In antiferromagnets critical behavior depends on the shape of the lattice (related to Frustration)
- Local order does not depend on the boundaries.

Frustration

• interactions in conflict



Picture taken from [Moessner,Ramirez 2006]

Interest

Applications

Materials with new properties

• Quantum technologies

Fundamental Side

- Phases of matter
- Spin ices, spin liquids
- Ability of such condensed matter systems to mimic different systems (e.g. Artificial light)

Interest

Applications

Materials with new properties

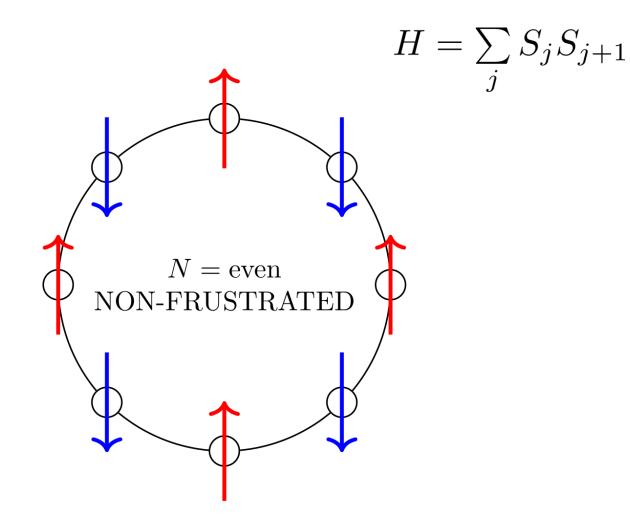
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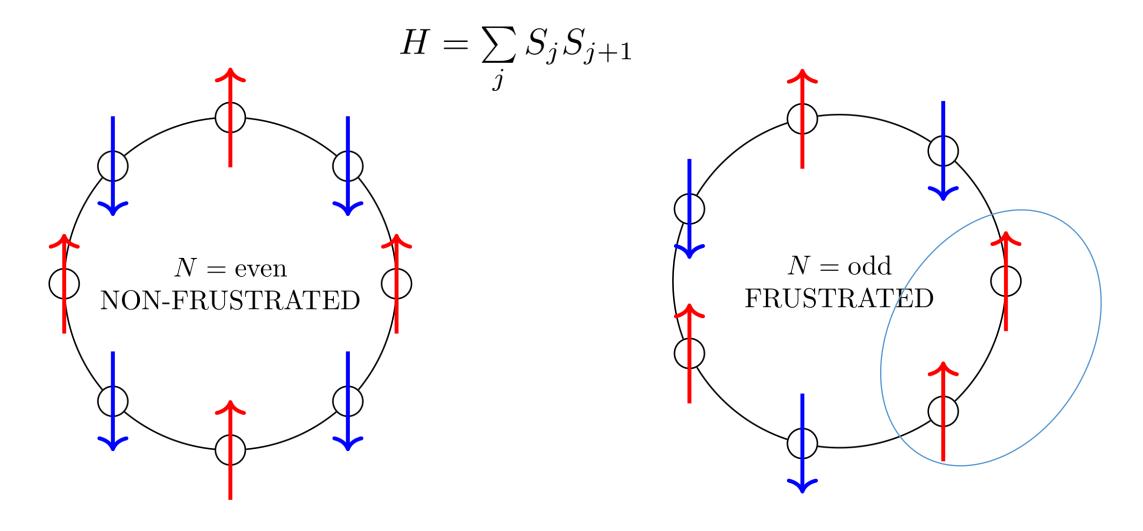
Frustration + Quantum Mechanics, Exact results?

1D: Frustration through Boundary Conditions



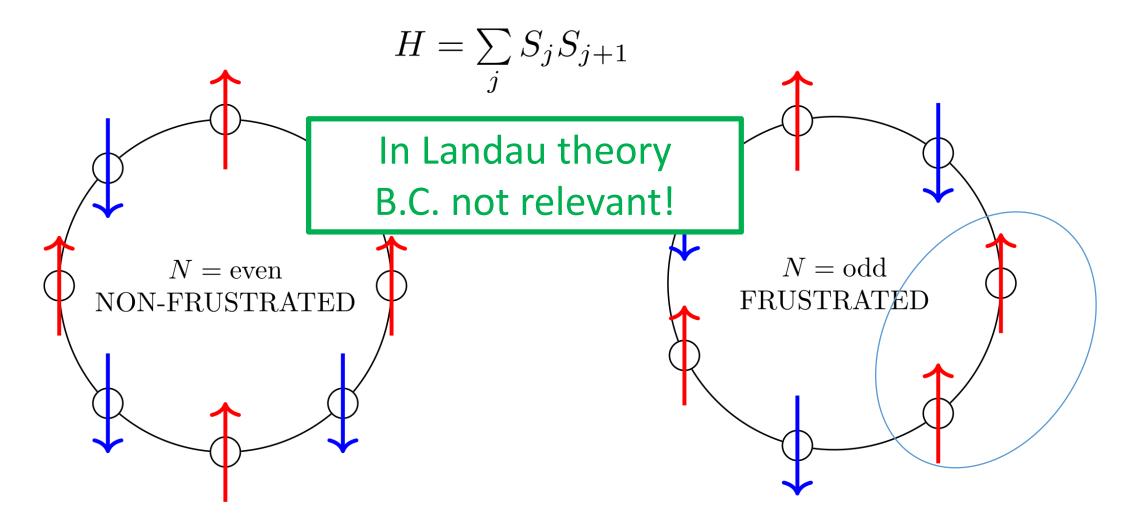
1D: Frustration through Boundary Conditions

• periodic boundary conditions and odd system size



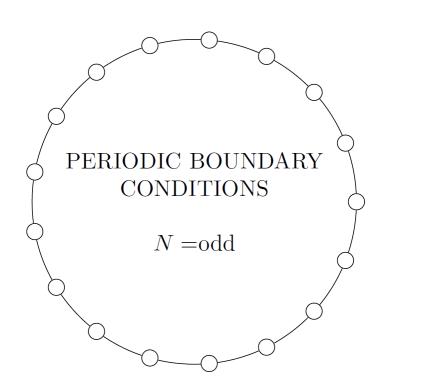
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Frustration + Quantum Mechanics

Quantum XY chain – xAFM, yFM



$$H = \sum_{j=1}^{N} \sigma_j^x \sigma_{j+1}^x - \lambda \sum_{j=1}^{N} \sigma_j^y \sigma_{j+1}^y, \ \lambda \in (0,1)$$

Order Parameter – (staggered) magnetization

$$\left\langle \sigma_{j}^{x} \right\rangle_{\mathrm{GS}} = ?$$

 Z_2 symmetry: $\sigma_j^x \to -\sigma_j^x$

Combination of analytical and numerical methods

How to diagonalize the model?
$$H = \sum_{j=1}^N \sigma_j^x \sigma_{j+1}^x - \lambda \sum_{j=1}^N \sigma_j^y \sigma_{j+1}^y$$
, $\lambda \in (0,1)$

Mapping spins to fermions – Jordan-Wigner Transformation, Fourier transform, Bogoliubov rotation

Z₂ symmetry:
$$\sigma_j^x \to -\sigma_j^x$$
 $[H, \Pi^z] = 0$ $\Pi^z = \prod_{j=1}^N \sigma_j^z$
 $H = \frac{1+\Pi^z}{2}H^+ \frac{1+\Pi^z}{2} + \frac{1-\Pi_z}{2}H^- \frac{1-\Pi_z}{2}$

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Mapping spins to fermions – Jordan-Wigner Transformation, Fourier transform, Bogoliubov rotation

$$Z_{2} \text{ symmetry: } \sigma_{j}^{x} \to -\sigma_{j}^{x} \qquad \left[H, \Pi^{z}\right] = 0 \qquad \Pi^{z} = \prod_{j=1}^{N} \sigma_{j}^{z}$$

$$H = \frac{1+\Pi^{z}}{2}H^{+}\frac{1+\Pi^{z}}{2} + \frac{1-\Pi_{z}}{2}H^{-}\frac{1-\Pi_{z}}{2}$$

$$H^{\pm} = \sum_{q \in \Gamma^{\pm}} \varepsilon(q) \left(\hat{a}_{q}^{\dagger}\hat{a}_{q} - \frac{1}{2}\right)$$

$$\epsilon(q) = |e^{i2q} - \lambda|, \ q \neq 0, \pi, \qquad \Gamma^{-} = \{2\pi k/N : k = 1..., N\}$$

$$\epsilon(0) = -\epsilon(\pi) = 1 - \lambda, \qquad \Gamma^{+} = \{2\pi(k + \frac{1}{2})/N : k = 1, ..., N\}$$

Construction of the ground states...

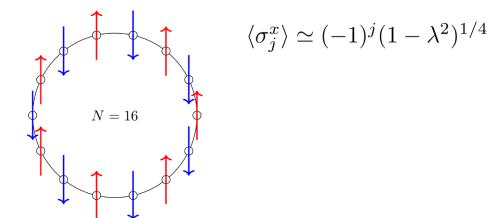
New method of computing the magnetization

Results

$$H = \sum_{j=1}^{N} \sigma_j^x \sigma_{j+1}^x - \lambda \sum_{j=1}^{N} \sigma_j^y \sigma_{j+1}^y, \ \lambda \in (0,1)$$

<u>Without frustration</u> (System size *N*=Even):

- Gapped
- Magnetization antiferromagnetic



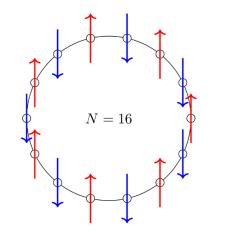
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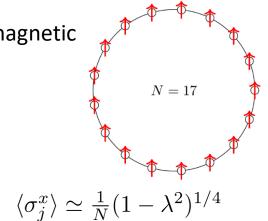
 $\langle \sigma_j^x \rangle \simeq (-1)^j (1-\lambda^2)^{1/4}$

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<u>With frustration (N=Odd)</u>:

- Gapless
- Magnetization decreases to zero with the system size
- Magnetization ferromagnetic



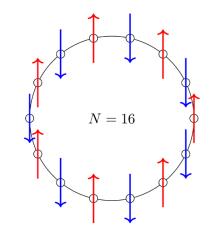
Mesoscopic Ferromagnetic Order

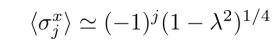
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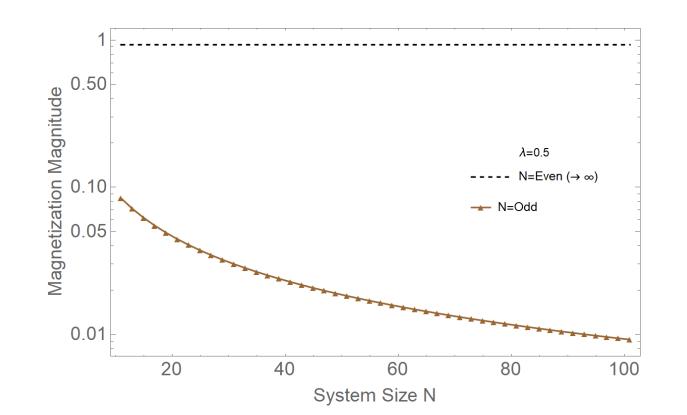
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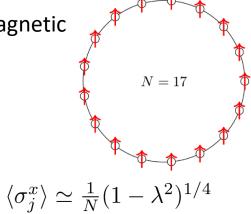




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<u>Without frustration</u> (System size *N*=Even):

 $\langle \sigma_j^x \rangle \simeq (-1)^j (1 - \lambda^2)^{1/4}$

Gapped

N = 16

Magnetization antiferromagnetic

0.01

20

With frustration (N=Odd):

- Gapless
- Magnetization decreases to zero with the system size
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100

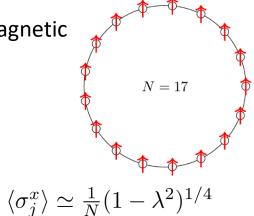
Not in agreement with the Landau theory!

40

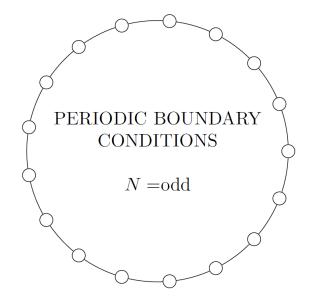
60

System Size N

80

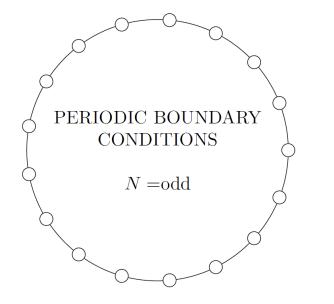


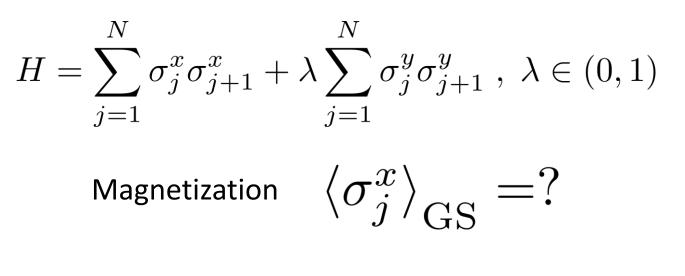
Mesoscopic Ferromagnetic Order XY chain – xAFM, yAFM



$$\begin{split} H &= \sum_{j=1}^{N} \sigma_{j}^{x} \sigma_{j+1}^{x} + \lambda \sum_{j=1}^{N} \sigma_{j}^{y} \sigma_{j+1}^{y} , \; \lambda \in (0,1) \\ \\ \text{Magnetization} \quad \left\langle \sigma_{j}^{x} \right\rangle_{\text{GS}} = ? \end{split}$$

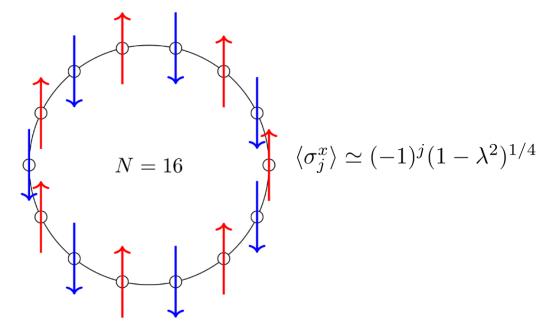
XY chain – xAFM, yAFM





Without frustration:

- Gapped
- Standard Antiferromagnetic order
- Two-fold ground state degeneracy

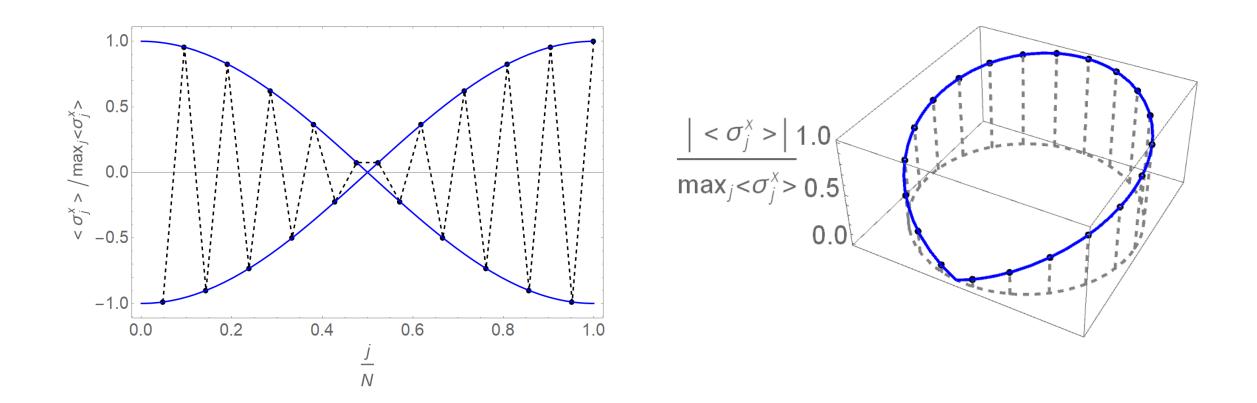


With Frustration: Breaking of Translational Symmetry

Gapless spectrum, Four-fold ground state degeneracy

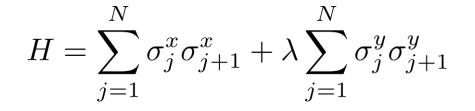
 $\frac{\langle \sigma_j^x \rangle}{\max_{j'} \langle \sigma_{j'}^x \rangle} = (-1)^j \cos\left(\pi \frac{j}{N}\right)$

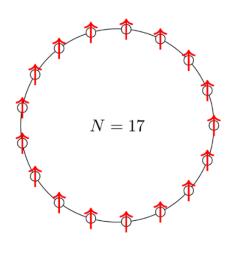
Magnetization non-zero



Two results combined

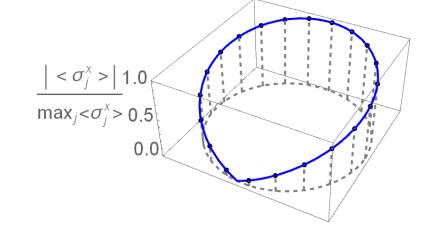
$$H = \sum_{j=1}^{N} \sigma_j^x \sigma_{j+1}^x - \lambda \sum_{j=1}^{N} \sigma_j^y \sigma_{j+1}^y$$





GS DEGENERACY=2

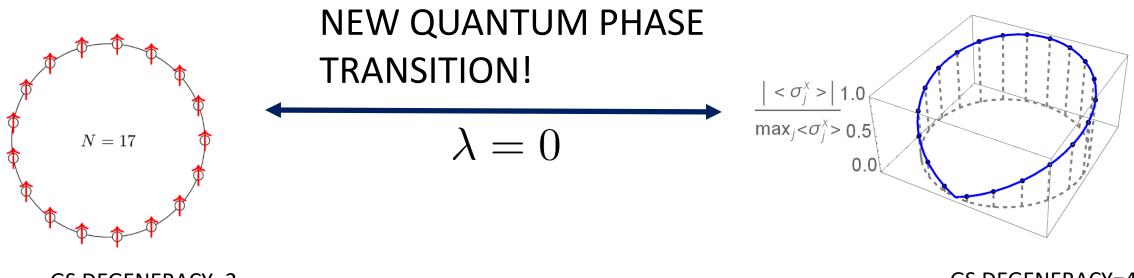
GS DEGENERACY=4



Two results combined

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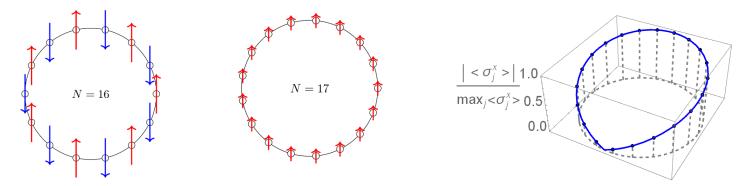
$$H = \sum_{j=1}^{N} \sigma_j^x \sigma_{j+1}^x + \lambda \sum_{j=1}^{N} \sigma_j^y \sigma_{j+1}^y$$



GS DEGENERACY=2

GS DEGENERACY=4

Conclusions



- Frustration with Quantum Mechanics leads to new types of order
 - Mesoscopic Ferromagnetic order, Breaking of translational symmetry, new Quantum Phase Transition
- Different behavior of systems of even and odd size, however large they are.
- Boundary conditions influence local order, however large system is.
- Incompletness of the Landau theory.

Reference: V. Marić, S. M. Giampaolo, D. Kuić, and F. Franchini. "The Frustration of being Odd: How Boundary Conditions can destroy Local Order". arXiv:1908.10876, 2019.

Reference: V. Marić, S. M. Giampaolo, D. Kuić, and F. Franchini. In preparation.

People involved in the project



Fabio Franchini



Salvatore Marco Giampaolo



Domagoj Kuić







• Thank you for your attention!