The Frustration of being Odd

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and more...

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- 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);
- arXiv:2101.07276;
- arXiv:2101.08807;
- arXiv:2105.06483; & work in progress

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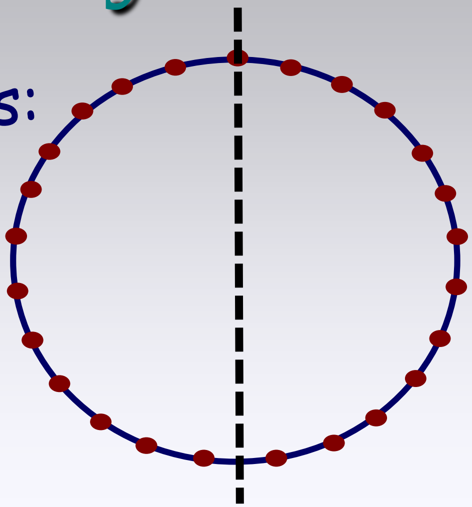
What's on the menu today…

- We revisit an old problem for spin chains:

  the effect of periodic b.c. with an ODD number of sites



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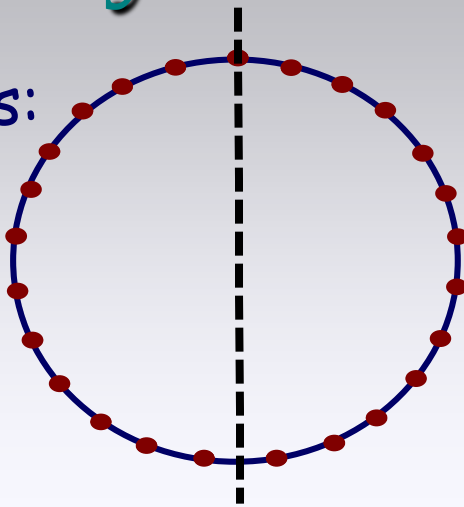


the effect of periodic b.c. with
an ODD number of sites

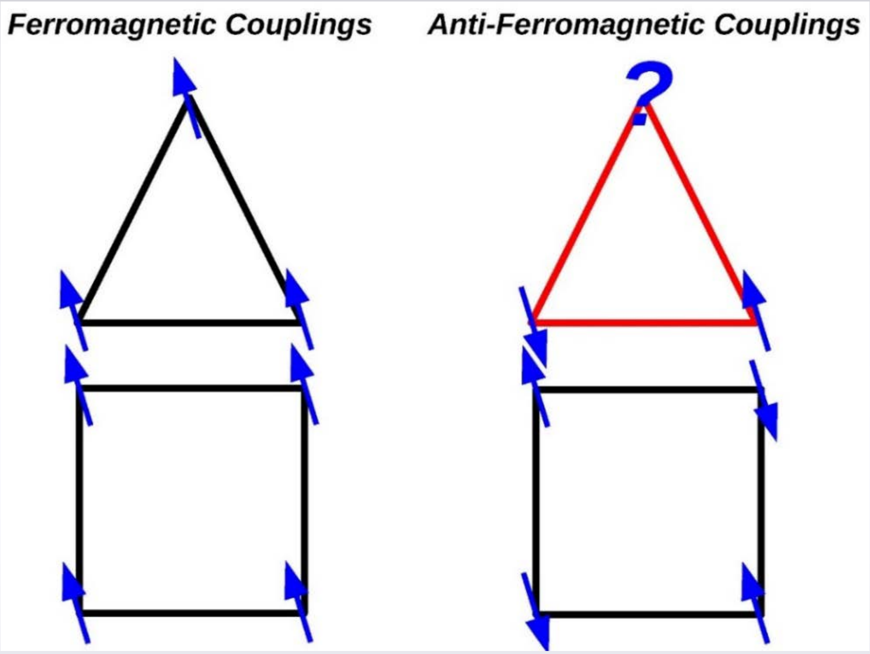
- We call them: Frustrated Boundary Conditions (FBC)
- Why such interest?
- From one side: b.c. can only matter in finite systems

(are we sure?)

- From another side: FBC are special

Geometrical Frustration

- Close loops generate frustration in classical systems:
  - Geometrical (topological) origin
  - Toulouse Criterion: a classical systems is frustrated if there is a close loop for which $-1^{\mathcal{N}_{AFM}} = -1$
  - More loops $\Rightarrow$ more frustration



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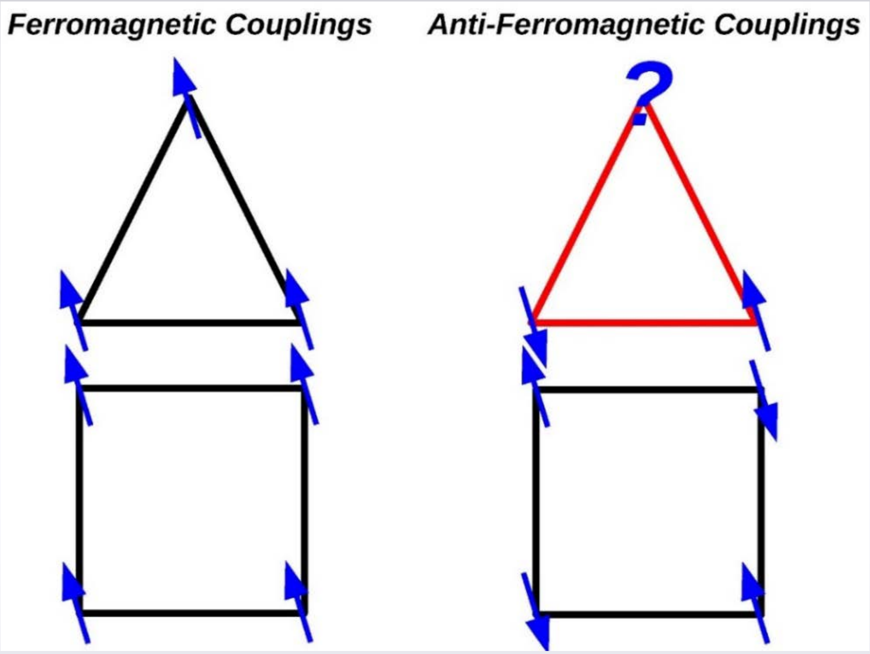
- Remark: adding one site changes GS degeneracy from 2 to 2N and vice versa (challenges perturbative picture)



Basics on Frustration

- Frustration:

  competing interactions favoring different orders

$\Rightarrow$ impossible to minimize all energy contributions

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  $\Rightarrow$ impossible to minimize all energy contributions

- Remark: all genuine quantum phases are frustrated (non-commuting terms promote diff. arrangements)

- E.g. Ising Chain: $H_{\text{Ising}} = \sum_{l=1}^{N} \left(\sigma_l^x \sigma_{l+1}^x - h\, \sigma_l^z \right)$

  $\left[\sigma_l^x \sigma_{l+1}^x, \sigma_l^z \right] \neq 0$: ground state as a trade-off

- However, typically we mean a conflict between local and global constraints

Frustrated Systems

- Certain degree of frustration is very common
- In any dimension, due to closed AFM loops

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- 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

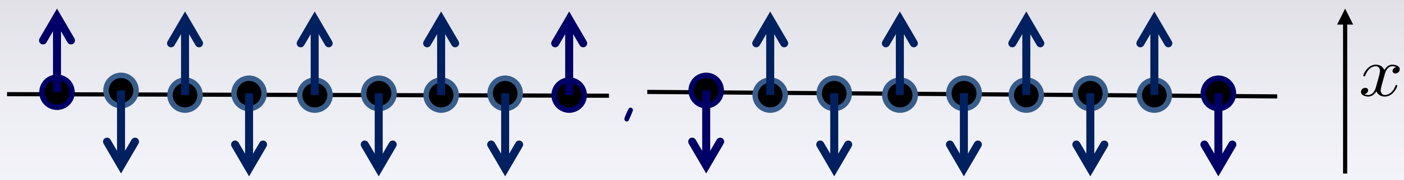
- We consider a simpler problem
- Loop (1D chain, pbc: $\sigma_{l+N}^{\alpha} = \sigma_l^{\alpha}$): non-extensive frustration

$$H = \frac{1}{2} \sum_{l=1}^{2M+1} \left[\left(\frac{1+\gamma}{2} \right) \sigma_l^x \sigma_{l+1}^x + \left(\frac{1-\gamma}{2} \right) \sigma_l^y \sigma_{l+1}^y + \frac{\Delta}{2} \sigma_l^z \sigma_{l+1}^z - h \, \sigma_l^z \right]$$

- Subtle interplay between geometrical frustration and quantum interactions

Frustrated Classical Ising

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

GS (Neel): 

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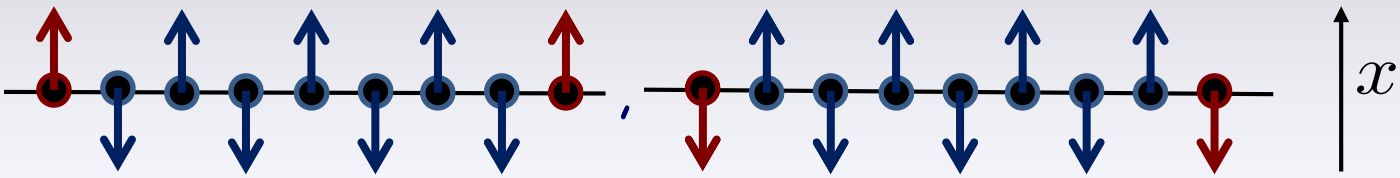
GS (Neel + 1 Domain wall):



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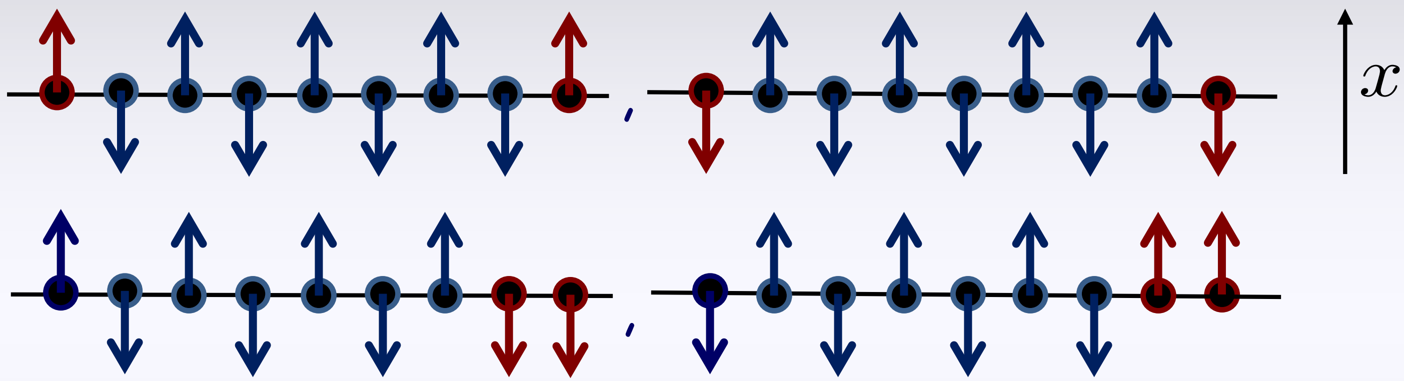

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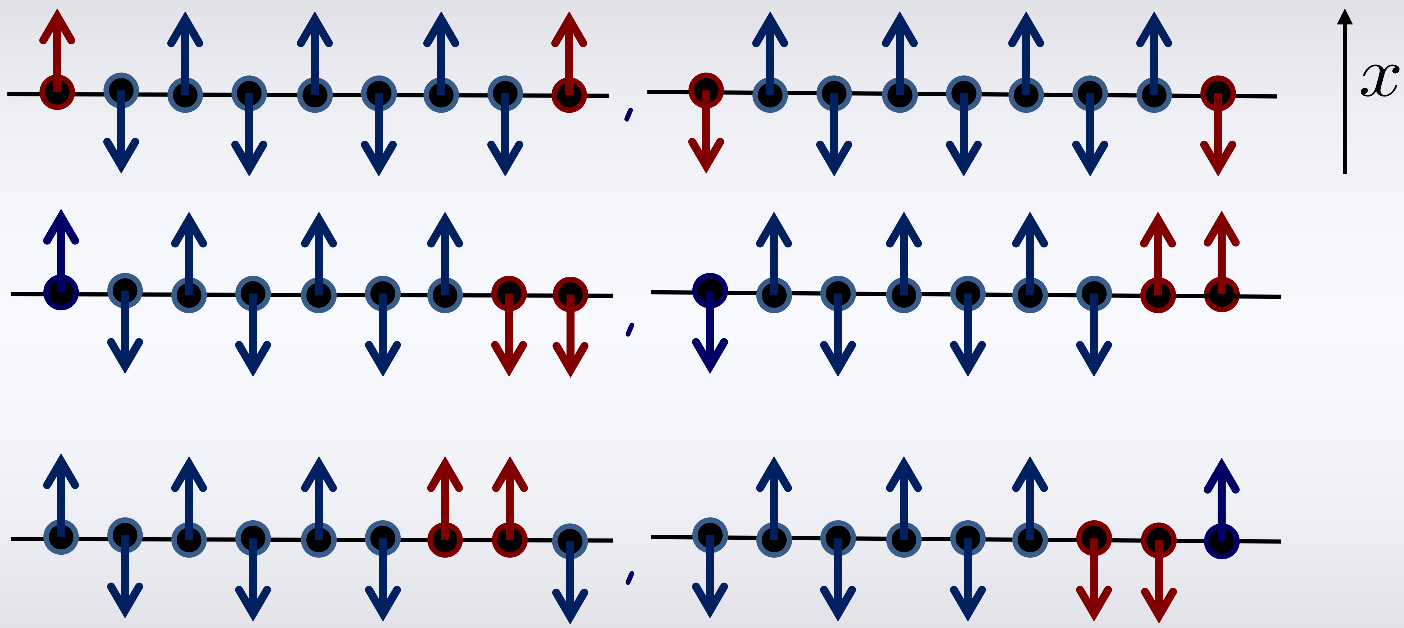

...

2N States!

Perturbative picture

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

- At λ=0: 2N-degenerate GS (2 x Neel with 1 domain wall)

  (compare to 2-degenerate for N even, i.e not frustrated)

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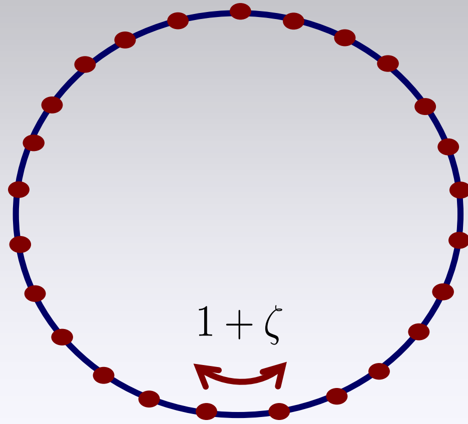
- At λ=0: 2N-degenerate GS (2 x Neel with 1 domain wall) (compare to 2-degenerate for N even, i.e not frustrated)
- Turn on λ≠0: it opens a small gap proportional $\frac{\lambda}{N^2}$
- Perturbative picture: low-energy eigenstates as a traveling domain wall with different momenta

⇒ quantum effects lift the massive degeneracy to a band of gapless states

Laumann et al, PRL (2012)

Frustrated Boundary Conditions

- Effects of FBC considered weak against local perturbations, however:



$$H = \frac{1}{2}\sum_{l=1}^{2M+1}\left(\sigma_l^x\sigma_{l+1}^x + \lambda\sigma_l^z\right) + \zeta\sigma_N^x\sigma_1^x$$

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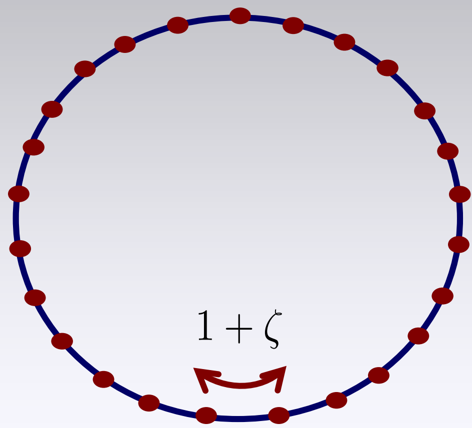

- A ferro defect ($\zeta<0$) localizes the domain wall
- An AFM defect stabilizes the traveling excitation

$\Rightarrow$ perfect FBC are a phase transition between a magnet and a kink phase (exponential vs algebraic gap closing)

Campostrini et al, PRE (2015)

Weakly frustrated Chain

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with PBC: $\sigma_{l+N}^{\alpha} = \sigma_l^{\alpha}$. For $|h| < 1$:

- $N = 2M$: No frustration $\Rightarrow$ SSB of Z_2 symmetry
  - Finite gap to first band
  - Exp. small gap for 2 GS $\rightarrow$ Spontaneous magnetization
  - Exponential decay of correlations

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- $N=2M+1$: Weak frustration + Z_2 quantum symmetry $\Rightarrow$
  - Gapless, but not relativistic (Galilean)
  - Algebraic gap $\rightarrow$ order parameter?
  - Mixture of exponential and algebraic correlations in 1/N

Loschmidt Echo

- Detect difference in spectrum through a Quantum Quench

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

- Loschmidt Echo: $\mathcal{L}(t) = |\, \langle g | e^{-\imath H_1 t} | g \rangle \,|^2$, $|g\rangle$ GS of H_0

G. Torre, V. Marić, D. Kuić, F. Franchini, S.M. Giampaolo, arXiv:2105.06483

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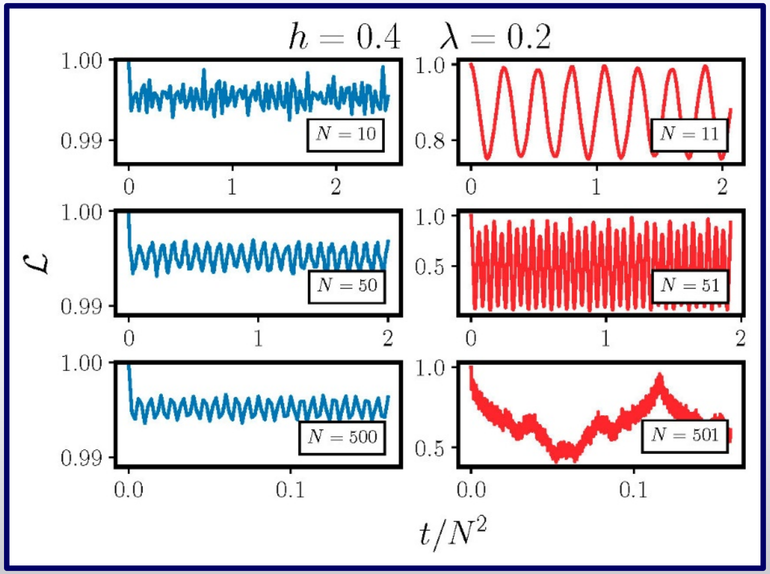

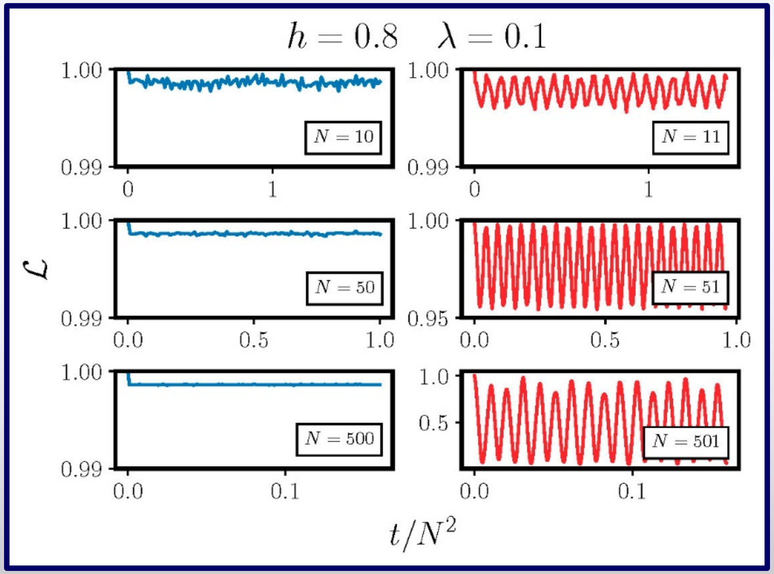

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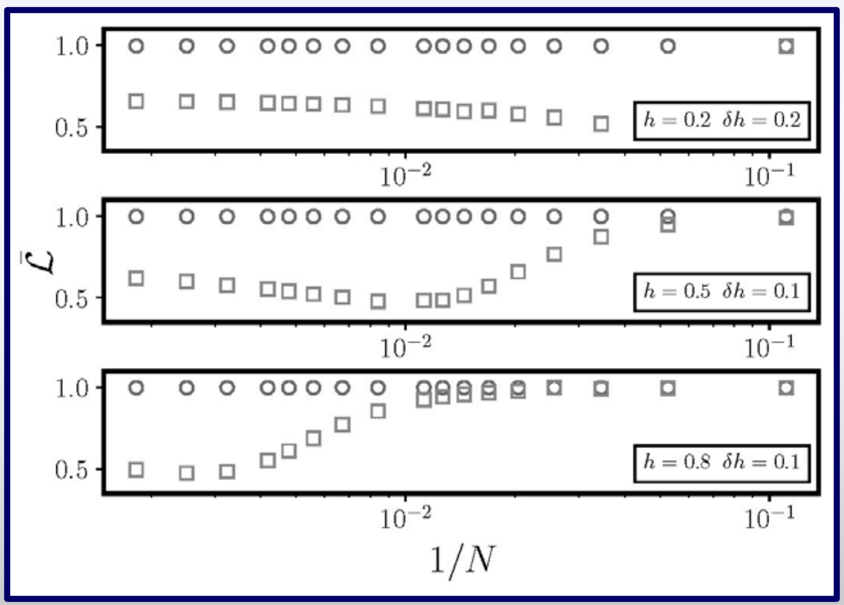

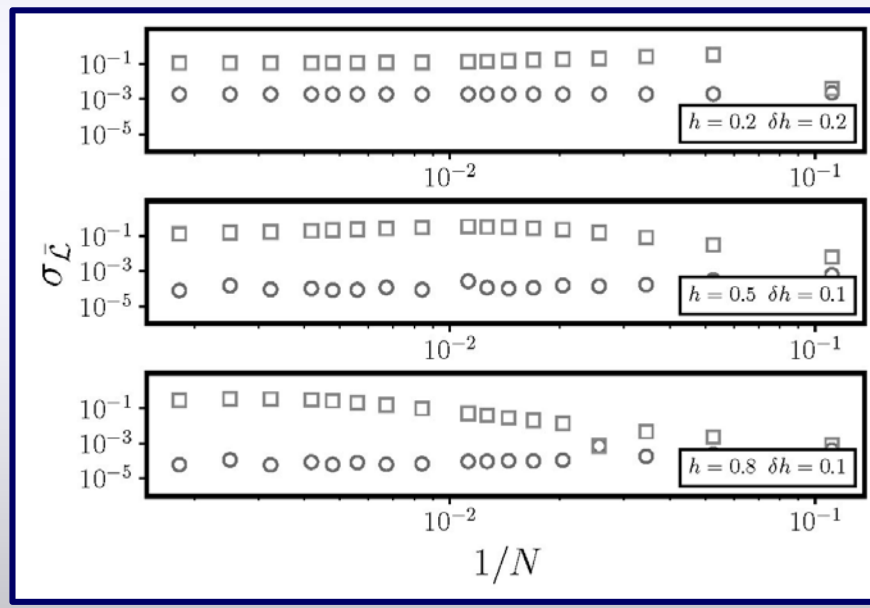

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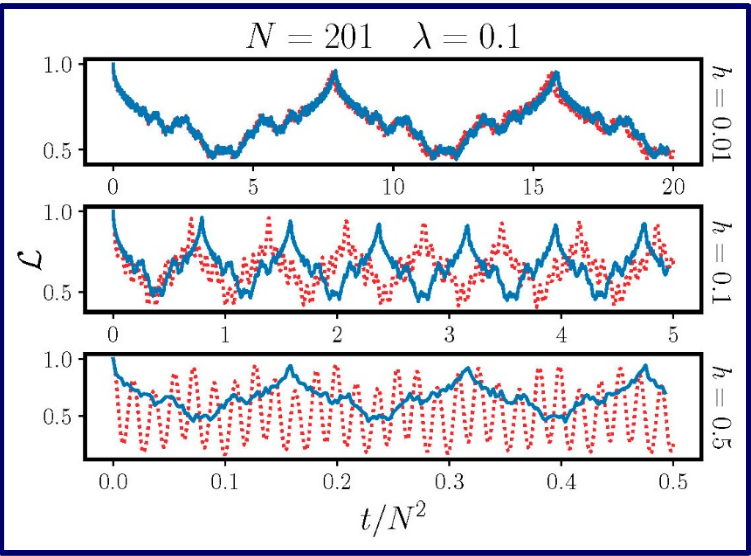
- Perturbative calculation (domain wall basis):

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

$$\begin{aligned} \mathcal{F}(x) &= \lim_{M\to\infty} \left| \frac{1}{2M^2} \sum_{k=1}^{M} \tan^2\left[\frac{(2k-1)\pi}{4M}\right] \times \right. \\ &\times \left. \exp\left\{ -\imath x (2M+1)^2 \cos\left[\frac{(2k-1)\pi}{2M}\right]\right\} \right|^2 \end{aligned}$$



- LE continuous, but nowhere differentiable

Torre, Marić, Kuić, Franchini, Giampaolo, arXiv:2105.06483

Order parameter

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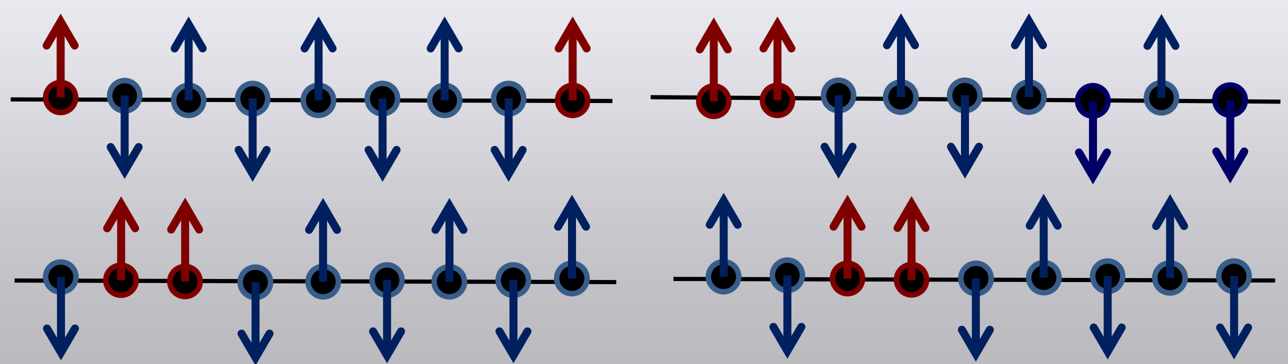

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  $\Rightarrow$ mesoscopic ferromagnetic magnetization
- Alternatively: non perfect staggerization (& modulation)

$$\langle \sigma_j^x \rangle = \mathrm{Re} \left[e^{\pi \left(1 \pm \frac{1}{N} \right) j + \theta} \right] m_x$$

Order Parameter & 2-Point function

- Order parameter from "connected component":

$$C^{xx}(R) \equiv \langle \sigma_l^x \sigma_{l+R}^x \rangle = (-1)^R \, m_x^2 \left[1 + c^x \, \frac{e^{-R/\xi}}{R^2} \right] \left(1 - \frac{2R}{N} \right)$$

Dong et al, JSTAT (2016), MPLB (2017), PRE (2018)

- Locally: indistinguishable from non-frustrated ones

Marić & Franchini, JPA 54 025201 (2020)

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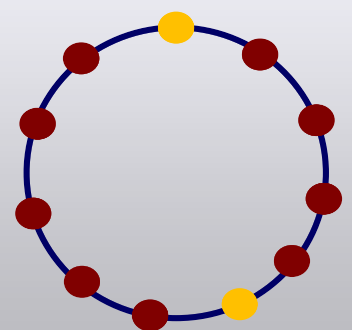

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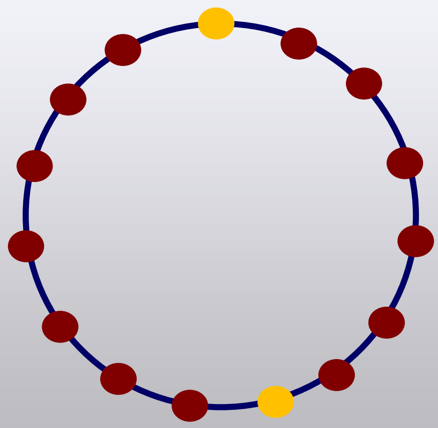

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- Locally: indistinguishable from non-frustrated ones
- Spontaneous Magnetization from antipodal points
- Order parameter: $\boxed{\langle \sigma^x \rangle = \lim_{N \to \infty} \sqrt{C^{xx}\left(\frac{N-1}{2}\right)} = 0}$
- Conflict between two approaches

Order parameter & Frustration

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

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- General, recent & old, puzzling arguments against perfect AFM staggered order
- Indeed, seemingly contradict Landau Theory
- We develop a new, exact, approach to this problem (and learn an interesting trick along the way)

XYZ Chain in zero field

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

- In absence of external fields, H commutes with all

  3 parities: $\Pi^\alpha \equiv \prod_{j=1}^{N} \sigma_j^\alpha, \; \alpha = x, y, z$ $\qquad [H, \Pi^\alpha] = 0$

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  3 parities: $\Pi^\alpha \equiv \prod_{j=1}^{N} \sigma_j^\alpha, \;\; \alpha = x, y, z \qquad [H, \Pi^\alpha] = 0$

- On odd # sites, parities do not commute: $\left\{ \Pi^\alpha, \Pi^\beta \right\} = 2\delta_{\alpha,\beta}$

  $\Rightarrow$ every states at least 2-fold degenerate

$$\Pi^z |\Psi\rangle = |\Psi\rangle, H|\Psi\rangle = E_\Psi |\Psi\rangle$$

$$\downarrow$$

$$|\tilde\Psi\rangle \equiv \Pi^x |\Psi\rangle \quad \to \quad \Pi^z |\tilde\Psi\rangle = -\Pi^x |\tilde\Psi\rangle, H|\tilde\Psi\rangle = E_\Psi |\tilde\Psi\rangle$$

- Exact, finite size, degeneracies (Kramer's deg)!

Spontaneous Magnetization

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- In zero field and N=2M+1, GS manifold with mixed parities

$\Rightarrow$ can develop finite magnetizations $\langle GS|\sigma_j^\alpha|GS\rangle$ at finite N

$$|g_z,\pm\rangle \longrightarrow |GS\rangle \equiv \alpha|g_z,+\rangle + \beta|g_z,-\rangle$$

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- Choosing one GS equivalent to switching on a symmetry breaking field and following its behavior to N $\rightarrow \infty$

Spontaneous Magnetization

- Use z-parity to classify states:

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- Normally: $|\langle GS|\sigma_j^x|GS\rangle| = \lim_{r\to\infty} \sqrt{\langle \sigma_j^x \sigma_{j+r}^x \rangle}$

- Here: $\Pi^x |g_z, +\rangle = |g_z, -\rangle$ (up to a phase)

$$\Rightarrow \qquad \langle GS|\sigma_j^x|GS\rangle = \alpha\beta^* \langle g_z, +|\sigma_j^x|g_z, -\rangle + \text{c.c.}$$

$$\langle g_z, +|\sigma_j^x|g_z, -\rangle = \langle g_z, +|\prod_{l\neq j}^N \sigma_l^x|g_z, +\rangle$$

- Can access directly 1-point function (on mixed states) from a string of operators (on single parity state)

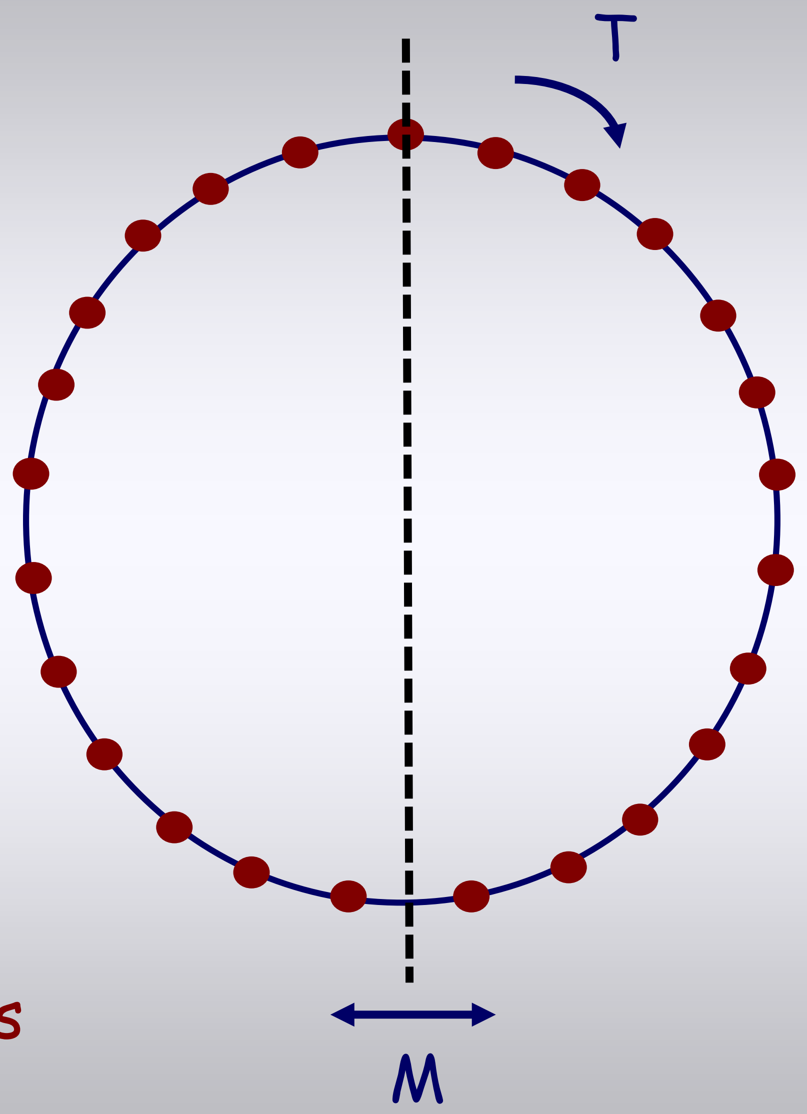
More Degeneracies

- On a ring with odd # sites reflection axes cross a vertex and a bond

$\Rightarrow$ Only states with 0 or π momentum can be simult. eigenstates M and T

- Other states come in (degenerate) doublets of opposite momentum or mirror

$\Rightarrow$ Exact finite size degeneracies (for any interaction!)



XYZ Chain in zero field

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

- On odd # sites, H has 2 sets of incompatible global symmetries:
  - Mirror (M) and lattice tranlation (T):

    $[H,M] = [H,T] = 0$, $MT|\Psi\rangle = TM|\Psi\rangle$ only if $M|\Psi\rangle = \pm|\Psi\rangle$

  - Parity operators: $\Pi^\alpha \equiv \prod_{j=1}^{N} \sigma_j^\alpha, \; \alpha = x, y, z$

    $[H, \Pi^\alpha] = 0 \qquad \{\Pi^\alpha, \Pi^\beta\} = 2\delta_{\alpha,\beta}$

$\Rightarrow$ Exact 2 or 4-fold GS degeneracy at finite N

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$$[H,\Pi^\alpha]=0 \qquad \left\{\Pi^\alpha,\Pi^\beta\right\}=2\delta_{\alpha,\beta}$$

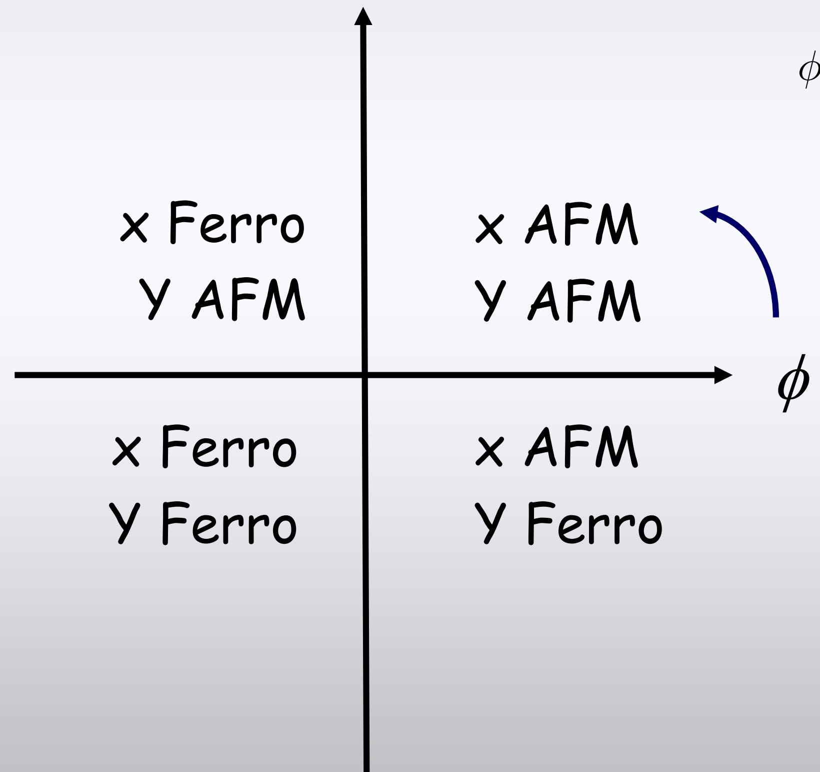
$\Rightarrow$ Exact 2 or 4-fold GS degeneracy at finite N

- Any GS choice necessarily break a symmetry of H

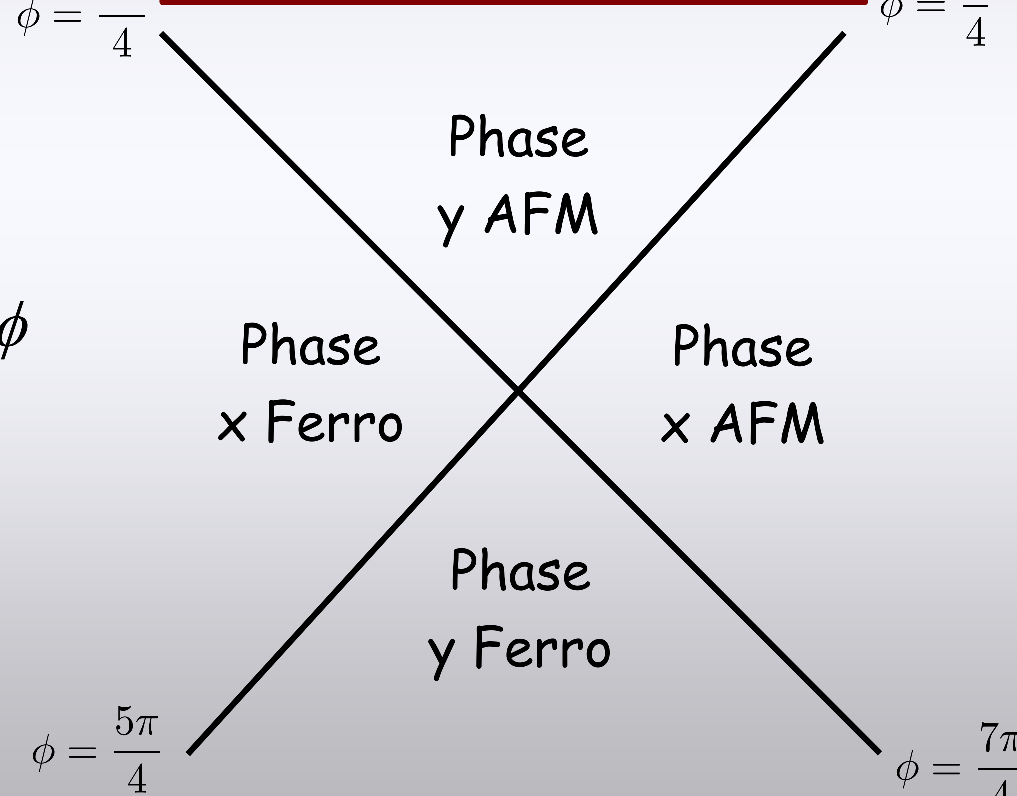
XYZ Chain in zero field

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

- Assume $\delta \in [0, \pi/2]$ (Ferro zz-interaction)



N=2M: not frustrated



XYZ Chain in zero field

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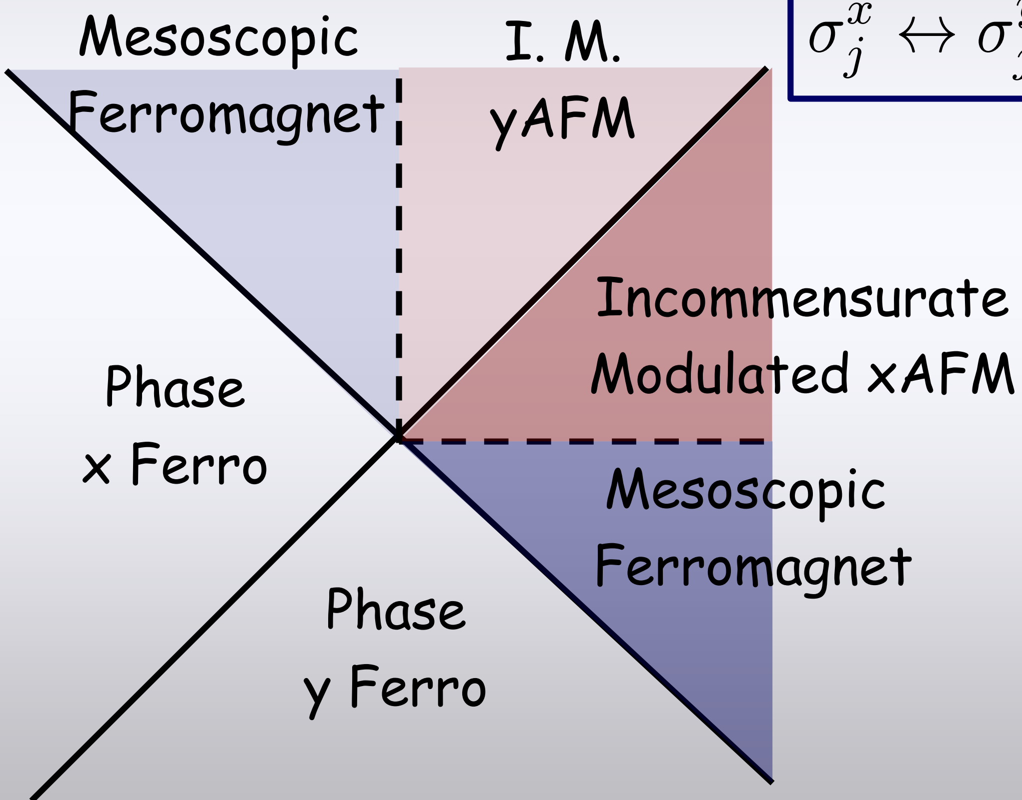
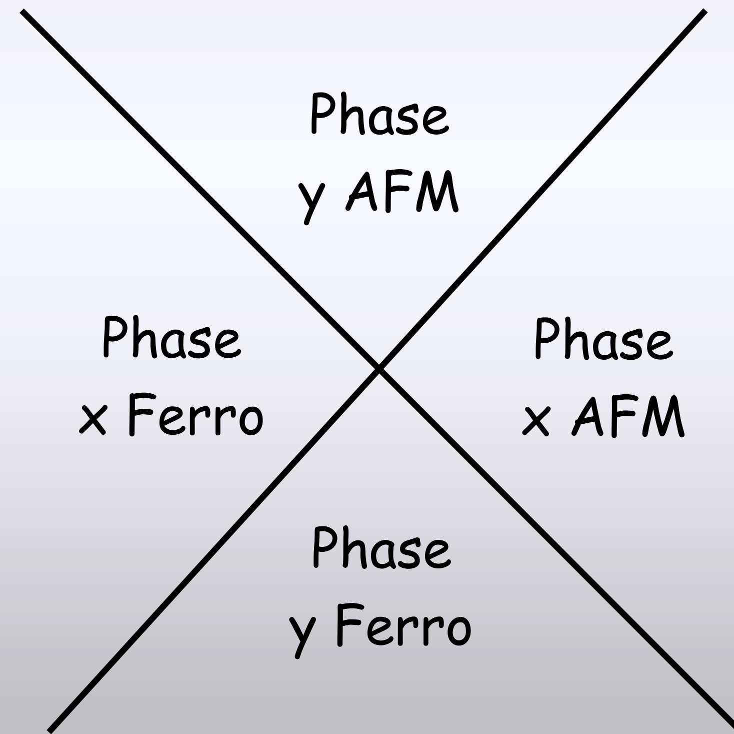
N=2M+1

Duality

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

N=2M: not frustrated





XYZ Chain in zero field

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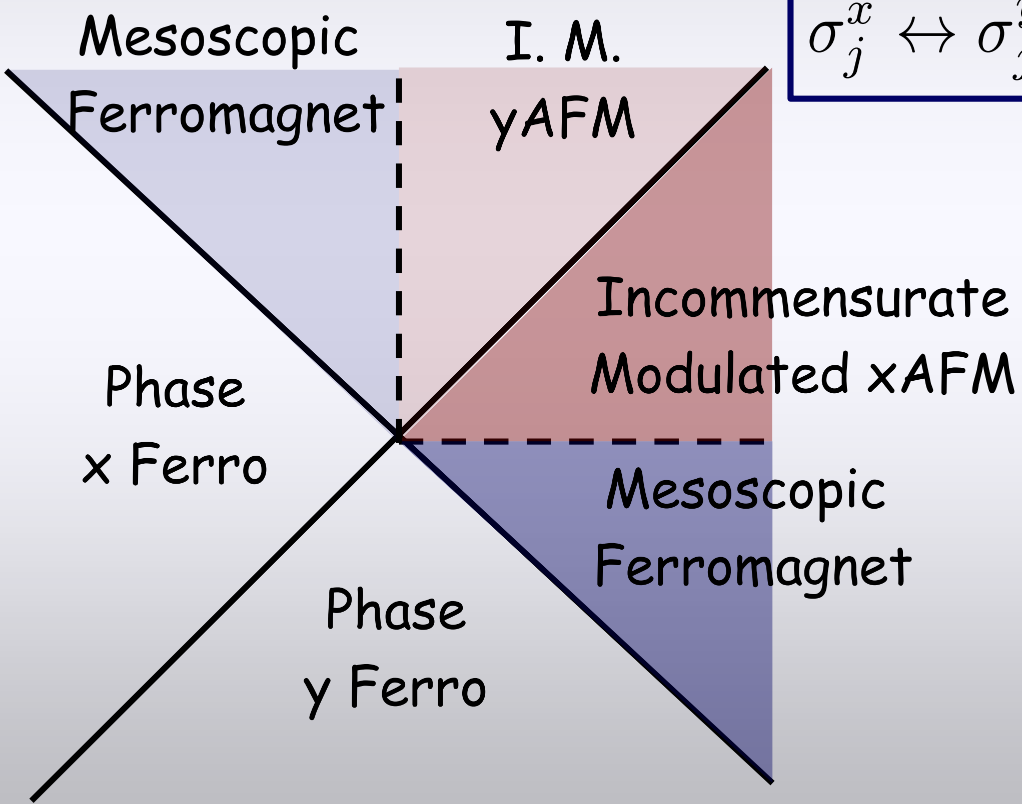


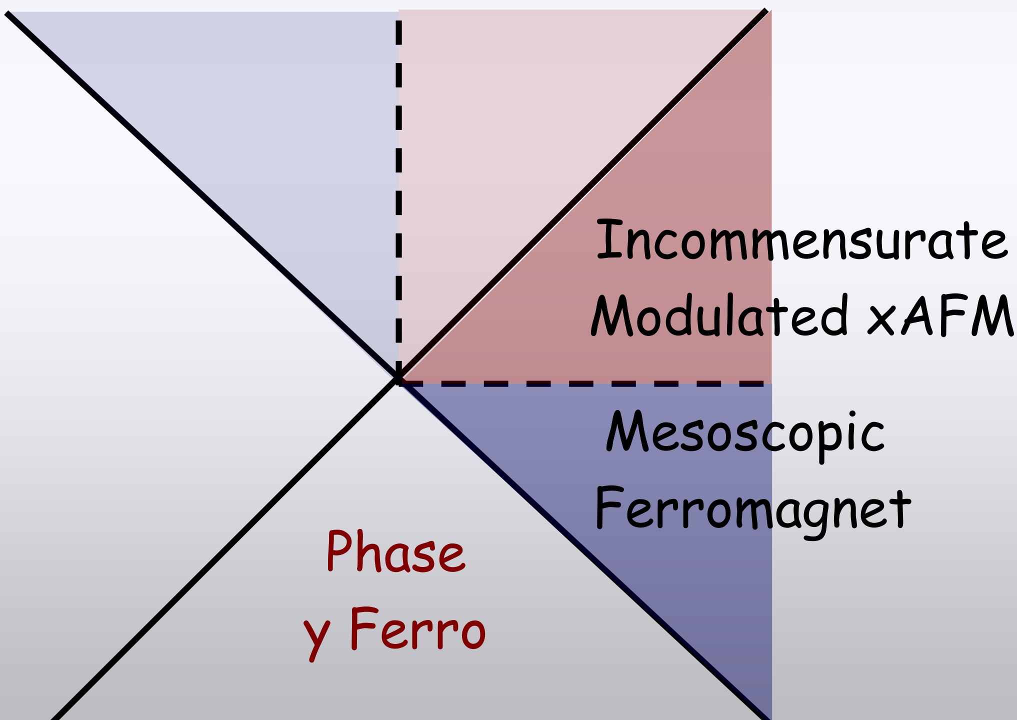
Duality $\sigma_j^x \leftrightarrow \sigma_j^y$

- Different bc induce changes in AFM phases
- Thanks to aformentioned symmetries/degeneracies we can calculate magnetization exactly
- Order in these regions compatible with perturbative picture

Ferromagnetic Phase

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

- y-FM: $\phi \in [-\pi/2, -\pi/4)$



Ferromagnetic Phase

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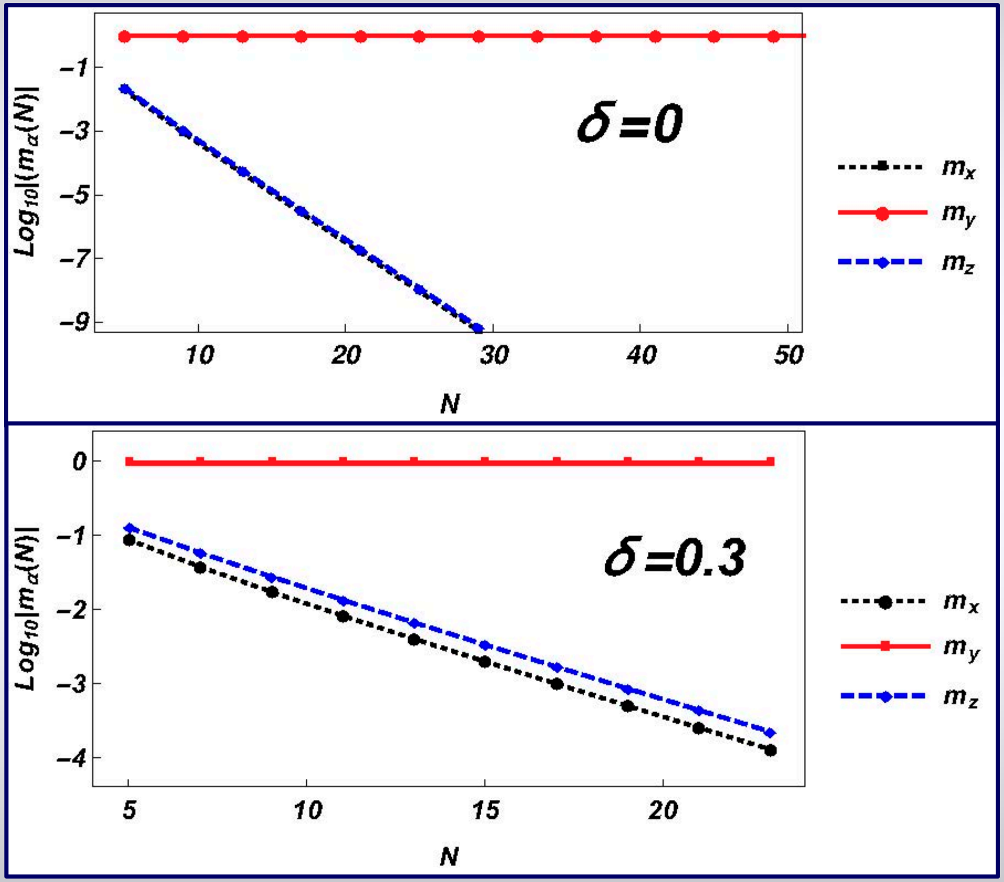
- y-FM: $\phi \in [-\pi/2, -\pi/4)$
- $|g_\alpha\rangle \equiv \frac{1}{\sqrt{2}} (1 + \Pi^\alpha) |g_z\rangle$
- $m_\alpha \equiv \langle g_\alpha | \sigma_j^\alpha | g_\alpha \rangle$

$$= \langle g_z | \prod_{l \neq j} \sigma_l^\alpha | g_z \rangle$$

$\Rightarrow m_x = m_z = 0$

$$m_y = \left(1 - \cot^2\phi\right)^{1/4}$$

in $N \to \infty$ limit



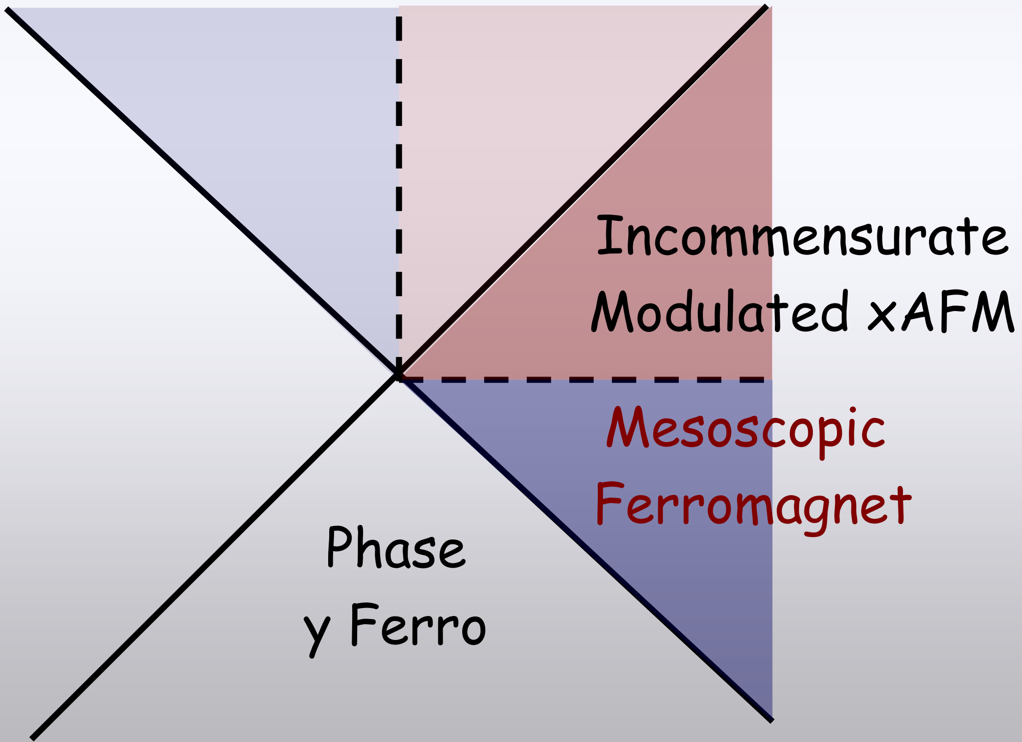
Consistency check on methodology!

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

Mesoscopic Ferromagnet

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

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



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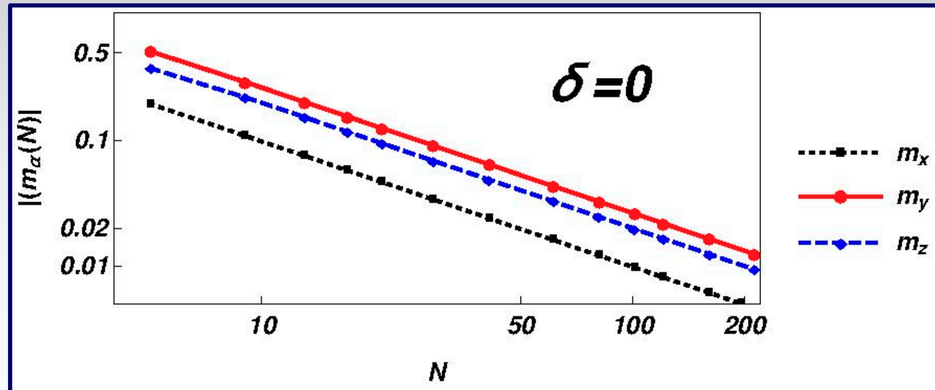
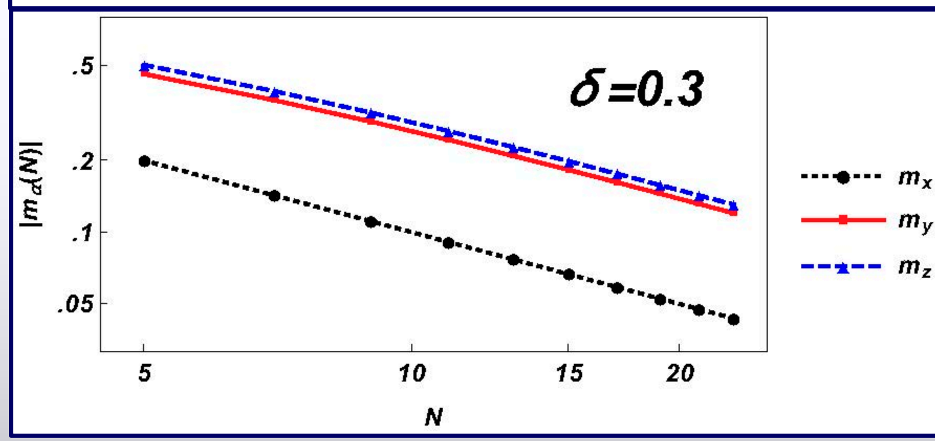
- MFM: $\phi \in (-\pi/4, 0)$
- $|g_\alpha\rangle \equiv \frac{1}{\sqrt{2}} (1 + \Pi^\alpha) |g_z\rangle$

$$m_\alpha \equiv \langle g_\alpha | \sigma_j^\alpha | g_\alpha \rangle = \langle g_z | \prod_{l \neq j} \sigma_l^\alpha | g_z \rangle$$

$$\Rightarrow m_\alpha \simeq \frac{\tilde{m}_\alpha}{N^\gamma} \stackrel{N \to \infty}{\longrightarrow} 0$$





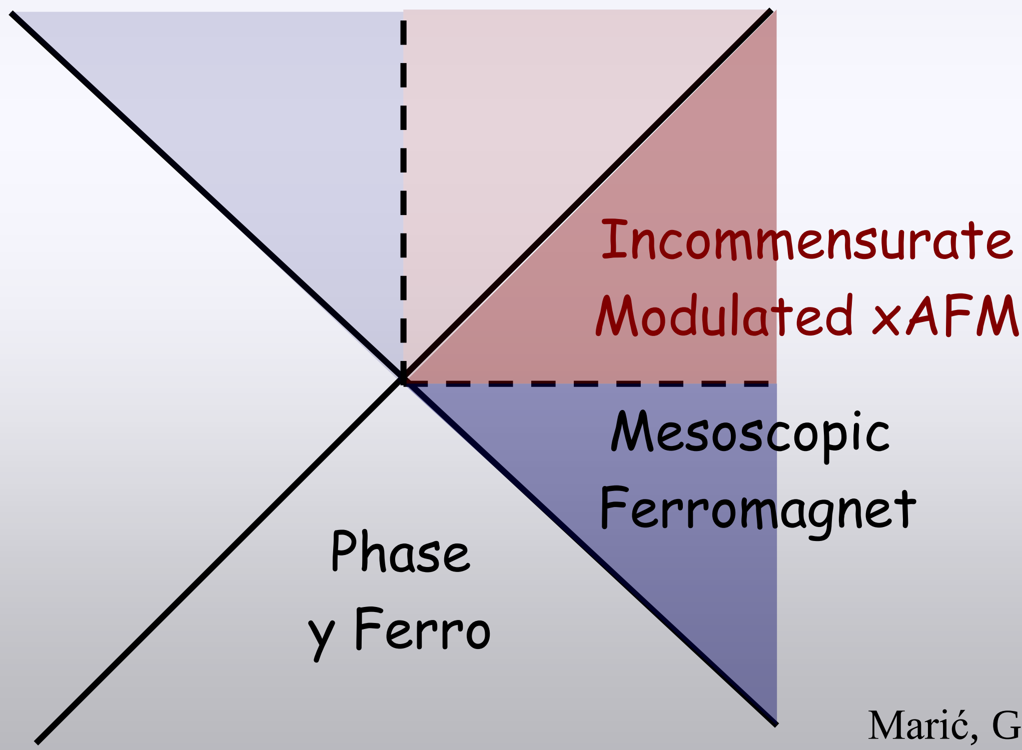
- All magnetizations decay algebraically to zero and are not staggered!

Marić, Giampaolo, Kuić, 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 competing (frustrated) AFM interactions
- Lowest energy states have finite momentum $\pm\pi/2$

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

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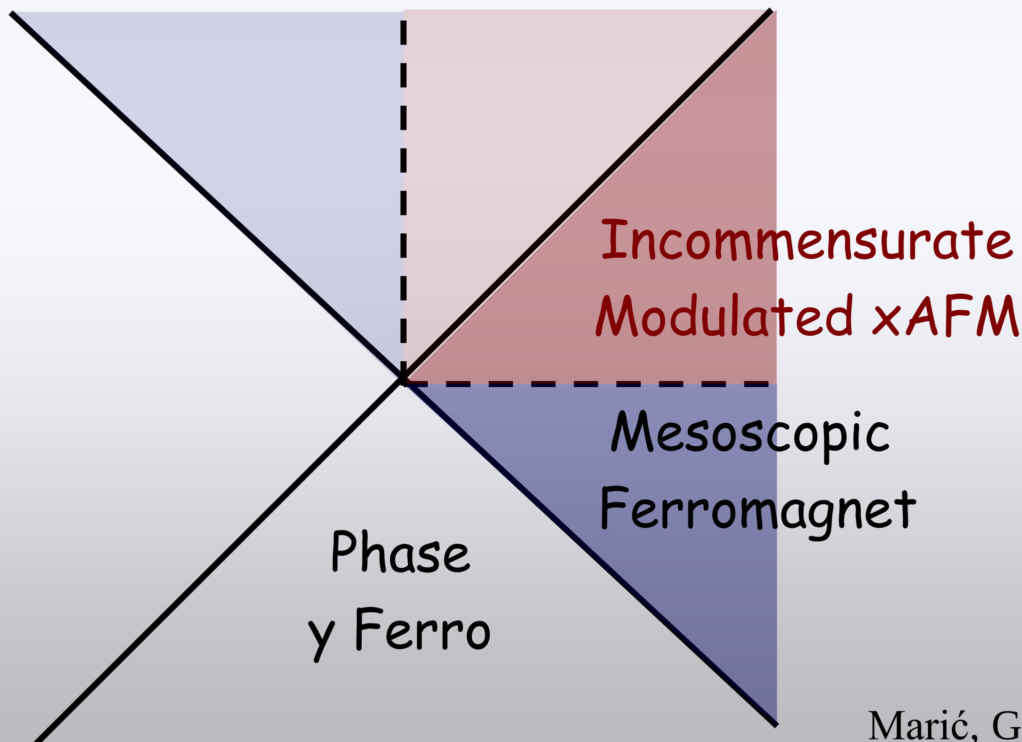

- 2 competing (frustrated) AFM interactions
- Lowest energy states have finite momentum ±π/2
- 4-fold degenerate GS (2x parities, 2x chiralities)
- GS can break transl. Inv.

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

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- Chose GS: $\frac{1}{\sqrt{2}}\left[|\pm p, +\rangle + e^{i\theta}|\pm p, -\rangle\right]$ $\Rightarrow$ Mesoscopic FM

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

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

$$\Rightarrow \qquad \langle \tilde{g} | \sigma_j^\alpha | \tilde{g}\rangle = \frac{1}{2}\left[e^{i\pi\left(1+\frac{1}{N}\right)j+\theta} \langle \pm p, + | \sigma_N^\alpha | \mp p, -\rangle + \text{c.c.}\right]$$

Use Transl. Inv.

$$f_\alpha \equiv |\langle \pm p, + | \sigma_N^\alpha | \mp p, -\rangle|$$

α=x: purely real
α=y: purely imaginary

Computable as a string as before

Incommensurate Modulated AFM

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

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

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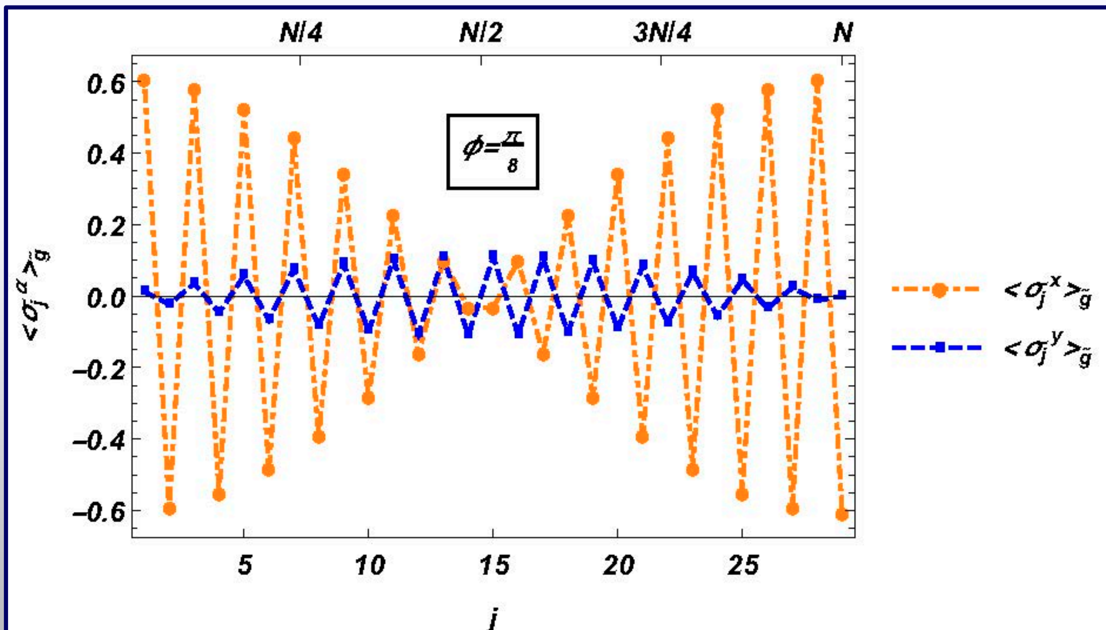

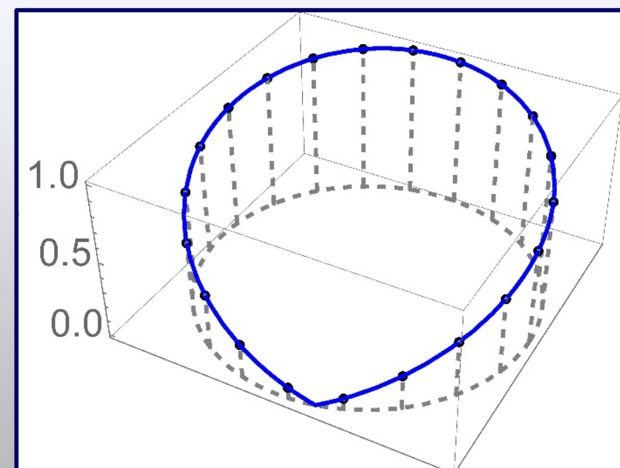

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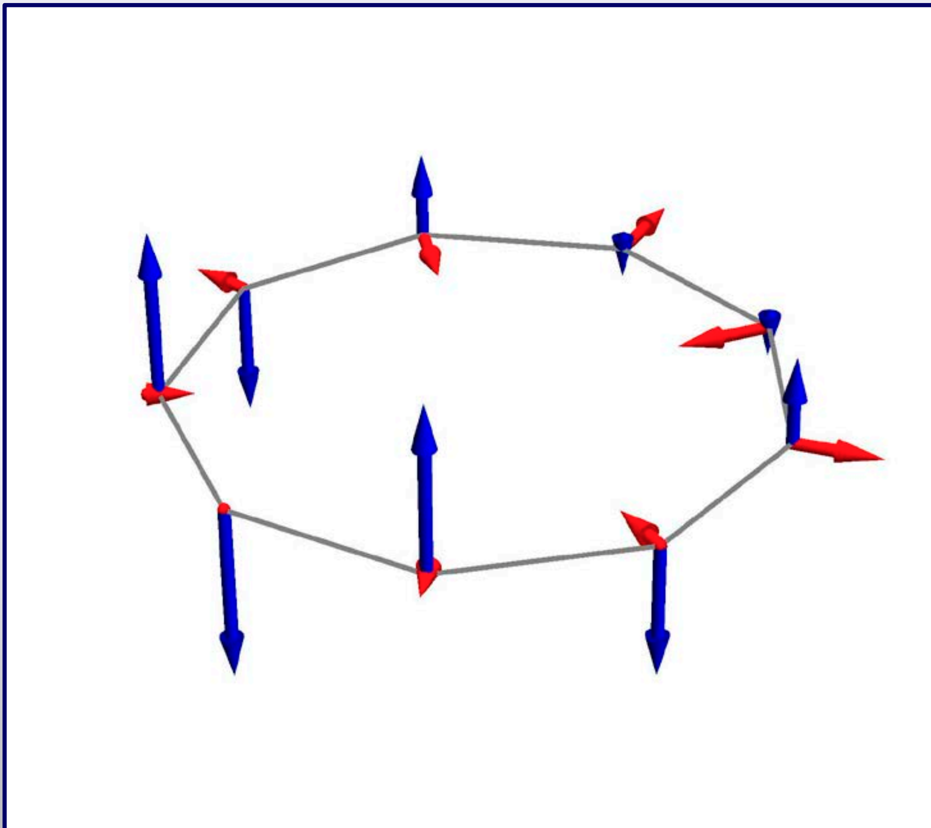

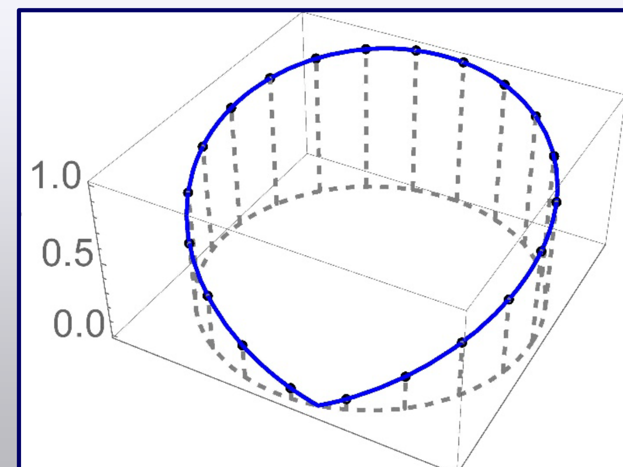

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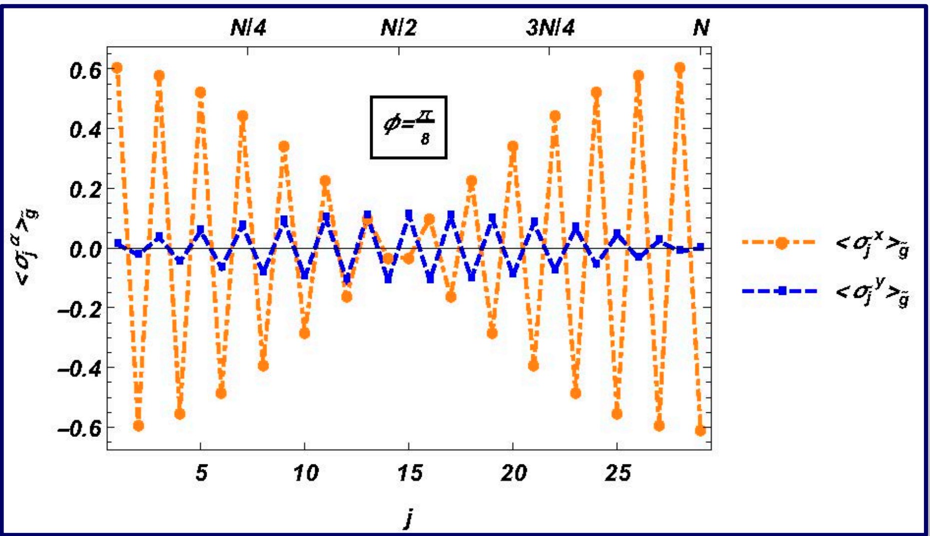
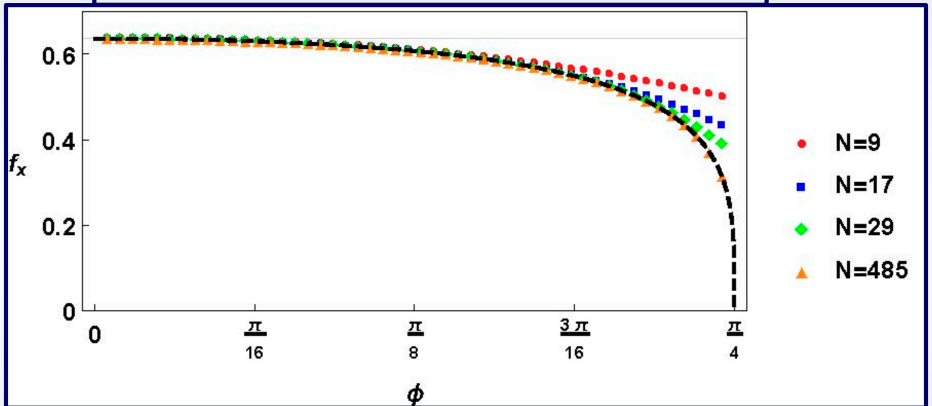
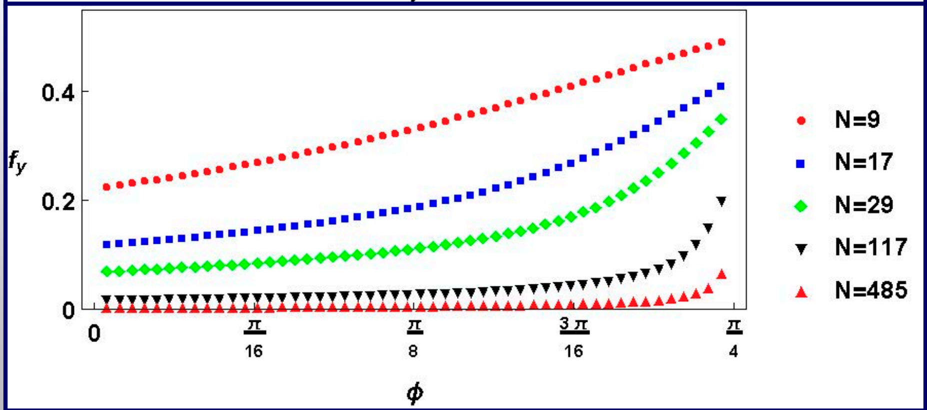
$$\langle \tilde{g} | \sigma_j^\alpha | \tilde{g} \rangle = (-1)^j \cos\left(\pi \frac{j}{N} + \tilde{\theta}_\alpha\right) f_\alpha$$

- Finite N: squeezed helical order



$$f_\alpha \equiv |\langle \pm p, + | \sigma_N^\alpha | \mp p, - \rangle|$$





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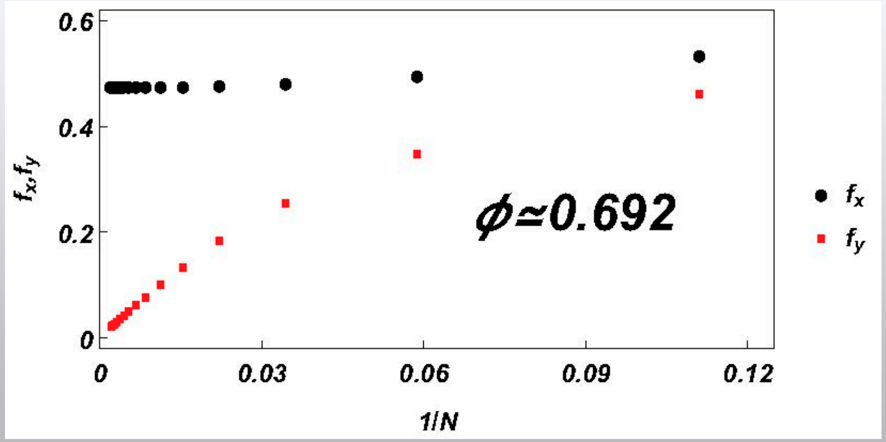
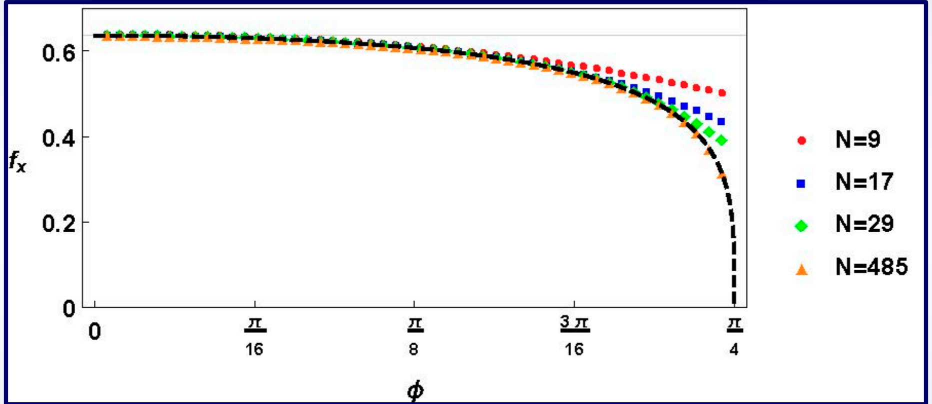
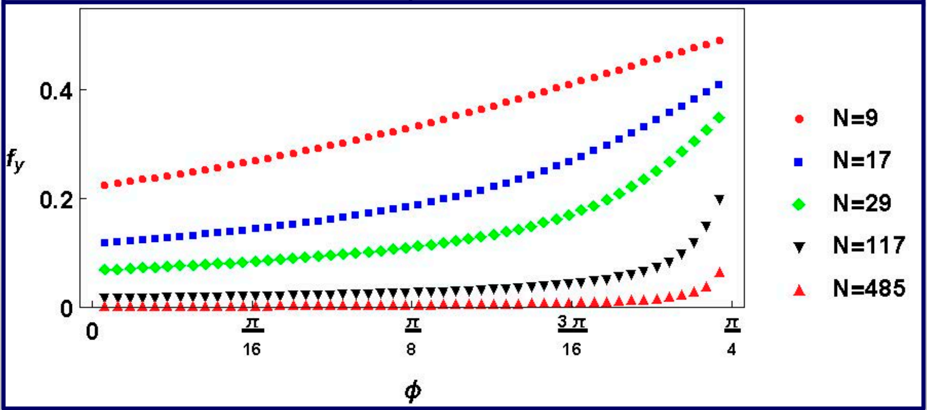
$$\boxed{\langle \tilde{g} | \sigma_j^\alpha | \tilde{g} \rangle = (-1)^j \cos\left(\pi \frac{j}{N} + \tilde{\theta}_\alpha\right) f_\alpha}$$

- y magn. suppressed in therm. limit but x remains finite!

$$\boxed{f_\alpha \equiv |\langle \pm p, + | \sigma_N^\alpha | \mp p, - \rangle|}$$



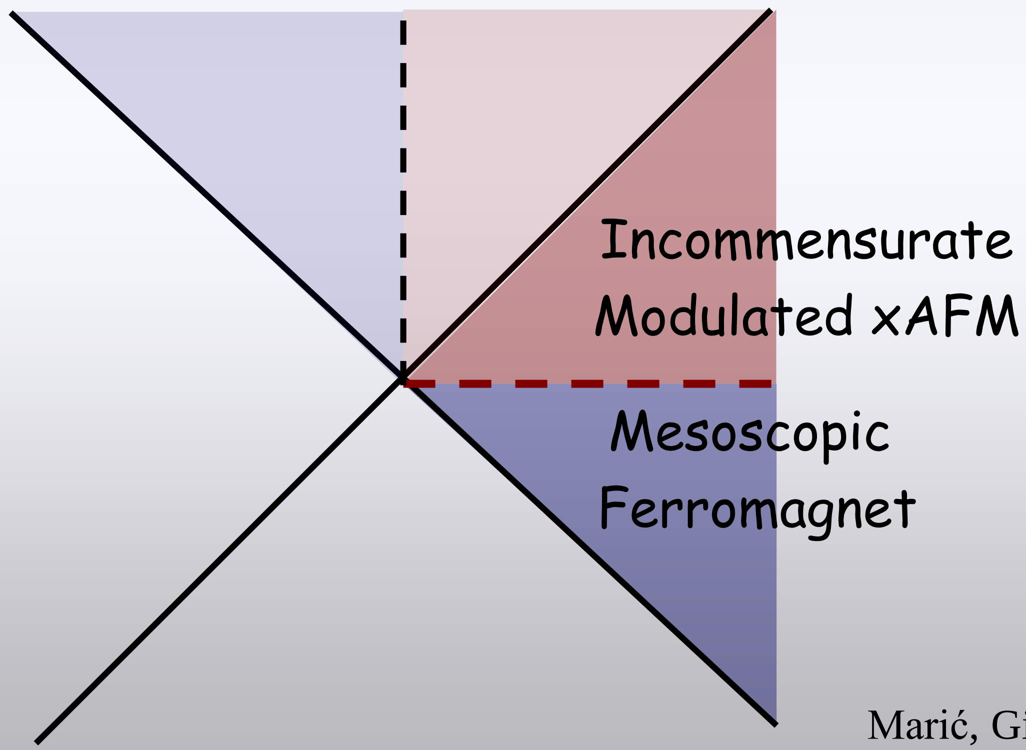




Quantum phase transition?

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

- ϕ =0 (classical Ising)
- Level crossing (change in GS degeneracy: 2 $\leftrightarrow$ 4)



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

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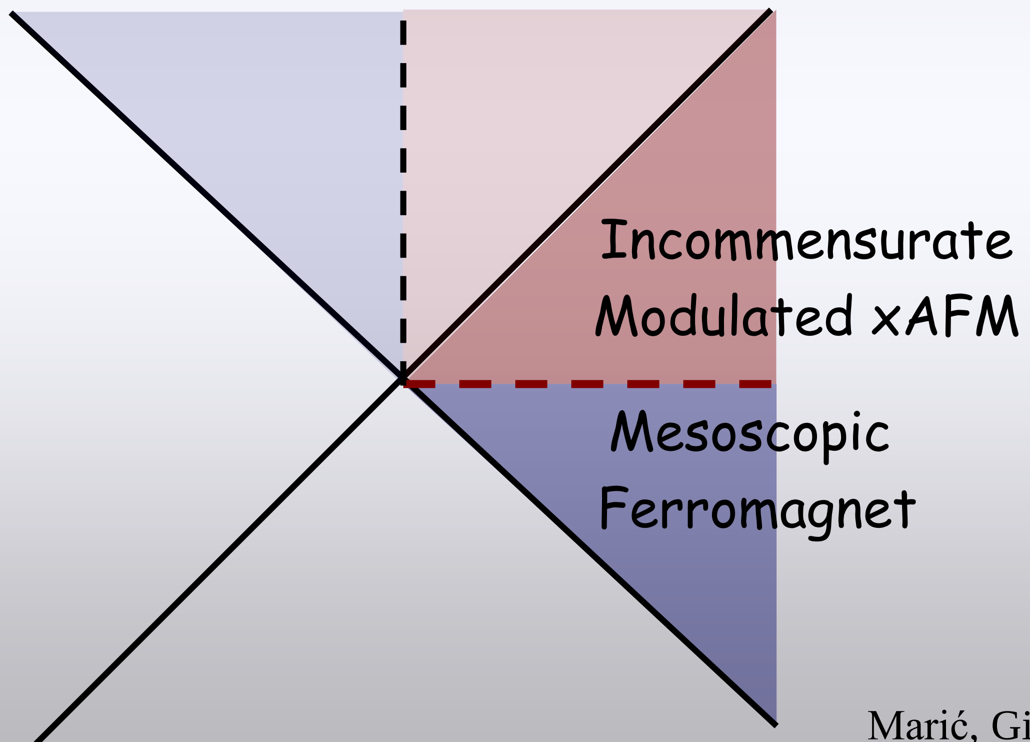
$$\left.\frac{dE_g}{d\phi}\right|_{\phi\to 0^-} - \left.\frac{dE_g}{d\phi}\right|_{\phi\to 0^+} = 2\left(1+\cos\frac{\pi}{N}\right)$$



- ϕ=0 (classical Ising)
- Level crossing (change in GS degeneracy: 2 ↔ 4)
- Finite discontinuity in 1° derivative of GS energy

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

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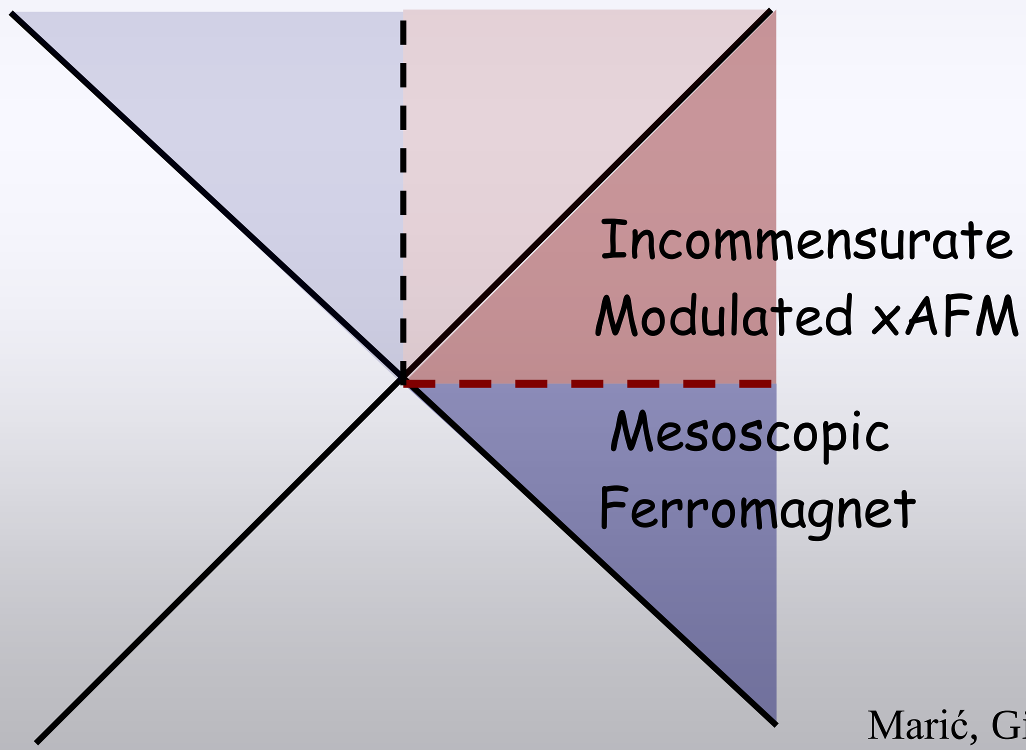

- ϕ=0 (classical Ising)
- Level crossing (change in GS degeneracy: 2 $\leftrightarrow$ 4)
- Finite discontinuity in 1° derivative of GS energy
- Akin to a 1° order b-QPT

$\Rightarrow$ Boundary-less b-QPT

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

Beyond integrabilty

- These results generalize to generic spin chains (in zero field)

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

- Theorem: No kind of order can exist with FBC in thermodynamic limit, except if GS admits 2 deg states with momenta

$$\boxed{p_1 - p_2 \overset{N\to\infty}{\simeq} \pi \left(1 \pm \frac{1}{N}\right)}$$

$\Rightarrow$ either mesoscopic or incommensurate AFM order is possible

Marić, Giampaolo, Franchini, arXiv:2101.07276

FBC change the nature of QPT

- Local order can be killed (mesoscopic) on both sides of a QPT
- E.g. 2-Cluster-Ising Chain:

$$H = \cos\phi \sum_{j=1}^{N} \sigma_j^x \sigma_{j+1}^x + \sin\phi \sum_{j=1}^{N} \sigma_{j-1}^y \sigma_j^z \sigma_{j+1}^z \sigma_{j+2}^y$$

Marić, Torre, Franchini, Giampaolo, arXiv:2101.08807

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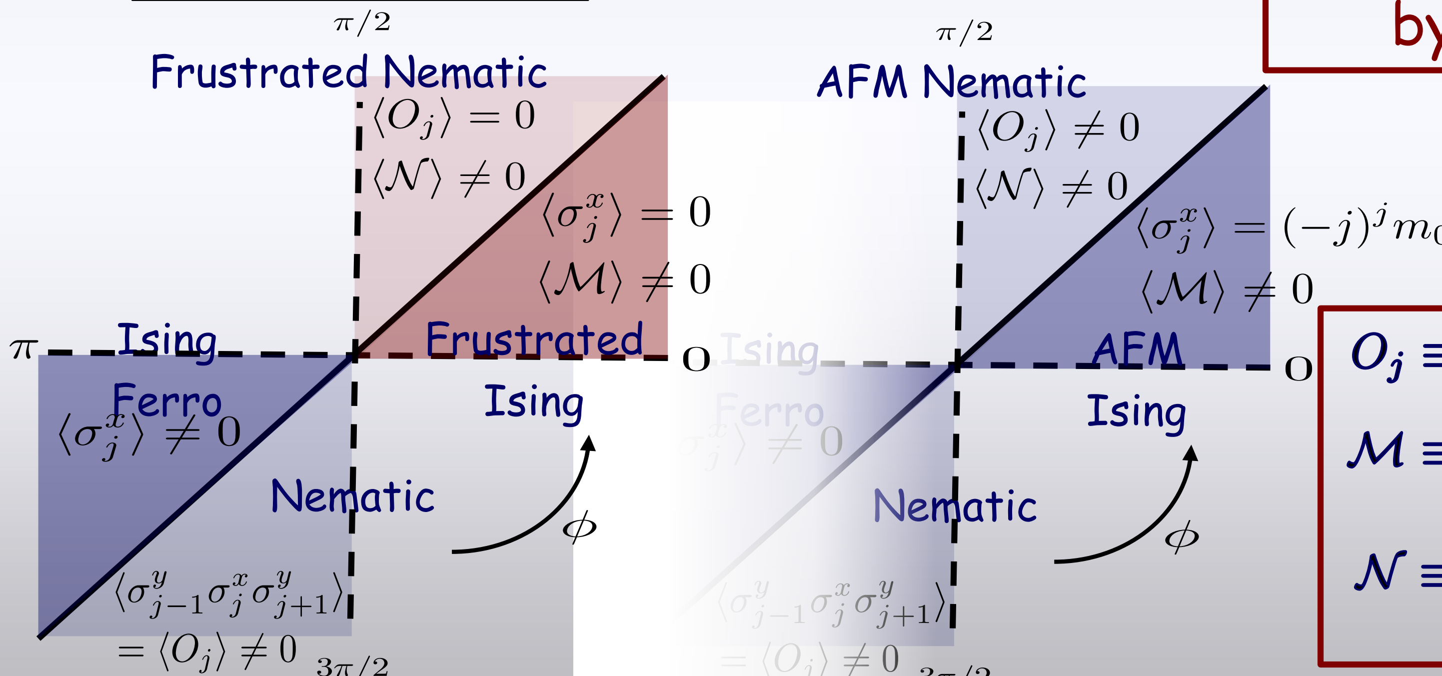
N=2M+1/FBC

N=2M/No FBC

Local order replaced by string one



$$O_j \equiv \sigma_{j-1}^y \sigma_j^x \sigma_{j+1}^y$$

$$\mathcal{M} \equiv \prod_k \left(\sigma_{4k-2}^x \sigma_{4k-1}^x\right)$$

$$\mathcal{N} \equiv \prod_k \left(O_{4k-2} O_{4k-1}\right)$$

Marić, Torre, Franchini, Giampaolo, arXiv:2101.08807

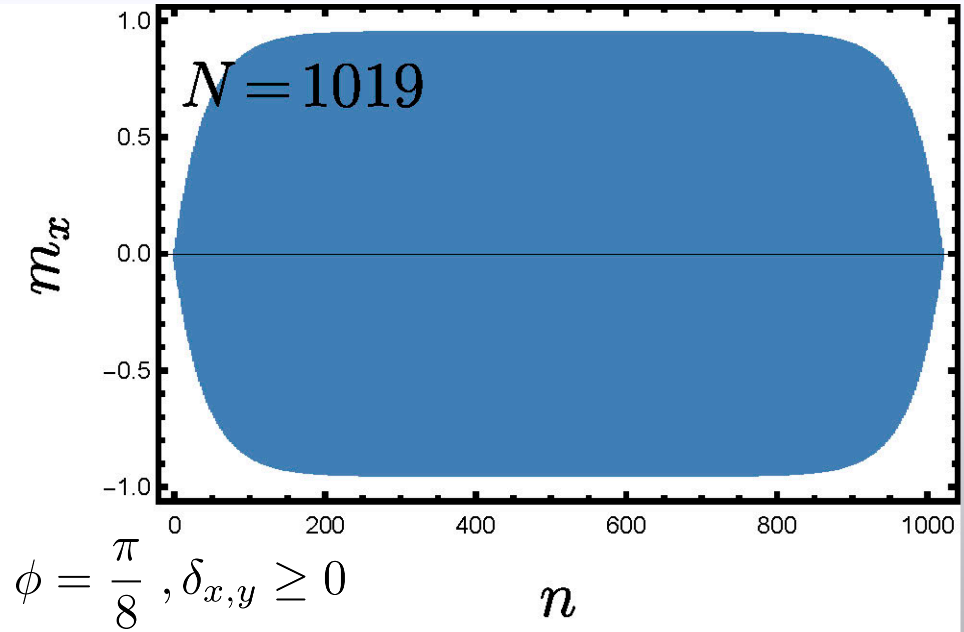
The effects of defects

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

- Physics discussed often dismissed as fragile
- Indeed a ferromagnetic defect simply pins one domain wall

$\rightarrow$ split classical point degeneracy and select one state

$\rightarrow$ far from defect standard AFM order is recovered



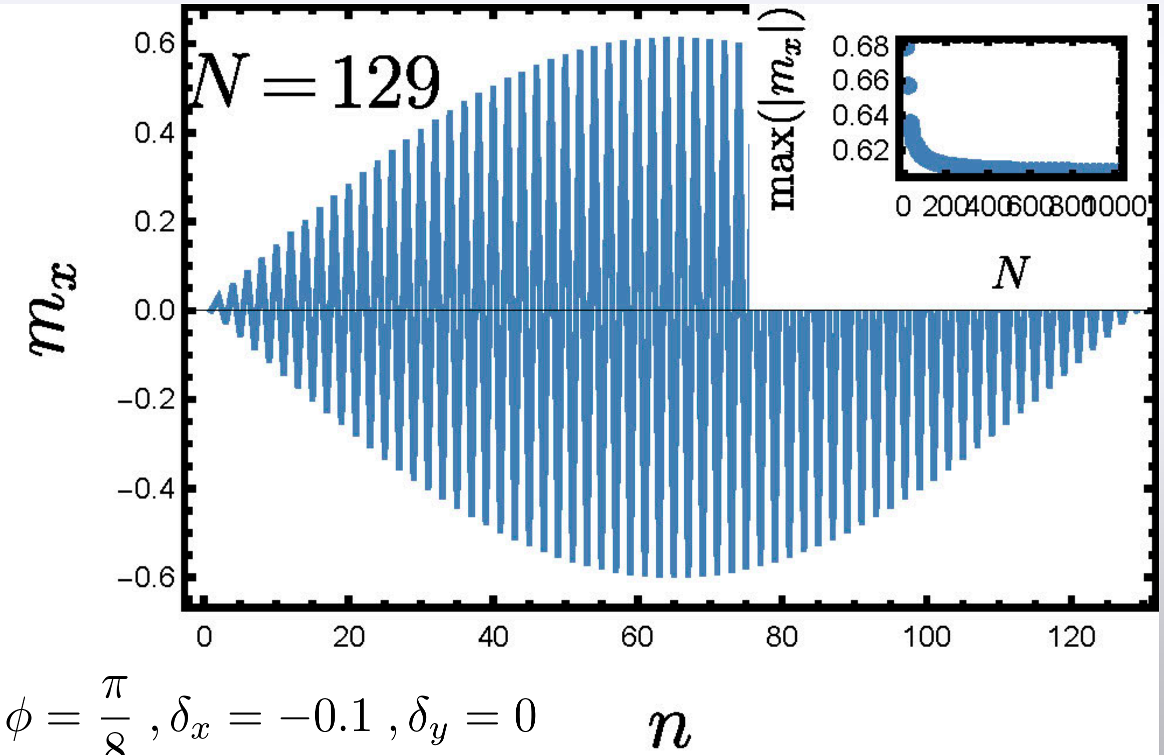
$\phi=\frac{\pi}{8}\,,\delta_{x,y}\geq 0$

Torre, Marić, Franchini, Giampaolo, Phys. Rev. B 103, 014429 (2021)

Defects

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

- Physics discussed so far often dismissed as fragile
- A single AFM defect stabilizes the incommensurate AFM order!



$$\phi = \frac{\pi}{8}\ , \delta_x = -0.1\ , \delta_y = 0$$

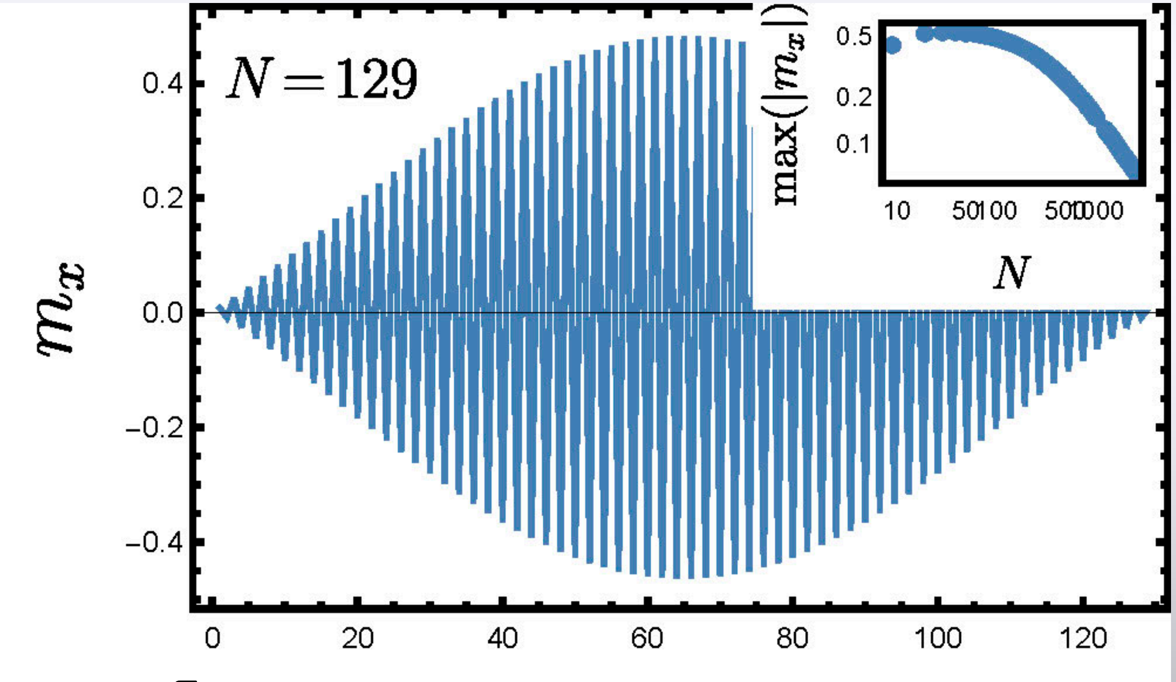
Torre, Marić, Franchini, Giampaolo, Phys. Rev. B 103, 014429 (2021)

Defects

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

- Physics discussed so far often dismissed as fragile
- However, other defects give rise to ever different orders

$\Rightarrow$ with FBC, usual AFM order becomes fragile!



$\phi = \frac{\pi}{8}$, $\delta_x = \delta_y = -0.1$

Torre, Marić, Franchini, Giampaolo, Phys. Rev. B 103, 014429 (2021)

Conclusions

- We studied the effect of frustrated boundary conditions on the local order of quantum spin chains
- Frustration knonw to give new physics in quantum systems
- FBC destroy perfect AFM order and replace it with:
  - Mesoscopic Ferromagnetic order for 1 AFM interaction
  - Incommensurate Modulated AFM order for 2 AFM int.
- Boundary-less b-QPT between the two

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Outlook: how can boundary conditions influence bulk properties?

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Outlook: how can boundary conditions influence bulk properties?

Thank you!

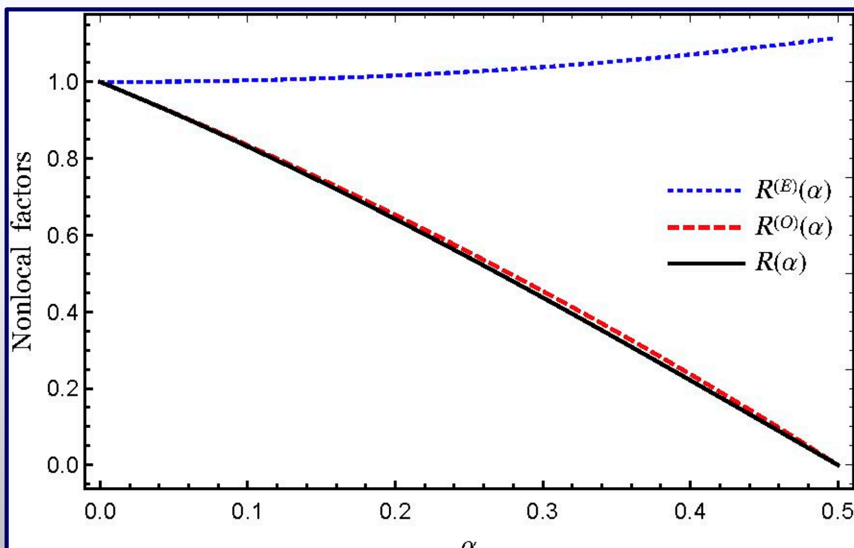
FBC at criticality

Li & He, PRE (2019)

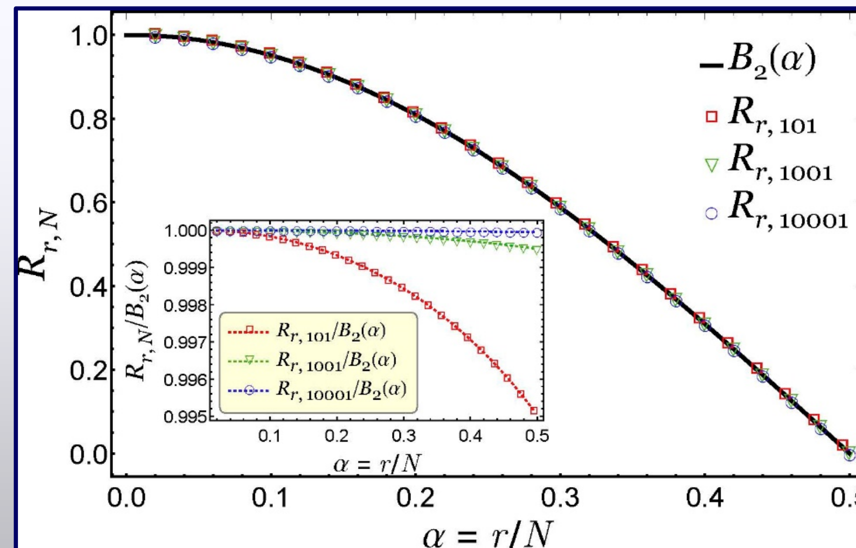
- Consider 2-point function of chains at criticality

$$C_{R,N} \equiv \langle \sigma^x_j \sigma^x_{j+R} \rangle \begin{cases} C_{R,\infty} \equiv C_{R,\lim_{N\to\infty} N} & \text{Usual} \\ C^{(O)}(\alpha) \equiv \lim\limits_{L\to\infty} C_{\alpha(2L+1),2L+1} & \text{PBC on odd \# (frustrated)} \\ C^{(E)}(\alpha) \equiv \lim\limits_{L\to\infty} C_{\alpha 2L,2L} & \text{PBC on even \#} \end{cases}$$

$$R^{(O)}(\alpha) \equiv C^{(O)}(\alpha)/C_{R,\infty} \qquad R^{(E)}(\alpha) \equiv C^{(E)}(\alpha)/C_{R,\infty} \qquad R(\alpha) \equiv C^{(O)}(\alpha)/C^{(E)}(\alpha)$$



Ising



XX

XY Chain

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

- Jordan-Winger transformation turns spins into spinless fermions:

$$\sigma_l^+ = e^{i\pi \sum_{j<l} \psi_j^\dagger \psi_j} \; \psi_l \, , \qquad \sigma_l^z = 1 - 2\psi_l^\dagger \psi_l$$

- Separate Hilbert space according to z-parity:

$$H = \frac{1+\Pi^z}{2} \, H^+ \, \frac{1+\Pi^z}{2} + \frac{1-\Pi^z}{2} \, H^- \, \frac{1-\Pi^z}{2} \qquad \Pi^z \equiv \prod_{l=1}^{N} \sigma_l^z$$

- Rotation in Fourier space (Bogoliubov rotation) to get:

$$H^\pm = \sum_{q \in \Gamma_\pm} \varepsilon\left(\tfrac{2\pi}{N} q\right) \left\{\chi_q^\dagger \chi_q - \frac{1}{2}\right\} , \qquad \Gamma_P = \left\{n + \frac{1+\Pi^z}{4}\right\}_{n=0}^{N-1}$$

$$\varepsilon(\alpha) \equiv 2 \left|\cos\phi \; e^{\imath 2q} + \sin\phi\right| \; , \quad \varepsilon(0) = -\epsilon(\pi) = 2\left(\cos\phi + \sin\phi\right)$$

can be negative!

XY Chain: FM phase

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

$$\varepsilon(\alpha) \equiv 2 \left| \cos\phi \; e^{\imath 2q} + \sin\phi \right|$$

- FM phase: $\phi \in [-\pi/2, -\pi/4)$

$$\varepsilon(0) = -\epsilon(\pi) = 2\,(\cos\phi + \sin\phi)$$

- $\epsilon(0) < 0$: belongs to odd parity sector

Bogoliubov vacuum

$\Rightarrow \quad |0\rangle$: lowest energy state in even parity sector

$\chi_0^\dagger |0'\rangle$: lowest energy state in odd parity sector

- Energy gap exponentially small in M (zero for h=0)
- Finite gap with other states

XY Chain: AFM phases

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

$$\varepsilon(\alpha) \equiv 2\left|\cos\phi \; e^{\imath 2q} + \sin\phi\right|$$

- FM phase: $\phi \in (-\pi/4, \pi/4)$

$$\varepsilon(0) = -\epsilon(\pi) = 2\,(\cos\phi + \sin\phi)$$

- $\epsilon(\pi) < 0$: belongs to even parity sector

Bogoliubov vacuum

$\Rightarrow \chi_\pi^\dagger |0\rangle$: lowest energy state in even parity sector

$|0'\rangle$: lowest energy state in odd parity sector

$\boxed{\text{Not compatible with parity constraint}}$

XY Chain: MFM

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

$$\varepsilon(\alpha) \equiv 2 \left| \cos\phi \; e^{\imath 2q} + \sin\phi \right|$$

- FM phase: $\phi \in (-\pi/4, 0)$

$$\varepsilon(0) = -\epsilon(\pi) = 2\left(\cos\phi + \sin\phi\right)$$

- $\epsilon(\pi) < 0$: belongs to even parity sector

Bogoliubov vacuum

$\Rightarrow \quad |0\rangle$: lowest allowed en. state in even parity sector

$\chi_0^\dagger |0'\rangle$: lowest allowed en. state in odd parity sector

- Energy gap algebraically small in M (zero for h=0)
- $\dfrac{1}{(2M+1)^2}$ closing gap with other states

XY Chain: IMAFM

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

$$\varepsilon(\alpha) \equiv 2 \left| \cos\phi \; e^{\imath 2q} + \sin\phi \right|$$

- FM phase: $\phi \in (0, \pi/4)$

$$\varepsilon(0) = -\epsilon(\pi) = 2\left(\cos\phi + \sin\phi\right)$$

- $\epsilon(\pi) < 0$: belongs to even parity sector

Bogoliubov vacuum

$\Rightarrow \chi^\dagger_{\pm\frac{\pi}{2}\left(1+\frac{1}{N}\right)} \chi^\dagger_\pi |0\rangle$: 2 deg. GS in even parity sector

$\chi^\dagger_{\pm\frac{\pi}{2}\left(1-\frac{1}{N}\right)} |0'\rangle$: 2 deg GS in odd parity sector

- Energy gap algebraically small in M (zero for h=0)
- $\dfrac{1}{(2M+1)^2}$ closing gap with other states

Even Parity

- Absolute GS → Bogoliubov vacuum: $\chi_q|GS\rangle = 0, \forall q \in \mathbb{N} + \frac{1}{2}$

  lowest energy allowed stat in even parity sector (P=1):

- For h<1, occupation of π-mode lowers the energy

$$|GS\rangle \to E_0 = -\frac{1}{2} \sum_{q=0}^{2M} \varepsilon \left[\tfrac{2\pi}{N}\left(q + \tfrac{1}{2}\right)\right] + 1 - h$$

excited states with P=1 lie arbitrarily close in energy to GS, forming a band with quadratic dispersion:

$$\chi^\dagger_{M+1/2}\chi^\dagger_{p+1/2}|GS\rangle \to E_p = -\frac{1}{2} \sum_{q=0}^{2M} \varepsilon \left[\tfrac{2\pi}{N}\left(q + \tfrac{1}{2}\right)\right] + \varepsilon \left[\tfrac{2\pi}{N}\left(p + \tfrac{1}{2}\right)\right]$$

$$E(k) \simeq E_0 + \frac{1}{2}\left(\frac{h}{1-h}\right)(k-\pi)^2 + \ldots$$

Odd Parity

- Vacuum does not belong to odd parity sector (P=-1):

$$\chi_q|0'\rangle = 0, \forall q \in \mathbb{N}$$

- Low energy states have one excitation: $\chi_p^\dagger|0'\rangle$
- Lowest energy state(s) for p=M/M+1:

$$\chi^\dagger_{M,M+1}|0'\rangle = |GS'\rangle \to E'_0 = -\frac{1}{2}\sum_{q=0}^{2M} \varepsilon\left[\tfrac{2\pi}{N}\left(q+\tfrac{1}{2}\right)\right] + \varepsilon\left(\pi \pm \frac{\pi}{N}\right)$$

which is bigger than E_0, closing in polynomially!

- Low energy states also form a band above |GS'> with quadratic dispersion, intertwining with that of the even parity sector
- In total: Even + Odd produce a gapless band of 2N states

Frustrated Ising Chain: Hilbert Space

- Ising Hilbert space exactly mappable into a FF Fock space
- In each parity sector: lowest energy state surmounted by N-1 state separated by a gap propotional to N^{-2}
- States in the two sectors intertwined with a similar energy splitting

$\Rightarrow$ GS part of a band of 2N gapless states in $N \to \infty$ limit

$\Rightarrow$ polynomial (not exp. !) energy split between parities

$\Rightarrow$ no SSB!

Order Parameter

$$H_{\text{Ising}} = \frac{1}{2} \sum_{l=1}^{2M+1} \left(\sigma_l^x \sigma_{l+1}^x - h\, \sigma_l^z \right)$$

$$P \equiv \prod_{l=1}^{N} \sigma_l^z \,,\, [H,P] = 0$$

- Parity eigenstates have vanishing order parameter: $\langle \sigma^x \rangle = \langle \sigma^+ + \sigma^- \rangle = 0$
- Non-zero magnetization only for degenerate GS of mixed parities: impossible at finite N
- Spontaneous Symmetry breaking by
  - Symmetry breaking field (not possible for gapless phases)
  - Long-range order in 2-point function:

$$C^{xx}(R) \equiv \langle \sigma_l^x \sigma_{l+R}^x \rangle$$

$$\lim_{R\to\infty} C^{xx}(R) = \langle \sigma^x \rangle^2$$

Correlation functions

$$H_{\text{Ising}} = \frac{1}{2}\sum_{l=1}^{2M+1}\left(\sigma_l^x\sigma_{l+1}^x - h\,\sigma_l^z\right)$$

$$\begin{aligned}\sigma_l^+ &= e^{i\pi\sum_{j<l}\psi_j^\dagger\psi_j}\ \psi_l\\ \sigma_l^z &= 1-2\psi_l^\dagger\psi_l\end{aligned}$$

- Correlation functions can be calculated starting from FF picture

- Introduce Majorana Fermions: $A_l \equiv \psi_l^\dagger + \psi_l\ , B_l \equiv i(\psi_l - \psi_l^\dagger)$

$$\langle A_l A_m\rangle = \langle B_l B_m\rangle = \delta_{l,m}\ ,$$

$$\langle A_{l+R} B_l\rangle = iG(R,J,h)\ ,$$

$$\nu(h,R) = \begin{cases} (-1)^R & h>0\\ -1 & h<0\end{cases}$$

$$G(R,J=1,h) = -G(R,J=-1,-h) + \frac{2}{N}\nu(h,R)$$

- Compared to the standard case, the frustrated GS correlators have 1 additional contribution as for 1 (π-)mode excited state

Local and Quasi-Local Correlators

$$\langle A_{l+R} B_l \rangle = i G(R,J,h) \,, \quad G(R,1,h) = -G(R,-1,-h) + \frac{2}{N} \nu(h,R)$$

- "Local" Correlation functions have a finite number of Majoranas

$$\langle \sigma^z_{l+R}\, \sigma^z_l \rangle = \langle A_{l+R} B_{l+R} A_l B_l \rangle$$
$$= m_z^2 - \frac{c_1^z(h)}{R^2} \left(\frac{h^2}{J^2} \right)^R + \frac{4 m_z}{N} \left[1 + c_2^z(h) (-1)^R \left| \frac{h}{J} \right|^R \right]$$

- "Quasi-local" one have # of Majorana growing with distances

(Dong et al. JSTAT '16)

$$\langle \sigma^x_{l+R}\, \sigma^x_l \rangle = \langle B_{l+R} A_{l+R-1} B_{l+R-1} \ldots A_{l-1} B_{l-1} A_l \rangle$$
$$= (-1)^R \left(1 - \frac{h^2}{J^2} \right)^{1/4} \left[1 + \frac{c^x(h)}{R^2} \left(\frac{h^2}{J^2} \right)^R \right] \left(1 - \frac{2R}{N} \right)$$

- The $\frac{1}{N}$ contributions add up to be finite at large distances
- Locality w.r.t Jordan-Wigner fermions

Correlation Functions

- "*Local*" correlators:

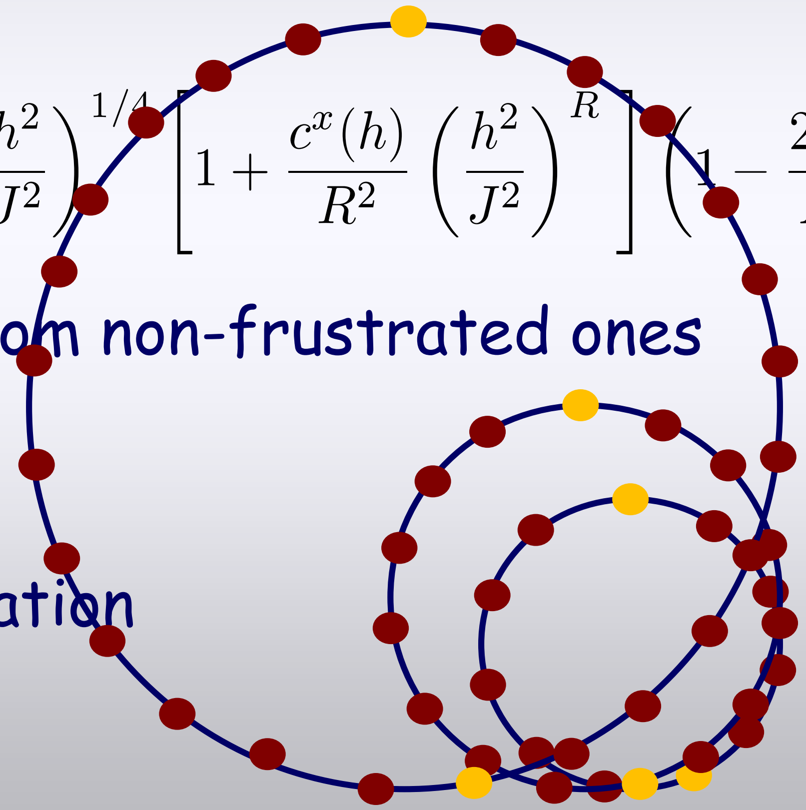
$$C^{zz}(R) \equiv \langle \sigma_l^z \sigma_{l+R}^z \rangle = m_z^2 - \frac{c_1^z(h)}{R^2} \left(\frac{h^2}{J^2} \right)^R + \frac{4m_z}{N} \left[1 + c_2^z(h)(-1)^R \left| \frac{h}{J} \right|^R \right]$$

- "*Quasi-Local*" correlators

$$C^{xx}(R) \equiv \langle \sigma_l^x \sigma_{l+R}^x \rangle = (-1)^R \left(1 - \frac{h^2}{J^2} \right)^{1/4} \left[1 + \frac{c^x(h)}{R^2} \left(\frac{h^2}{J^2} \right)^R \right] \left(1 - \frac{2R}{N} \right)$$

- Locally: indistinguishable from non-frustrated ones

- Order parameter/
    Spontaneous Magnetization



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$$C^{zz}(R) \equiv \langle \sigma_l^z \sigma_{l+R}^z \rangle = m_z^2 - \frac{c_1^z(h)}{R^2} \left(\frac{h^2}{J^2} \right)^R + \frac{4 m_z}{N} \left[1 + c_2^z(h) (-1)^R \left| \frac{h}{J} \right|^R \right]$$

- "*Quasi-Local*" correlators

$$C^{xx}(R) \equiv \langle \sigma_l^x \sigma_{l+R}^x \rangle = (-1)^R \left(1 - \frac{h^2}{J^2} \right)^{1/4} \left[1 + \frac{c^x(h)}{R^2} \left(\frac{h^2}{J^2} \right)^R \right] \left(1 - \frac{2R}{N} \right)$$

- Locally: indistinguishable from non-frustrated ones

- Order parameter: $\boxed{\langle \sigma^x \rangle = \lim_{N \to \infty} \sqrt{C^{xx}\left(\frac{N-1}{2} \right)} = 0}$

- <u>Inconsistent</u> with thermodynamic Limit ($N \to \infty$)

Scaling Thermodynamic Limit

$$C^{xx}(R) \equiv \langle \sigma_l^x \sigma_{l+R}^x \rangle = (-1)^R \left(1 - \frac{h^2}{J^2}\right)^{1/4} \left[1 + \frac{c^x(h)}{R^2} \left(\frac{h^2}{J^2}\right)^R\right] \left(1 - \frac{2R}{N}\right)$$

- Local behavior cannot depend on even/oddness of large chain
- Yet, the order parameter does $\boxed{\langle \sigma^x \rangle = \lim_{N\to\infty} \sqrt{C^{xx}\left(\frac{N-1}{2}\right)} = 0}$
- Traditional therm. limit restores finite order parameter
- To account for the frustrated behavior we consider a

  <u>Scaling Thermodynamic Limit</u>: $N \to \infty$ as $\boxed{r \equiv \frac{R}{N} = \text{const}}$
- In this way, signatures of a new "pseudo-phase"
- Let us look at the entanglement entropy in the STL

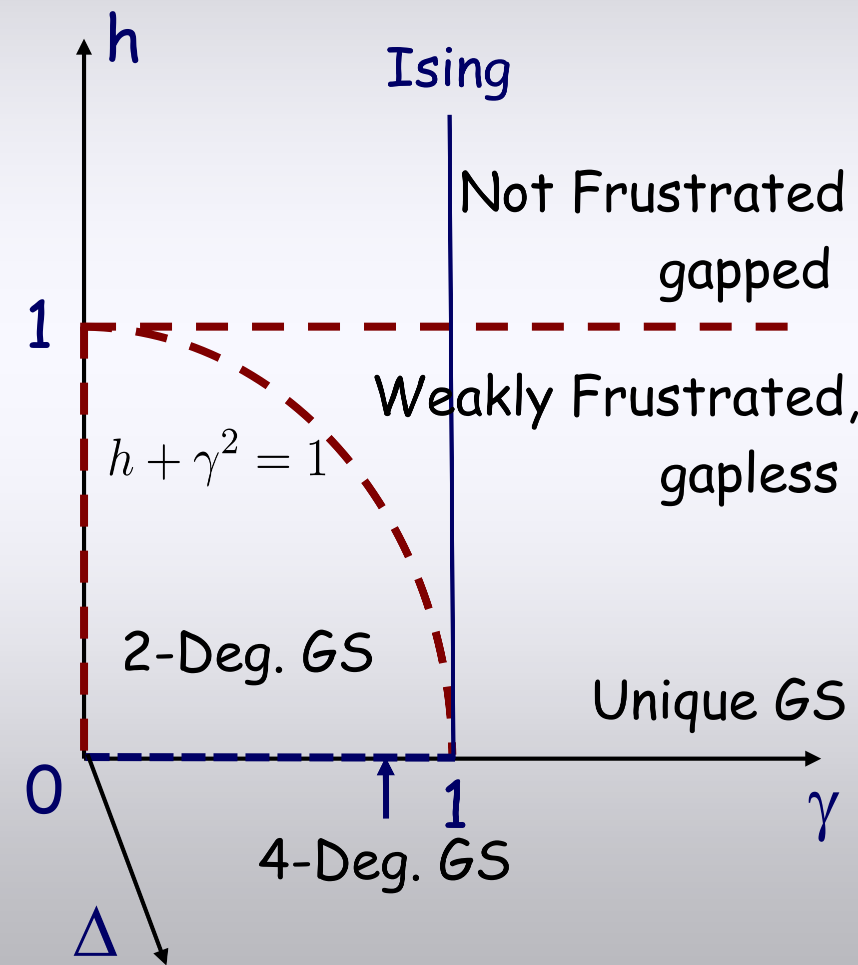
Weak Frustration's Phase Diagram

$$H = \frac{1}{2}\sum_{l=1}^{N}\left[\left(\frac{1+\gamma}{2}\right)\sigma_l^x\sigma_{l+1}^x + \left(\frac{1-\gamma}{2}\right)\sigma_l^y\sigma_{l+1}^y\right] + \frac{\Delta}{2}\sum_{l=1}^{N}\sigma_l^z\sigma_{l+1}^z - \sum_{l=1}^{N} h\,\sigma_l^z$$

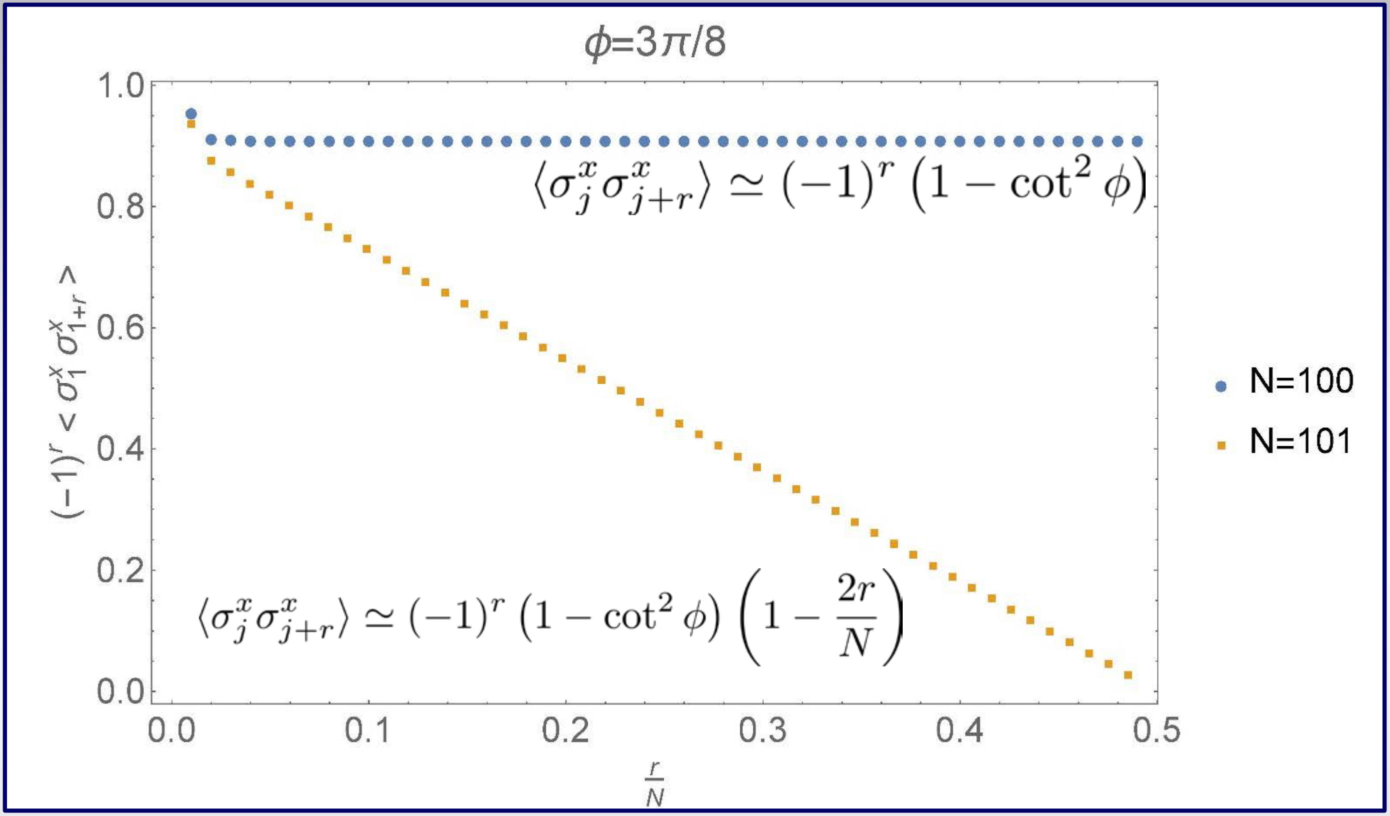
- Frustration can give GS a finite momentum

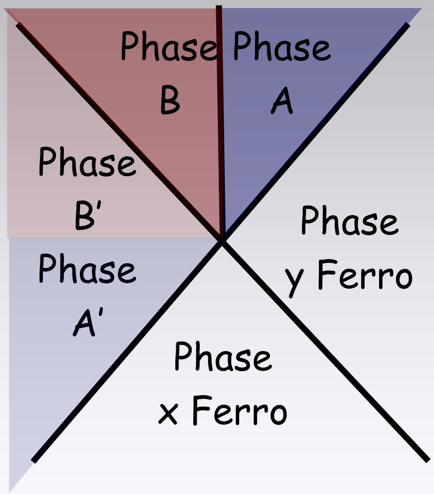
$\Rightarrow$ GS 2-fold degenerate

- Exact, geometrical, finite size degenaricy, for any interaction
- Spontaneous breaking of translational invariance



2-point function

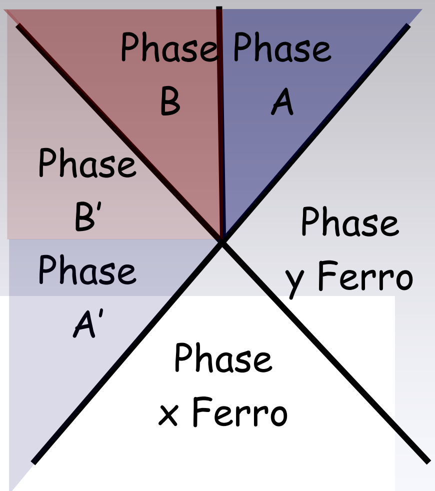


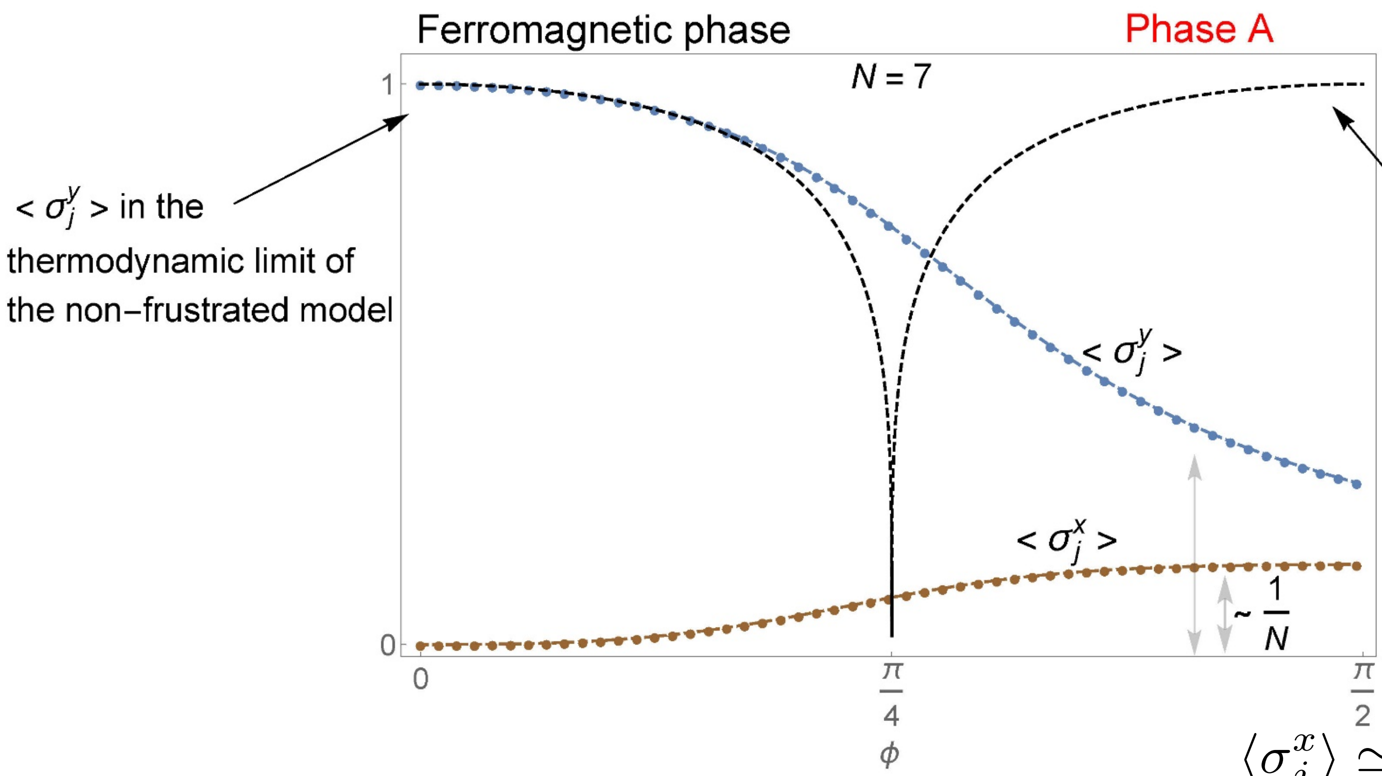


- Behavior of 2-point function in regions A & B analogue to Ising

Phase A: mesoscopic magnetization

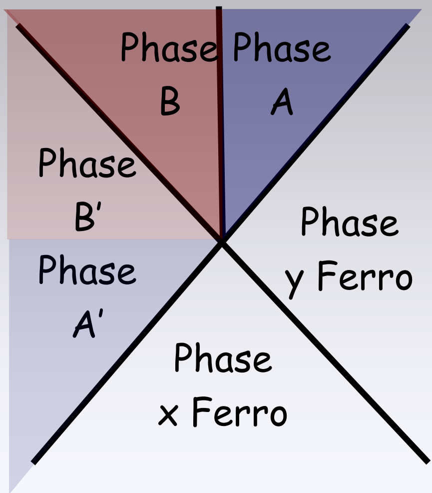
- Finite magnetization in finite system
- Clearly different from non-frustrated





$$\langle \sigma_j^x \rangle \simeq \frac{1}{N} \left(1 - \cot^2 \phi\right)^{\frac{1}{4}}$$

Phase B: Lost Translational Inv.

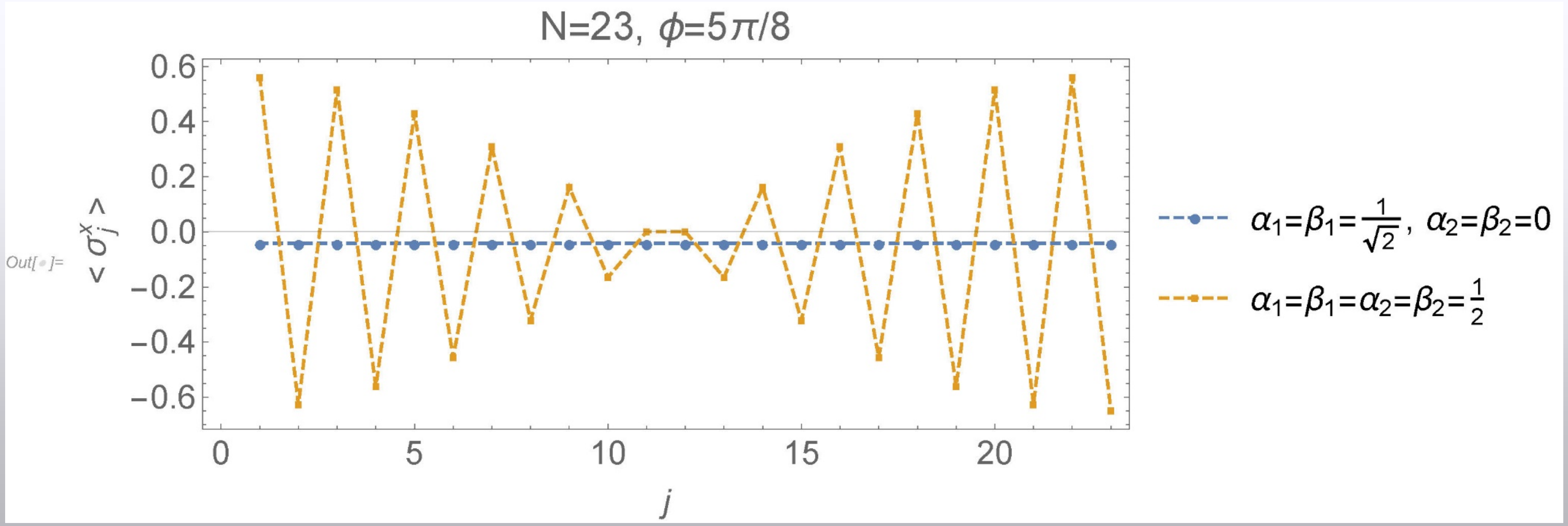


- 4-fold deg. GS:

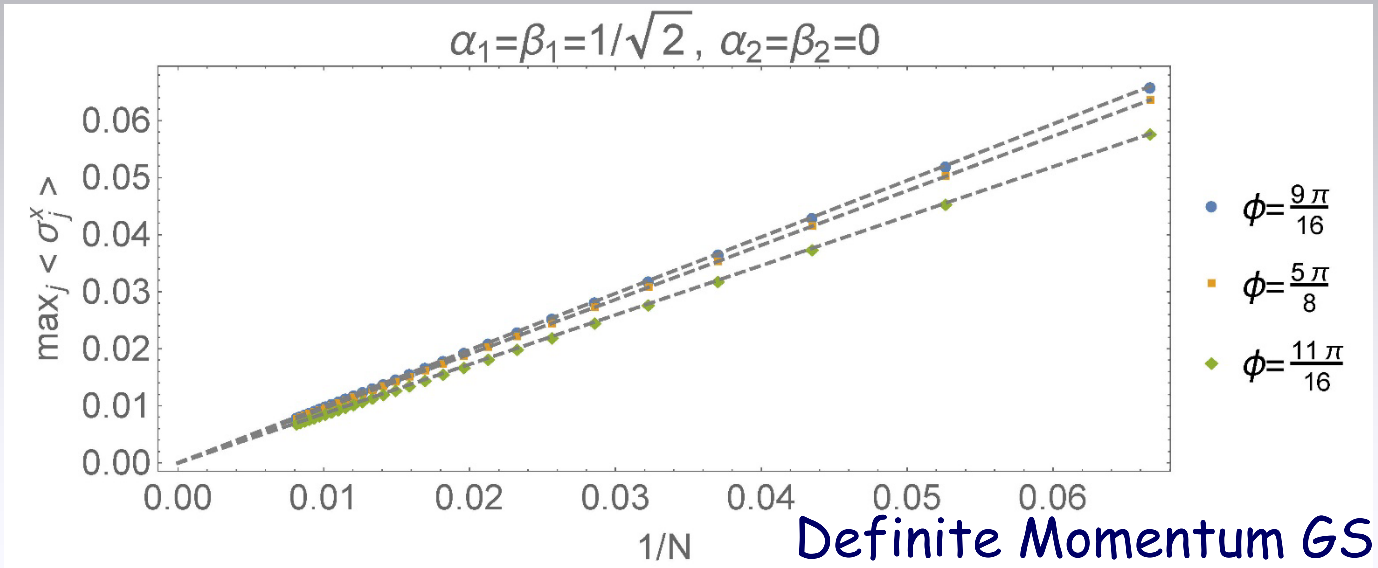
$$|GS\rangle \equiv \sum_{l=1}^{2} \alpha_l |GS_l, +\rangle + \beta_l |GS_l, -\rangle, \ \sum_{l=1}^{2} \alpha_l^2 + \beta_l^2 = 1$$

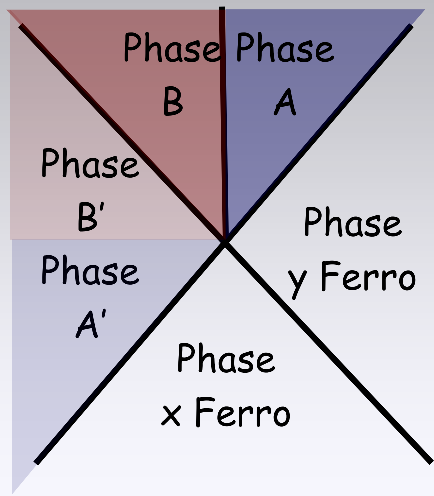
$$P|GS_l, \pm\rangle = e^{\pm \frac{i\pi}{2}\left(1 \pm \frac{1}{N}\right)} |GS_l, \pm\rangle$$

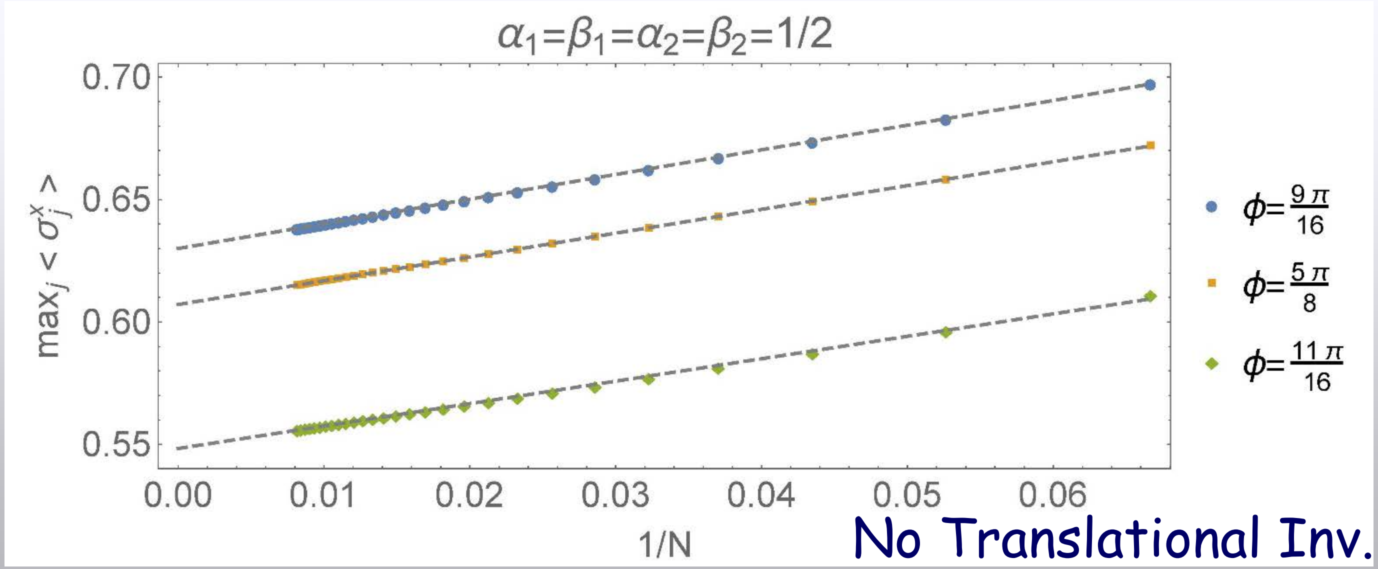
- Magnetization for $\alpha_l = \beta_l$



Phase B: Finite-Size Scaling

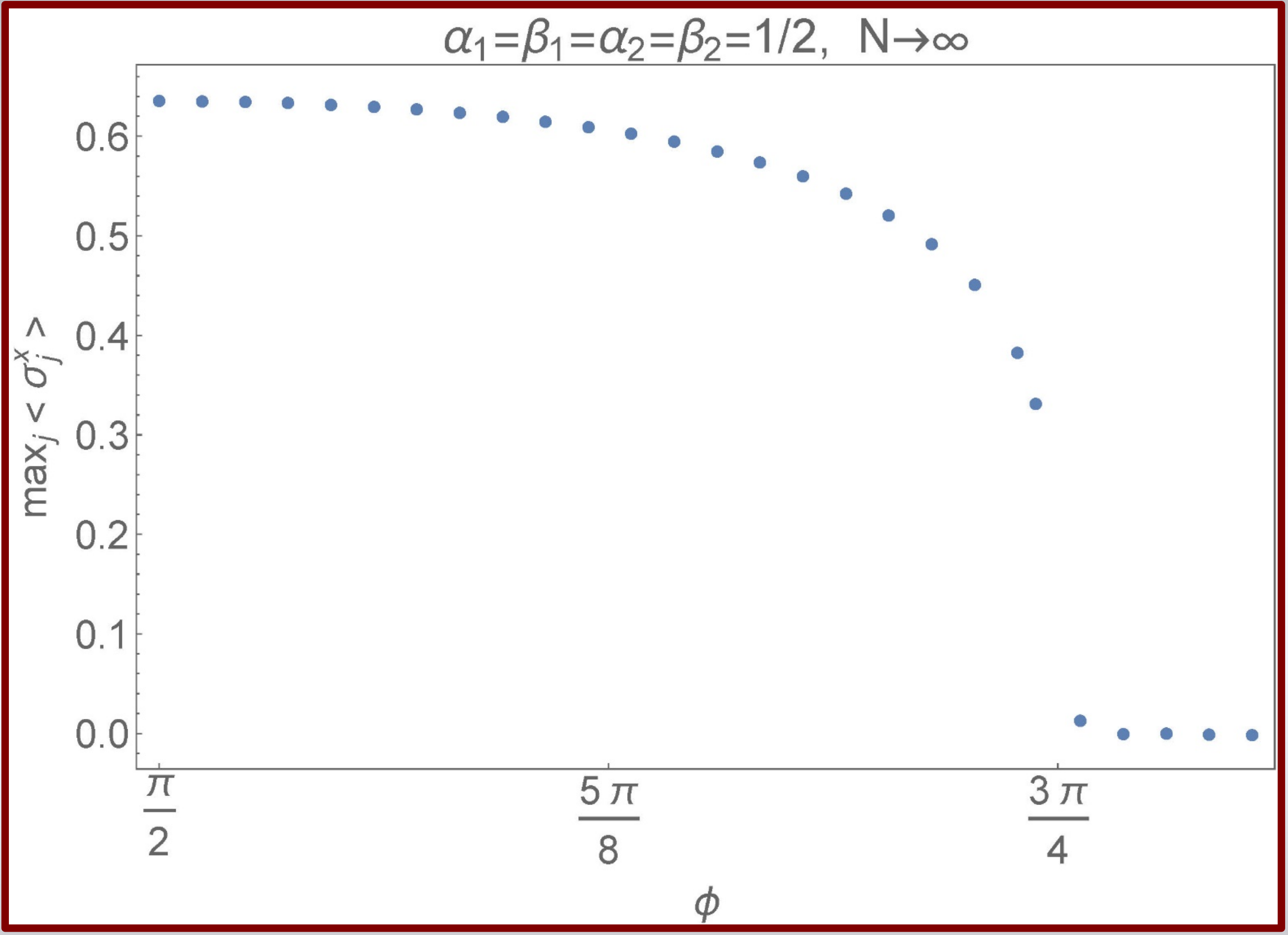


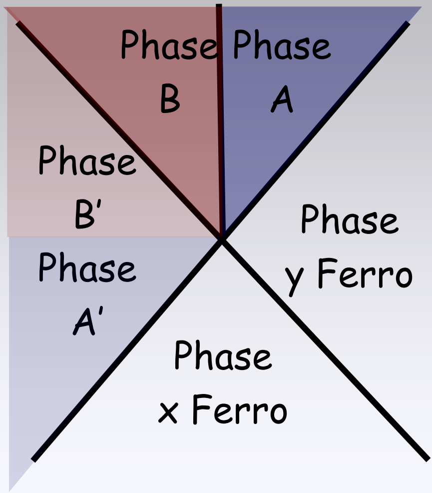




- Finite intercept in therm. limit: single particle?!?

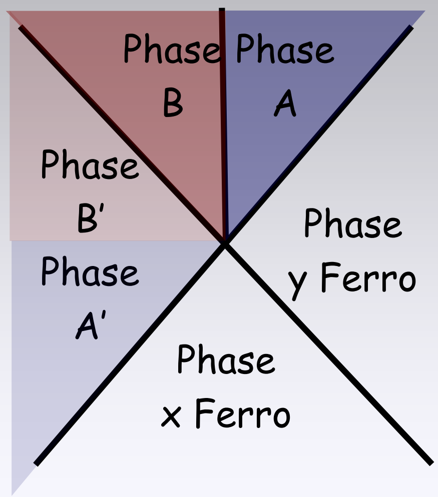
Order Parameter?





- $\max\langle\sigma_j^x\rangle$ (in therm. limit) acts as an order parameter

Magnetization: Summary



- y-Ferro phase: GS deg=2

$$\langle \sigma_j^x \rangle \stackrel{N\to\infty}{\to} 0, \; \langle \sigma_j^y \rangle \stackrel{N\to\infty}{\to} \left(1 - \cot^2\phi\right)^{\frac{1}{4}}$$

- Phase A: GS deg = 2

$$\langle \sigma_j^x \rangle, \langle \sigma_j^y \rangle \sim \frac{1}{N}$$

- Phase B: GS deg = 4 (broken translational invariance)

$$\max_j \langle \sigma_j^x \rangle \sim a + \frac{b}{N}$$

$$\max_j \langle \sigma_j^y \rangle \sim \frac{1}{N}$$

Quantifying Frustration

- First quantify "quantum" frustration:
  - Write Hamiltonian as sum of local terms
  - Find GS of H and of all the H_j separately and construct projectors

$$H = \sum_j H_j \longrightarrow \begin{cases} H \to \Pi \equiv |GS\rangle\langle GS| \\ H_j \to \Pi_j \equiv \sum_\alpha |GS_j^\alpha\rangle\langle GS_j^\alpha| \end{cases}$$

  - Measure Hilbert-Schmidt distance between them

$$\boxed{F_j \equiv Tr\left(\Pi_j \Pi\right)}$$

  - If translational invariance: $F \equiv F_j$

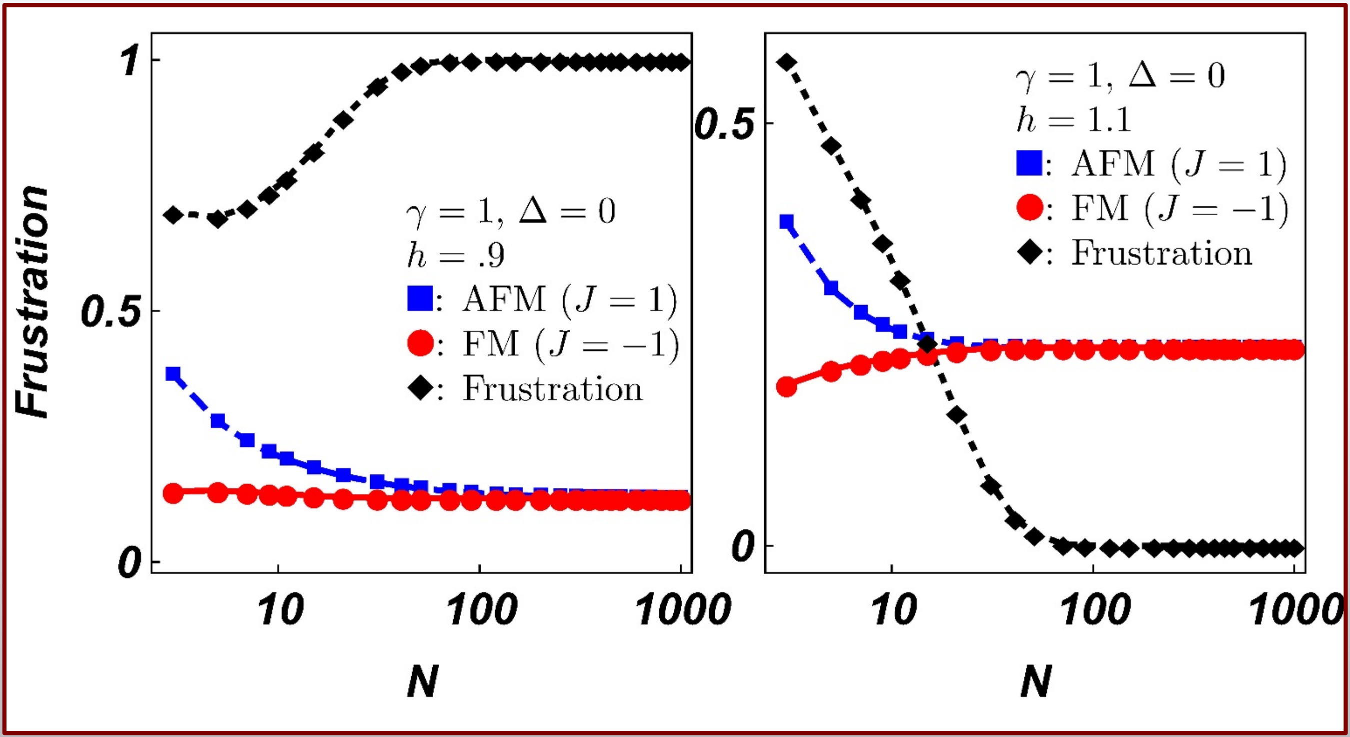
(Giampaolo et al. PRL '11)

Quantifying Frustration

- Consider frustration of Ferromagnetic (J=-1) $F(J=-1)$

  and AFM system (J=1) $F(J=1)$

- Geometrical frustration: $g_F = \sum_{j=1}^{N} \left[F(J=1) - F(J-1) \right]$



Frustration does not increase with the system's length and vanishes in non-frustrated phase

Approaching h→1

- CFT behavior up to (non-frustrated) correlation length scale & deviation beyond it