

# Energy Spectroscopy of Quantum Critical Systems

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Support: **FWF**



Foundations and Applications of Quantum Science



# Outline of this talk

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- Introduction: Quantum Many Body Systems / Spectroscopy
- Torus Energy Spectra and Quantum Critical Points ?
- Spectrum of the standard 2+1D Ising transition
- Topological Phase Transitions
- Gross-Neveu-Yukawa fixed points
- Outlook

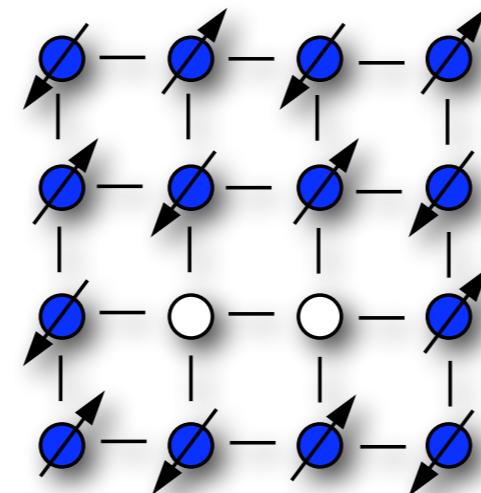
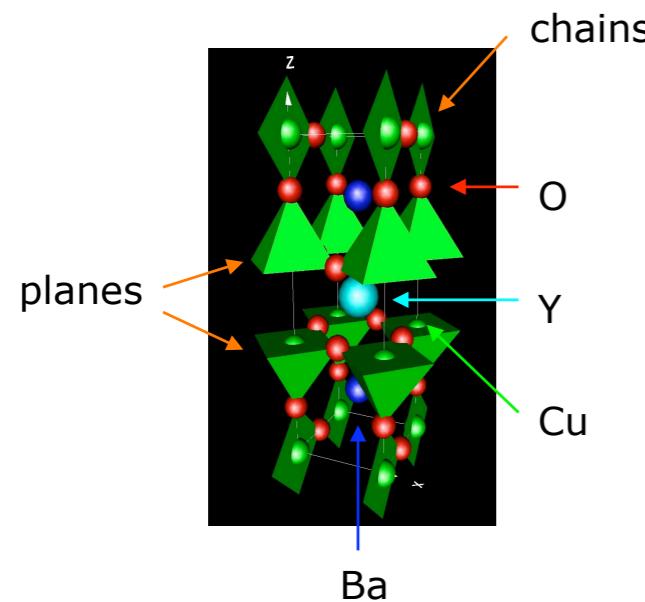
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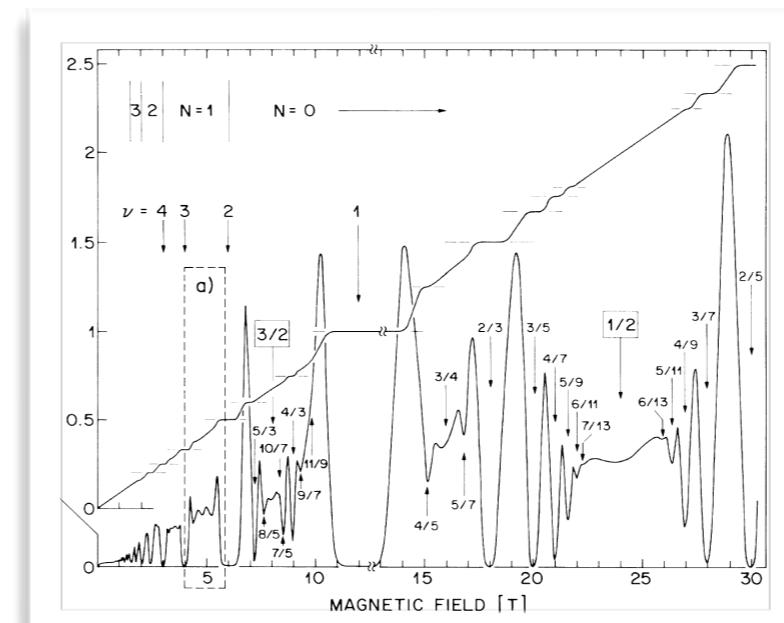
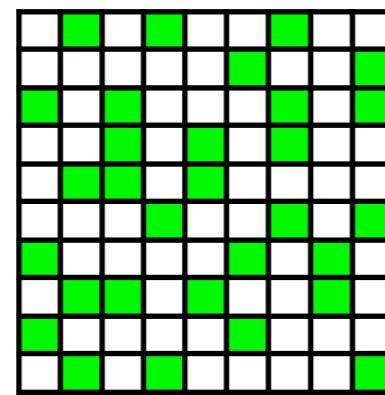
# Quantum Matter: Strongly correlated electrons in solids

- High T<sub>c</sub> superconductors & Quantum Magnets

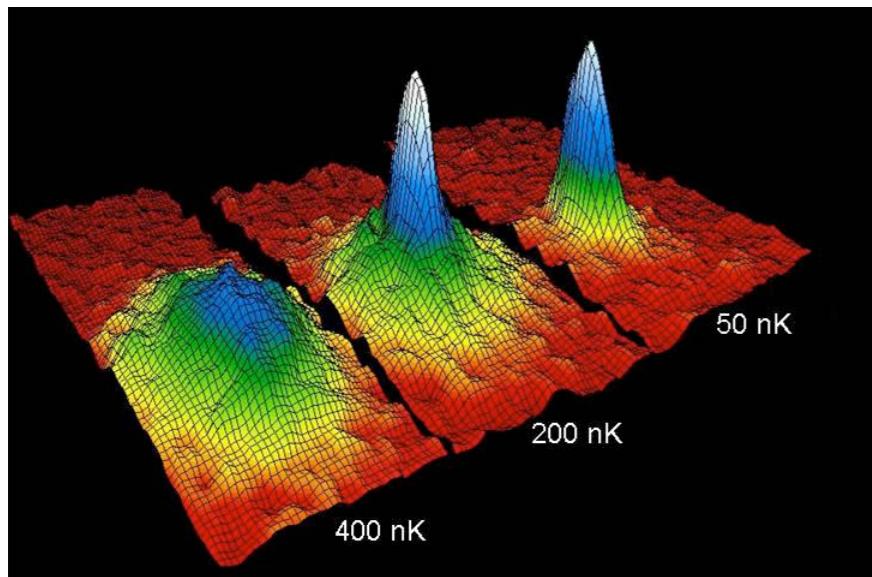


- Fractional Quantum Hall Effect

$$\nu = 1/3$$

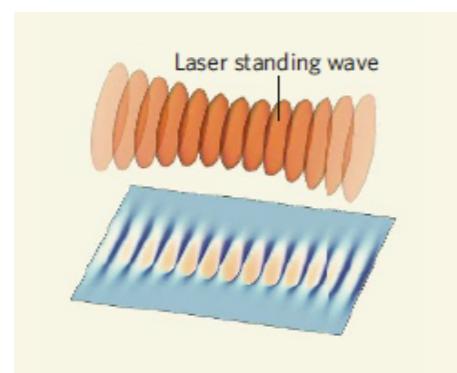


# Quantum Matter: Ultracold atomic gases



From weakly interacting Bose gases

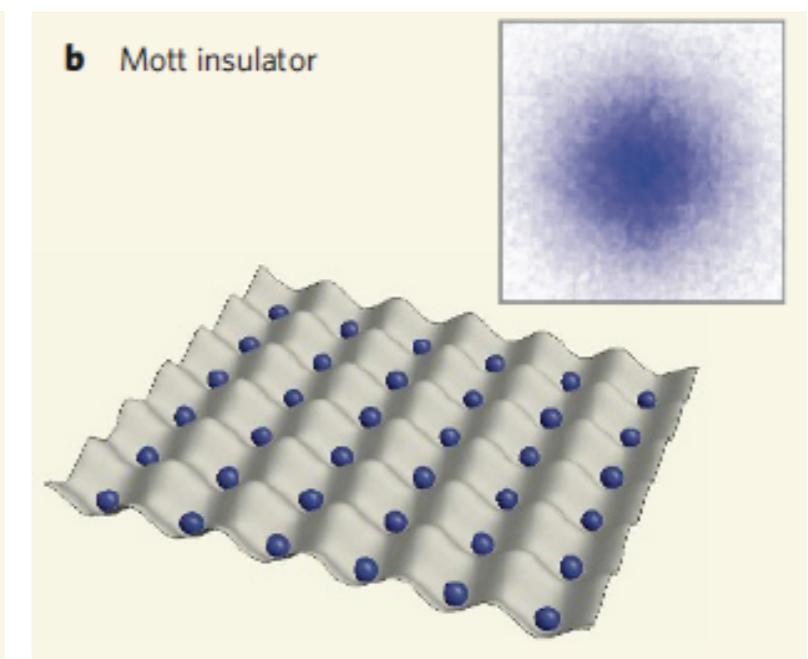
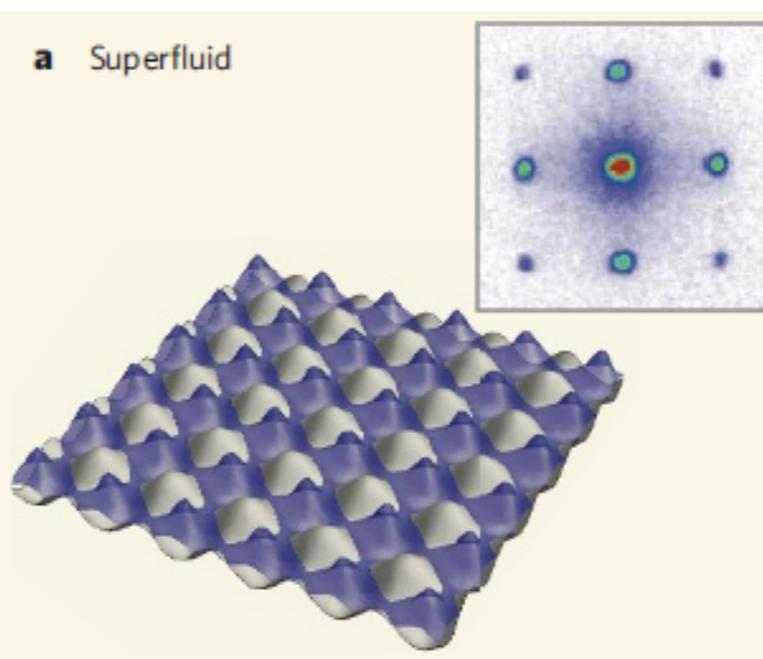
to strongly interacting gases in optical lattices



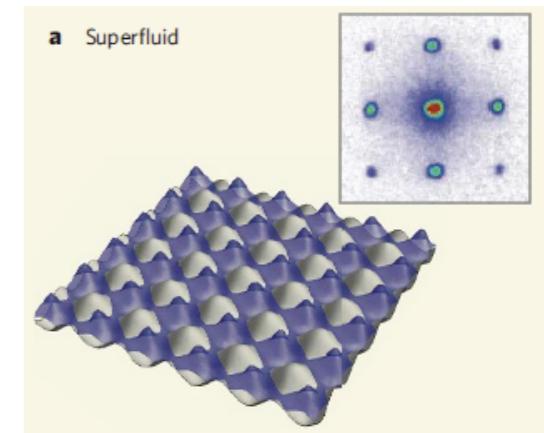
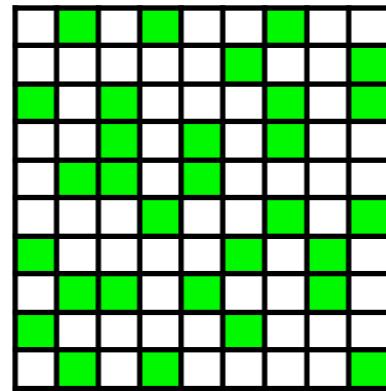
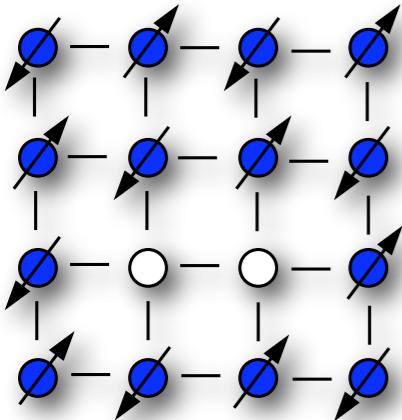
$$H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c.) + \frac{U}{2} \sum_i n_i(n_i - 1)$$

D. Jaksch et al., PRL (1998)

M. Greiner et al., Nature (2002)



# Quantum Matter

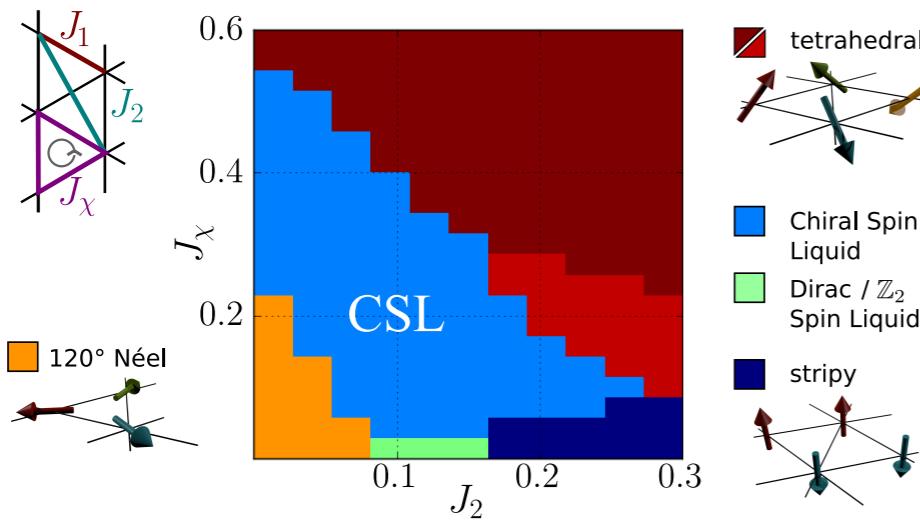


- We would like to understand phase diagrams of complex systems, but whose Hamiltonians are often reasonably well known.
- Quantum phase transitions occur. What is their universality class & field theoretical description ?
- New tools welcome to diagnose/characterize QFTs at phase transitions

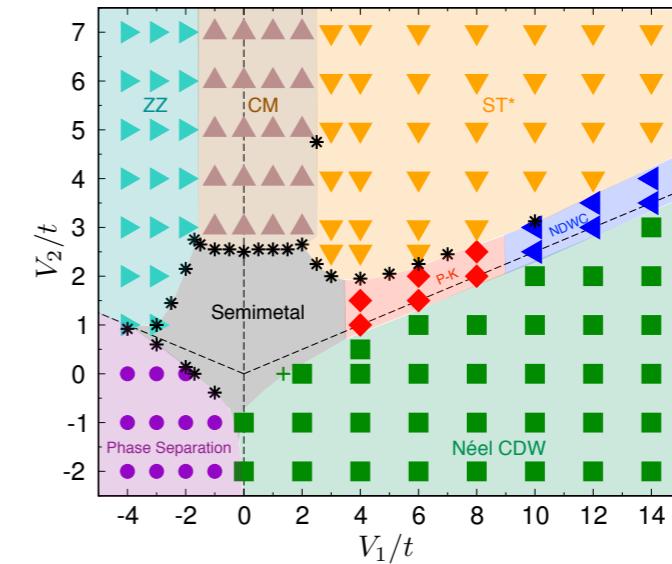


# Example of Microscopic Condensed Matter Models

- From microscopic models:



Phys. Rev. B **95**, 035141 (2017)



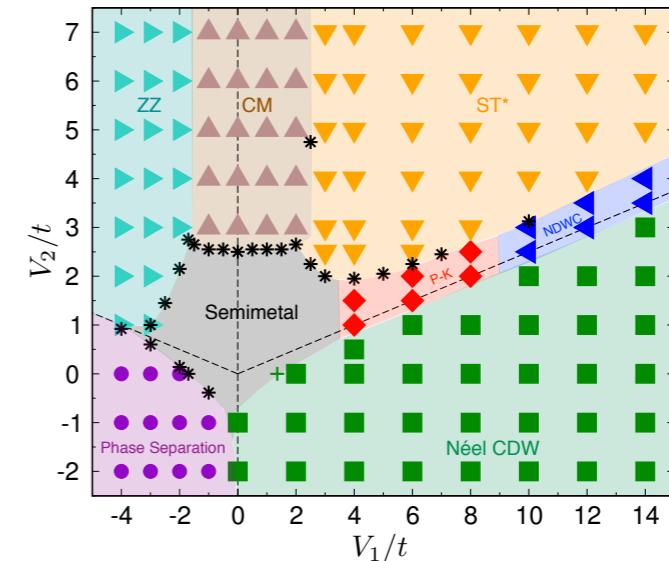
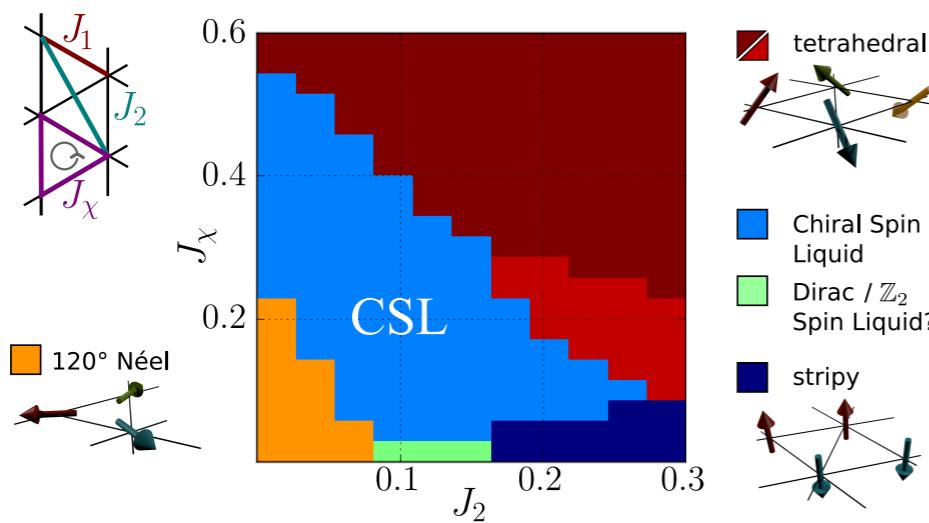
Phys. Rev. B **92**, 085146 (2015)

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j + J_\chi \sum_{i,j,k \in \Delta} \vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k)$$

$$\begin{aligned} \mathcal{H} = & -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + h.c.) \\ & + V_1 \sum_{\langle ij \rangle} (n_i - 1/2)(n_j - 1/2) \\ & + V_2 \sum_{\langle\langle ij \rangle\rangle} (n_i - 1/2)(n_j - 1/2) \end{aligned}$$

- To quantum phase transitions: Wilson Fisher CFTs, QED<sub>3</sub>, Gross Neveu, ...

# Quantum Matter

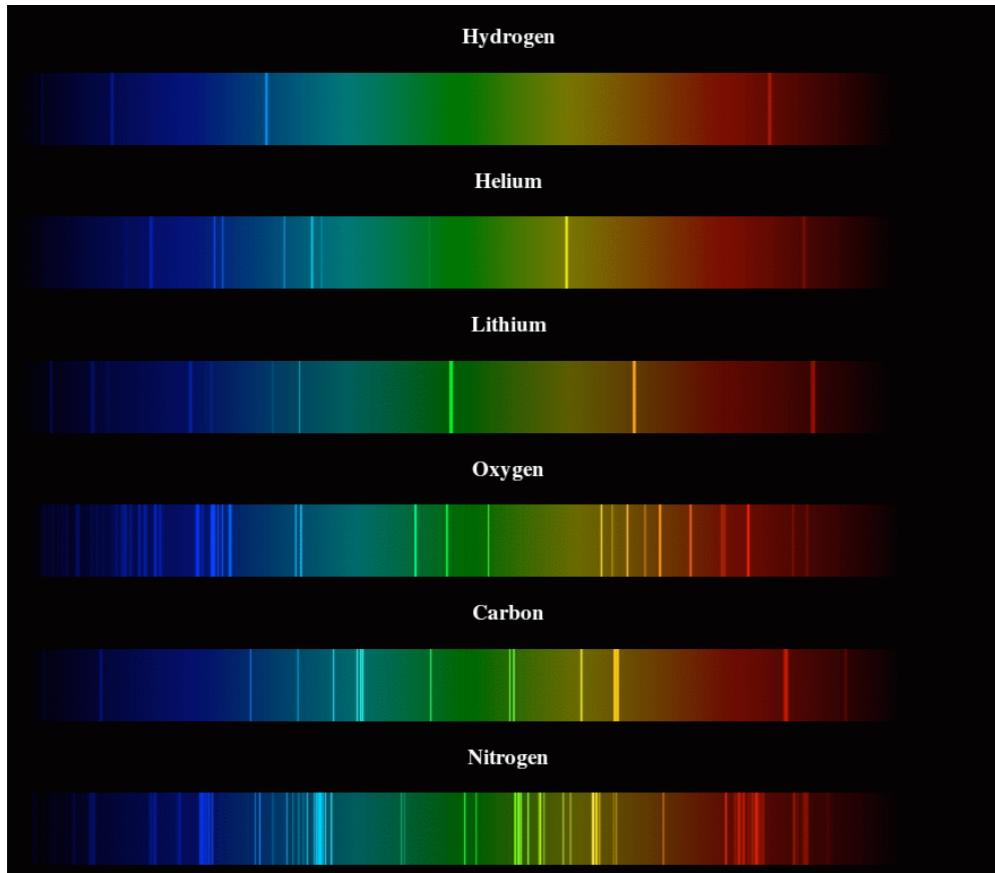


- Standard Approach: Simulate system on a computer, calculate correlation functions, order parameter, and determine critical exponents. Can work very well, but does not have to...
- Here want to investigate whether the **Energy Spectrum** of a quantum many body system at criticality reveals its universality class (Spectroscopy) ?

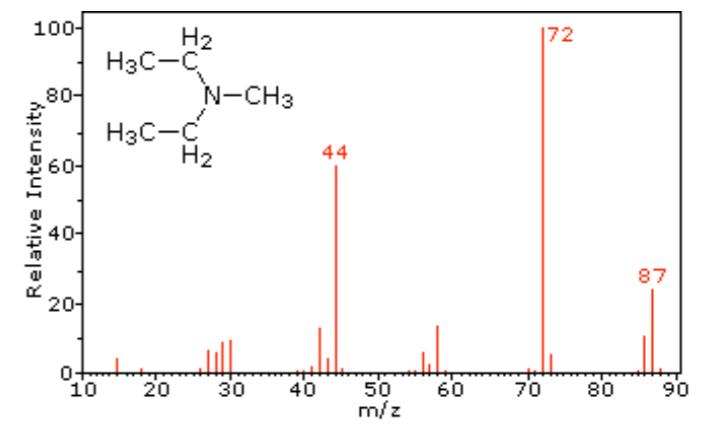
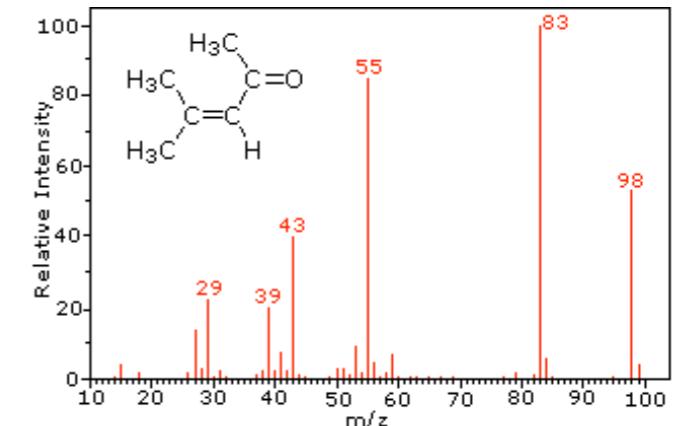


# Spectroscopy in other areas:

- For example in optics and mass spectroscopy one measures spectra, and then compares with a catalogue of known spectra to infer the nature of an “unknown” substance.



<http://www.astro.rug.nl>



<https://www2.chemistry.msu.edu>

- Can we do the same with Quantum Field Theories at Quantum Critical Points ?

# “Can one hear the shape of a drum” ?

- Can one infer the shape of a domain from the spectrum of the Laplacian ?  
(not unambiguously, there are non-congruent shapes with the same spectrum)

## CAN ONE HEAR THE SHAPE OF A DRUM?

MARK KAC, The Rockefeller University, New York

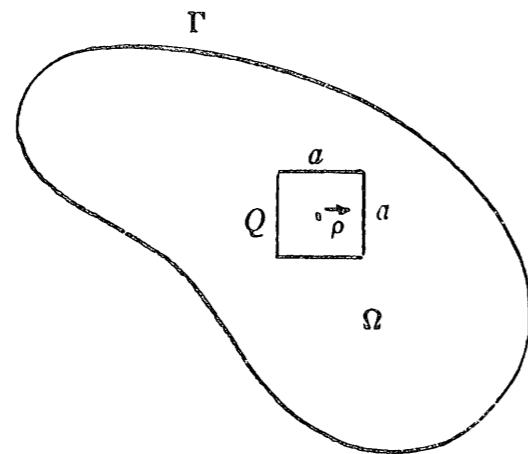
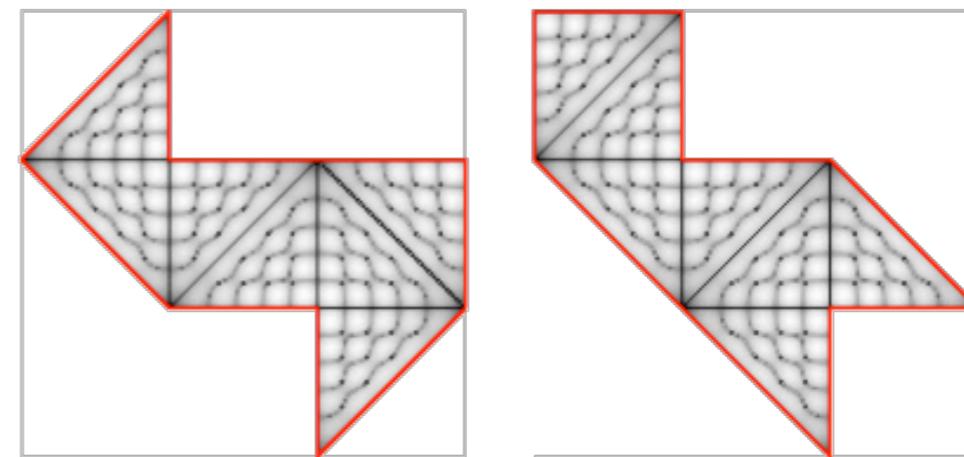


FIG. 1

[Amer. Math. Monthly 73, 1-23, 1966.](#)



<http://mathworld.wolfram.com/IsospectralManifolds.html>

- We would ask a related, but somewhat different question:  
Given a shape, can we “hear” the nature of the (massless) field theory  
confined to this shape ?

# Exact Diagonalization: Main Idea

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- Solve the Schrödinger equation of a quantum many body system numerically

$$\mathcal{H}|\psi\rangle = E|\psi\rangle$$

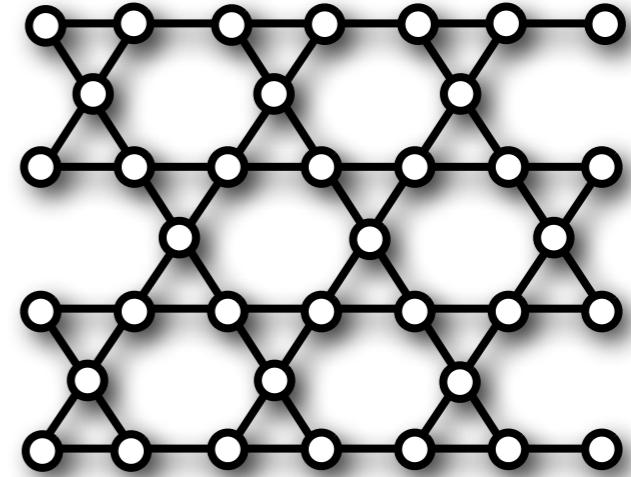
- Sparse matrix, but for quantum many body systems the vector space dimension grows exponentially!
- But the amount of information one is able to extract is worth the effort:

Powerful Quantum Mechanics Toolbox

# Hilbert space sizes

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- The Hilbert space of a quantum many body system grows exponentially in general
- For  $N$  spin 1/2 particles, the complete Hilbert space has  $\text{dim} = 2^N$  states
  - 10 spins  $\text{dim} = 1'024$
  - 20 spins  $\text{dim} = 1'048'576$
  - 30 spins  $\text{dim} = 1'073'741'824$
  - 40 spins  $\text{dim} = 1'099'511'627'776$
  - 50 spins  $\text{dim} = 1'125'899'906'842'624 \dots$
- The quantum mechanical wave function is a vector in this Hilbert (vector) space and we would like to know the ground state and a few other low lying eigenstates
- Current limit for  $S=1/2$  spin models on regular lattice, **50 spins** ! (MPI + Supercomputer)  
actual dimension  $\sim 3 \times 10^{11}$ .



○  $|\uparrow\rangle$  or  $|\downarrow\rangle$

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# Operator spectrum in conformal field theories

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- A local operator has a scaling dimension:

$$\mathcal{O}_i \rightarrow \Delta_i = \text{scaling dimension}$$

- The scaling dimension determines the decay of the 2-point correlation function:

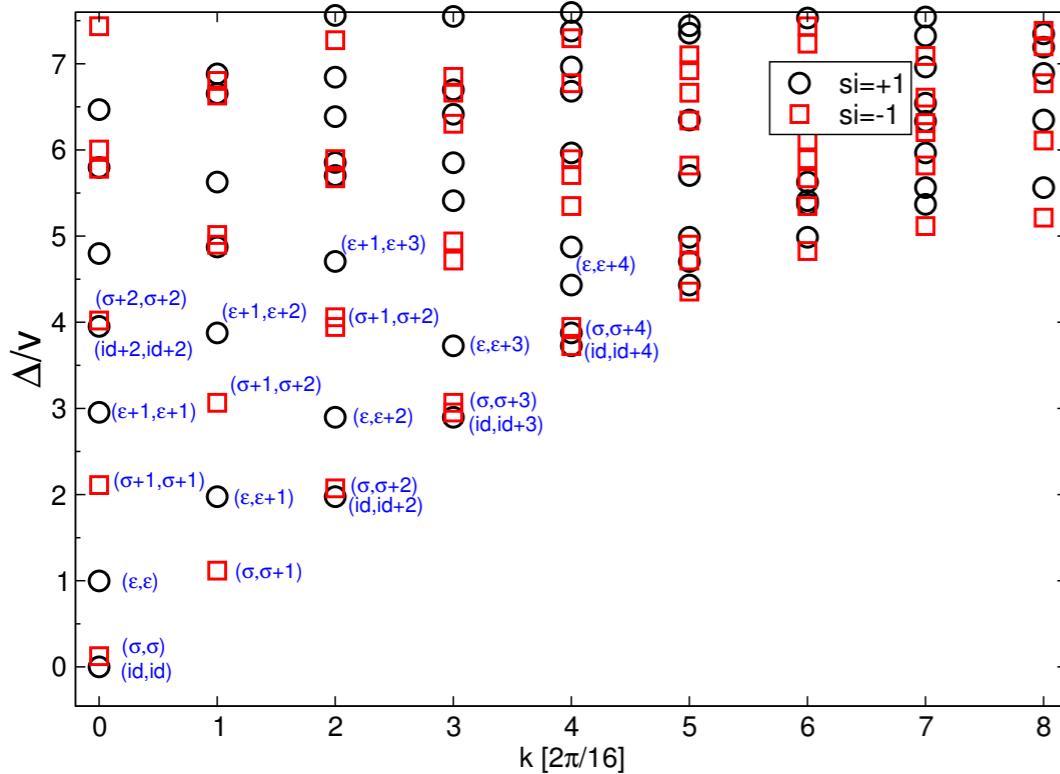
$$\langle \mathcal{O}_i(x) \mathcal{O}_i(0) \rangle = \frac{c}{|x|^{2\Delta_i}}$$

- It seems interesting and important to know the various fields with their corresponding scaling dimensions.

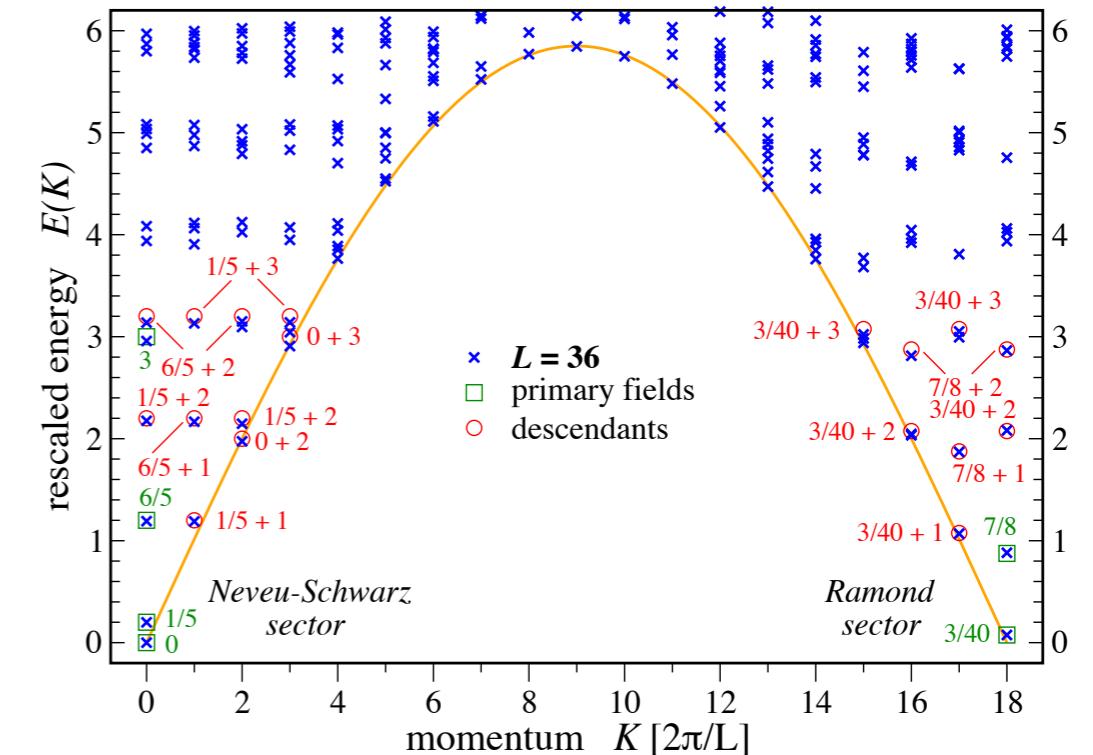
- Where can we find those in numerics ?

# 1D Torus (Circle) Energy Spectra

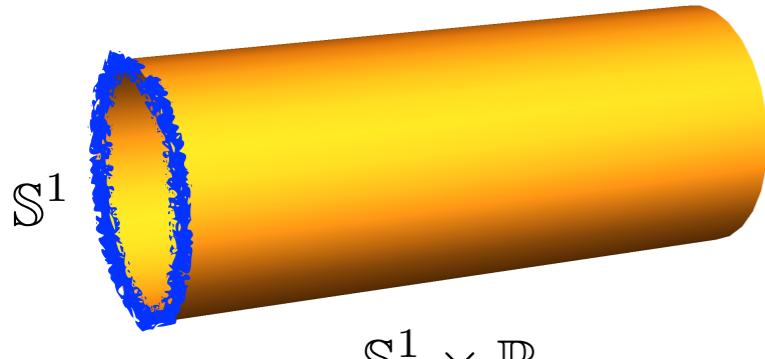
- For CFTs energy spectra of finite size (1+1D) systems arrange into conformal towers !



TFI chain  $L=16$   
2D Ising CFT Spectrum



A. Feiguin et al. PRL 2007  
tricritical Ising CFT Spectrum in anyon chains



$$\mathbb{R}^2 \leftrightarrow S^1 \times \mathbb{R}$$

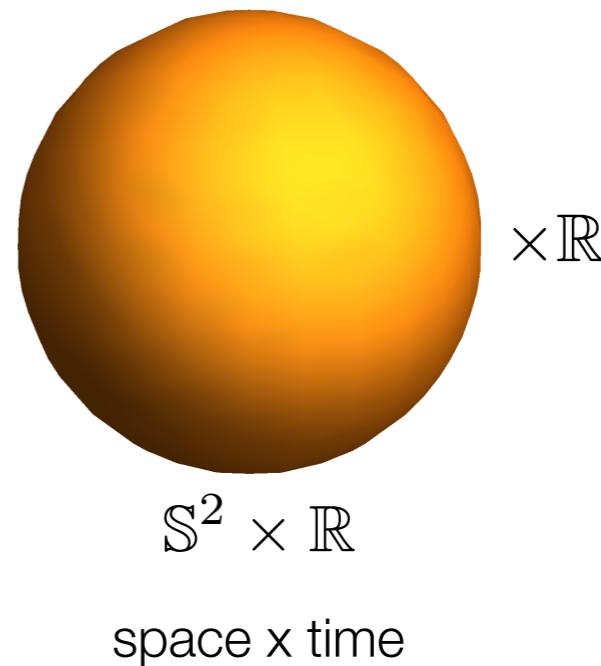
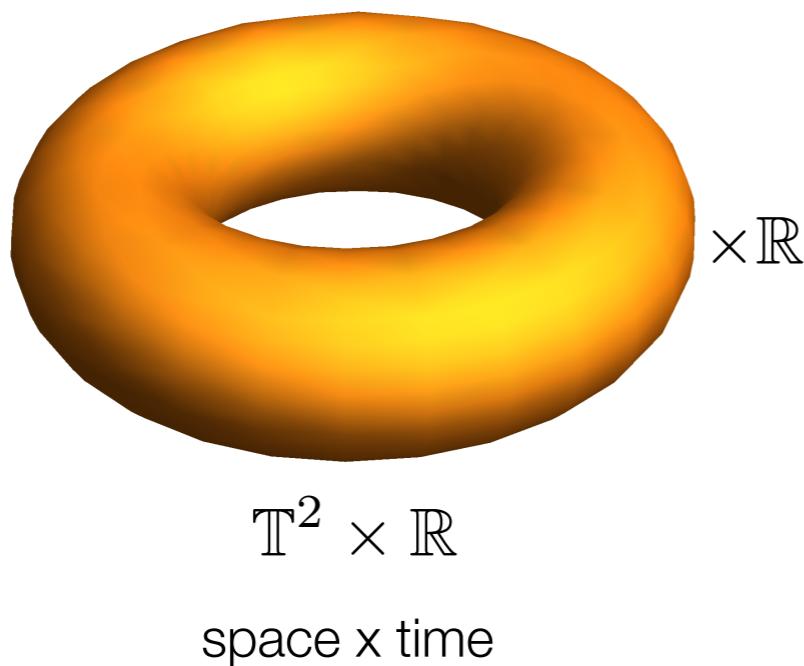
- Spectrum of scaling dimensions of CFT maps to Hamiltonian spectrum on a circle.

# Energy spectra and CFTs in more than 1+1D ?

- In more than 1+1D, this relation does not hold for tori anymore, only for the sphere !

$$\mathbb{R}^d \leftrightarrow S^{d-1} \times \mathbb{R} \quad (\neq \mathbb{T}^{d-1} \times \mathbb{R}, \ d > 2)$$

- First mapping: radial quantisation, can reveal scaling dimensions in higher d, but not easily accessible to numerics (although several efforts over the decades).



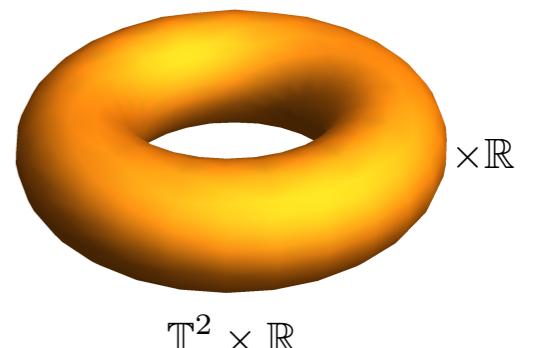
# Energy spectra and CFT in more than 1+1D ?

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- In more than 1+1D, this is not expected to hold anymore for tori !

$$\mathbb{R}^d \leftrightarrow S^{d-1} \times \mathbb{R} \quad (\neq \mathbb{T}^{d-1} \times \mathbb{R}, \ d > 2)$$

- First mapping: radial quantization, can reveal scaling dimension in higher d, but not easily accessible to numerics (although several efforts over the decades).
- What about energy spectra on tori, which are numerically accessible?
- Is there a universal low-energy spectrum (and is it accessible numerically) ?
- How does it look like ?
- Any analogy to the spectrum of scaling dimensions ?



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  - M. Schuler, S. Whittsitt, L.-P. Henry, S. Sachdev & AML  
Phys. Rev. Lett. 2016
- Topological Phase Transitions
  - S. Whittsitt, M. Schuler, L.-P. Henry, AML & S. Sachdev  
Phys. Rev. B. 2017
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## 2+1D “standard” Ising CFT

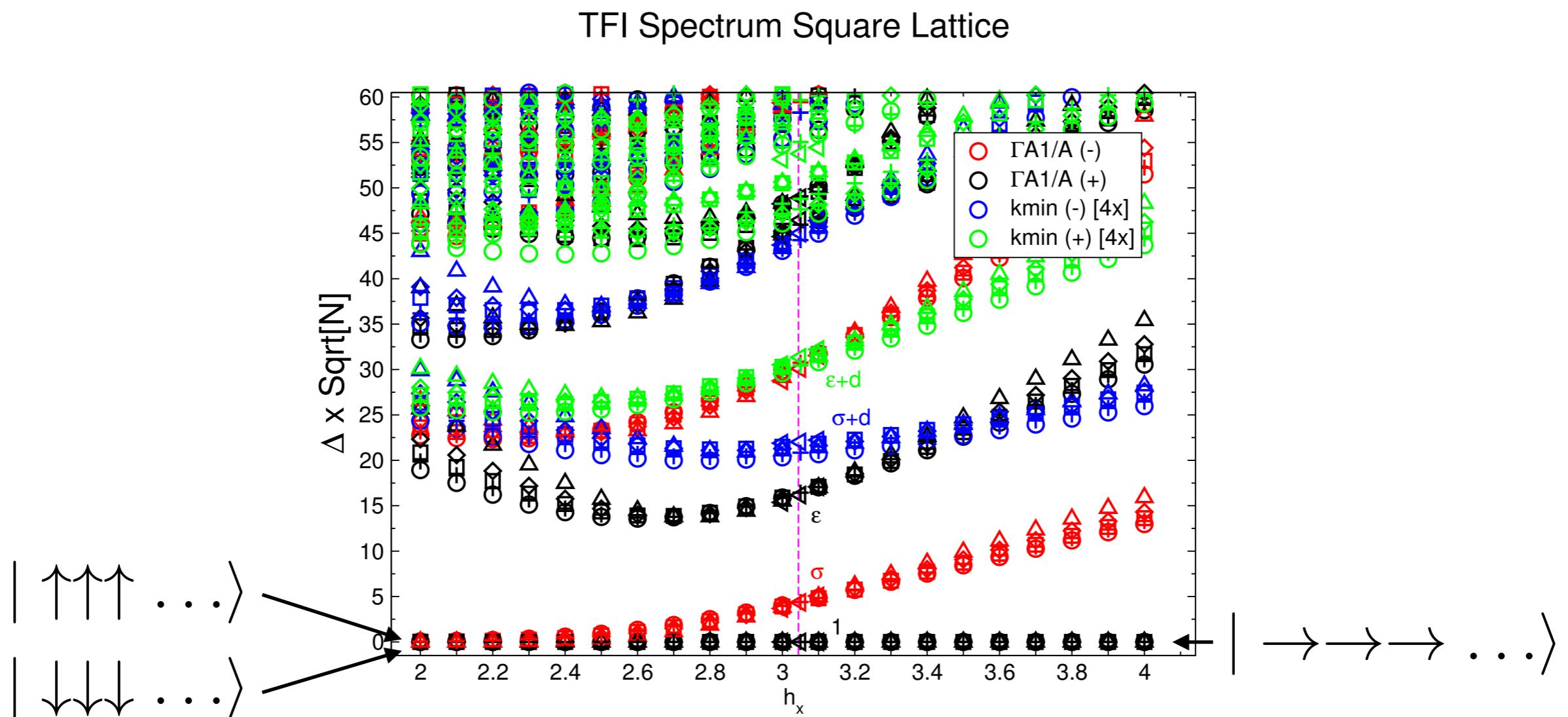
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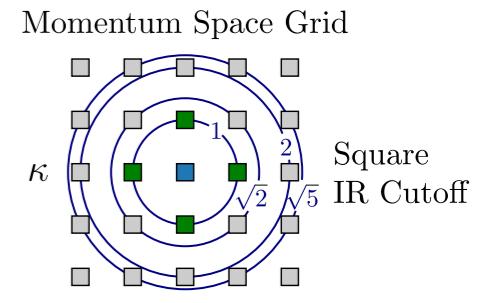
- We want to investigate the torus energy spectrum at a quantum critical point.
- While we do not expect to find the exact spectrum of scaling dimensions, the spectrum is still expected to be universal, i.e. UV cutoff independent.
- The spectrum could however depend on the IR-cutoff (shape of torus)  
(c.f. “hearing the shape of the drum”)
- We start with a  $Z_2$  symmetry breaking transition, and consider the transverse field Ising (TFI) model as a particular microscopic realization

$$H_{\text{TFI}} = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$

# “Raw” energy spectrum across the transition

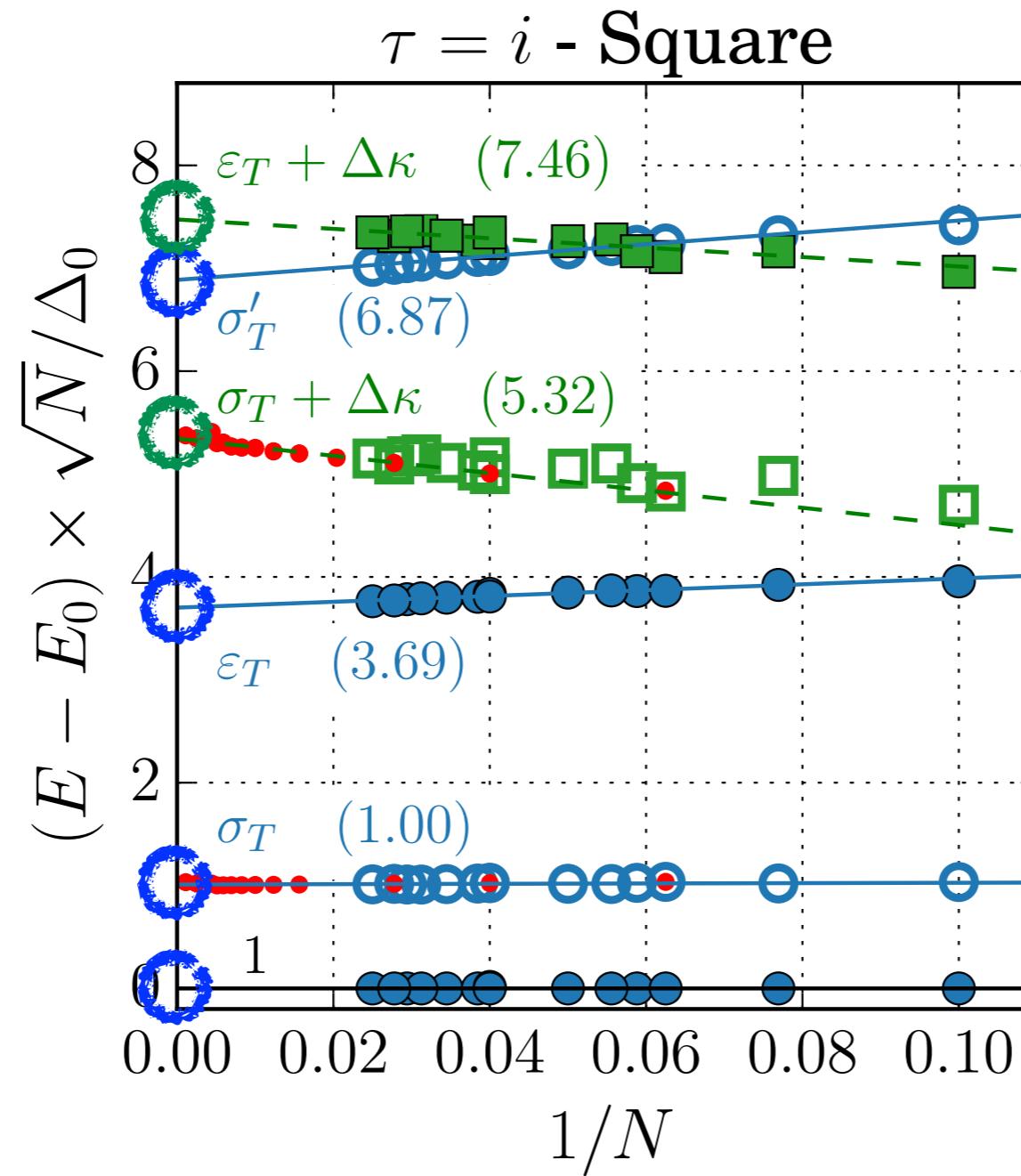
- small field: approx. 2-fold degeneracy due to  $Z_2$ -symmetry breaking.
- large field: unique ground state in paramagnetic phase.



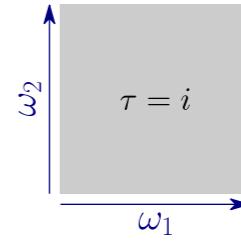


# Detailed finite size scaling

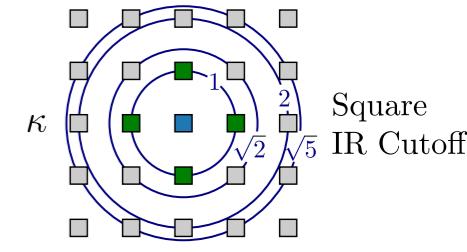
- Square lattice at critical transverse field  $h_c$ :



Torus Shape

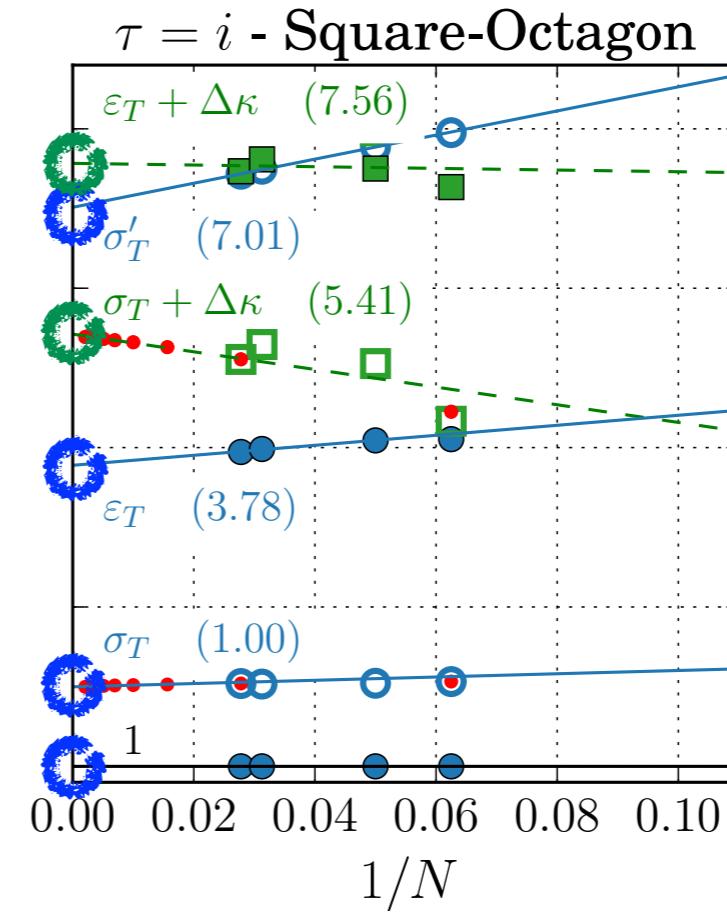
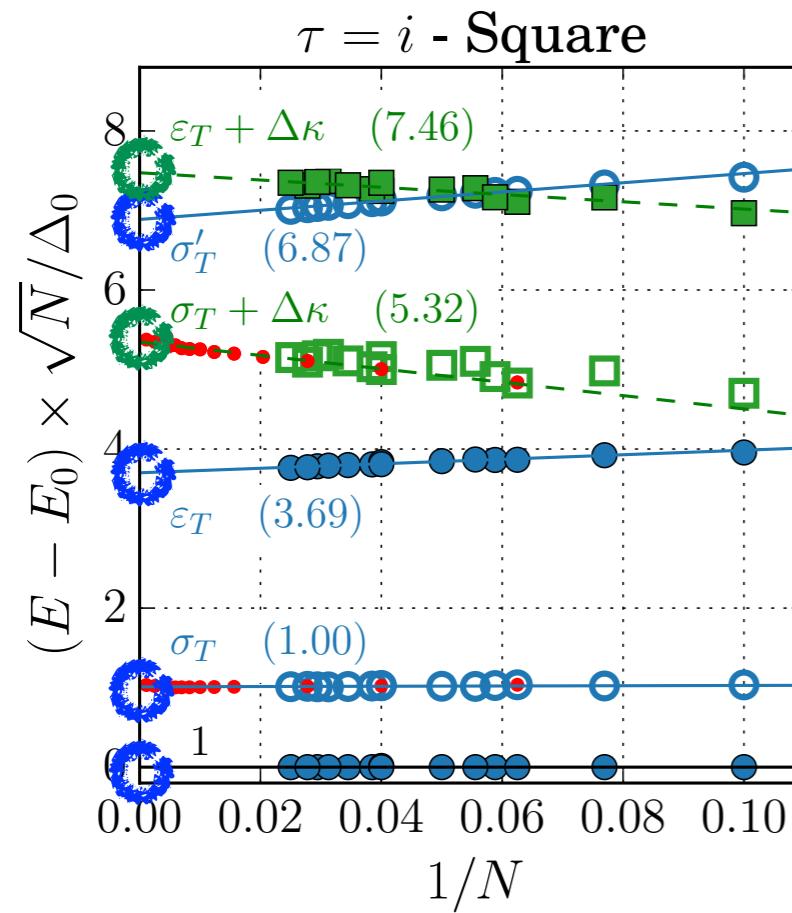


Momentum Space Grid

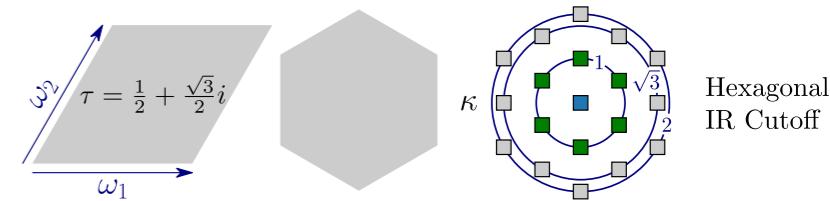


# Comparison with a different lattice

- Square lattice and Square-Octagon lattice at their critical point:

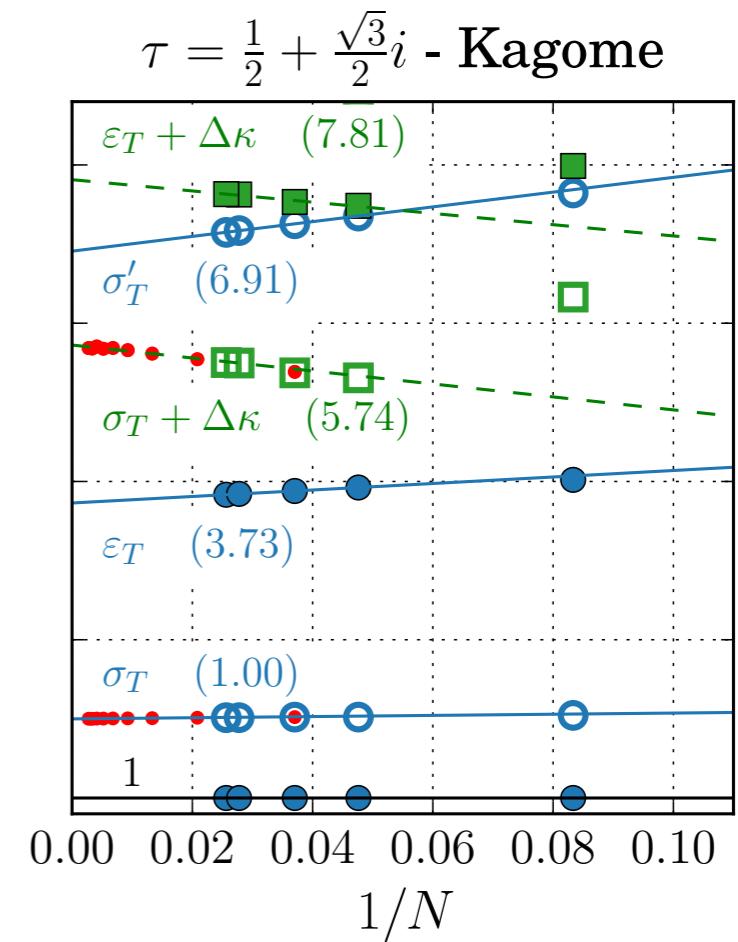
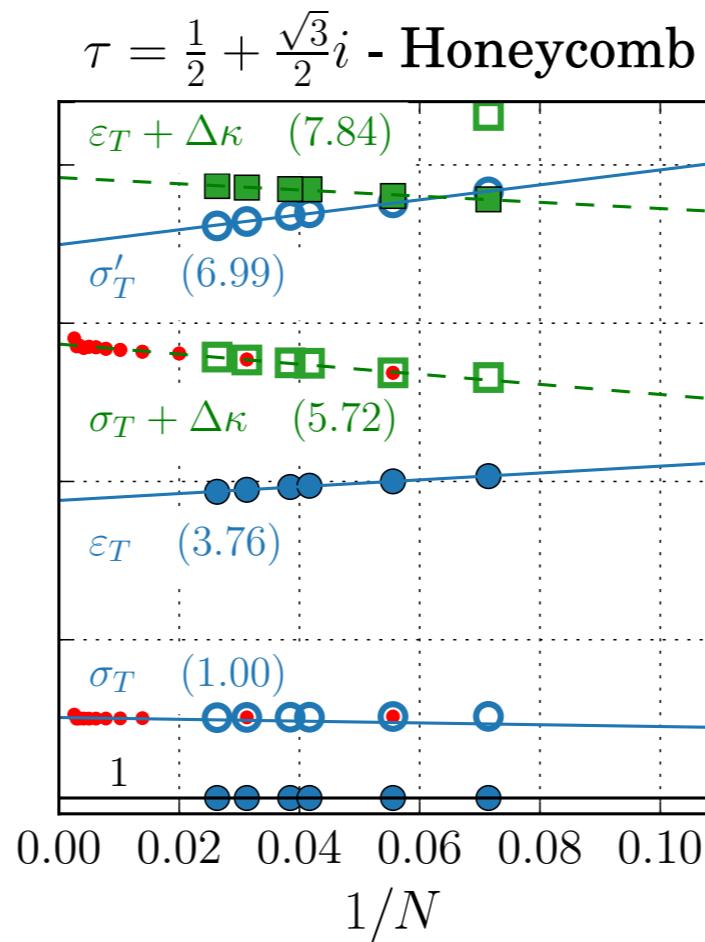
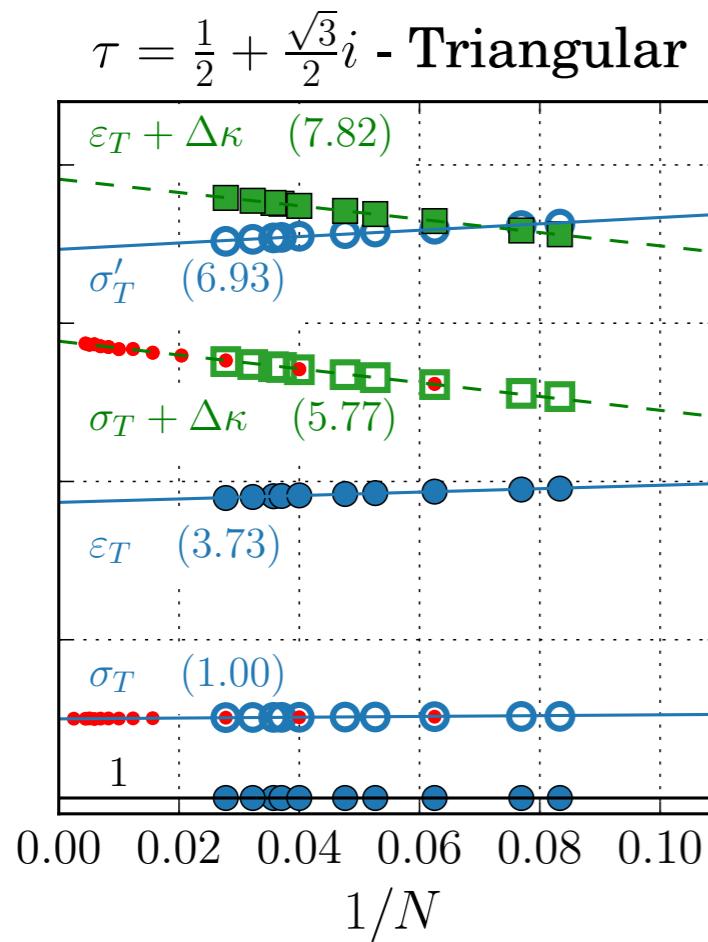


- The spectra are identical after finite-size extrapolation!  
This is thus the genuine 3D Ising CFT spectrum on a **square** torus !



# Comparison with different modular parameter

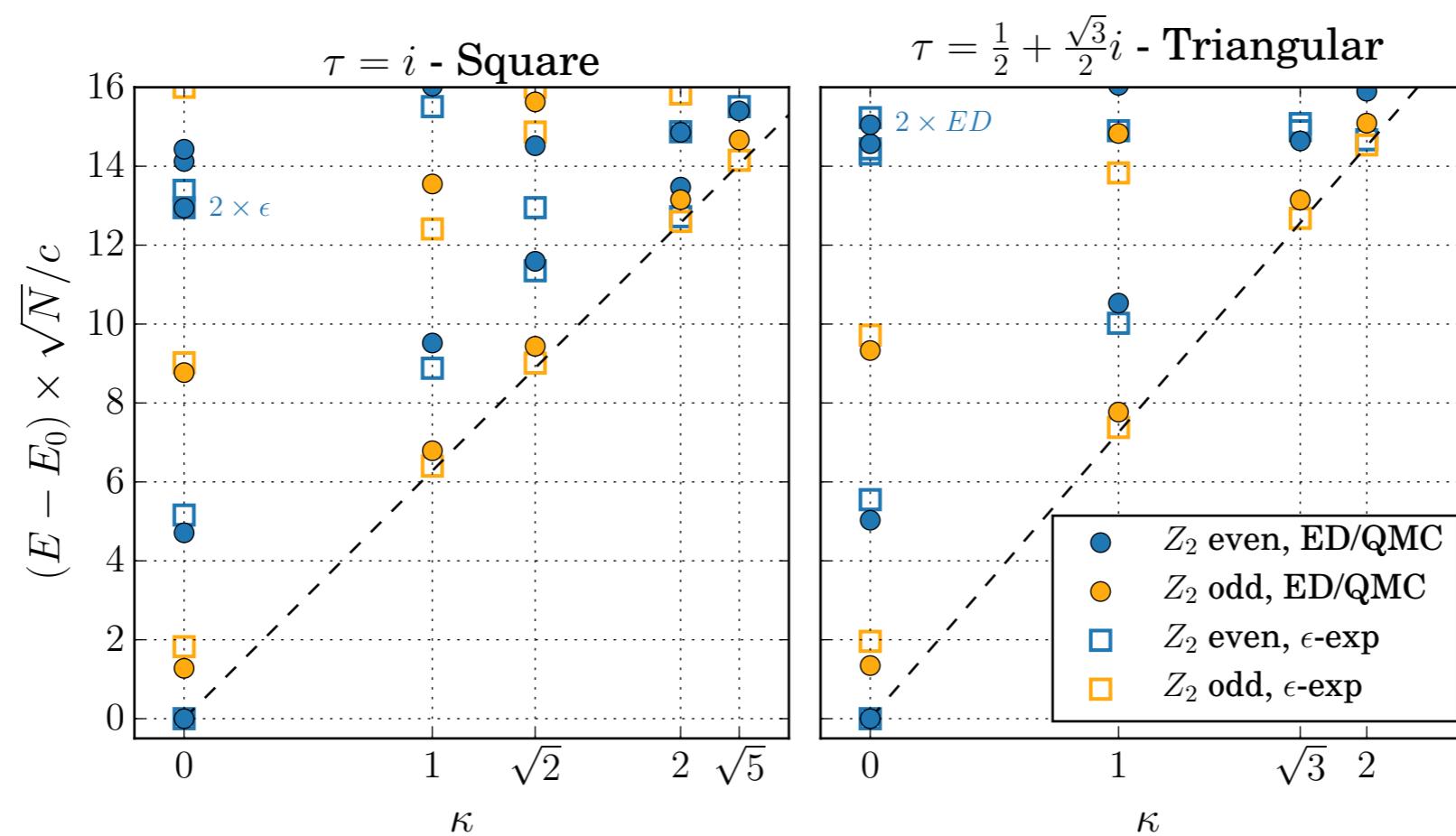
- Triangular, honeycomb and kagome lattice at their critical point:



- The spectra are identical after finite-size extrapolation!  
This is thus the genuine Ising CFT spectrum on a [hexagonal torus](#) !

# Analytical approach: (4-epsilon)-expansion

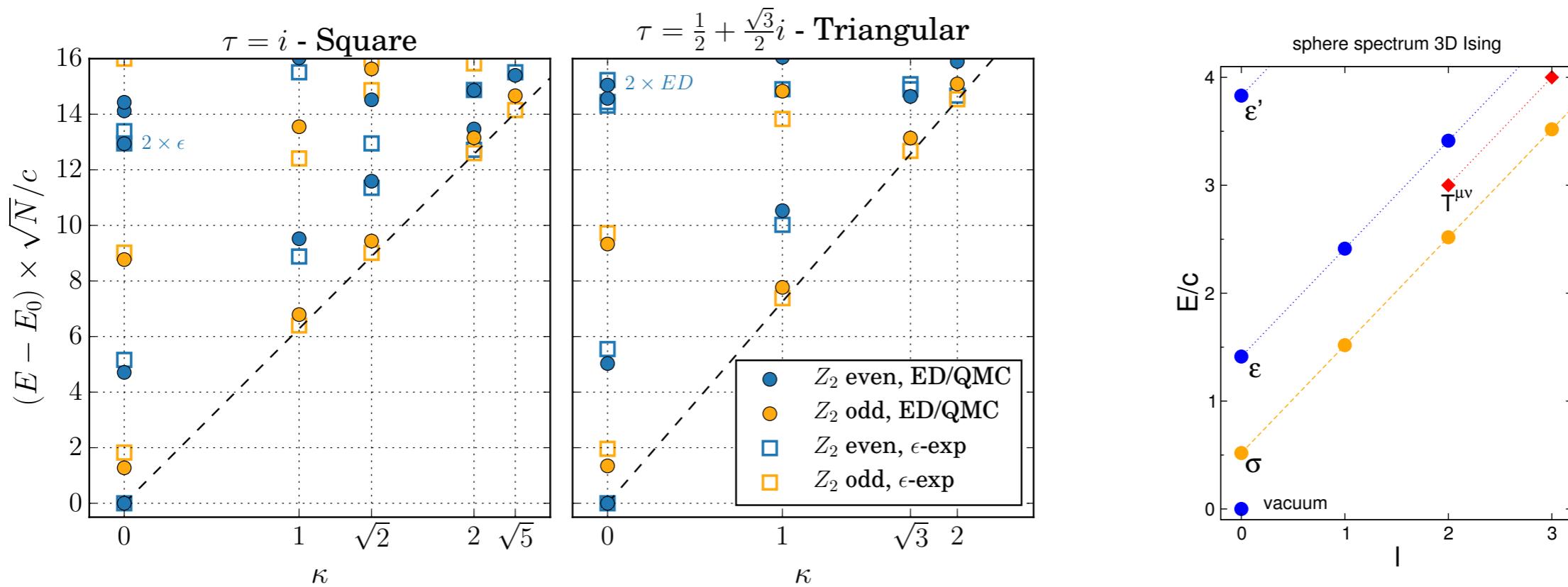
- Work done by S. Withsett and S. Sachdev. Lowest non-trivial order in epsilon.
- Rather good agreement between analytics and numerics.
- Zero-mode is most important in (4-epsilon)-expansion, anharmonic oscillator.



$$\mathcal{H} = \int d^d x \left[ \frac{1}{2} \Pi^2 + \frac{1}{2} (\nabla \phi)^2 + \frac{s}{2} \phi^2 + \frac{u}{4!} \phi^4 \right]$$

# Comparison between torus and sphere spectra

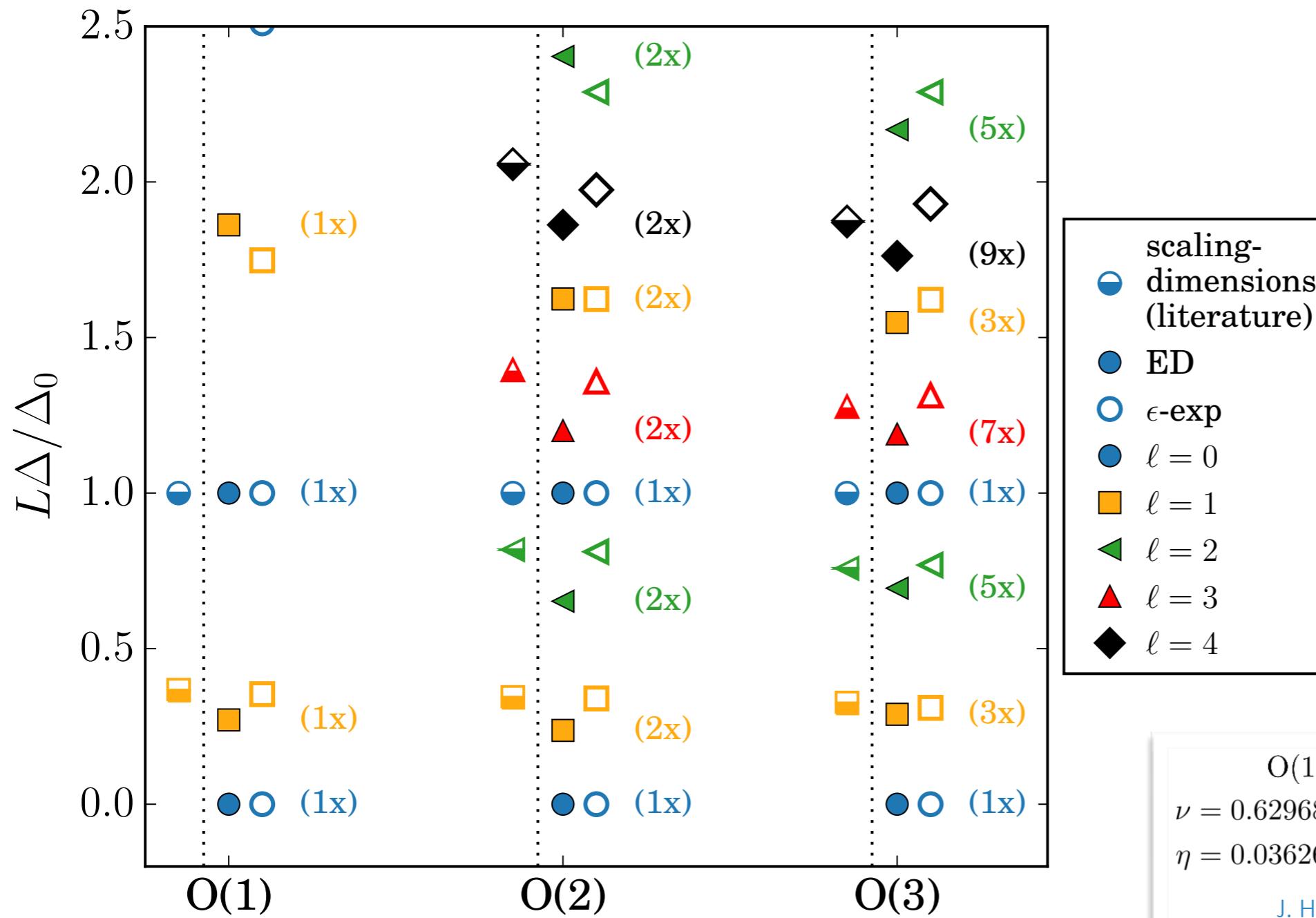
- Torus spectra at low energy per sector resemble the spectrum on the sphere:



- We believe this handwaving resemblance might be more generally the case:  
“light states on the sphere have a light analogon on the torus”
- But likely no state operator correspondence on the torus.

# Wilson-Fisher $Z_2$ / O(2) / O(3) Results

- Universality classes differ by amount of multiplets and their size!



O(1)	O(2)	O(3)
$\nu = 0.62968(66)$	$0.67195(97)$	$0.7113(21)$
$\eta = 0.03626(10)$	$0.03810(20)$	$0.03750(50)$

J. High Energ. Phys. (2014) 2014: 91

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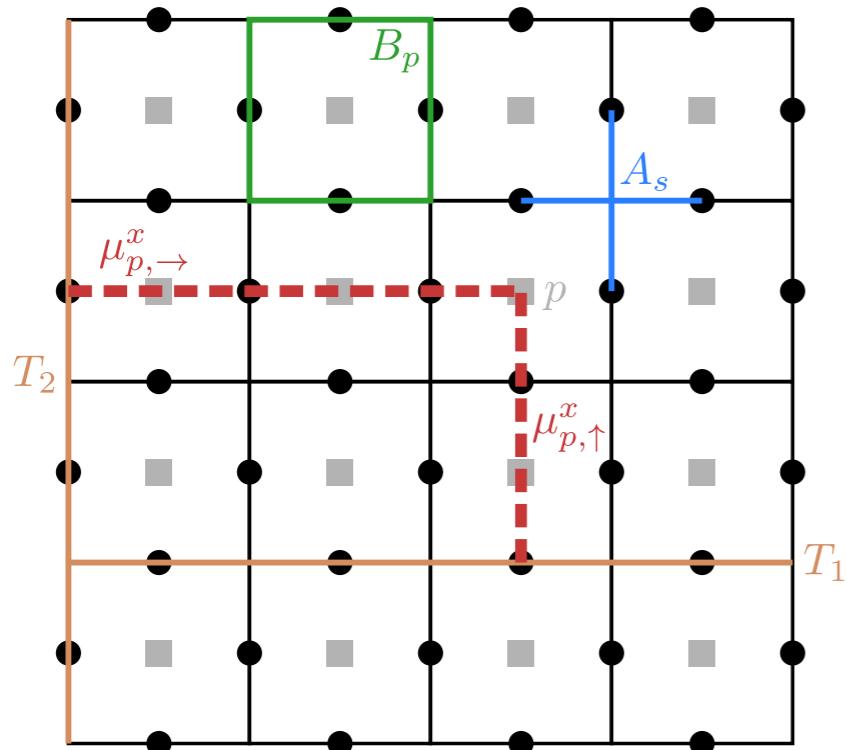
# Confinement transition

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- $Z_2$  spin liquids are among the simplest topological phases.
- They are phases with a four-fold ground state degeneracy on a torus, but the degeneracy is topological, and not related to symmetry breaking.
- One of the simplest incarnations of this phase appears in the Toric Code model by Kitaev.
- By an appropriate perturbation the topological phase (“deconfined”) gives way to a simple paramagnetic phase (“confined”). The transition is a confinement transition and is expected to be in the  $2+1D = 3D$  Ising universality class.
- Q: Is the torus spectrum at criticality identical to the symmetry breaking case ?

# Toric code in a magnetic field

- We study the following microscopic model (but results will be independent of specific model):
- Toric code with a longitudinal magnetic field ([S. Trebst et al., J. Vidal et al, ...](#)):



$$H = -J \sum_s A_s - J \sum_p B_p - h \sum_i \sigma_i^x$$

$$A_s = \prod_{i \in s} \sigma_i^x, \quad B_p = \prod_{i \in p} \sigma_i^z$$

$$\mu_p^z = B_p$$

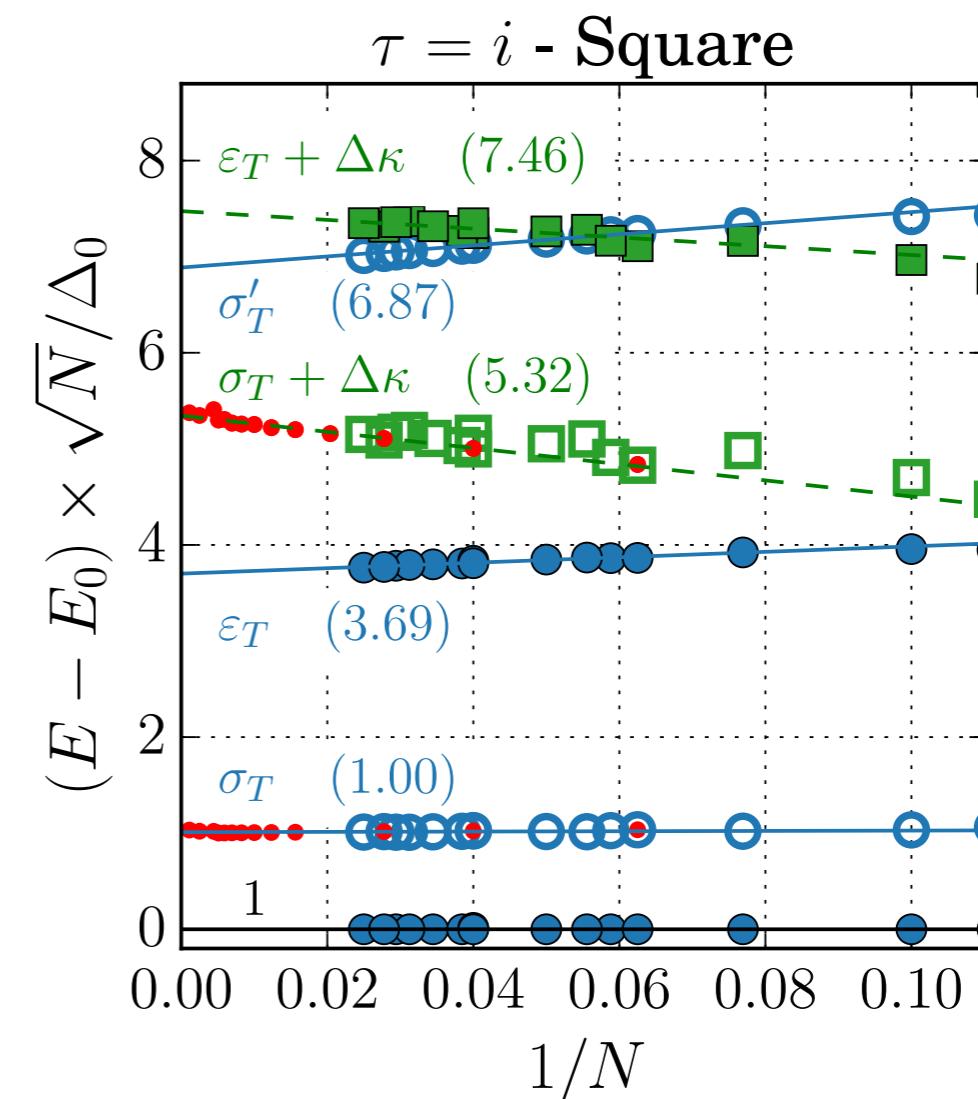
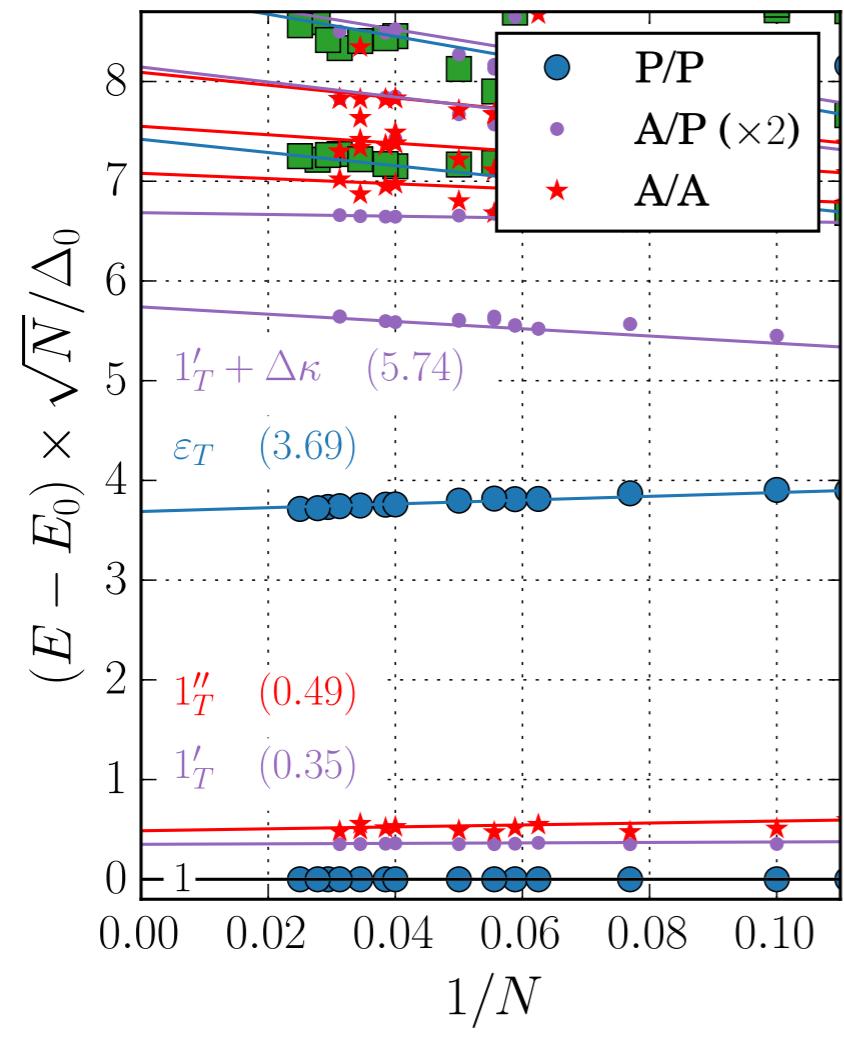
$$\mu_{p,\rightarrow(\uparrow)}^x = \prod_{i \in c_{p\rightarrow(\uparrow)}} \sigma_i^x$$

TFI boundary conditions imposed by  $T_1, T_2$  loops !

$$H_{TFI} = -h \sum_{\langle p,q \rangle} \mu_p^x \mu_q^x - J_p \sum_p \mu_q^z + const.$$

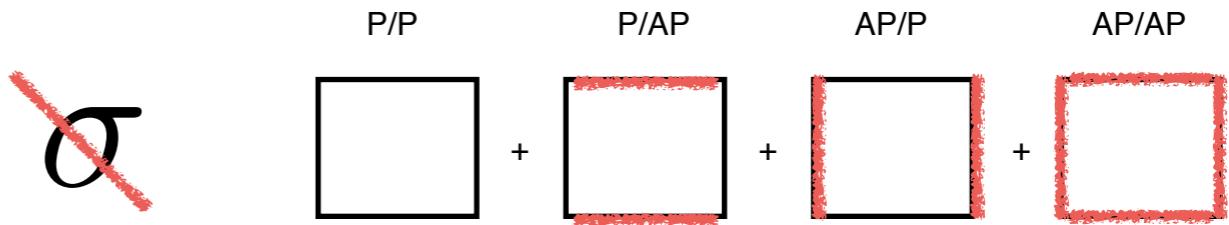
# Numerics at criticality

- Left: data for the TC at criticality, Right: Symmetry breaking



- The spectra at criticality do not agree ! What is going on ?

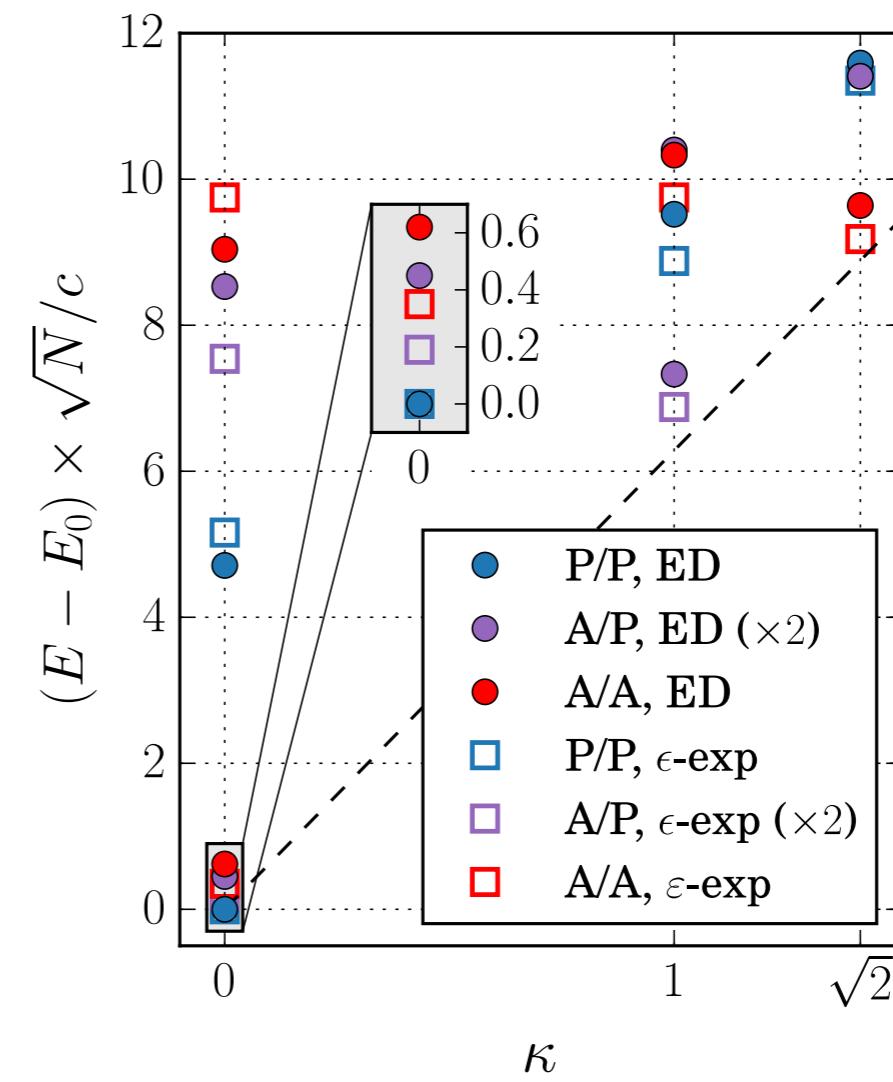
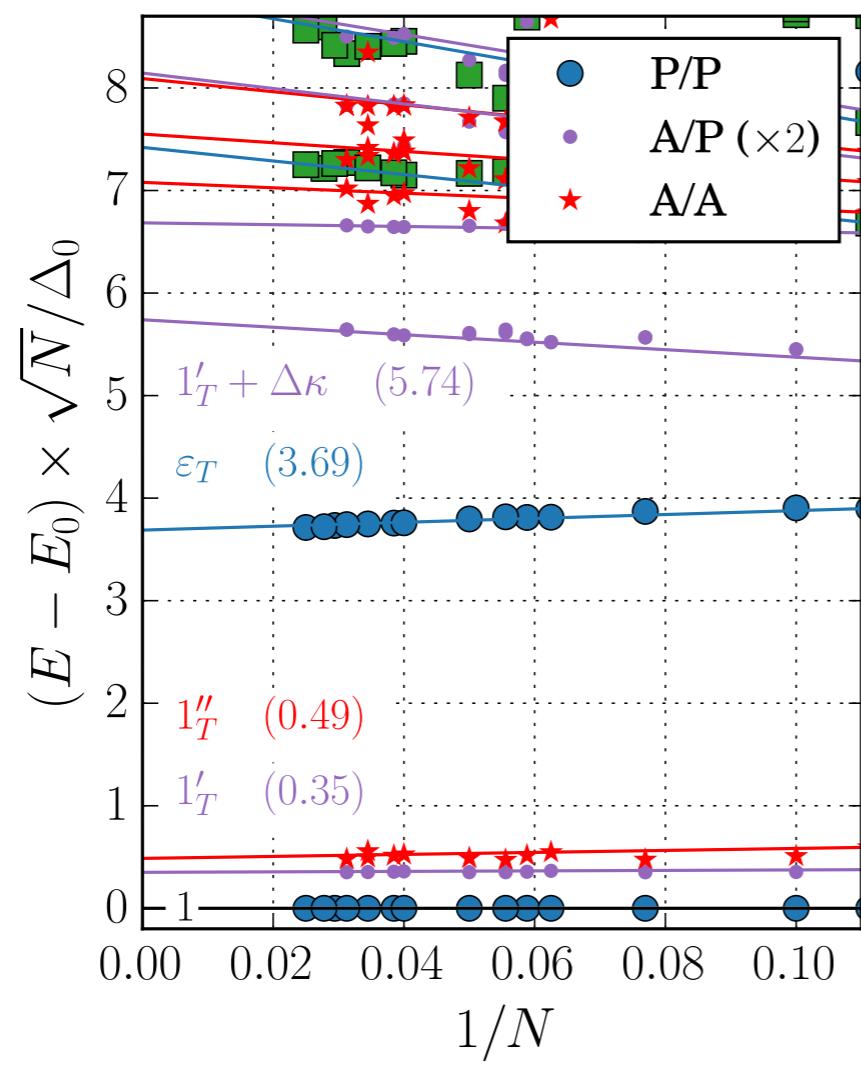
# The Ising\* transition



- The explanation is that the operator content of the two transitions are different:
- In the  $Z_2$  symmetry breaking case we have  $Z_2$  even and odd levels and only one set of boundary conditions (fixed by the lattice model).
- In the confinement transition (Ising\*), only  $Z_2$  even levels are allowed, and for periodic boundary conditions in the Toric Code, four different boundary conditions of the CFT become simultaneously apparent.
- This can be understood at the microscopic level in the Toric Code Hamiltonian and is supported by general field theoretical considerations.
- In the Ising\* case the magnetic sector is completely absent, and the torus energy spectrum reflects this fact.

# The Ising\* transition

- comparison between numerics and epsilon-expansion:
- At criticality the 4 “topological sectors” scale also as  $1/L$ , but are much closer together than the next level above them.



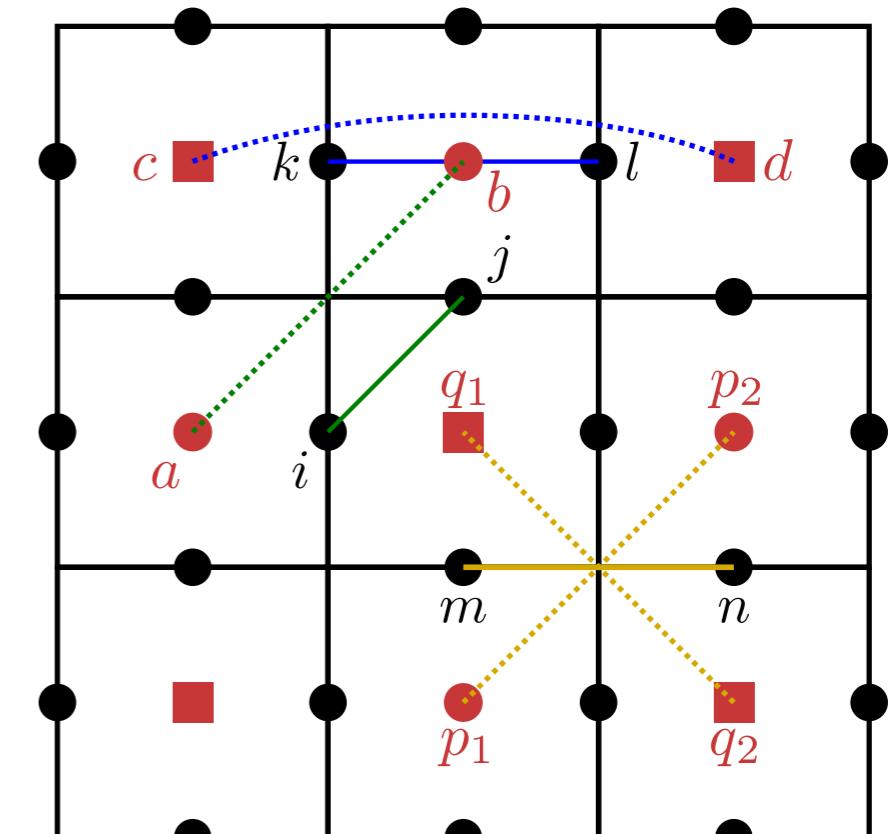
# Toric code with Ising interactions

- Want to study a possible quantum phase transition between  $Z_2$  topological order and spontaneous global  $Z_2$  symmetry breaking.
- Toric code plus additional Ising interactions:

$$H = - J \sum_s A_s - J \sum_p B_p$$

$$- J_I \sum_{\langle i,j \rangle} \sigma_i^x \sigma_j^x - J_{I_2} \sum_{\langle\langle i,j \rangle\rangle} \sigma_i^x \sigma_j^x$$

$$A_s = \prod_{i \in s} \sigma_i^x \quad B_p = \prod_{i \in p} \sigma_i^z$$



$$\sigma_i^x \sigma_j^x \rightarrow 2\mu_a^x \mu_b^x$$

$$\sigma_k^x \sigma_l^x \rightarrow \mu_c^x \mu_d^x$$

$$\sigma_m^x \sigma_n^x \rightarrow 2\mu_{p1}^x \mu_{p2}^x \mu_{q1}^x \mu_{q2}^x$$

# Toric code with Ising interactions

- Toric code plus additional Ising interactions:

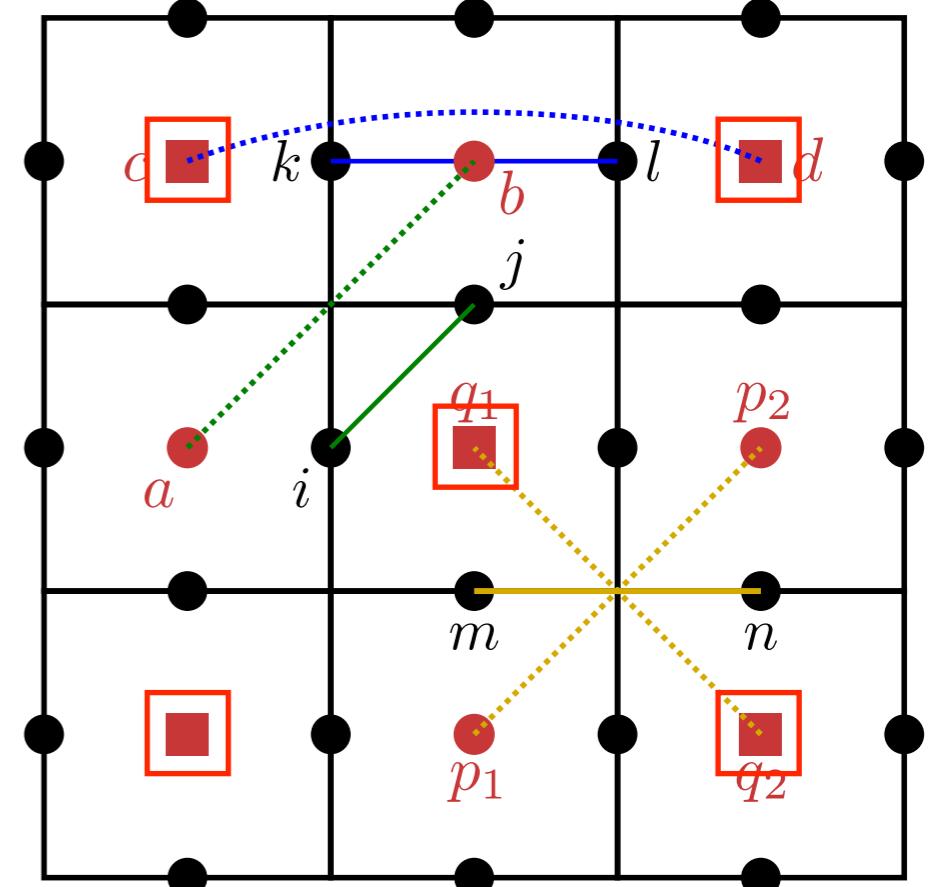
$$H = - J \sum_s A_s - J \sum_p B_p - J_I \sum_{\langle i,j \rangle} \sigma_i^x \sigma_j^x - J_{I_2} \sum_{\langle\langle i,j \rangle\rangle} \sigma_i^x \sigma_j^x$$

$$A_s = \prod_{i \in s} \sigma_i^x \quad B_p = \prod_{i \in p} \sigma_i^z$$

- Maps onto a particular 2+1D quantum Ashkin-Teller (AT) model:

$$H_{AT} = - J \sum_i \mu_i^z - 2J_I \sum_{\langle\langle i,j \rangle\rangle} \mu_i^x \mu_j^x - J_{I_2} \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} \mu_i^x \mu_j^x - 2J_{I_2} \sum_i \mu_i^x \mu_{i+\hat{\mathbf{x}}}^x \mu_{i+\hat{\mathbf{y}}}^x \mu_{i+\hat{\mathbf{x}}+\hat{\mathbf{y}}}^x \quad (\text{A6})$$

- This model has a two checkerboard lattice spatial structure, yielding the two AT-sublattices



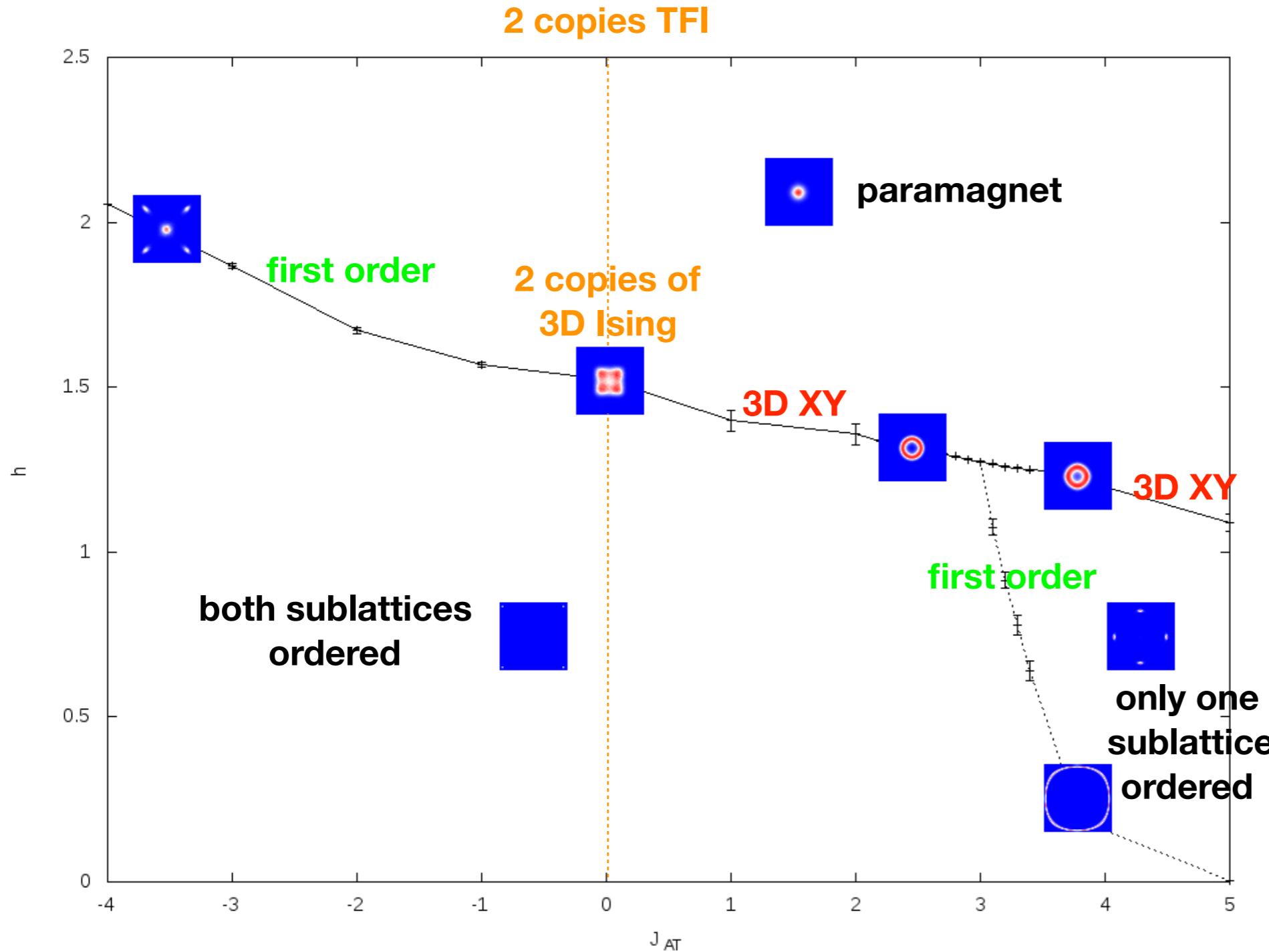
$$\sigma_i^x \sigma_j^x \rightarrow 2\mu_a^x \mu_b^x$$

$$\sigma_k^x \sigma_l^x \rightarrow \mu_c^x \mu_d^x$$

$$\sigma_m^x \sigma_n^x \rightarrow 2\mu_{p1}^x \mu_{p2}^x \mu_{q1}^x \mu_{q2}^x$$

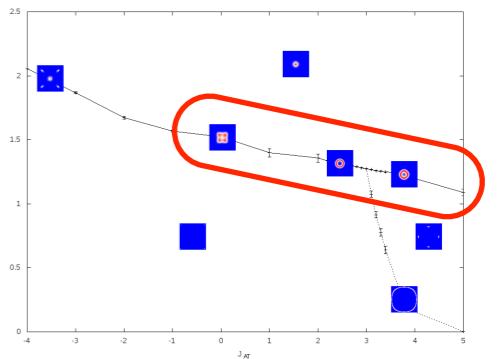
# Phase diagram of the Quantum Ashkin-Teller model

- Rather poorly studied in the past, so here we perform a new QMC study:

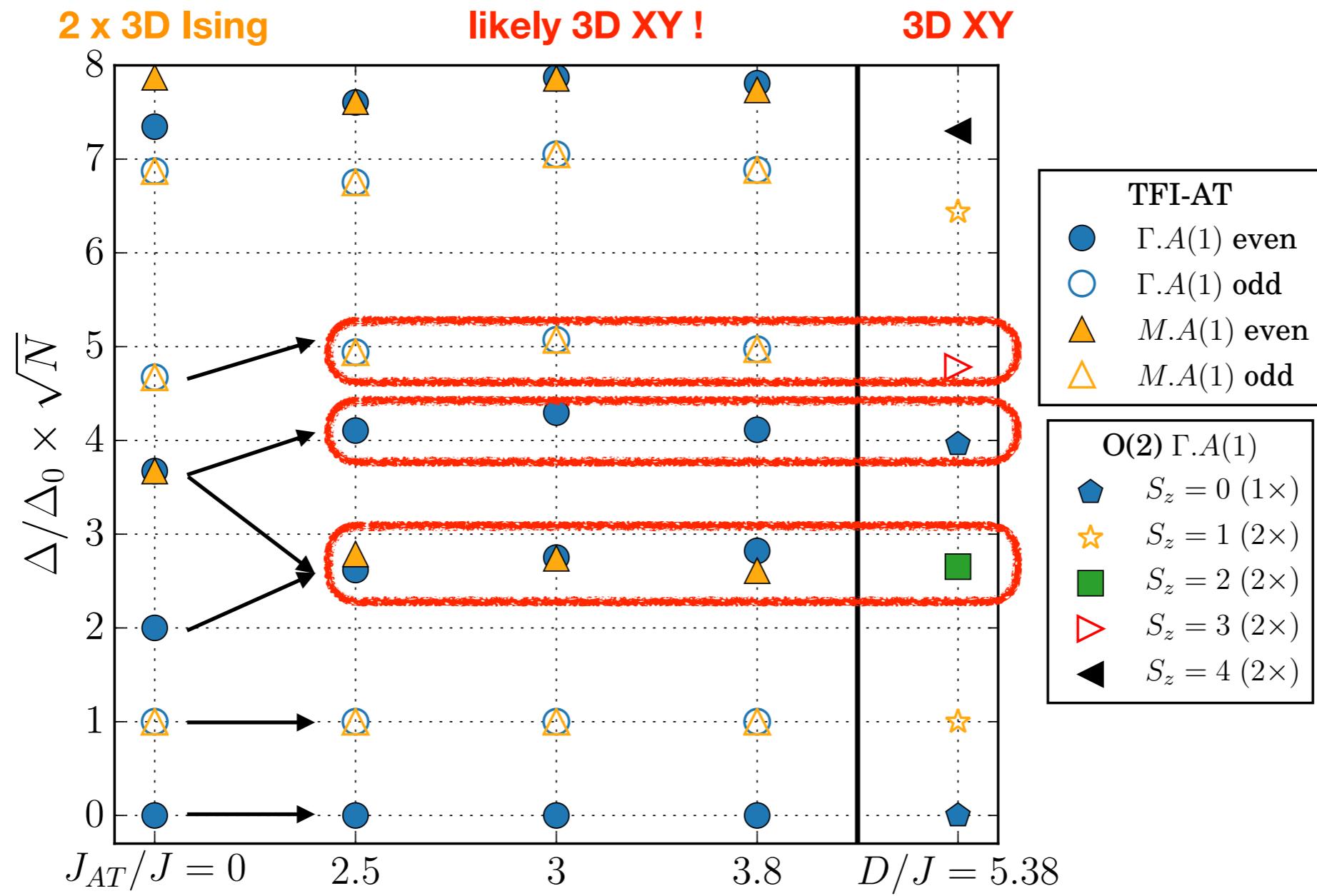


- Phase structure in agreement with QFT results of  $N_c=2$   $\phi^4$  theory with cubic anisotropy.

# Spectroscopy of QCP

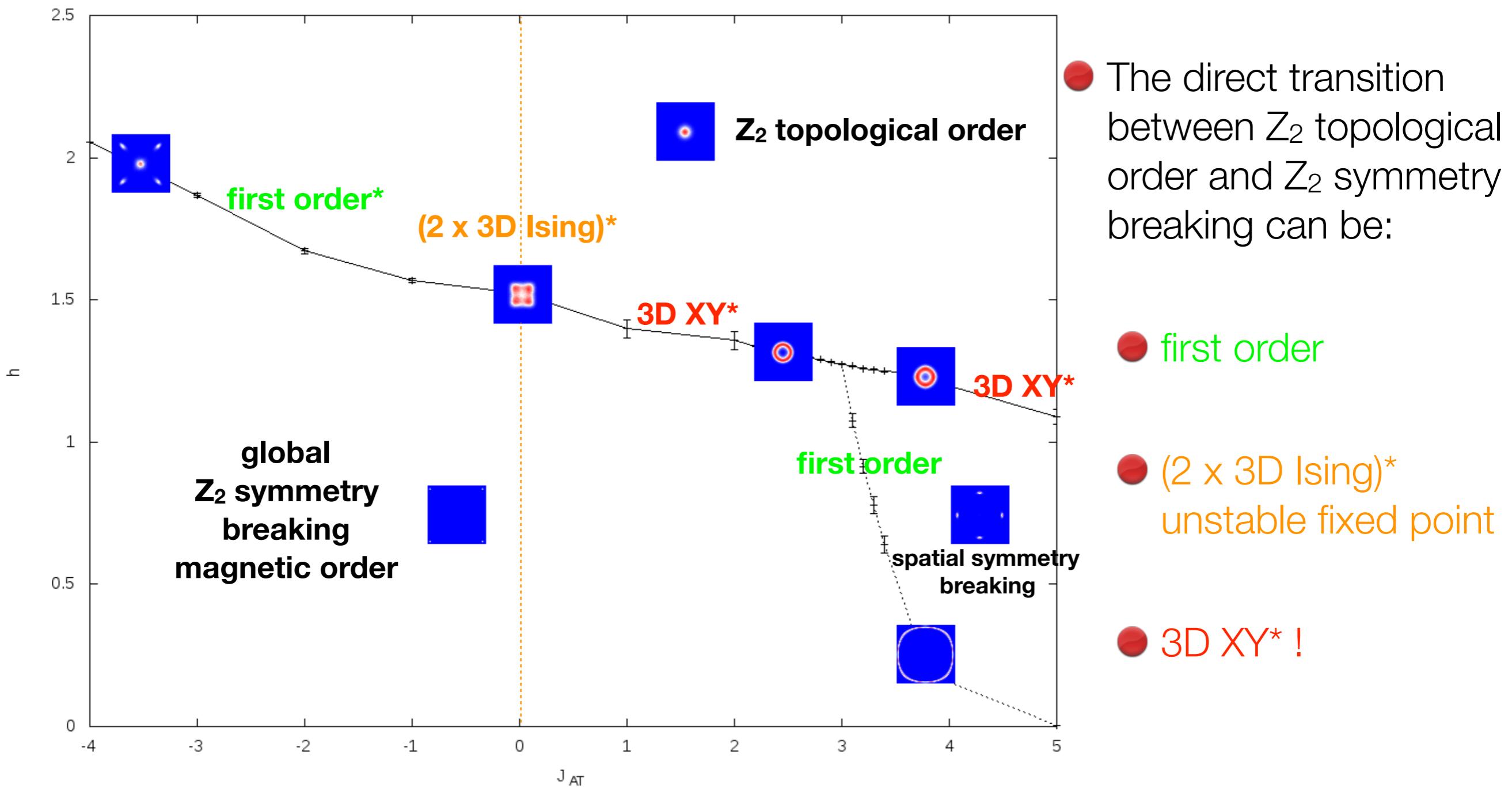


- ED Torus Spectra in the Quantum Ashkin-Teller model at criticality:



# Phase diagram of the Toric Code + Ising interactions

- Translate the Ashkin-Teller results back to the Toric code + Ising:



# Outline of this talk

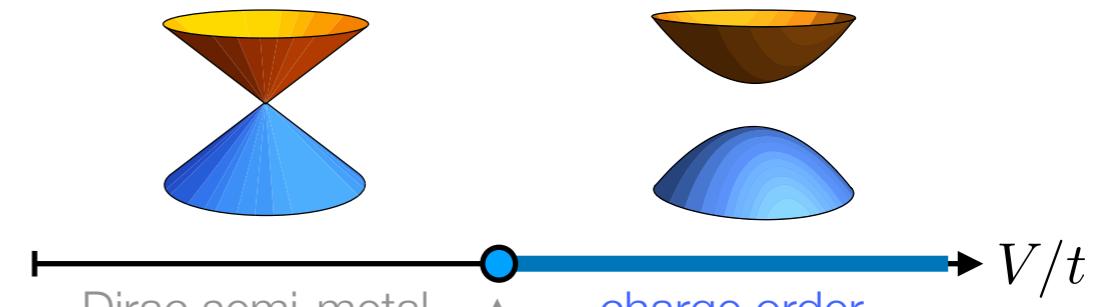
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- Introduction: Quantum Many Body Systems / Spectroscopy
- Torus Energy Spectra and Quantum Critical Points ?
- Spectrum of the standard 2+1D Ising transition
- Topological Phase Transitions
- Gross-Neveu-Yukawa fixed points
- Outlook

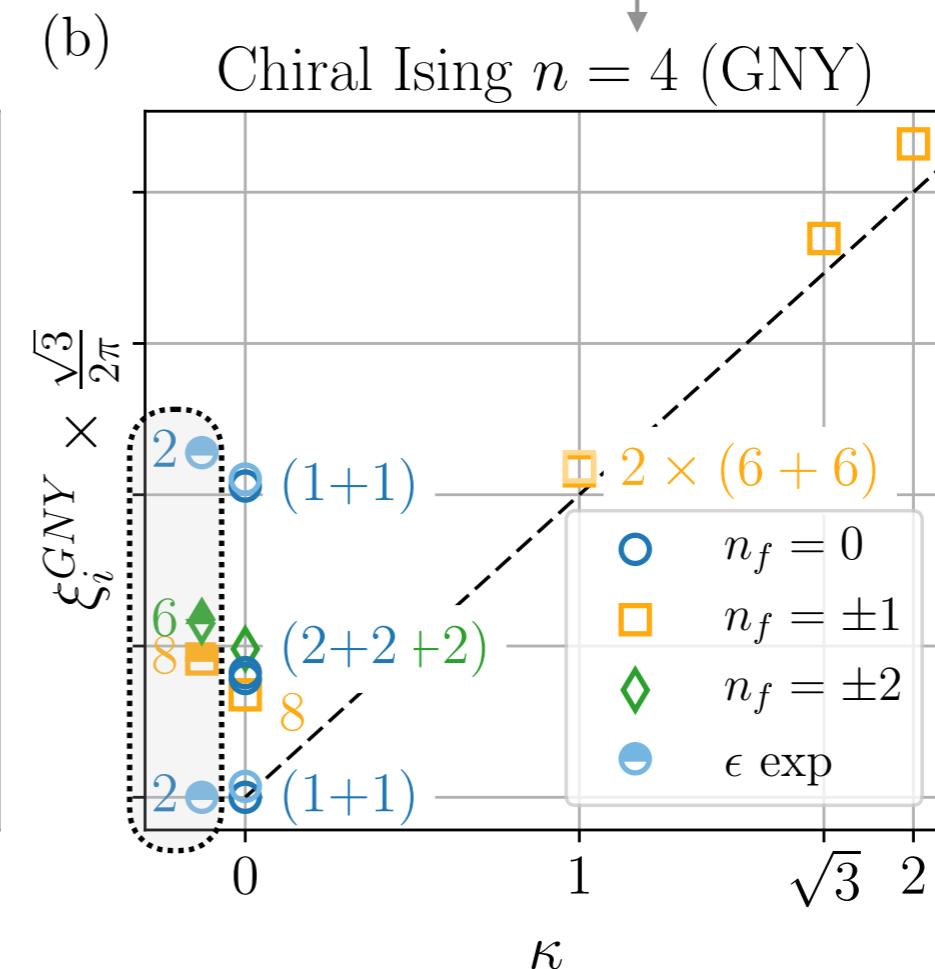
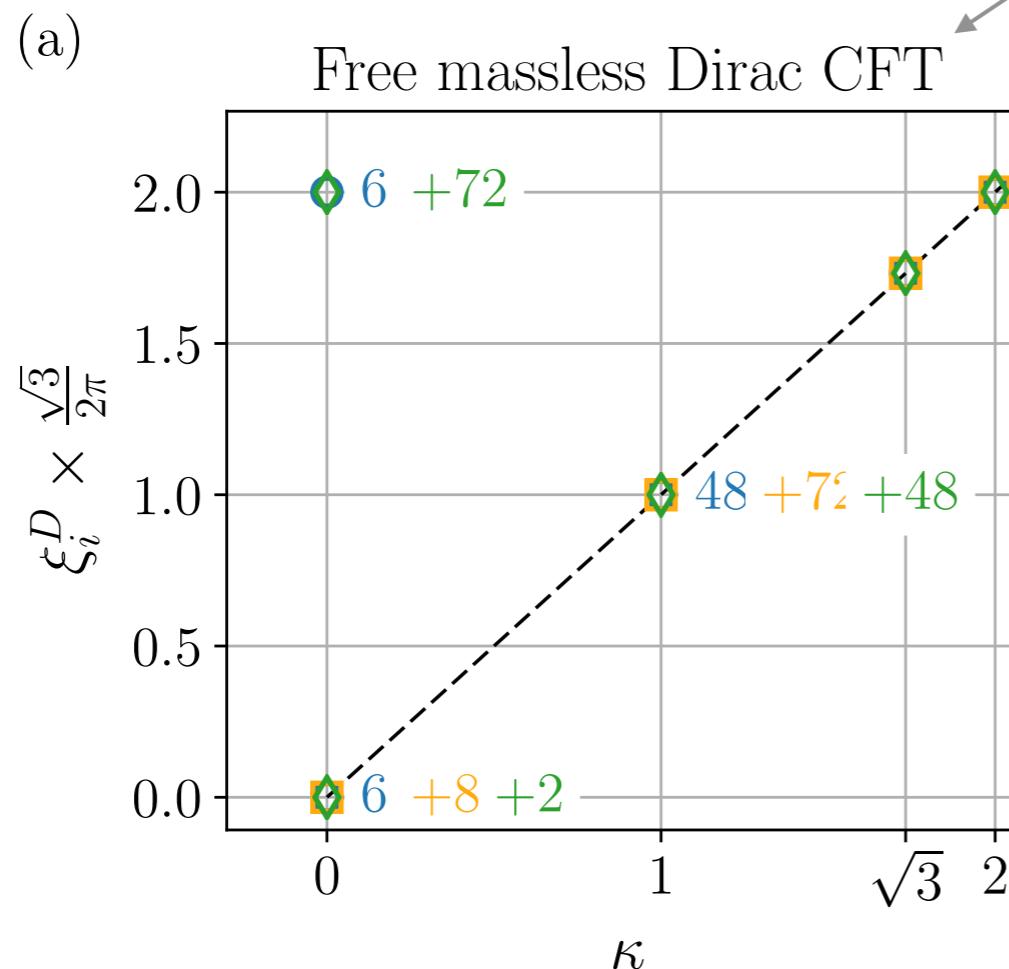
M. Schuler, S. Hesselmann, T.C. Lang, S. Wessel & AML  
arXiv:1907.05373

# Gross-Neveu-Yukawa: Chiral Ising

- Spinless fermions on a honeycomb lattice:

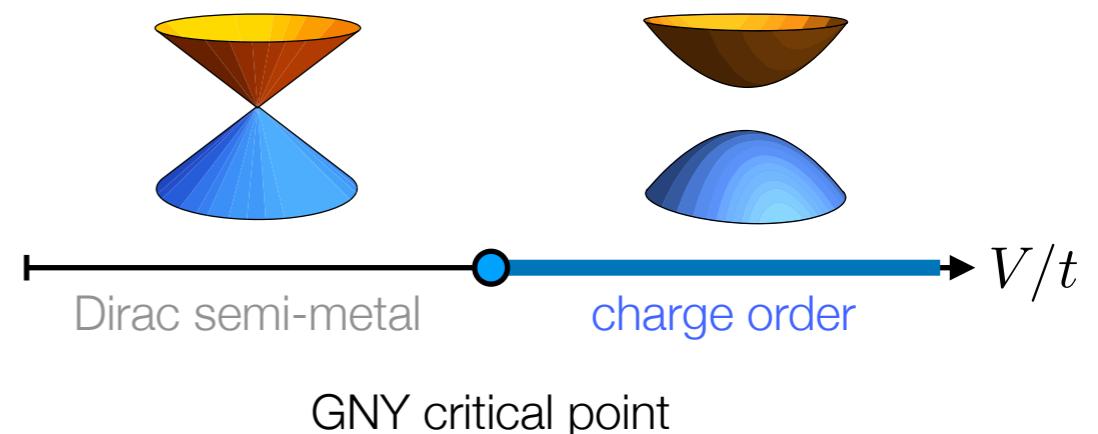


- Gross-Neveu-Yukawa  $N_f=4$  CFT



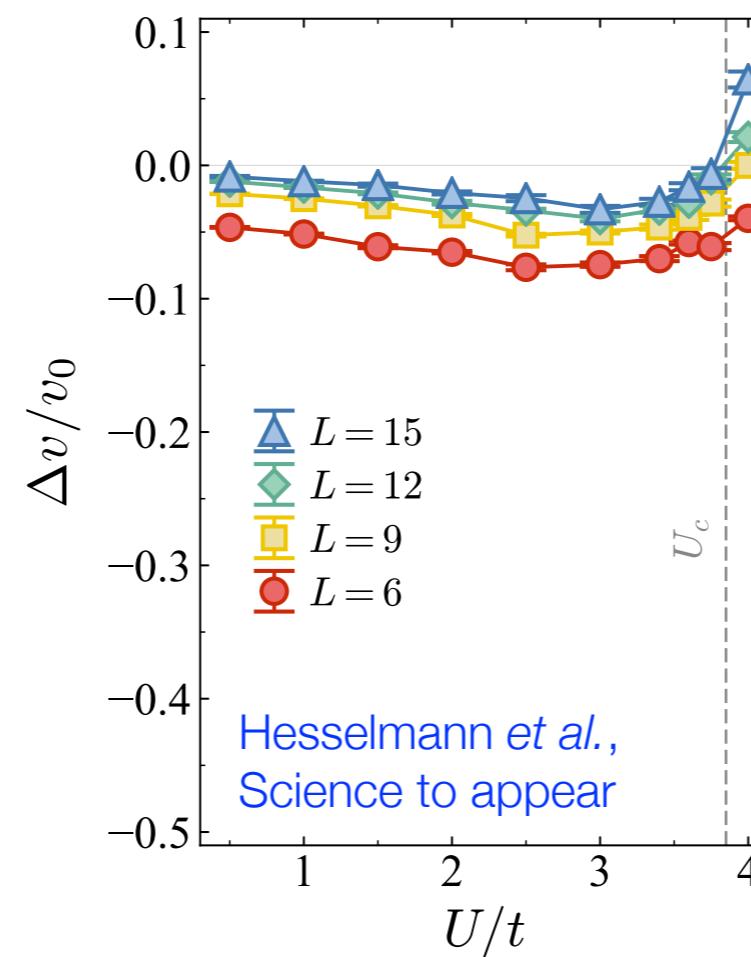
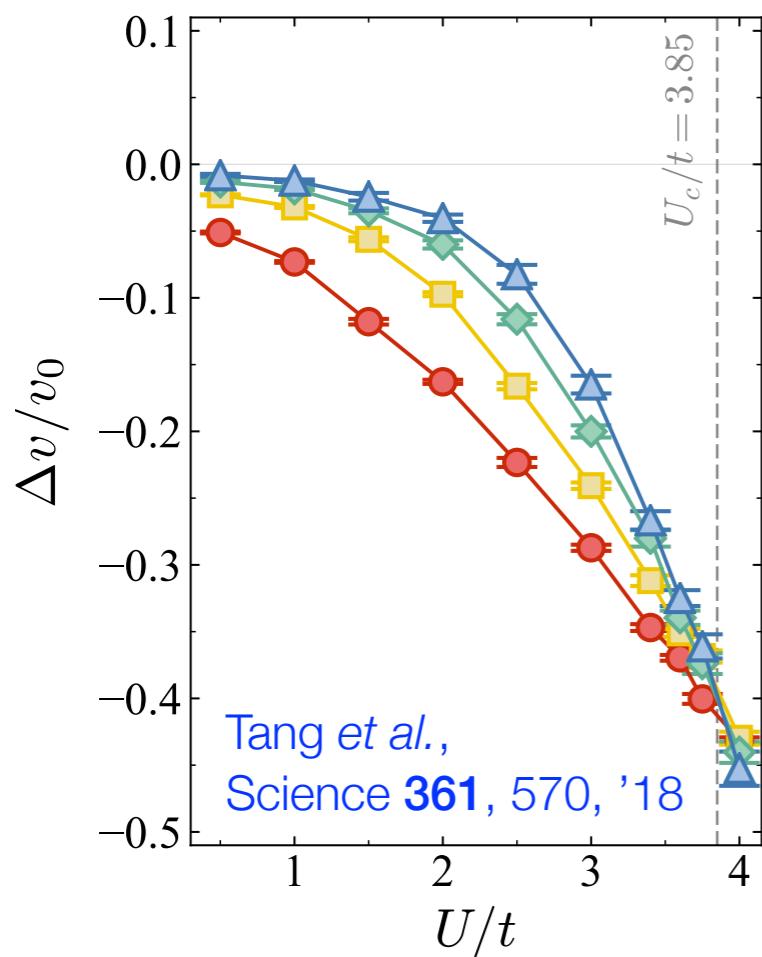
# Gross-Neveu-Yukawa: Chiral Ising

- Can one infer the “speed of light” from energy spectrum ?



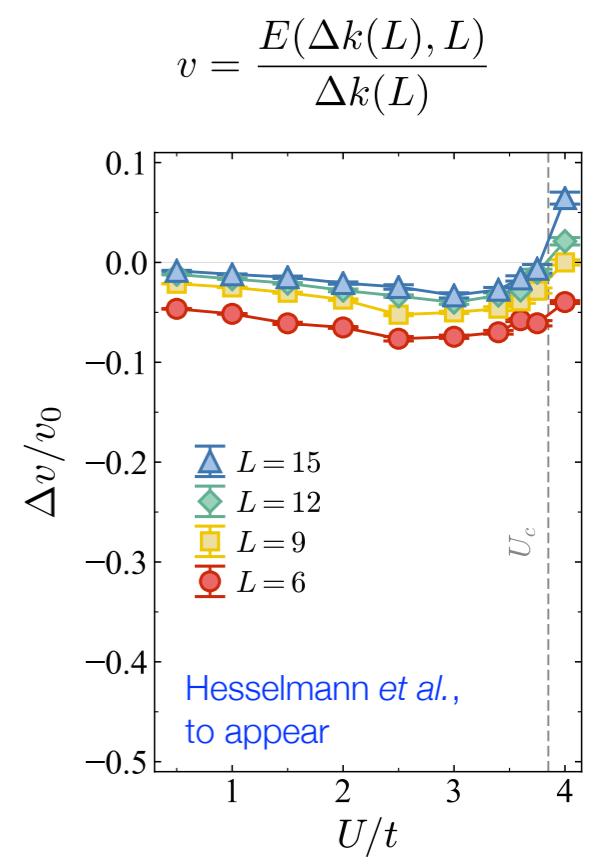
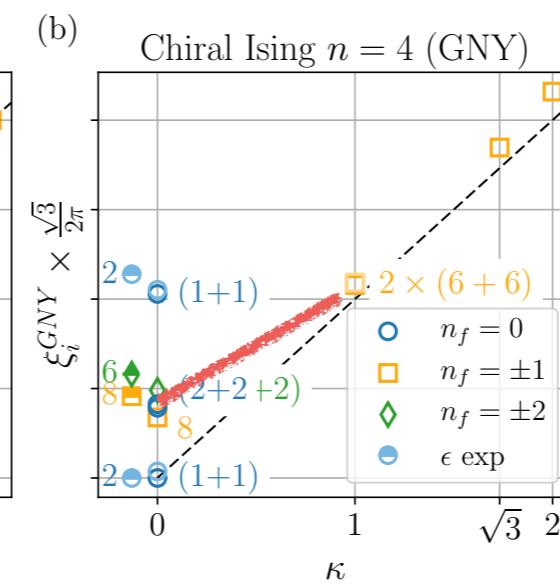
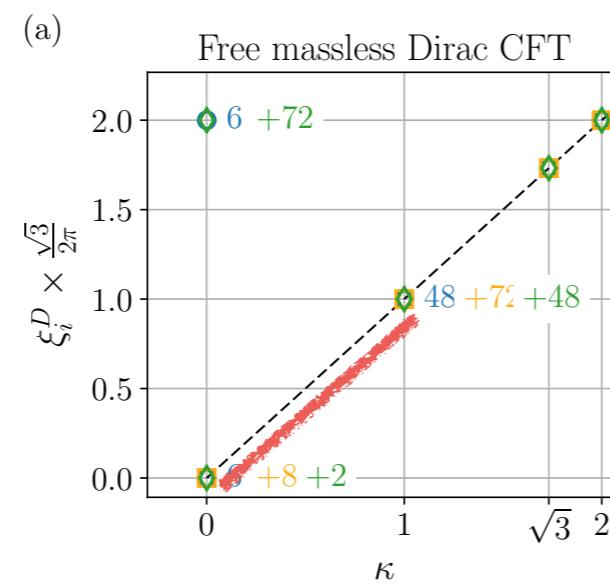
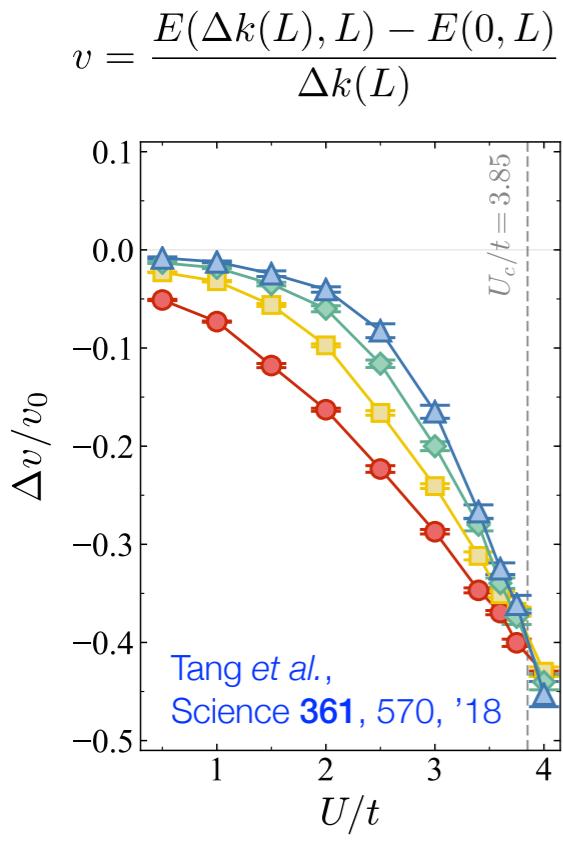
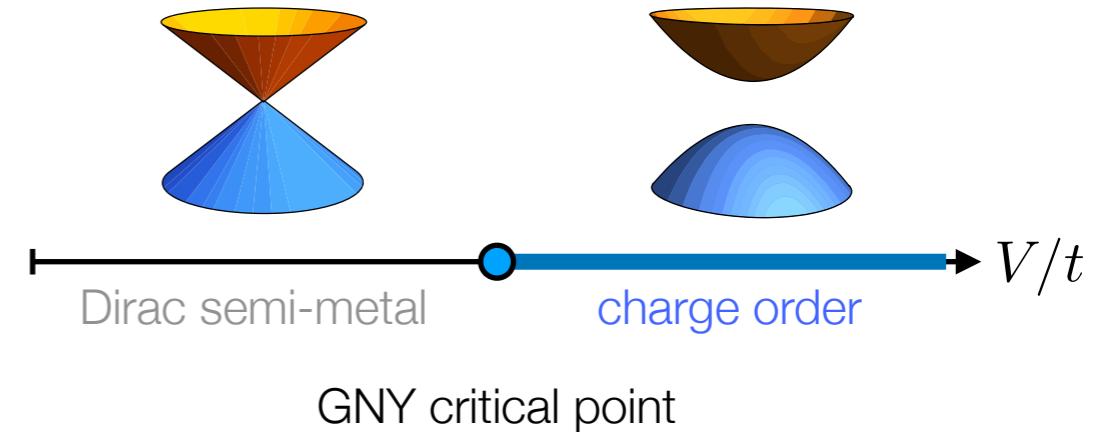
$$v = \frac{E(\Delta k(L), L) - E(0, L)}{\Delta k(L)}$$

$$v = \frac{E(\Delta k(L), L)}{\Delta k(L)}$$



# Gross-Neveu-Yukawa: Chiral Ising

- Can one infer the “speed of light” from energy spectrum ?



# Outline of this talk

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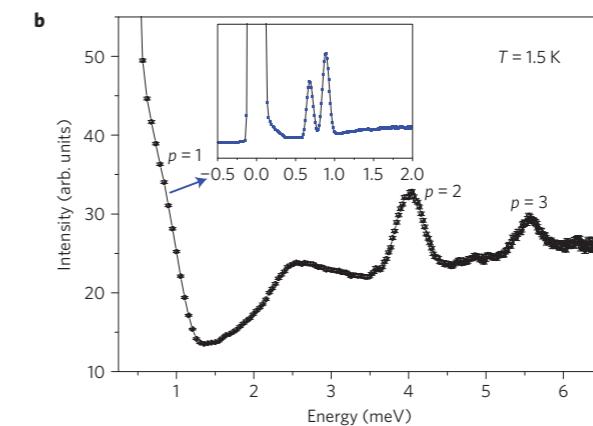
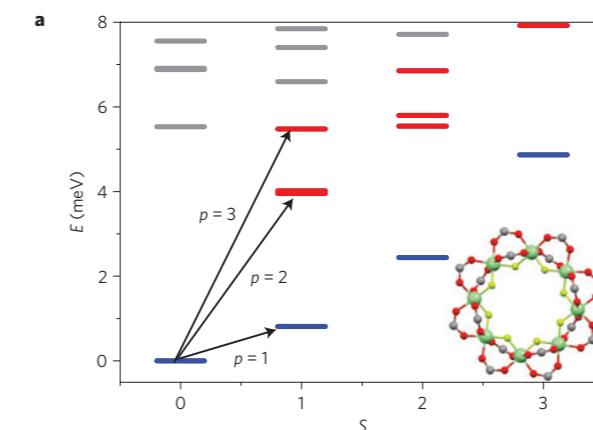
# Experimental Prospects ?

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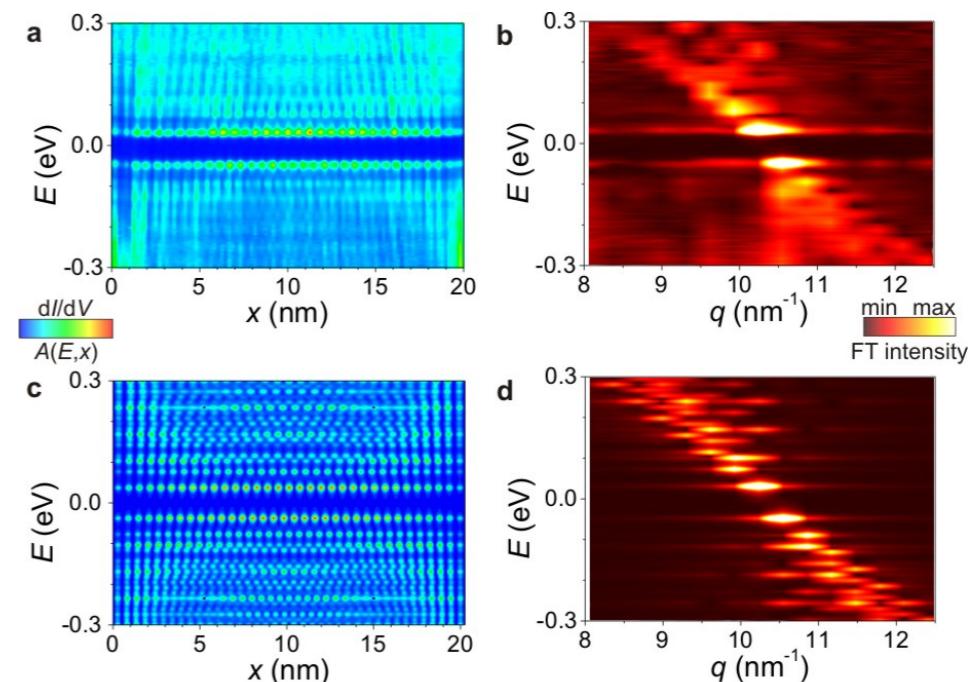
- In large, bulk materials, the many body energy spectrum is mostly extremely dense.
- In mesoscopic systems the finite energy spacing starts playing a role
- Our results show that the precise relative position of energy levels at the edge of the spectrum carries valuable information.
- Can one access some of this information using experimental probes ?

# Experimental Prospects ?

- Some of the energy levels can be seen in some inelastic scattering experiments on *mesoscopic* samples.
- in 1D, ring magnetic molecules provide a nice example of this approach.
- New STM experiments on interacting 1D metals reveal spin-charge separation based on real-space LDOS measurements.



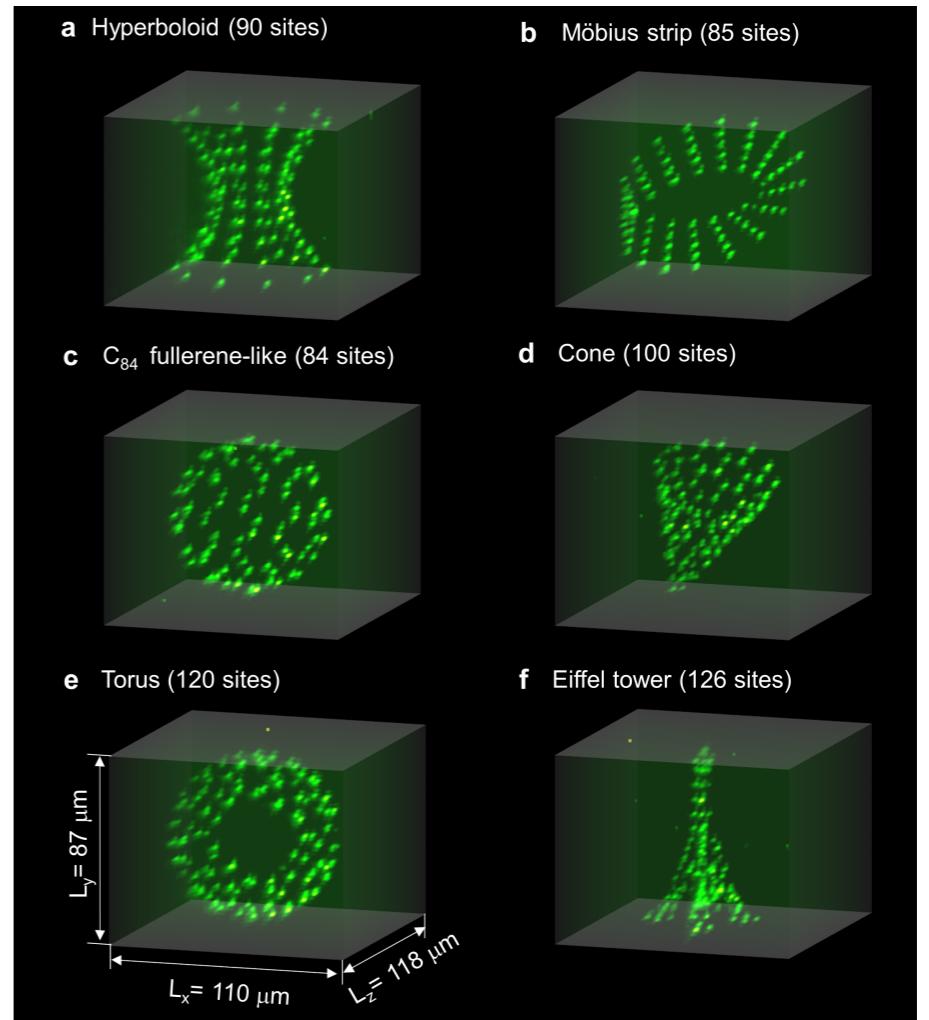
M.L. Baker et al. Nat. Phys. 2012



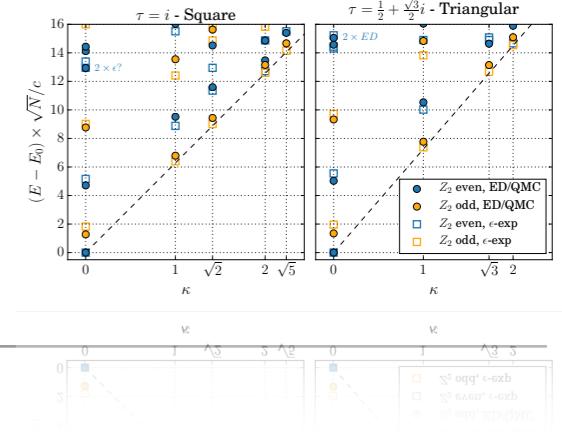
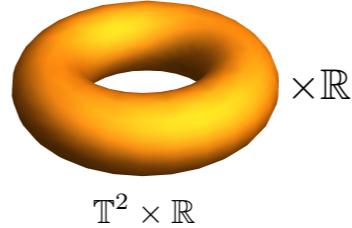
W. Jolie et al., Phys. Rev. X 2019

# Experimental Prospects ?

- In 2D tori are perhaps not readily available in condensed matter systems, but we plan to extend our analysis to systems with open boundaries, but the analysis might become involved.
- In synthetic (AMO) systems tori might become accessible for some Hamiltonians.



# Conclusion / Outlook



- We have shown that the universal torus energy spectrum of the CFT describing quantum critical points is accessible numerically.
- The torus energy spectrum contains valuable information on the “operator content”. It is e.g. able to discriminate the Ising from the Ising\* universality class, and  $2 \times$  Ising from 3D XY
- We have results for O(2)/O(3) Wilson-Fisher fixed points and for several Gross-Neveu-Yukawa critical points.
- Results from CFT side ?
- Spectra for QED<sub>3</sub>, Fermi surface + U(1) gauge field ?



# Collaborators

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PostDoc ▶ TU Wien



Louis-Paul Henry  
PostDoc ▶ Hamburg

## ● Harvard University



Seth Whitsitt  
PhD Student  
▶ JQI Maryland



Subir Sachdev



Thank you for your attention !

