Exact Field Induced Ground States of the Quantum Compass Model

Erik S. Sørensen, McMaster University

Canada

- ADS Richards - McMaster

- ADS Richards, ESS, PRB 109, L241116 (2024), arXiv:2310.01384

- ESS, J. Ridell, H.-Y. Kee, Phys. Rev. Research 5, 013210 (2023)
- ESS, J. Gordon, J. Ridell, T. Yang, H.-Y. Kee, Phys. Rev. Research 5, L012027 (2023)

2D Quantum Compass Model - Bond-Directional Interactions

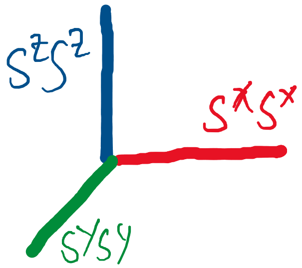
Directional Interactions

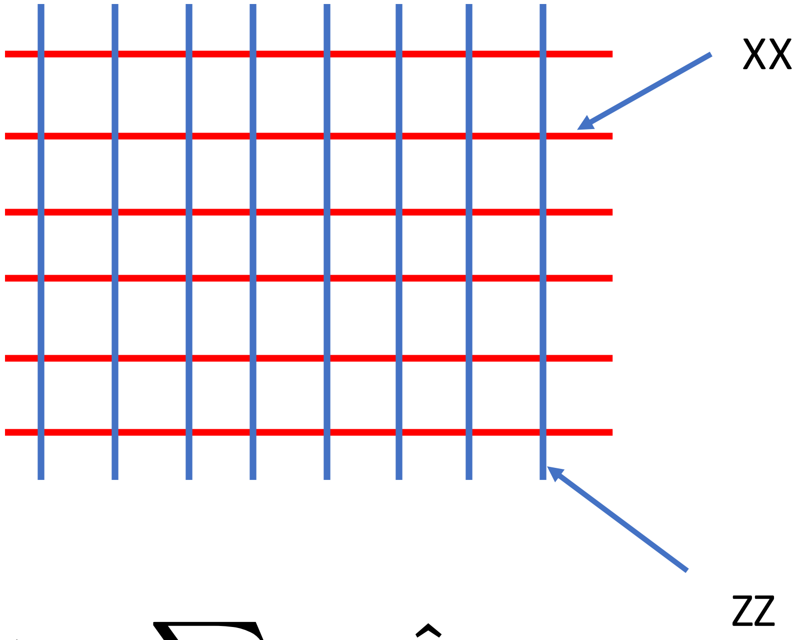
Early Eighties: Compass Models

I. Kugel' and D. I. Khomskii, Superexchange ordering of degenerate orbitals and magnetic structure of dielectrics with jahn–teller ions, JETP Letters 15, 446 (1972).

Review: Compass models.
Z. Nussinov, J.v.d. Brink
RMP 87, 1 (2015)

Ising interactions that depend on the bond direction





$$\mathcal{H} = J\sum_{\mathbf{r}}(\hat{S}^x_{\mathbf{r}}\hat{S}^x_{\mathbf{r}+e_x} + \hat{S}^z_{\mathbf{r}}\hat{S}^z_{\mathbf{r}+e_z}) - \sum_{\mathbf{r}}\mathbf{h}\cdot\hat{\mathbf{S}}_{\mathbf{r}}.$$

Conserved Quantities

$$\mathcal{H} = J \sum_{\mathbf{r}} (\hat{S}^x_{\mathbf{r}} \hat{S}^x_{\mathbf{r}+e_x} + \hat{S}^z_{\mathbf{r}} \hat{S}^z_{\mathbf{r}+e_z}) - \sum_{\mathbf{r}} \mathbf{h} \cdot \hat{\mathbf{S}}_{\mathbf{r}}.$$

J>0, matters for non-zero h

$$P_j = \Pi_i \sigma^z_{i,j} \qquad Q_i = \Pi_j \sigma^x_{i,j}$$

Row product — Column product

Nussinov, Ortiz, Cobanera, Ann. Phys. 2012

Equivalent to Xu-Moore model (Nussinov, Fradkin PRB 2005)

Which can be mapped to the toric code in a transverse field (Vidal et al, PRB 2009)

All eigen-states are at least 2-fold degenerate. In thermodynamic limit GS is $2\text{x}2^L$ degenerate.

Quantum Compass Models (sq lattice) Dorier, Becca, Mila PRB **72**, 024448 (2005). Doucot et al PRB (2005)

Why should we care ?

Toric Code

Fault-tolerant quantum computation by anyons

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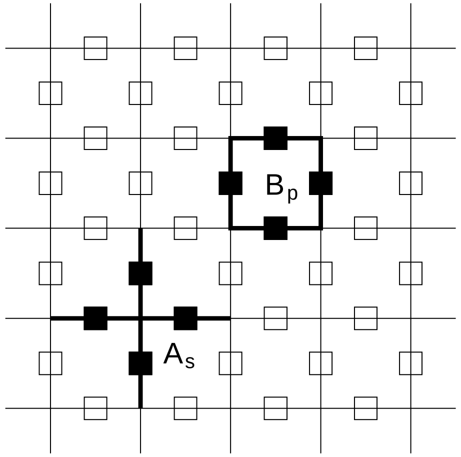
Received 20 May 2002

Abstract

A two-dimensional quantum system with anyonic excitations can be considered as a quantum computer. Unitary transformations can be performed by moving the excitations around each other. Measurements can be performed by joining excitations in pairs and observing the result of fusion. Such computation is fault-tolerant by its physical nature.

Annals of Physics 303 (2003) 2–30



$$H = -J_c \sum_s A_s - J_m \sum_p B_p$$

$$A_s = \prod_{j \in star} \sigma_j^x$$

$$B_p = \prod_{j \in \partial p} \sigma_j^z$$

Kugel’, Khomskiĭ, Sov. Phys Uspekhi (1982)

Kitaev Honeycomb Model

Anyons in an exactly solved model and beyond

Alexei Kitaev *

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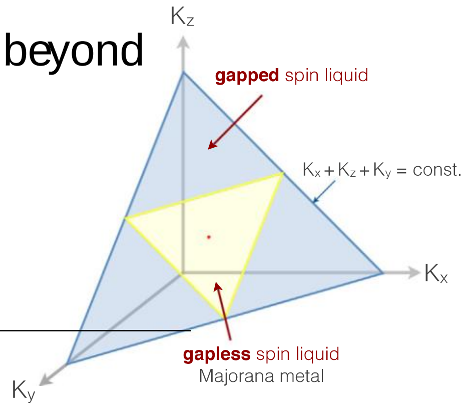
Received 21 October 2005; accepted 25 October 2005

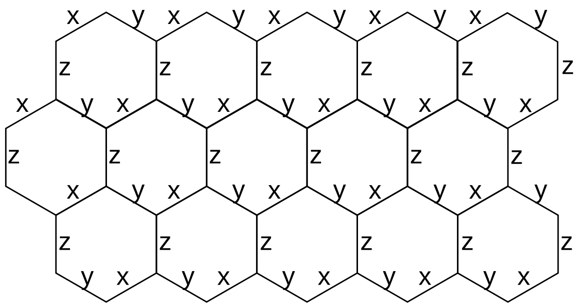


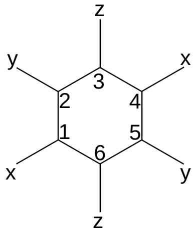
Abstract

A spin-1/2 system on a honeycomb lattice is studied. The interactions between nearest neighbors are of XX, YY or ZZ type, depending on the direction of the link; different types of interactions may differ in strength. The model is solved exactly by a reduction to free fermions in a static Z_2 gauge

Annals of Physics 321 (2006) 2–111

$$H = J_x \sum_{x\ links} S_j^x S_k^x + J_y \sum_{y\ links} S_j^y S_k^y + J_z \sum_{z\ links} S_j^z S_k^z$$





$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$$

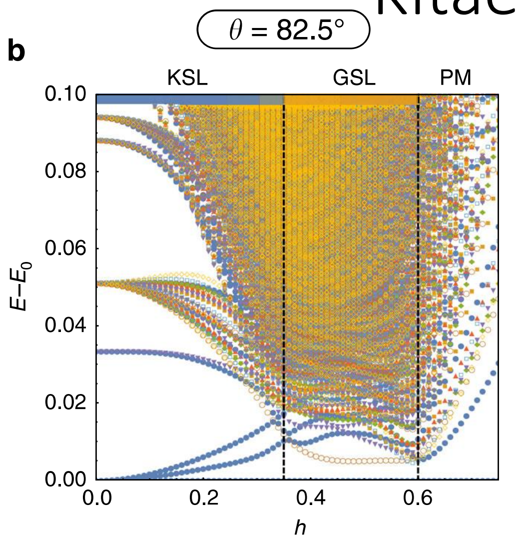
$$[H, W_p] = 0$$

Quantum Compass Models (sq lattice) Dorier, Becca, Mila PRB **72**, 024448 (2005). Doucot et al PRB (2005)

Kitaev Honeycomb

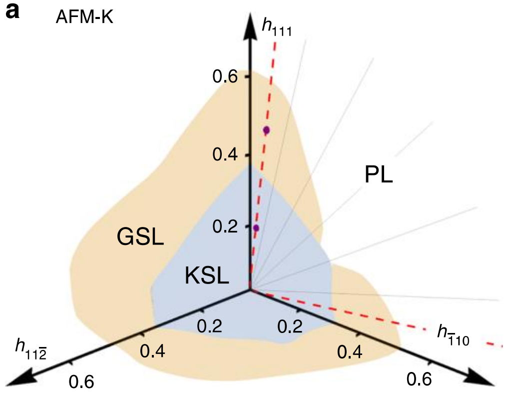
α-RuCl3

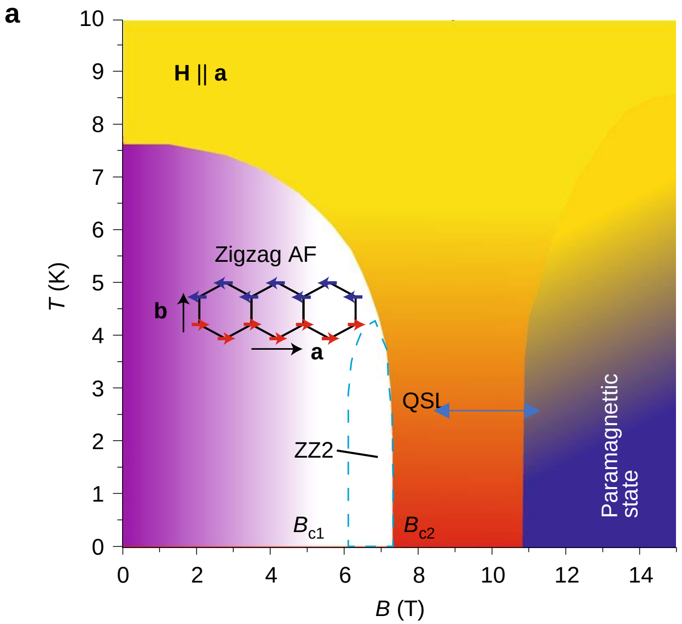
Experiments



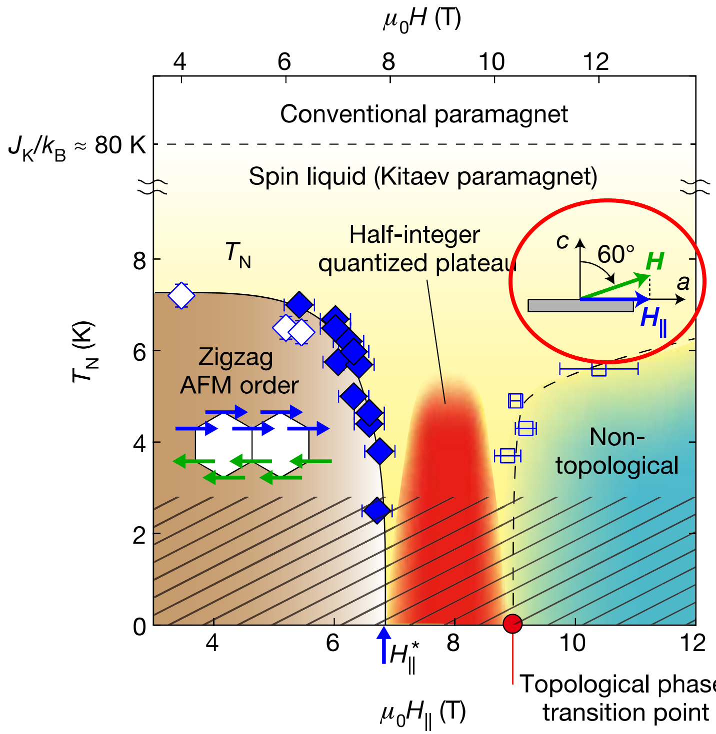
Hickey, Trebst, Nat. Phys. (2019).

Numerics





Czajka et al Nature Physics, 17, 915 (2021)
ArXiv:2201.0787
"incompatible with half-quantization of κxy/T"



Kasahara, Nature 559, 227 (2018)

PRL 102, 017205 (2009) PHYSICAL REVIEW LETTERS week ending 9 JANUARY 2009

Mott Insulators in the Strong Spin-Orbit Coupling Limit: From Heisenberg to a Quantum Compass and Kitaev Models

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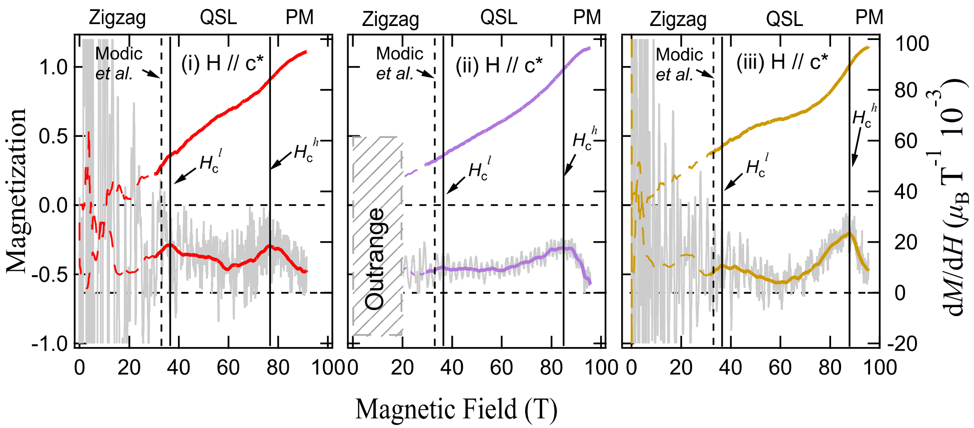
(Received 21 August 2008; published 6 January 2009)

Quantized (or not quantized) thermal hall effect..
PA Lee www.condmatjclub.org Nov 2021

Zhou et al ArXiv:2201.04597, Nat Commun 14, 5613 (2023)



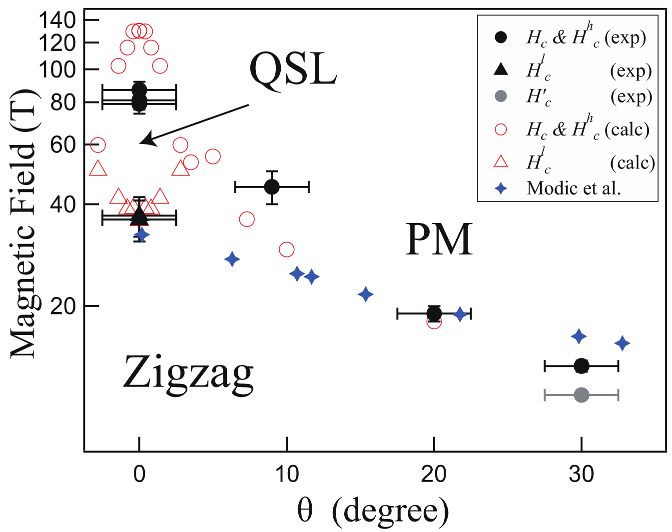


FIG. 4. The field-angle phase diagram that summarizes the values of transition fields determined from both the experimental (black and grey solid markers) and the calculated data (red open ones). We also plot the low-field results (blue stars) taken from Ref. [43] as a supplement. The zigzag antiferromagnetic, paramagnetic (PM), and the quantum spin liquid (QSL) phases are indicated.

Why should we care ?

2d Quantum compass model is the simplest 2D model with bond-directional interactions

- What phases are possible in a magnetic field
- What excitations.

The Exact Ground-States

With PBC in can absorb the field term

At $h_x^\star = h_z^\star = 2JS$ Write Hamiltonian as

$$\mathcal{H} = J\sum_{\mathbf{r}}(\hat{S}^x_{\mathbf{r}}\hat{S}^x_{\mathbf{r}+e_x} + \hat{S}^z_{\mathbf{r}}\hat{S}^z_{\mathbf{r}+e_z}) - \sum_{\mathbf{r}} \mathbf{h}\cdot\hat{\mathbf{S}}_{\mathbf{r}}$$

$$\mathcal{H} = \mathcal{H}_p - 2NJS^2$$

Only possible due to the Bond-directional interactions

$$\mathcal{H}_p = J\sum_{\mathbf{r}}\left[\underbrace{\left(S - \hat{S}^x_{\mathbf{r}}\right)\left(S - \hat{S}^x_{\mathbf{r}+e_x}\right) + \left(S - \hat{S}^z_{\mathbf{r}}\right)\left(S - \hat{S}^z_{\mathbf{r}+e_z}\right)}_{\text{Positive Semidefinite}}\right]$$

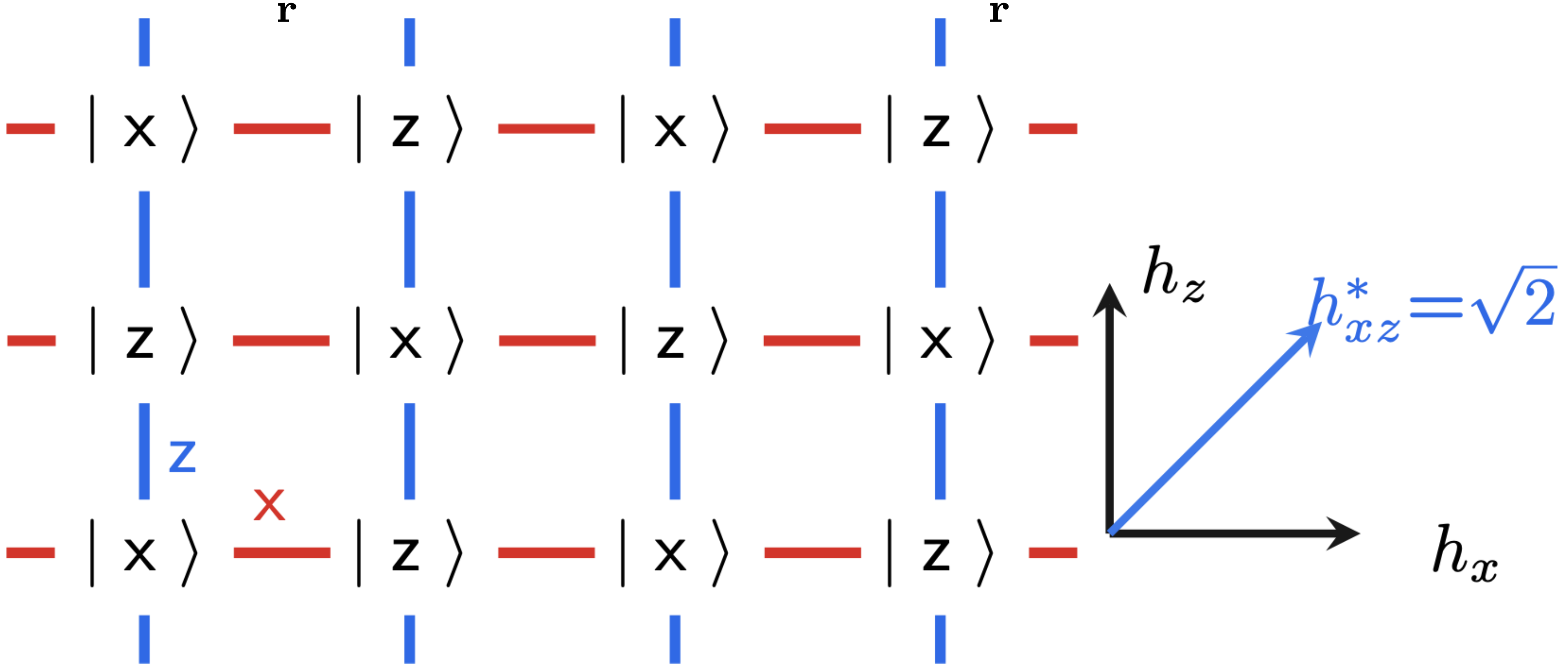
Just need to find states where the positive H_p gives 0 !!

Decorate the lattice to obtain a classical product state

Exact Ground-States for PBC

Only works for low co-ordination
For instance, not the 3D QCM

$$\mathcal{H} = J\sum_{\mathbf{r}}(\hat{S}^x_{\mathbf{r}}\hat{S}^x_{\mathbf{r}+e_x} + \hat{S}^z_{\mathbf{r}}\hat{S}^z_{\mathbf{r}+e_z}) - \sum_{\mathbf{r}} \mathbf{h}\cdot\hat{\mathbf{S}}_{\mathbf{r}}$$



2 degenerate classical product states should occur for any value of S=1/2,1,3/2,2,…. at h*

For a Lx by Lz lattice exact for finite lattice with Lx and Lz even !

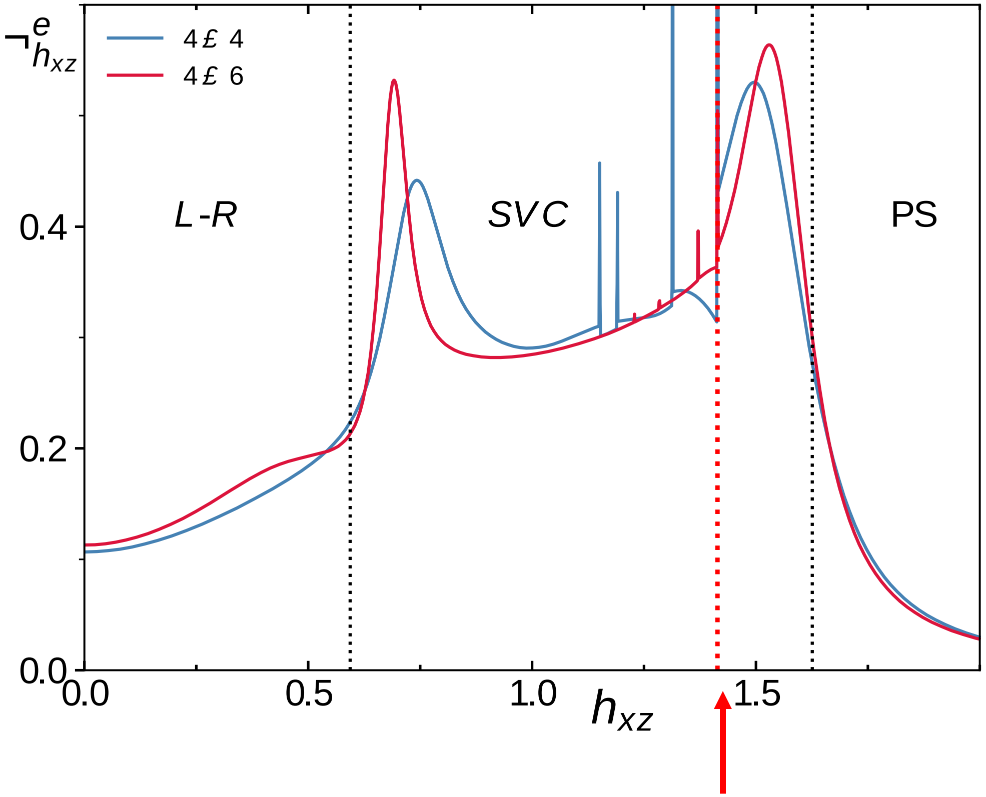
Extreme Ising state

Zero entanglement

Coupling Term is cancelled

2D Quantum Compass model in-plane magnetic field hx=hz

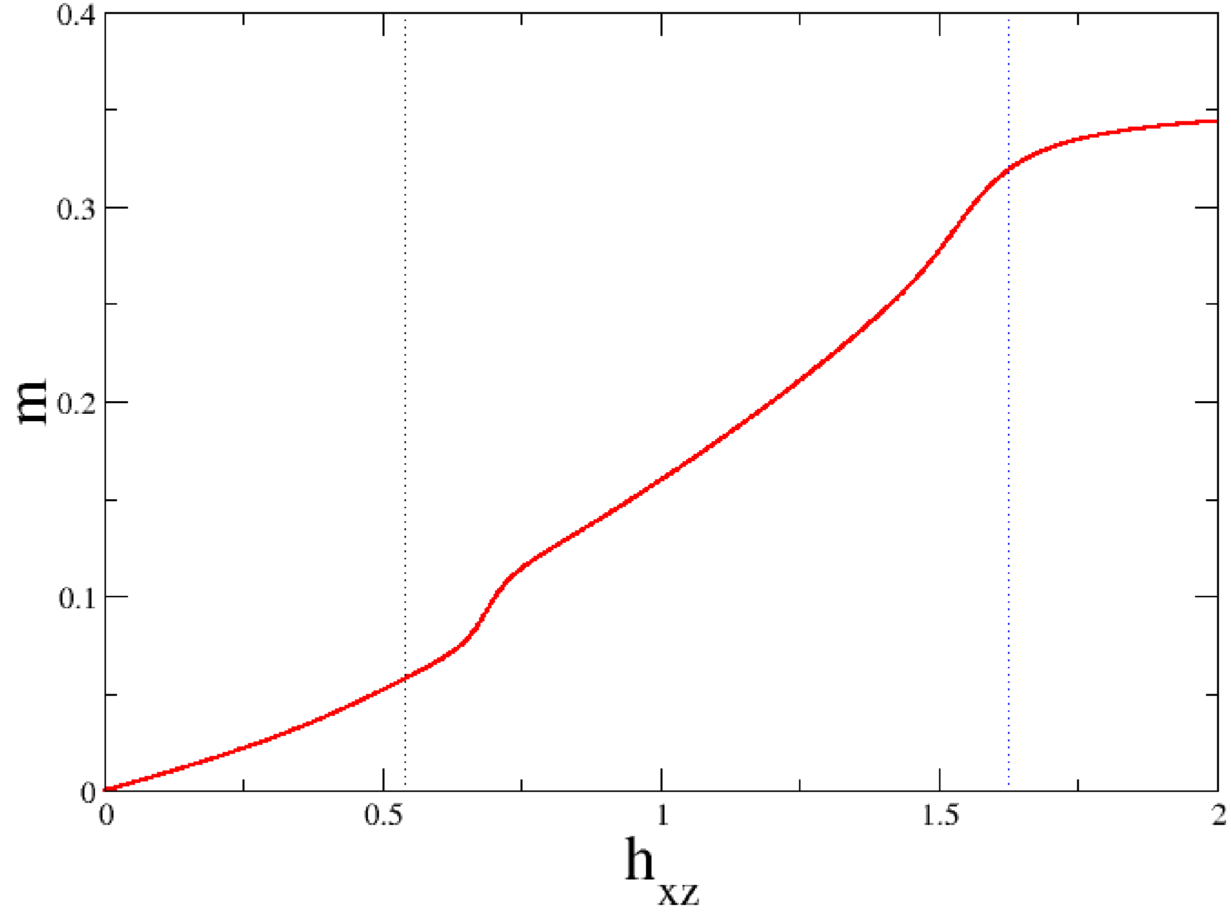
$$\chi_h^e = -\frac{\partial^2 e_0}{\partial h^2}$$



Exactly solvable point

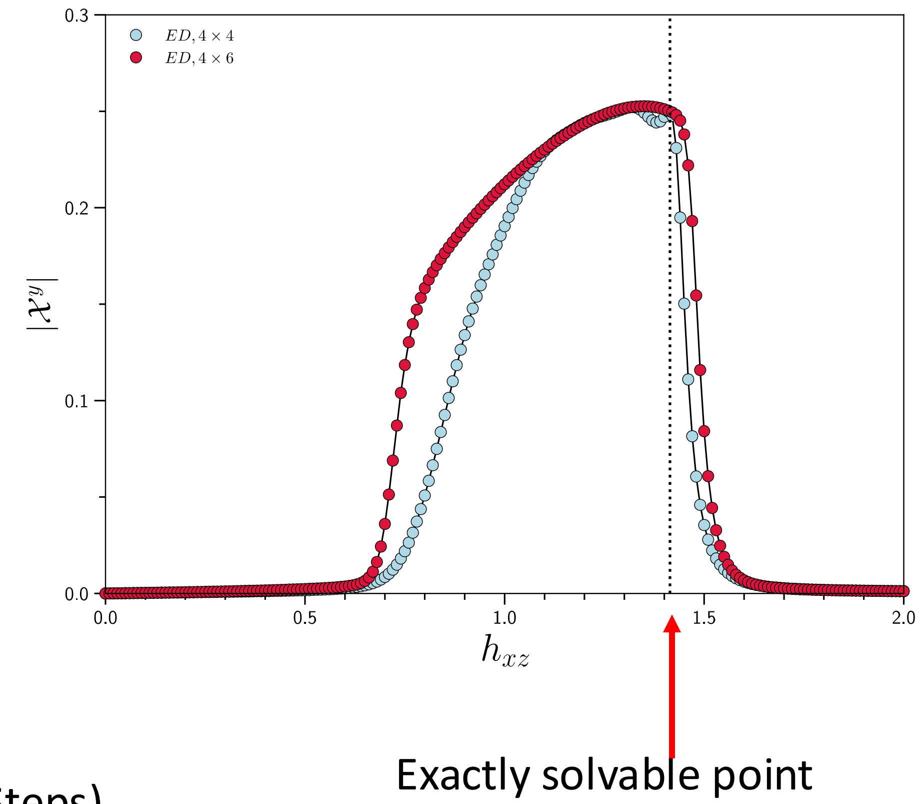
$$\chi^e \sim L^{2/\nu-(d+z)}$$

Magnetization, staggered vector chirality

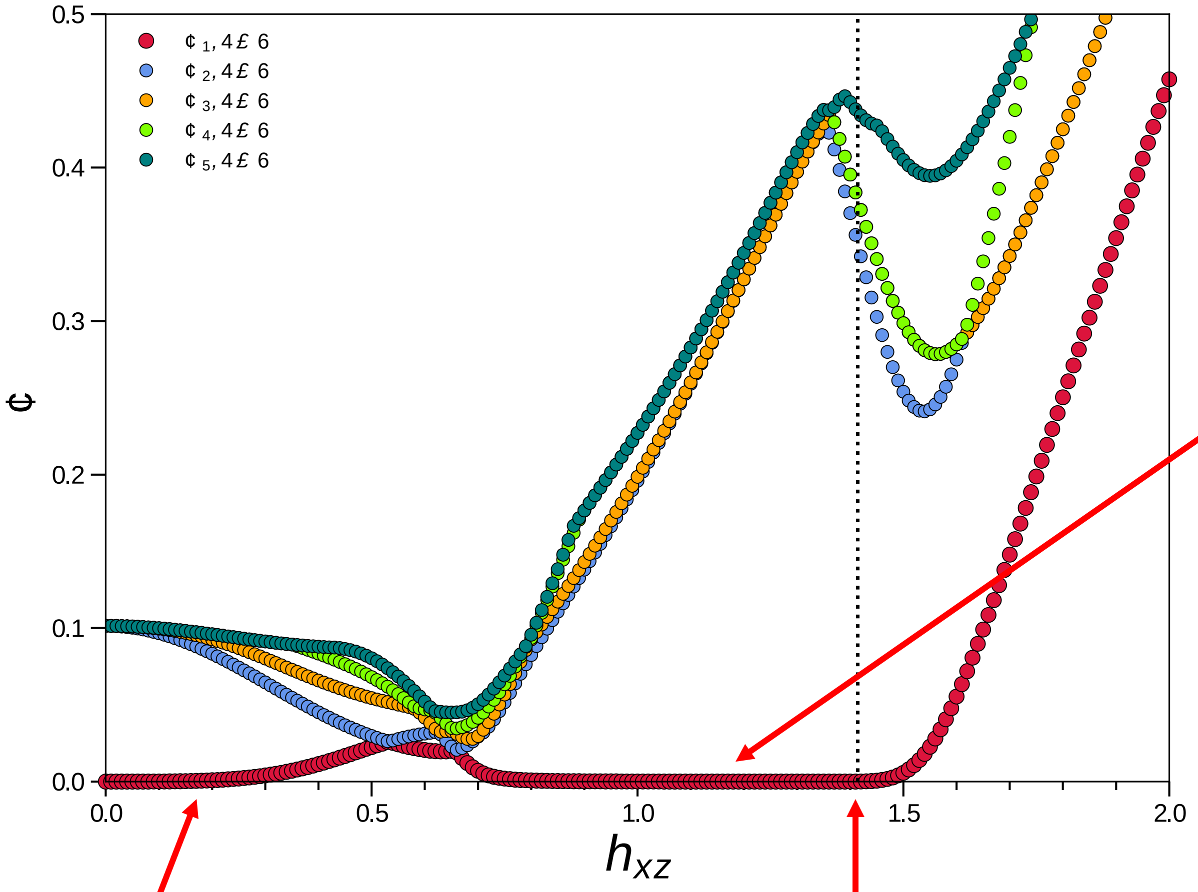


Magnetization versus in-plane field for a 4x6 periodic lattice. (no Steps)

$$\mathcal{X}_\alpha^y = \langle \vec{S}_{\mathbf{r}} \times \vec{S}_{\mathbf{r}+\mathbf{e}_\alpha} \rangle^y \quad \alpha = x, z$$



ED Energy Gaps 2D Quantum Compass models hx=hz=hxz



Two-Fold degenerate GS

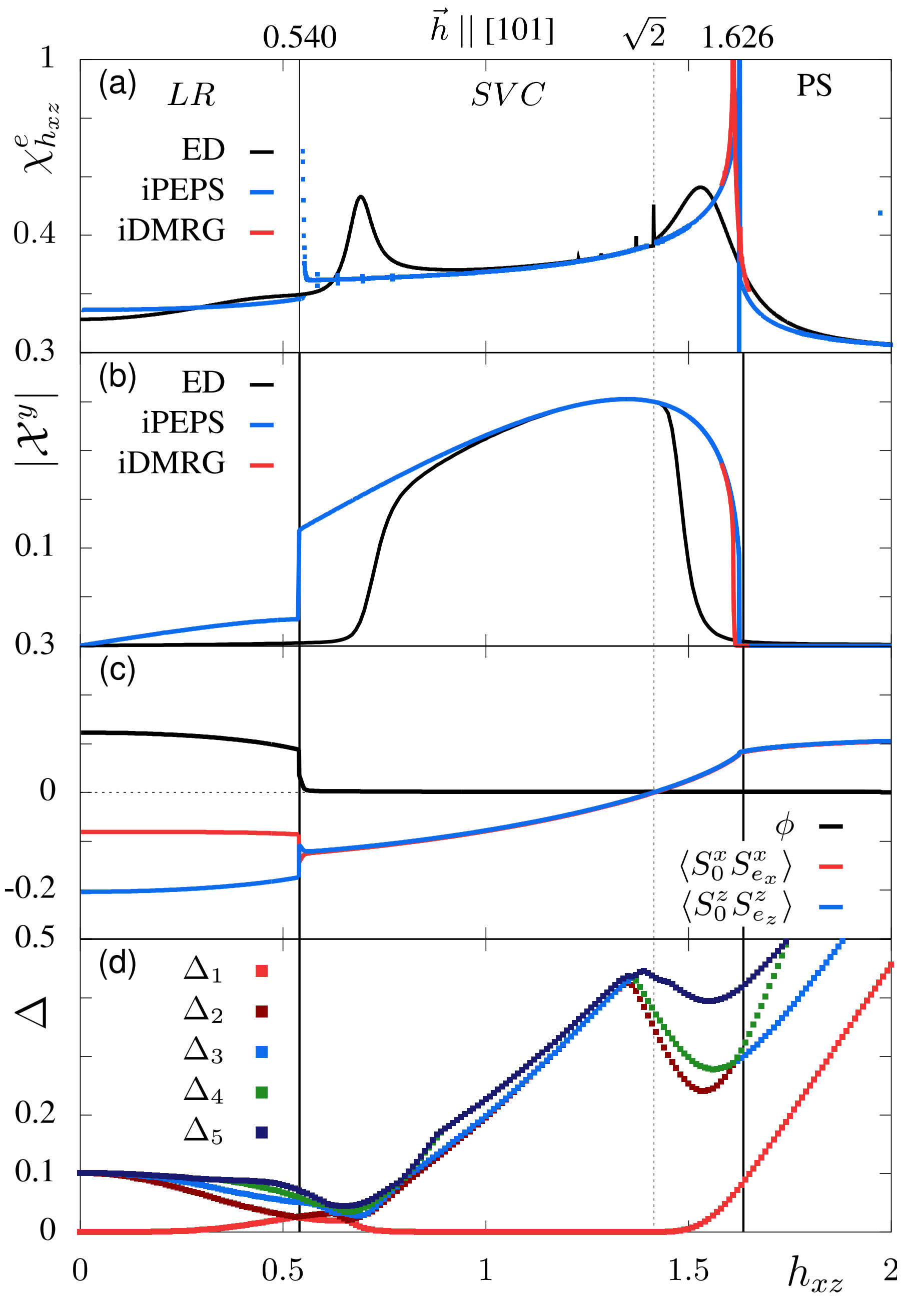
(GS not shown)

Gapless

Exactly solvable point

iPEPS Results

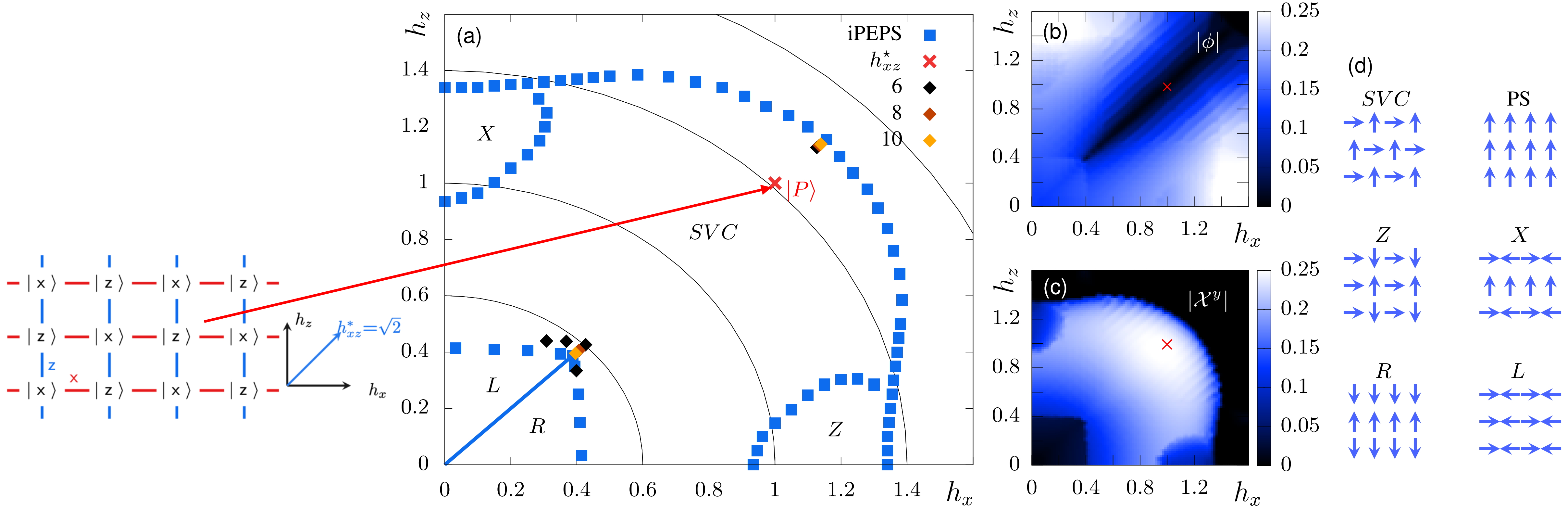
Y. Motoyama, T. Okubo, K. Yoshimi, S. Morita, T. Kato, N. Kawashima,
TeNeS: Tensor network solver for quantum lattice systems, Computer Physics Communications, **279** (2022)



Bond Correlators

2D Quantum Compass Model

$$\mathcal{H} = J\sum_{\mathbf{r}}(\hat{S}^x_{\mathbf{r}}\hat{S}^x_{\mathbf{r}+e_x} + \hat{S}^z_{\mathbf{r}}\hat{S}^z_{\mathbf{r}+e_z}) - \sum_{\mathbf{r}} \mathbf{h}\cdot\hat{\mathbf{S}}_{\mathbf{r}}.$$



Excitations: What can we learn from one Dimension = Kitaev Spin Chain

Kitaev Honeycomb Model

Anyons in an exactly solved model and beyond

Alexei Kitaev *

California Institute of Technology, Pasadena, CA 91125, USA

Received 21 October 2005; accepted 25 October 2005

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Annals of Physics 321 (2006) 2–111

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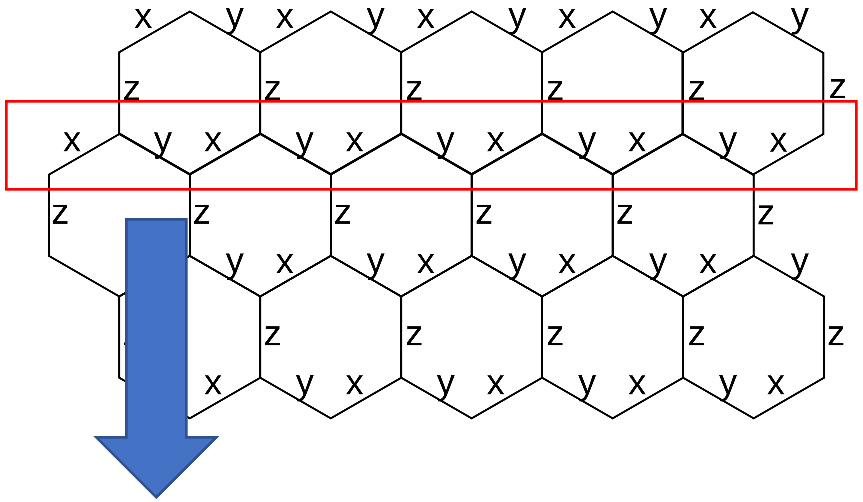


$$H = K \sum_j \left(S^x_{2j+1} S^x_{2j+2} + S^y_{2j+2} S^y_{2j+3} \right) - \sum_j \mathbf{h} \cdot \mathbf{S}_j$$

$$\mathbf{h} = h(\cos\phi_{xy} \cos\theta_z, \sin\phi_{xy} \cos\theta_z, \sin\theta_z)$$

h=0 and h=(0,0,h) solvable. No phase transitions

Phase Diagram, S=1/2

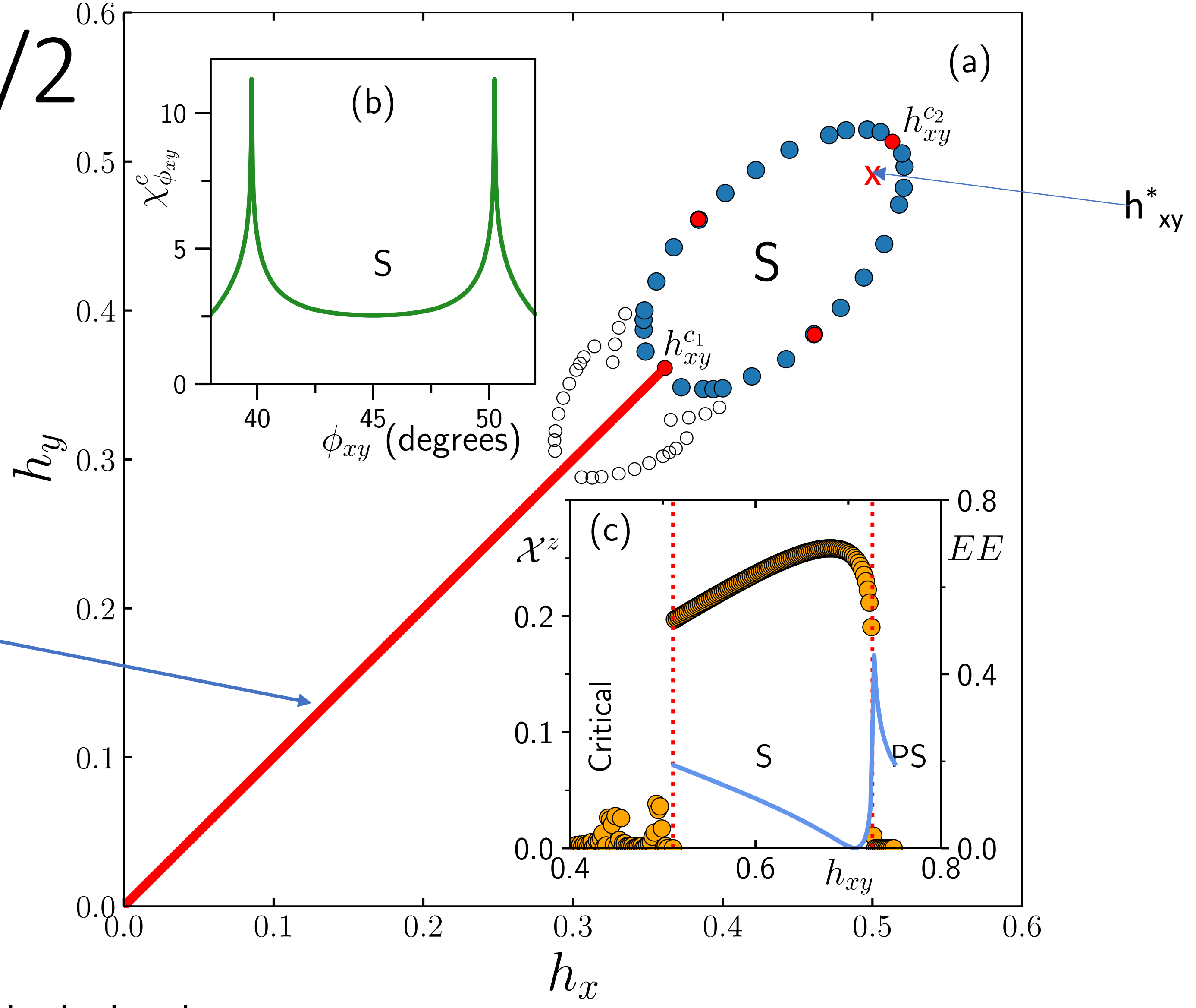
Vector Chirality

$$X^{z} = (-1)^{j} \langle (S_j \times S_{j+1})^{z} \rangle$$

Critical line

$$R^{xy} = \exp(i\pi (S^x + S^y)/\sqrt{2})$$

Non-symmomorphic symmetry (Glide-line) $R^{xy} \otimes T$

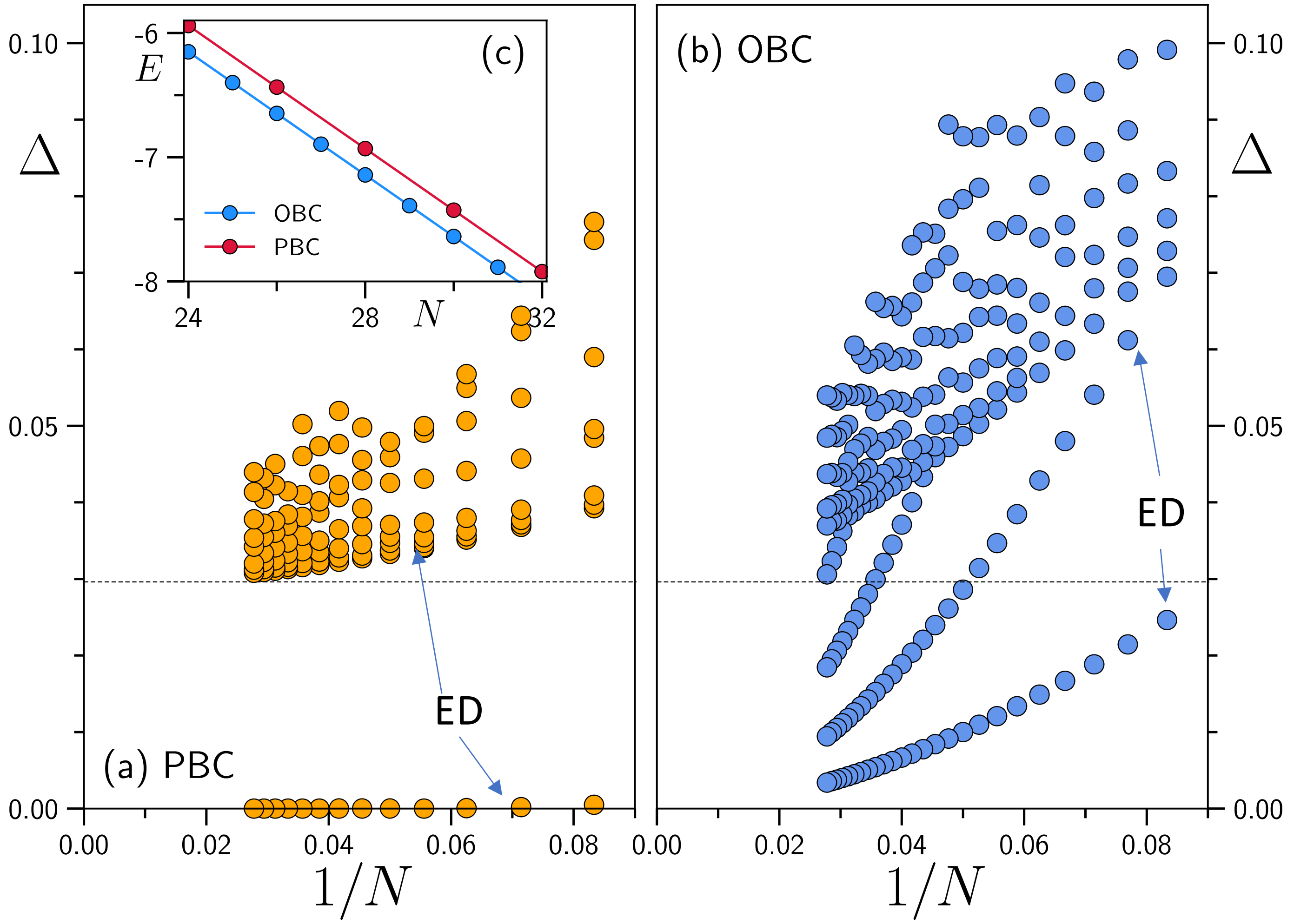


S-phase also extends out of the hx,hy plane

Unusual Spectrum from ED

- PBC is gapped
- OBC appears gapless
- OBC lowers the energy !
- h_{xy}=0.7 Inside Soliton Phase

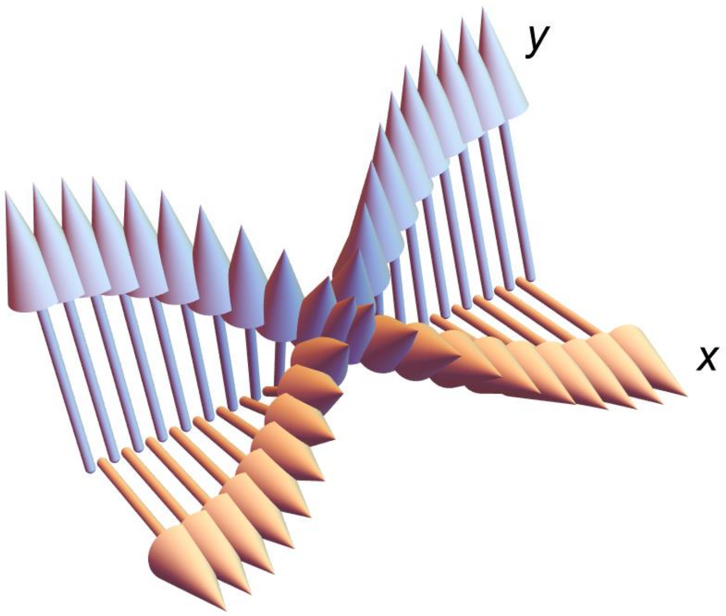
Gap for PBC is ~ 0.03 K

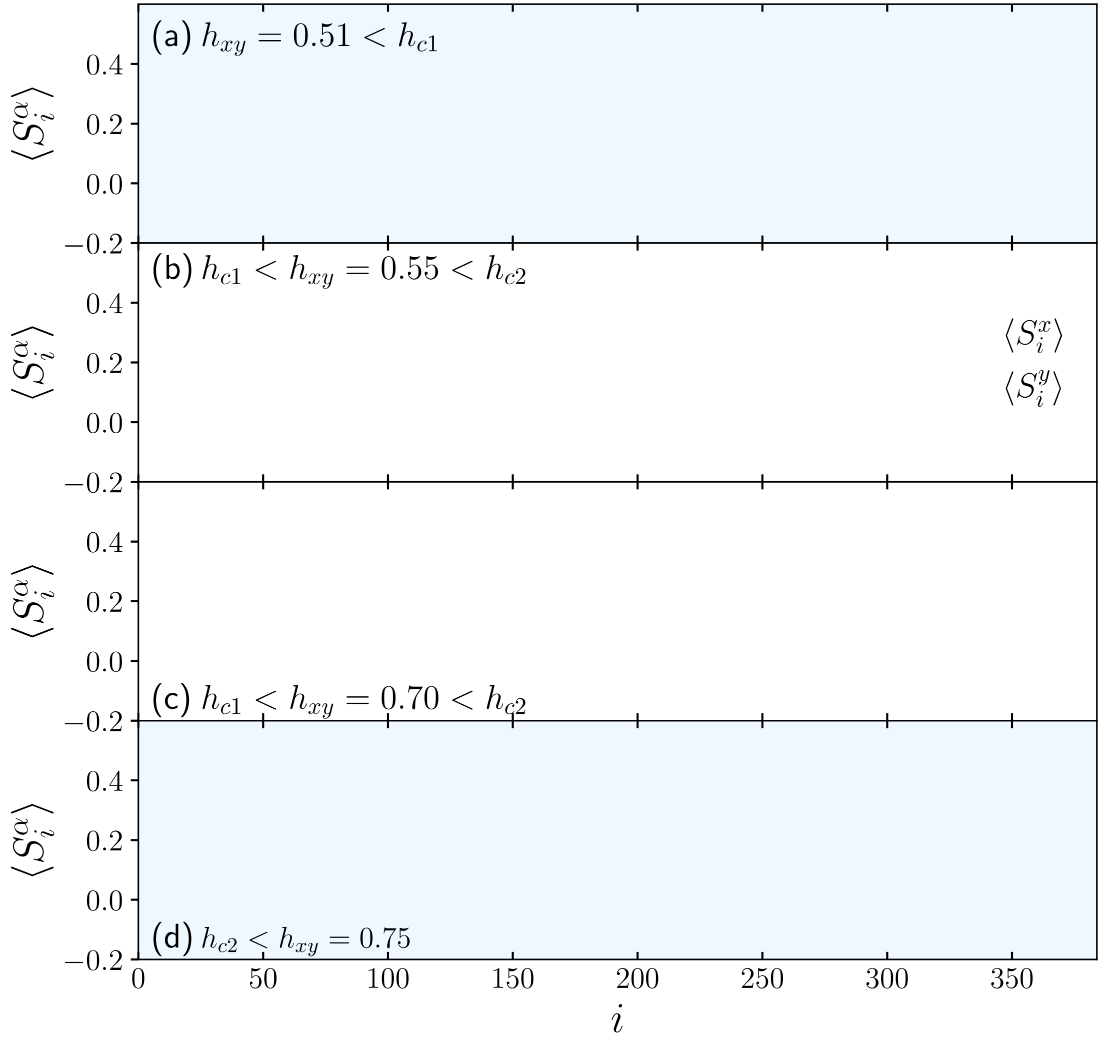


Solitons: OBC

Topological Soliton, connecting 2 degenerate ground-states

- Only every second point is shown
- DMRG Results – Almost Exact





Variational Picture

Removed YY-Bond !

$S_i^x S_{i+1}^x \quad S_{i+1}^y S_{i+2}^y$

$$|b\rangle = |YX\ldots \nearrow_i \ldots XY\rangle$$ Soliton

Asymmetry

Lowers Energy

$$|\psi_b(i)\rangle = |y - x - y - \nearrow_i - x - y - x - y - x - y\rangle,$$

$$|\psi_b(i)\rangle = |y - x - y - x - \nearrow_i - y - x - y - x - y\rangle,$$

At h* all bond operators are 0

Zeeman term on site I lowers energy

$$\langle X|S^y S^y|\nearrow\rangle = 0$$

$$\langle Y|S^x S^x|\nearrow\rangle = 0$$

$$|B\rangle = |XY\ldots \nearrow_i \ldots YX\rangle$$ Anti-Soliton

Raises Energy more

$$|\psi_B(i)\rangle = |x - y - x - \nearrow_i - y - x - y - x - y - x\rangle,$$

$$|\psi_B(i)\rangle = |x - y - x - y - \nearrow_i - x - y - x - y - x\rangle,$$

bond operators [i-1,i] and [I,i+1]

Very costly, Zeeman term on site I cannot compensate

Remember all bond interactions are AF

Variational Subspace OBC

Watch Out !

$$|\Psi_b\rangle = \sum_{k=1}^{N} a_k |b(k)\rangle, \qquad |\Psi_B\rangle = \sum_{l=2}^{N-1} g_l |B(l)\rangle$$

J1-J2 chain: Shastry, Sutherland, Phys. Rev. Lett. **47**, 964 (1981)

Basis states are non-orthogonal: Generalized eigenvalue problem

$$H_{kl} = h\ \ _b(k)|H|\ \ _b(l)i \quad \text{and} \quad M_{kl} = h\ \ _b(k)|\ \ _b(l)i,$$

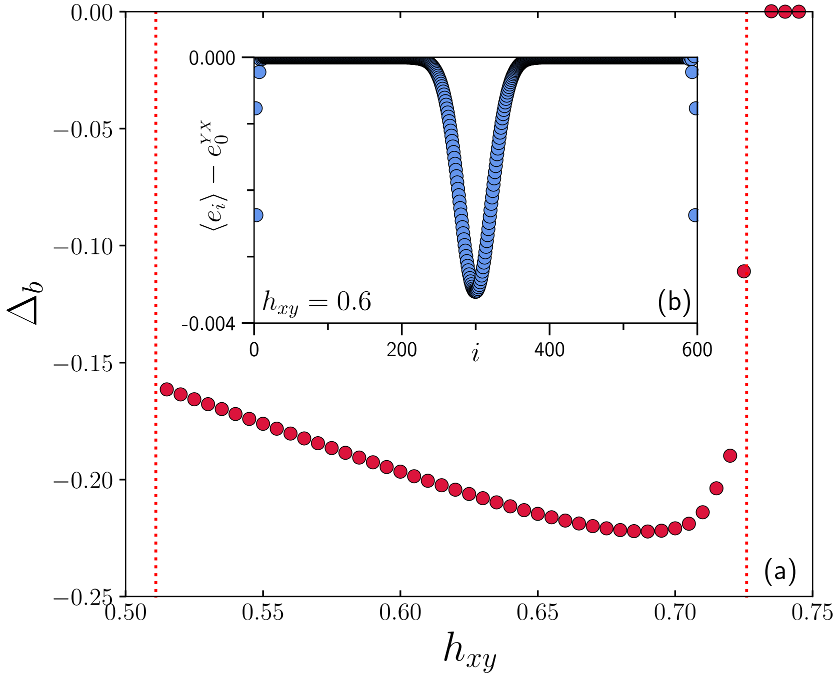
Dense Matrices

The Soliton Masses: From Variational and DMRG Calculations.

$$\Delta_b = \sum_i \left(\langle e_i \rangle - e_0^{\text{bulk}}\right)$$

$$\Delta_b < 0 \quad \Delta_B > 0$$

$$\Delta_b + \Delta_B > 0$$



Spin Gap for PBC

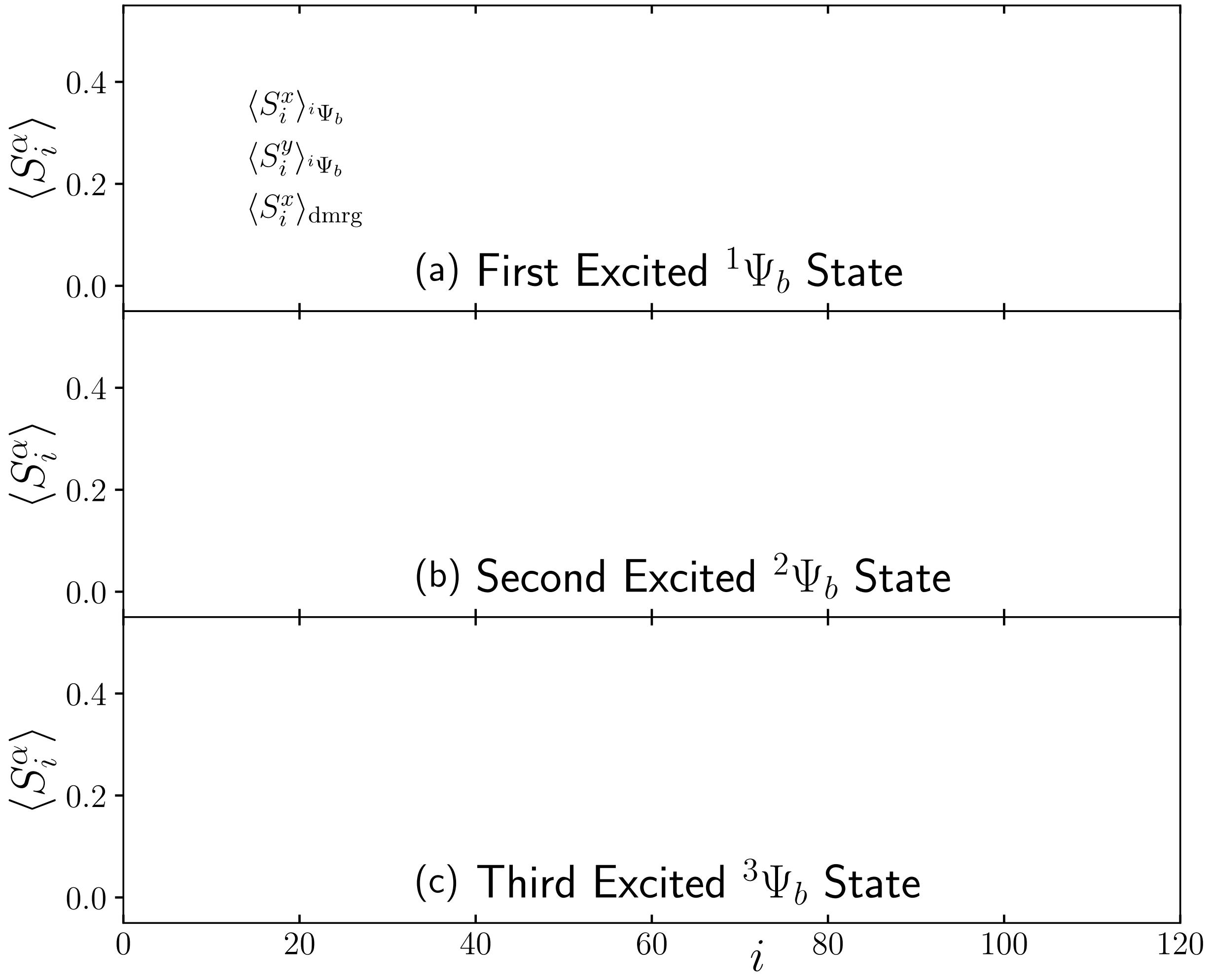
h_{xy}=0.7 $\Delta_b = -0.2044K$ $\Delta_B = 0.2455K$ Compared to DMRG $\Delta_{PBC} = 0.02962K$

$$\Delta_{PBC}^{Var} \sim 0.04K$$

Excited States OBC

h_{xy}=0.7 Inside Soliton Phase

Low Energy Excitations for OBC



Two Soliton bB states for PBC

$$| \;_{bB}(i, j)i = |y^0 - \%_i - x^0 - y^0 - x^0 - y^0 - \%_j - x^0 - y^0 - x^0 i$$

J1-J2 chain: Shastry, Sutherland, Phys. Rev. Lett. **47**, 964 (1981)

$$| \;_{bB}\, i = \sum_{i \neq j} a_{i,j} | \;_{bB}(i, j)i$$

Variational Results : Gap with PBC

Unusual Spectrum from ED

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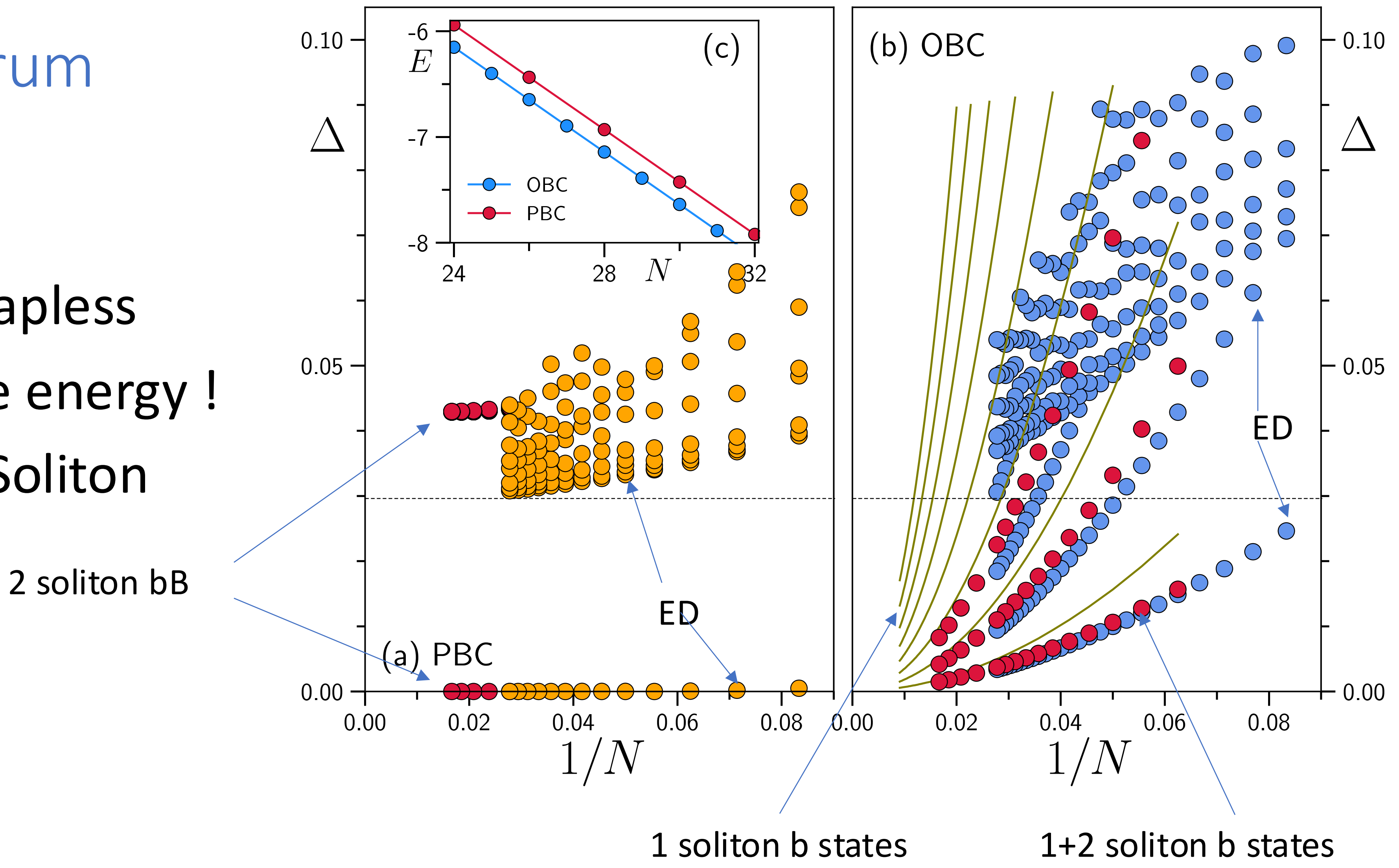

- Exact Ground-States in a field
- Surrounding Gapped Phase
- Single Soliton ground-states in 1D with OBC

- Thanks !

Open Questions:

- Experimental Realization Ba_2IrO_4 ?
- Rigourous proof of Gap ?
- Excitations (Generalization of Solitons ?)

- ADS. Richards, ESS, arXiv:2310.01384
- ESS, J. Ridell, H.-Y. Kee, Phys. Rev. Research 5, 013210 (2023)
- ESS, J. Gordon, J. Ridell, T. Yang, H.-Y. Kee, Phys. Rev. Research 5, L012027 (2023)
- ESS, A Catuneanu, JS Gordon, HY Kee Physical Review X 11 (1), 011013 (2021)