清華大學
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State Key Laboratory of
Low Dimensional Quantum Physics

Conference "Entanglement in Strongly Correlated Systems"
(Aug. 7 - 18, 2023)

Tensor network approach to 2D fully frustrated XY spin model

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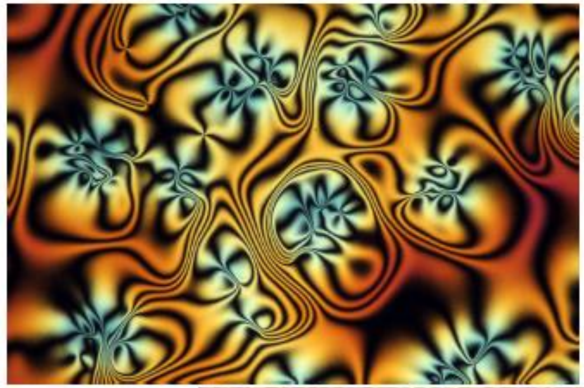
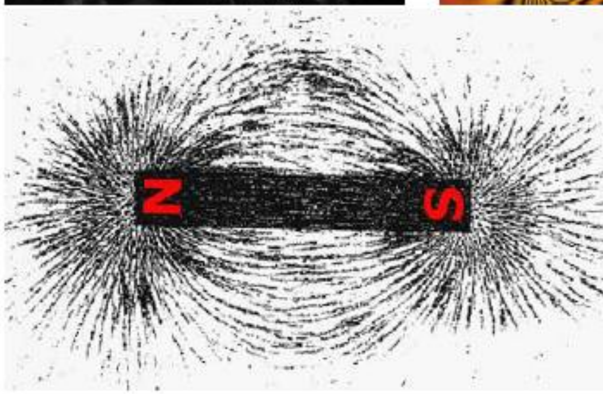
7 Aug., 2023 @ Benasque, Spain

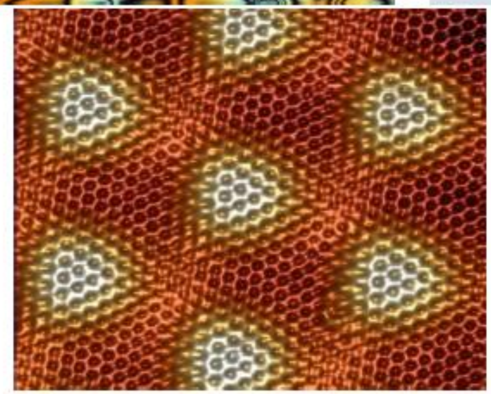
Outline

- **Introduction: Landau paradigm and BKT transition**
- **Tensor network approach for 2D XY spin models**
- **Fully frustrated XY spin model on a Kagome lattice**
- **Conclusion**

Landau paradigm of phase transitions

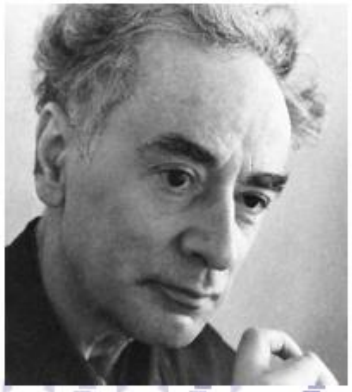






- Rich forms of matter ← rich types of orders
- A deep insight from Landau: **different orders come from different symmetry breaking.**

  → Symmetry breaking theory of orders

  → A corner stone of condensed matter physics

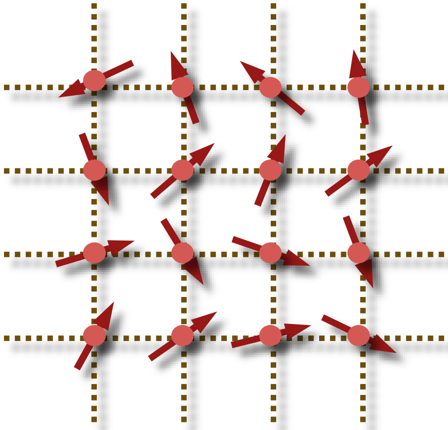


Berezinskii-Kosterlitz-Thouless phase transition

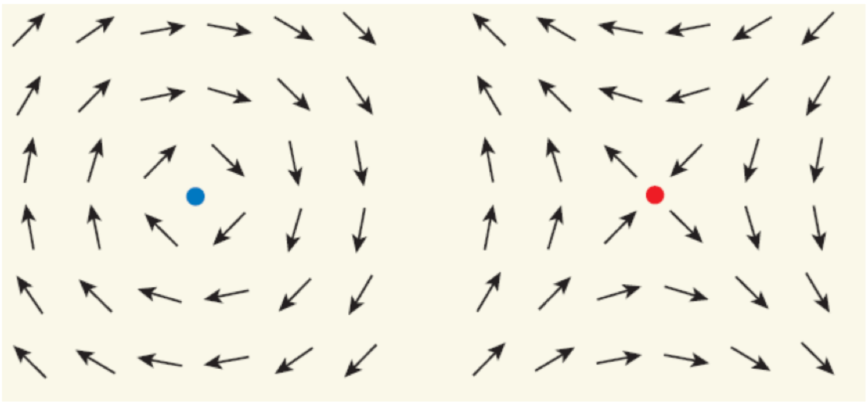
2D classical XY model with U(1) symmetry

$$H = -\sum_{\langle i,j \rangle} \vec{s_i} \cdot \vec{s_j} = -\sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)$$

Mermin-Wagner Theorem:
No continuous symmetry broken phase at finite temperature in any 1D and 2D systems.

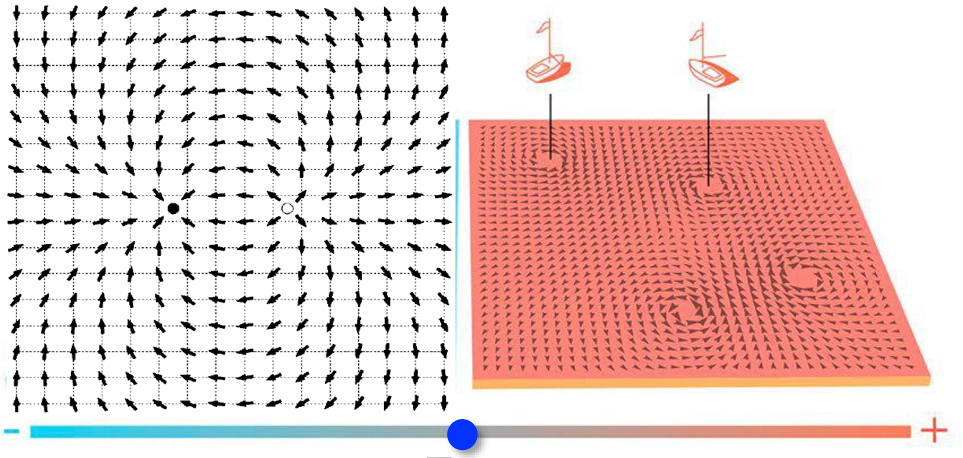


Thouless/Haldane/Kosterlitz



Topological charge
***q*= +1**

Topological charge
***q*= -1**



T_{BKT}

Low T **High T**

Key features of BKT transition

spin-spin correlation function characterizes the binding of vortex pairs

above T_{BKT},

$$G(r) = \langle e^{-i\varphi(r)} e^{i\varphi(0)} \rangle \sim e^{-r/\xi(T)}$$

$$\xi(T) \sim e^{b/\sqrt{T-T_{BKT}}}, b > 0$$

below T_{BKT},

$$G(r) \sim \left(\frac{r}{a}\right)^{\eta(T)}$$

spin stiffness

$$\rho_s = \frac{\partial^2 f}{\partial v^2}\Big|_{v=0}$$

twist field

$$\theta(\vec{r}) \to \theta(\vec{r}) + \vec{v} \cdot \vec{r}$$

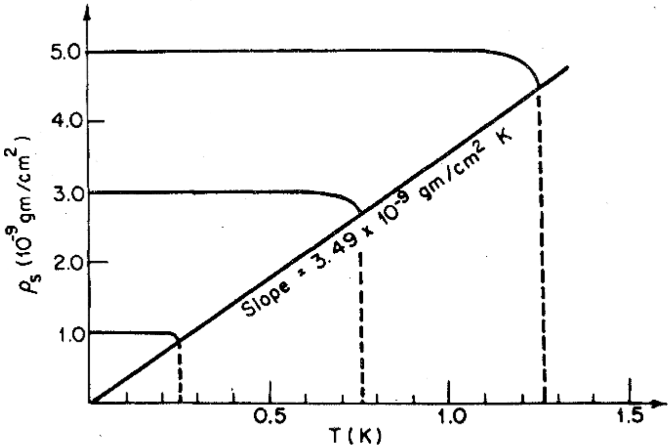
a universal jump in spin stiffness

$$\lim_{T \to T_{BKT}} \rho_s(T) = \frac{2}{q^2 \pi} T_{BKT}$$

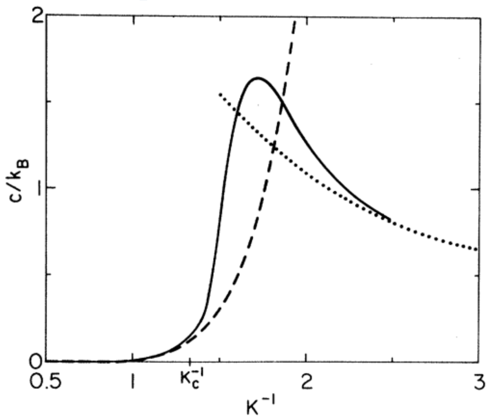
specific heat

infinite order phase transition

$$C_V \sim \xi^{-2}(T_+)$$



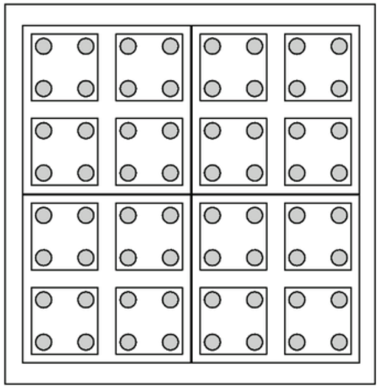
D. J. Bishop et al., PRB 22, 5171 (1980)



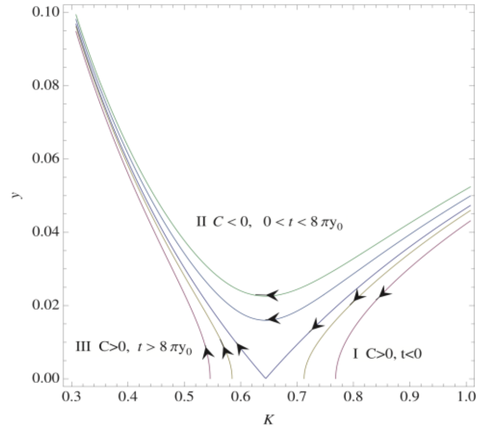
Sara A. Solla et al., PRB 23, 6008(1981)

RG method and Mont Carlo simulation

renormalization group Kosterlitz, Rep. Prog. Phys. 79 026001 (2016)



self-similarity

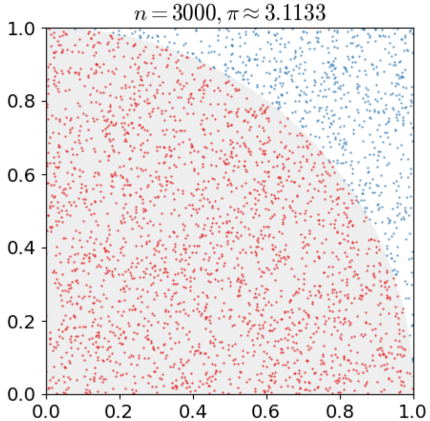


RG flow for XY model

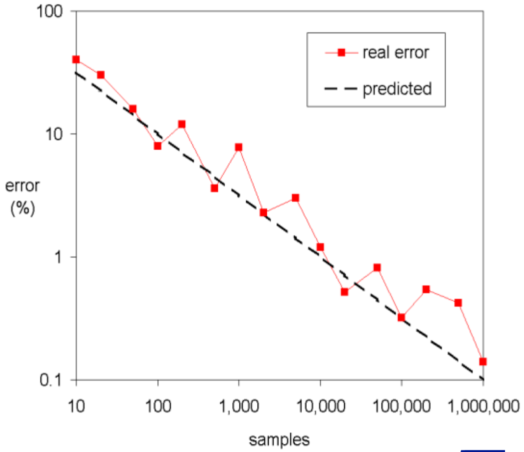
limitations:

- information only near fixed points
- hard to handle multiple topological defects

Monte Carlo method



evaluations of π



errors reduced by $1/\sqrt{N}$

limitations:

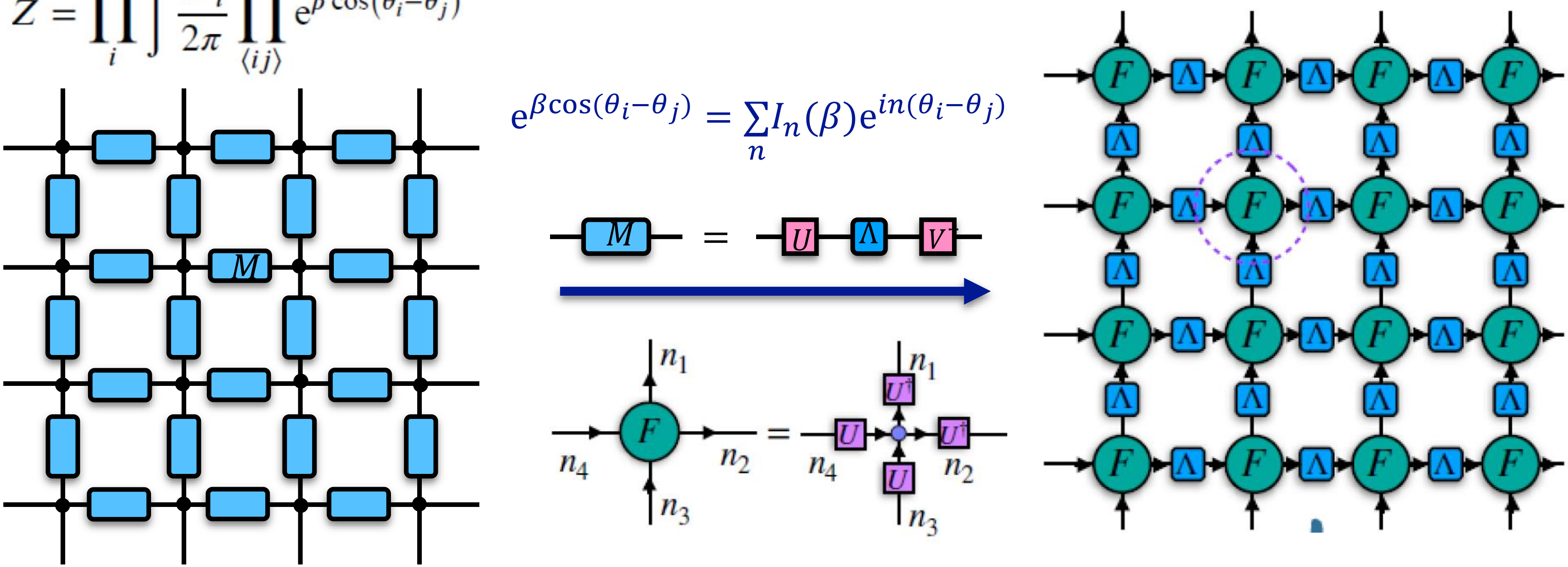
- finite size effect
- inefficiency in reaching the low-energy phase space
- No sharp criterion for transition

Tensor network approach to the 2D XY spin models

Approaching the Kosterlitz-Thouless transition for the classical XY model with tensor networks

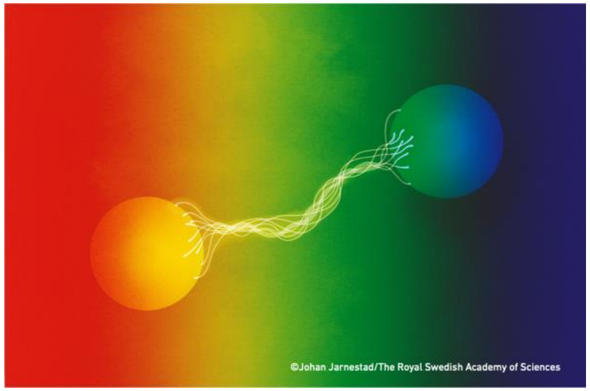
Laurens Vanderstraeten,[1,*] Bram Vanhecke,[1] Andreas M. Läuchli,[2] and Frank Verstraete[1]
[1] *Department of Physics and Astronomy, University of Ghent, Krijgslaan 281, 9000 Gent, Belgium*
[2] *Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria*

$$Z = \prod_i \int \frac{d\theta_i}{2\pi} \prod_{\langle ij \rangle} e^{\beta \cos(\theta_i - \theta_j)}$$



Key physical idea in our study

quantum entanglement: a powerful tool



Ill. Niklas Elmehed © Nobel Prize Outreach
Alain Aspect

Ill. Niklas Elmehed © Nobel Prize Outreach
John F. Clauser

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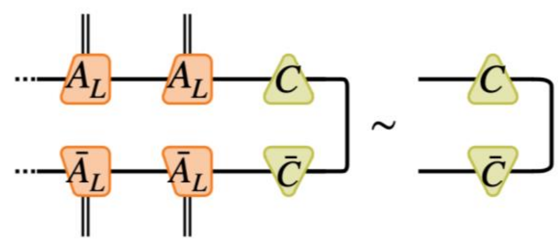
Anton Zeilinger

1D quantum correspondence

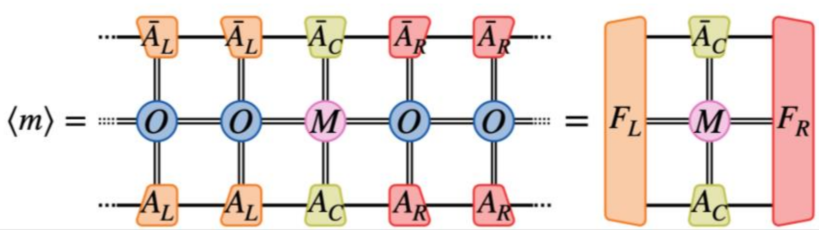
$$Z_{2D} = \mathrm{Tr}(\hat{T}^N), \quad \hat{H}_{1D} = -\frac{1}{\beta}\ln\hat{T} \qquad \hat{T}|\Psi\rangle = \Lambda_{max}|\Psi\rangle$$

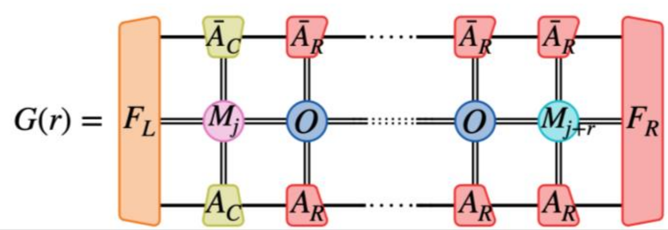
entanglement entropy

$$S_E = -\mathrm{Tr}(\rho_L \ln \rho_L), \qquad \rho_L = \mathrm{Tr}_R|\Psi\rangle\langle\Psi| =$$



expectational values



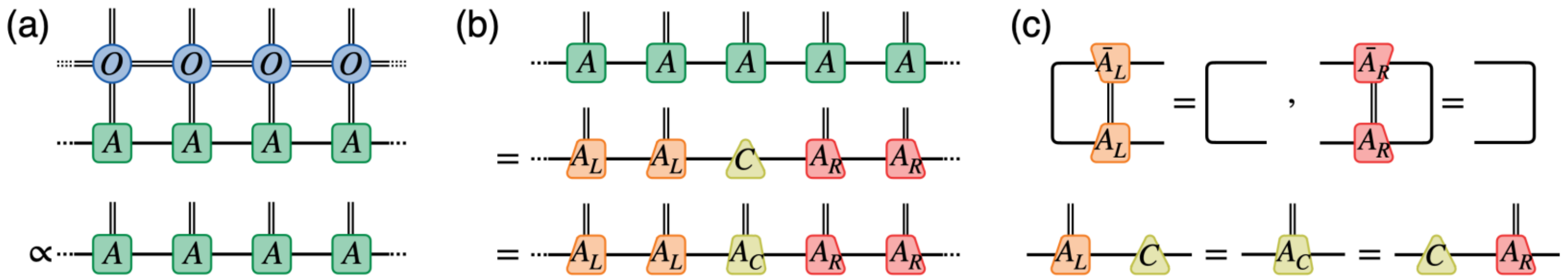


Uniform variational matrix product state

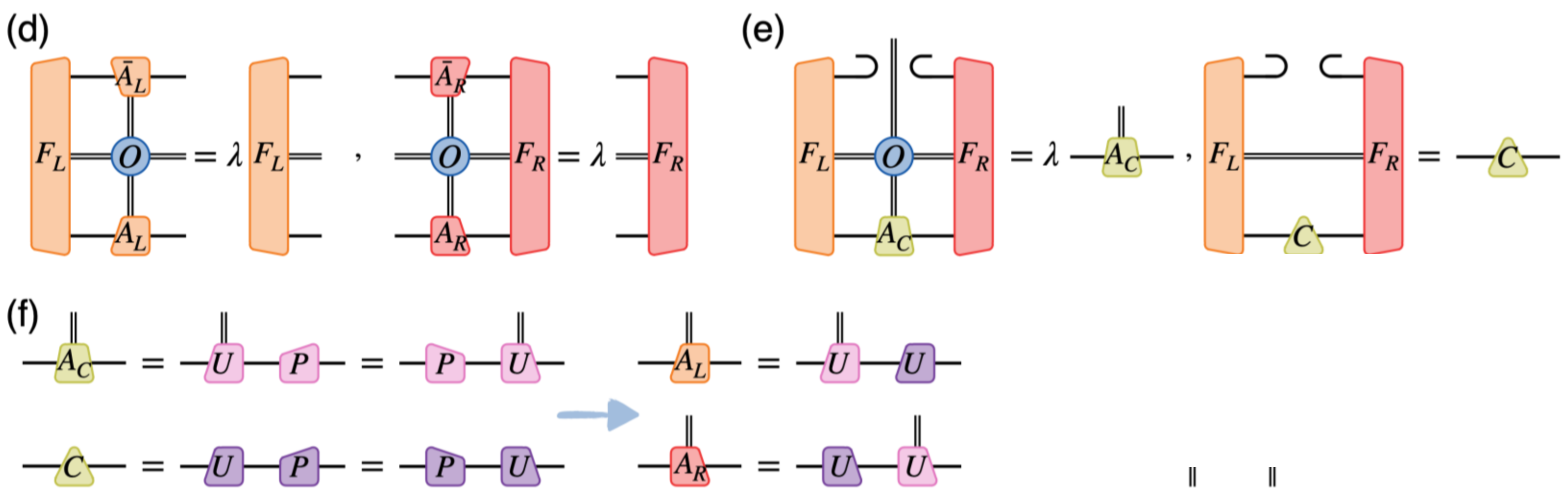
M. T. Fishman, L. Vanderstraeten, V. Zauner-Stauber, J. Haegeman, and F. Verstraete, Phys. Rev. B **98**, 235148 (2018).

$$\hat{T}|\Psi(A)\rangle = \Lambda_{max}|\Psi(A)\rangle \longleftrightarrow max\frac{\langle\Psi(A)|\hat{T}|\Psi(A)|\rangle}{\langle\Psi(A)|\Psi(A)\rangle}$$

mixed canonical form

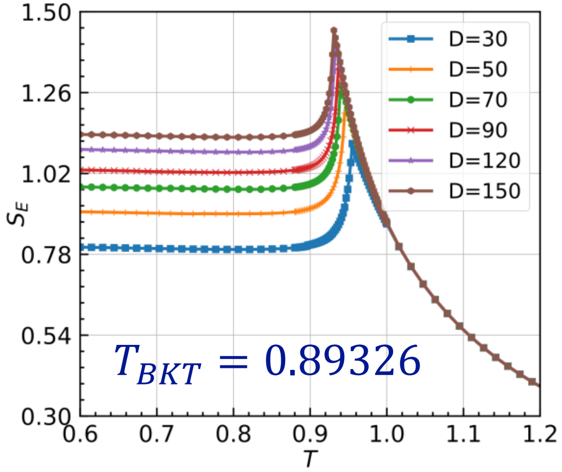


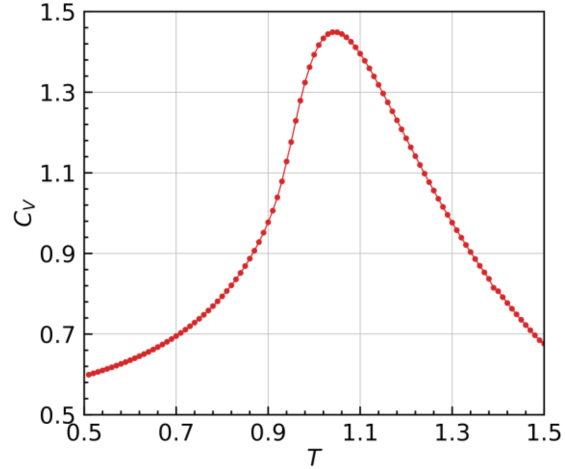
variational approximation process

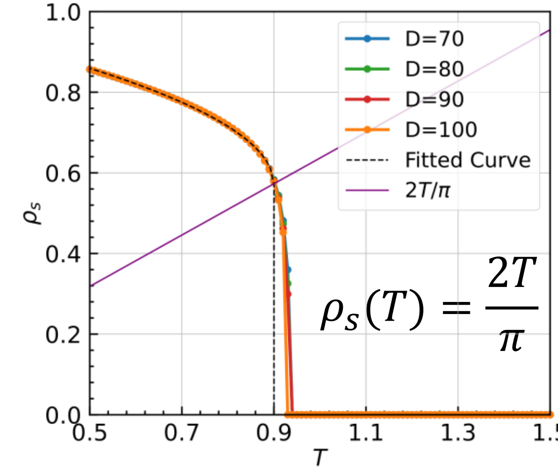


2D XY spin model: BKT transition

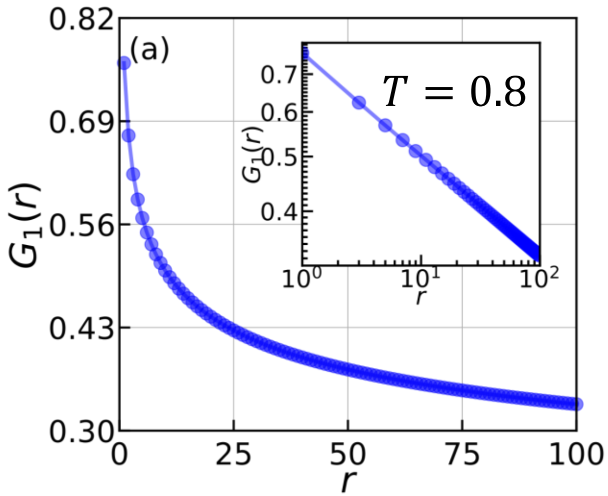
entanglement and thermodynamics

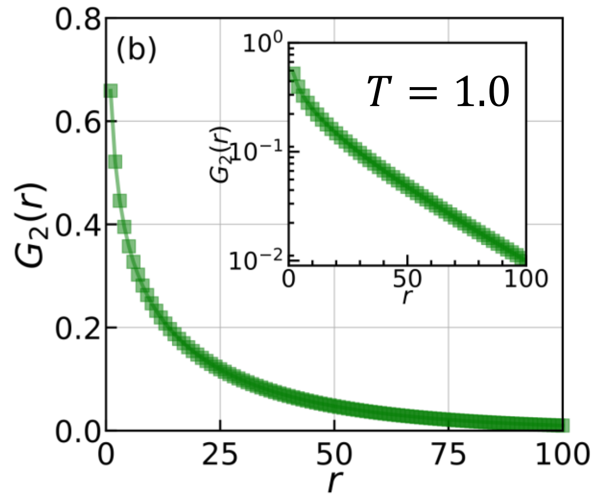


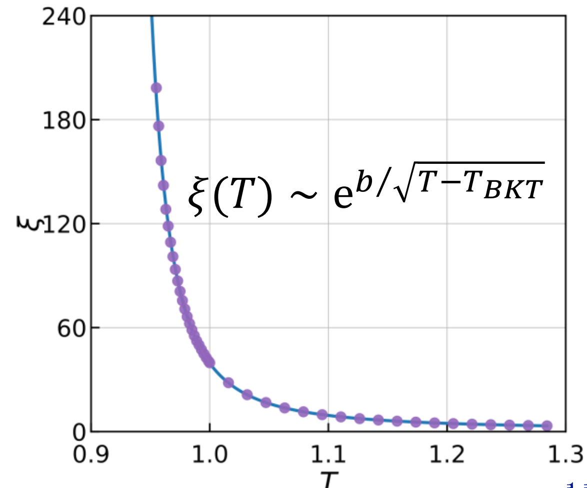




correlation properties







Our works on various problems of 2D XY spin models

- Hybrid Berezinskii-Kosterlitz-Thouless and Ising topological phase transition in the generalized two-dimensional XY model using tensor networks
  Feng-Feng Song & Guang-Ming Zhang, Phys. Rev. B **103**, 024518 (2021)

- Phase coherence of pairs of Cooper pairs as quasi-long-range order of half-vortex pairs in a two-dimensional bilayer system
  Feng-Feng Song & Guang-Ming Zhang, Phys. Rev. Lett. **128**, 195301 (2022)

- Two-stage melting of an inter-component Potts long-range order in two dimensions
  Feng-Feng Song & Guang-Ming Zhang, Phys. Rev. B **107**, 165129 (2023)

- Tensor network approach to the two-dimensional fully frustrated XY model and a chiral ordered phase
  Feng-Feng Song & Guang-Ming Zhang, Phys. Rev. B **105**, 134516 (2022)

- Tensor network approach to the fully frustrated XY model on a Kagome lattice with a fractional vortex-antivortex pairing transition
  Feng-Feng Song & Guang-Ming Zhang, Phys. Rev. B **108**, 014424 (2023)

Fully frustrated XY spin model on a Kagome lattice

F. F. Song & G. M. Zhang, Phys. Rev. B **108**, 014424 (2023).

PHYSICAL REVIEW RESEARCH **3**, 013041 (2021)

Solving frustrated Ising models using tensor networks

Bram Vanhecke,[1,*] Jeanne Colbois,[2,†] Laurens Vanderstraeten,[1] Frank Verstraete,[1] and Frédéric Mila[2]
[1] *Department of Physics and Astronomy, University of Ghent, Krijgslaan 281, 9000 Gent, Belgium*
[2] *Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*

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Motivated by the recent success of tensor networks to calculate the residual entropy of spin ice and kagome Ising models, we develop a general framework to study frustrated Ising models in terms of infinite tensor networks that can be contracted using standard algorithms for infinite systems. This is achieved by reformulating the problem as local rules for configurations on overlapping clusters chosen in such a way that they relieve the frustration, i.e., that the energy can be minimized independently on each cluster. We show that optimizing the choice of clusters, including the weight on shared bonds, is crucial for the contractibility of the tensor networks, and we derive some basic rules and a linear program to implement them. We illustrate the power of the method by computing the residual entropy of a frustrated Ising spin system on a kagome lattice with next-next-nearest-neighbor interactions, vastly outperforming Monte Carlo methods in speed and accuracy. The extension to finite temperatures is briefly discussed.

Antiferromagnetic Ising model on a Kagome/triangular lattice

Phase coherence of Cooper pairs of Kagome superconductors

From the Ginsburg-Landau free energy density of superconductivity in the external gauge field,

$$\mathcal{F}_{GL} = a|\psi|^2 + \frac{b}{2}|\psi|^4 + \frac{1}{2m^*}\left|\left(\frac{\hbar}{i}\nabla - \frac{e^*}{c}\vec{A}\right)\psi\right|^2,$$

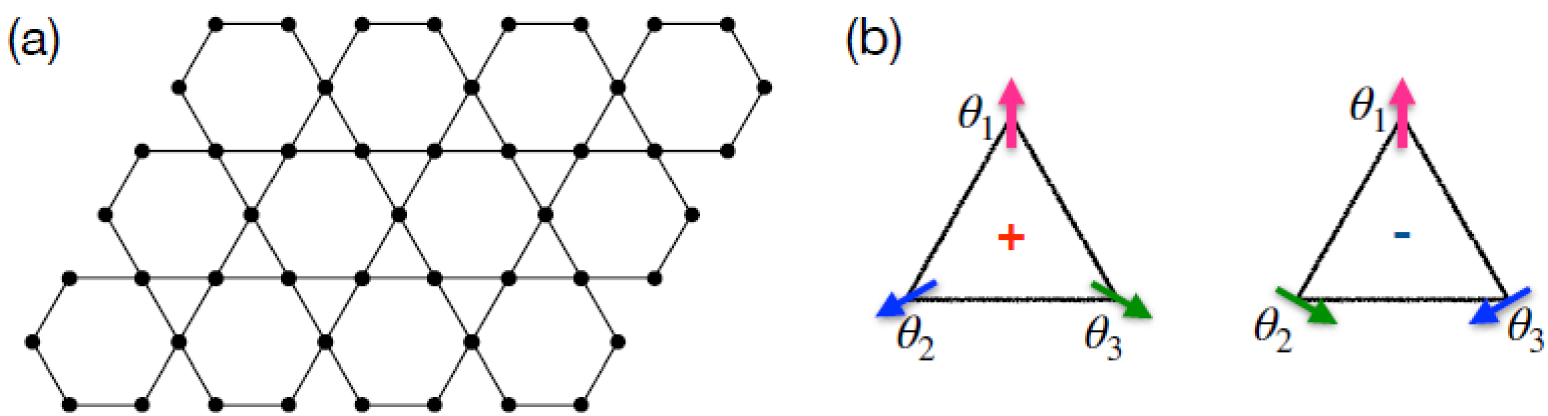
where $\psi(\vec{r}) = \langle c_\uparrow^\dagger(\vec{r}) c_\downarrow^\dagger(\vec{r})\rangle$ $\psi(\vec{r}) = |\psi(\vec{r})| e^{i\theta(\vec{r})}$

When the magnitude of the local order parameter field is frozen and the external gauge field makes half quantum flux per triangular plaquette, $\sum_{\langle i,j\rangle\in\triangle} A_{ij} \equiv \pi \pmod{2\pi}$,

the phase fluctuations of the Cooper pairs is effectively described by

$$H = J_1 \sum_{\langle i,j\rangle} \cos(\theta_i - \theta_j),$$

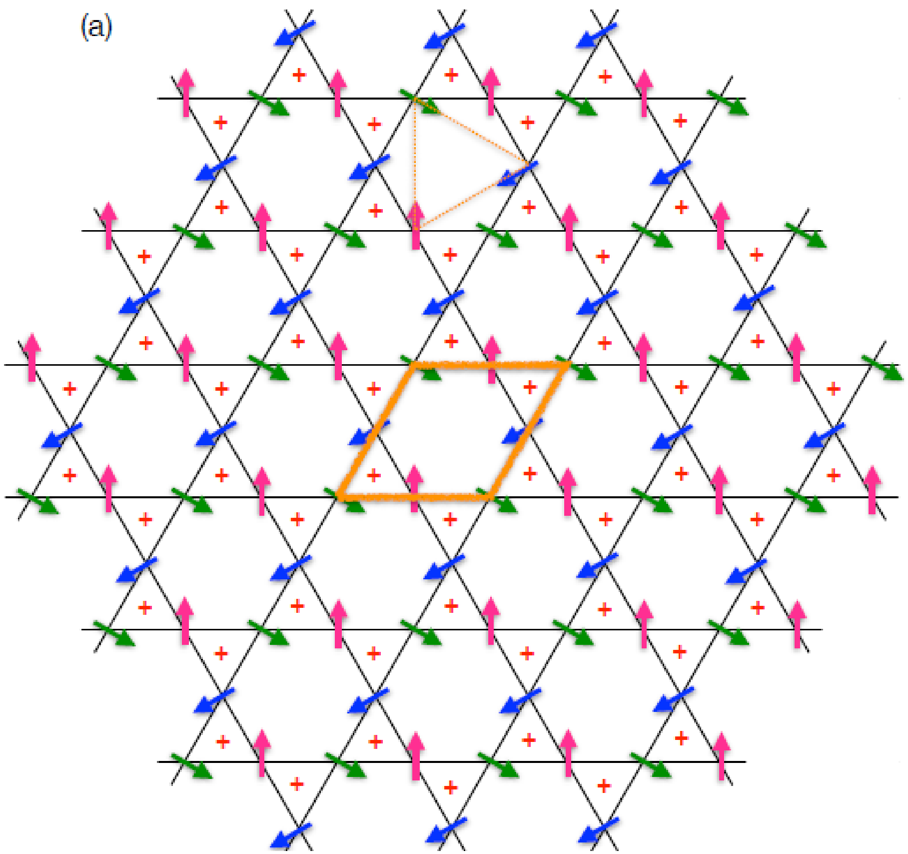
$J_1 > 0$ denotes a **fully frustrated** XY model.



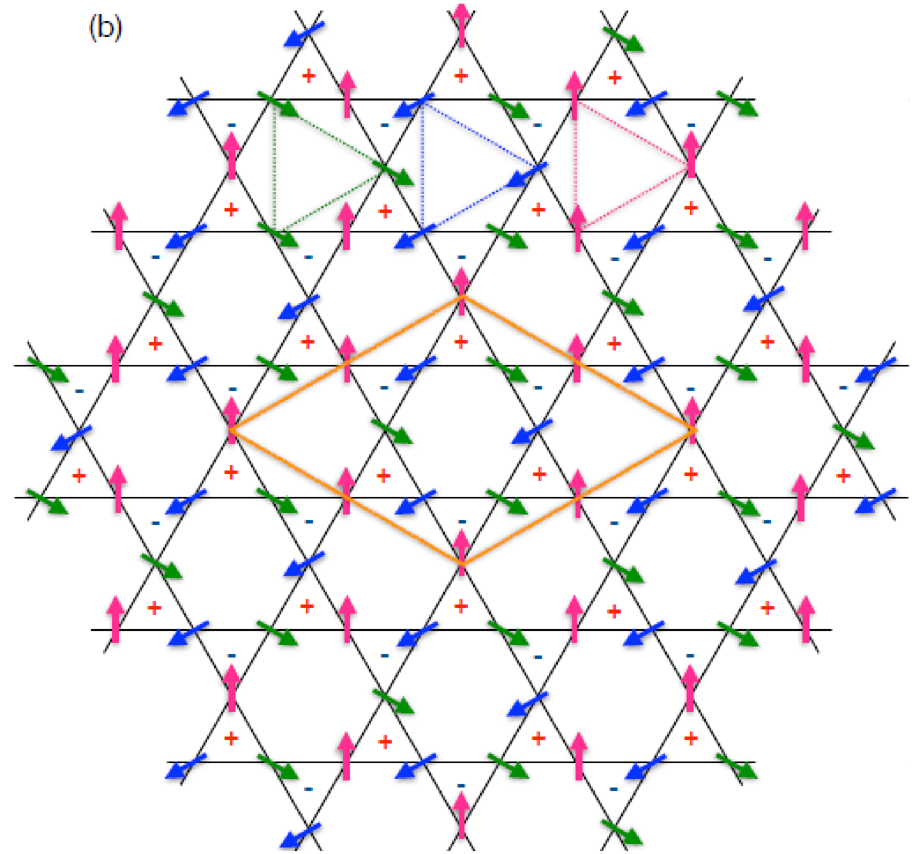
The ground state has a massive degeneracy due to the presence of chirality degrees of freedom.

Two periodic pattern of chirality as the possible ground states

$$H = J_1 \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) + J_2 \sum_{\langle\langle i,j \rangle\rangle} \cos(\theta_i - \theta_j),$$

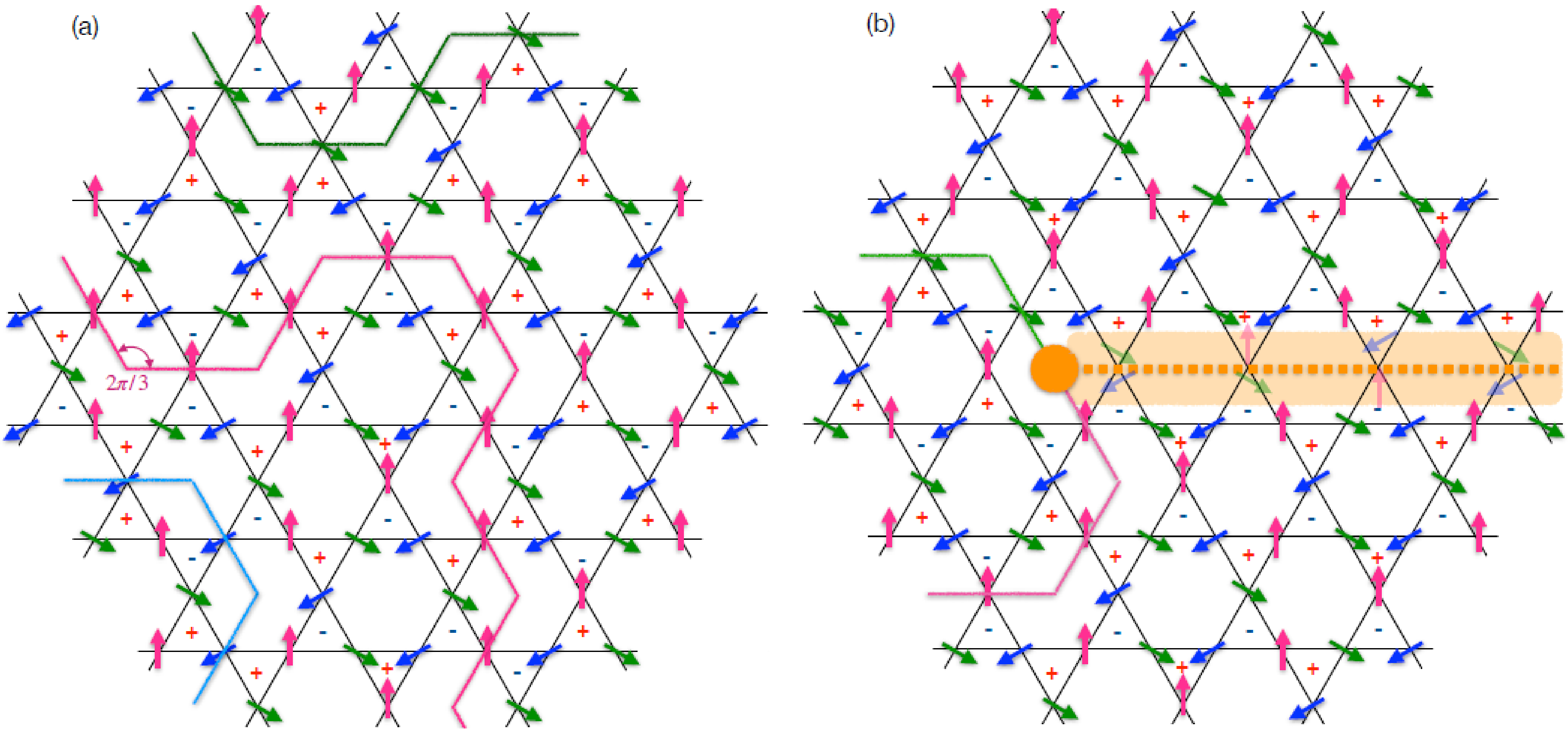


"q=0" **pattern for** $J_2 > 0$

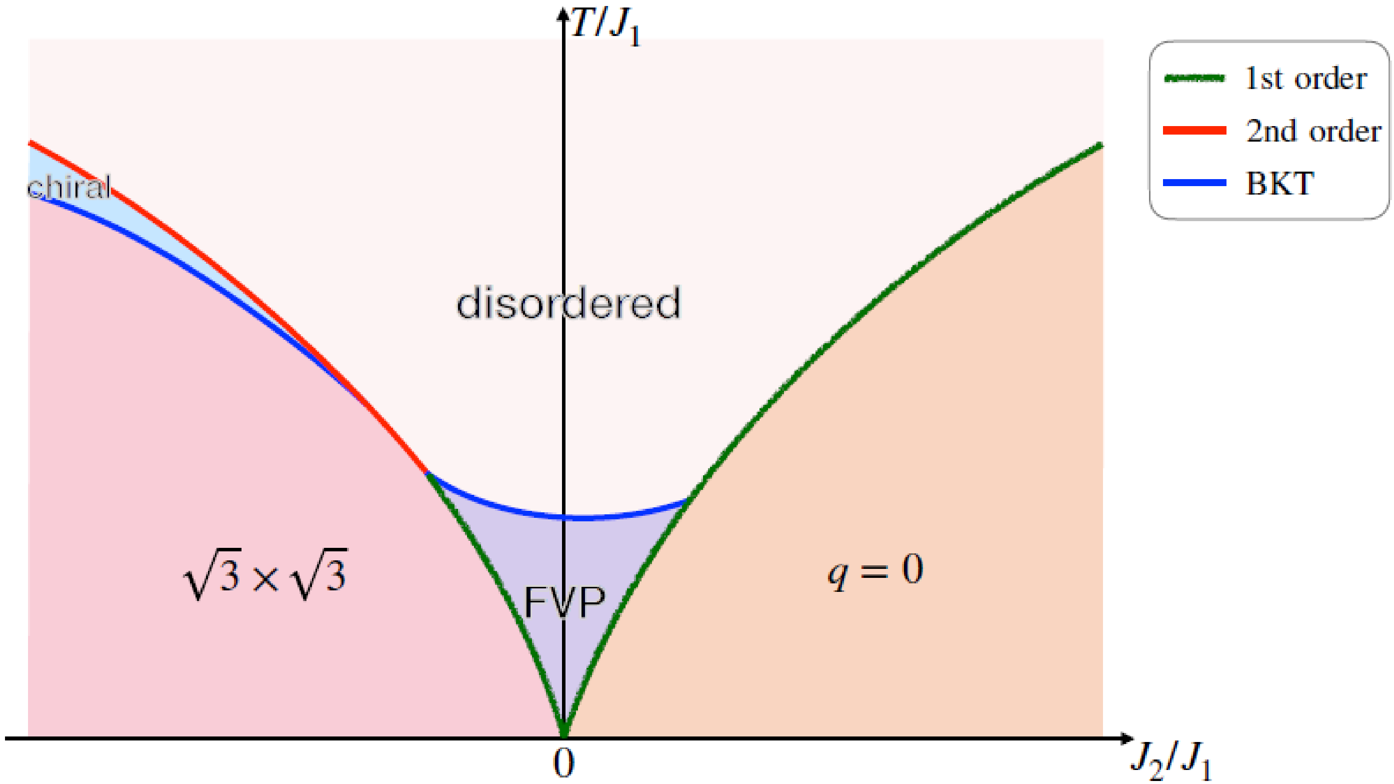


$\sqrt{3} \times \sqrt{3}$ **pattern for** $J_2 < 0$

For the model with a finite J_2, there are domain wall excitations and 1/3 fractional vortex excitations in the low-temperature phase.

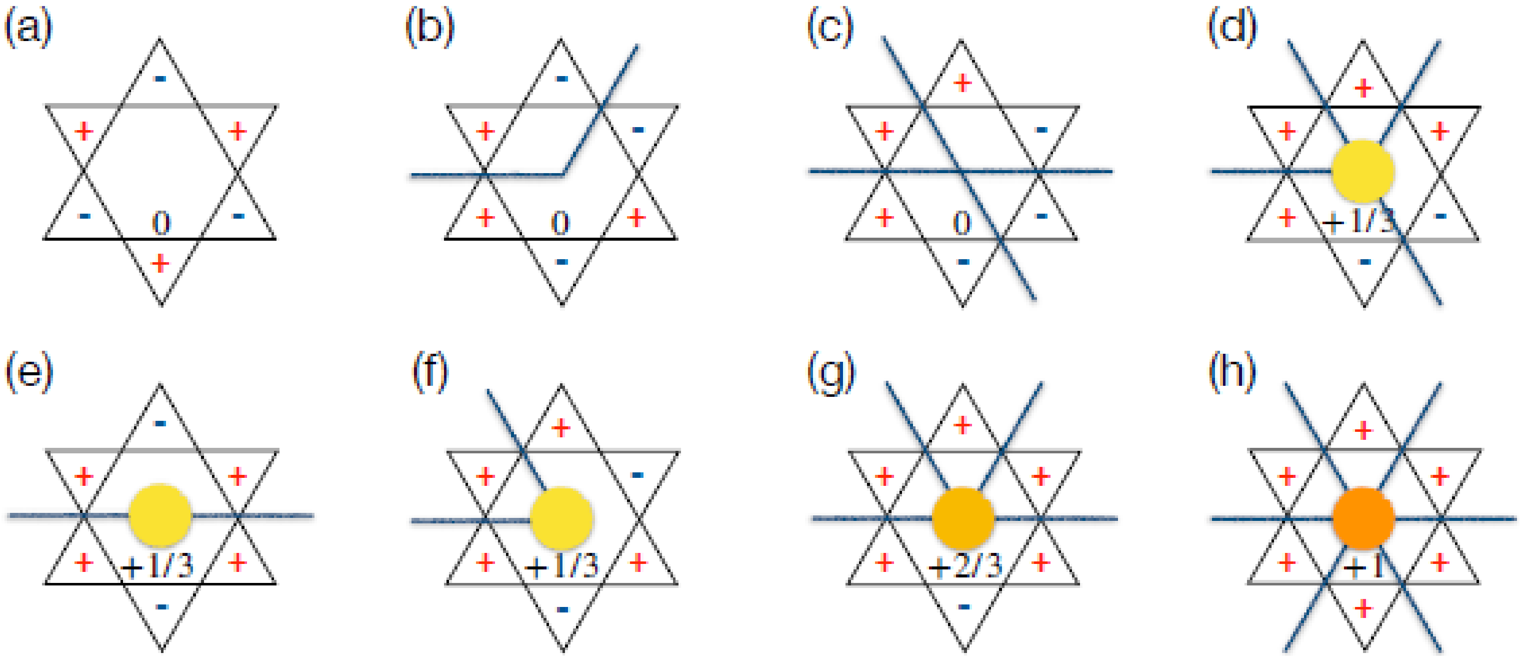


Proposed phase diagram for the general fully frustrated model



$J_2=0$ corresponds to the disordered pattern of chirality.

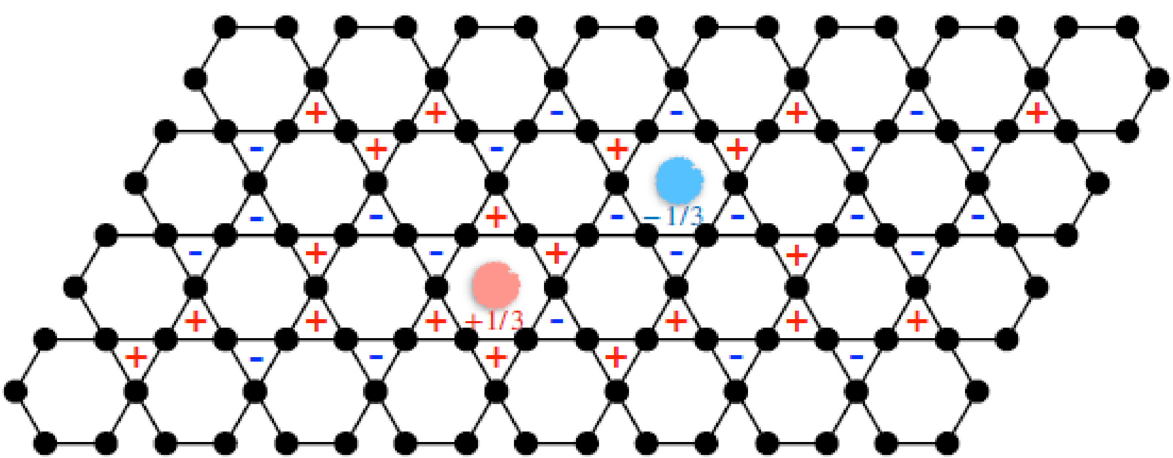
Simplified representation of various topological excitations



$$q_h = \frac{1}{3}\sum_{t=1}^{6} q_t,$$

$$q_t = \pm\frac{1}{2}$$

a charge neutral pair of 1/3 vortex and anti-vortex

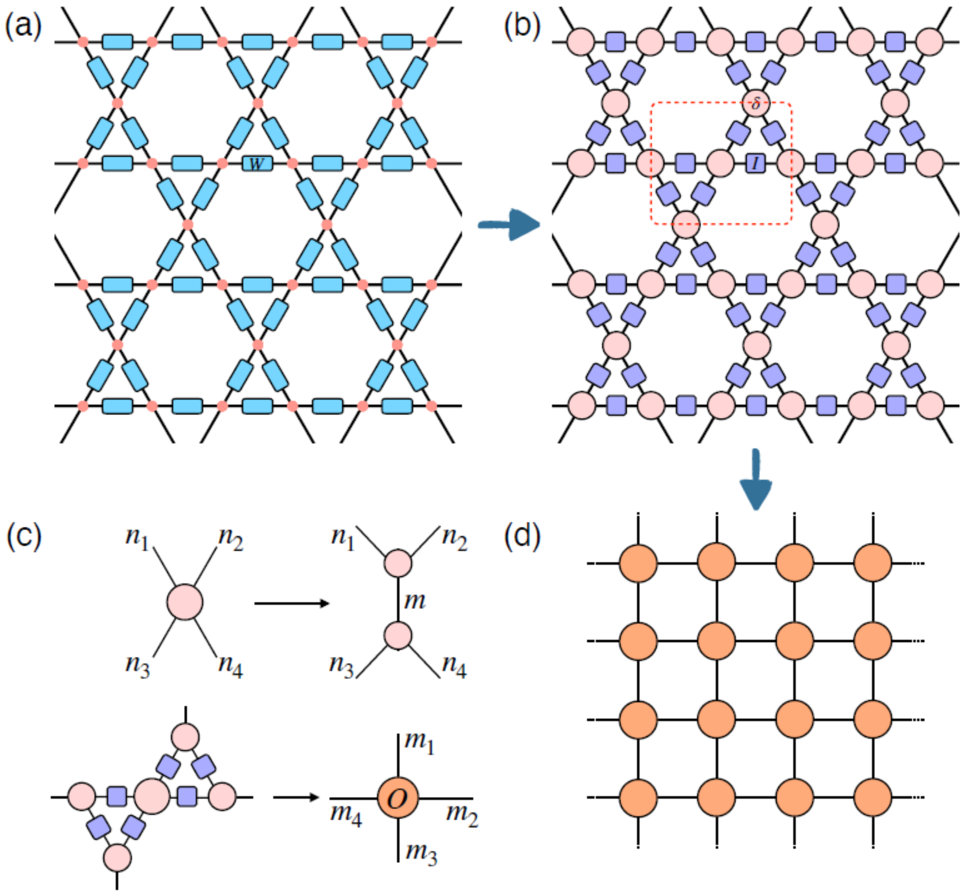


The 1/3 fractional vortex or anti-vortex is related to a cluster of three Cooper pairs, and their bounded neutral pair with algebraic correlation represents the phase coherence of the so-called "charge-6e superconductivity".

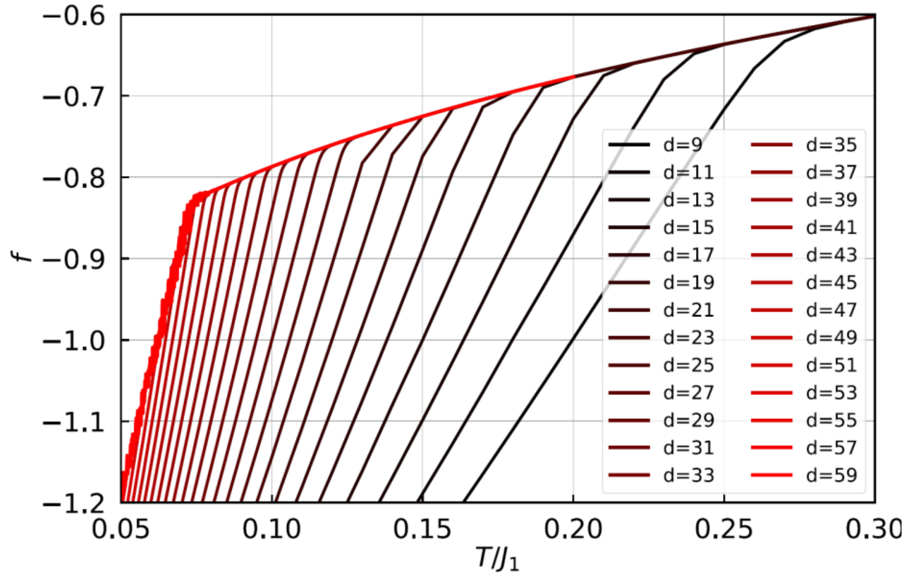
Tensor network representation of the partition function

$$Z = \prod_i \int \frac{d\theta_i}{2\pi} \prod_{\langle i,j \rangle} W(\theta_i, \theta_j),$$

$$W(\theta_i, \theta_j) = e^{-\beta J_1 \cos(\theta_i - \theta_j)} = \sum_{n_l} I_{n_l}(-\beta) e^{i n_l (\theta_i - \theta_j)},$$



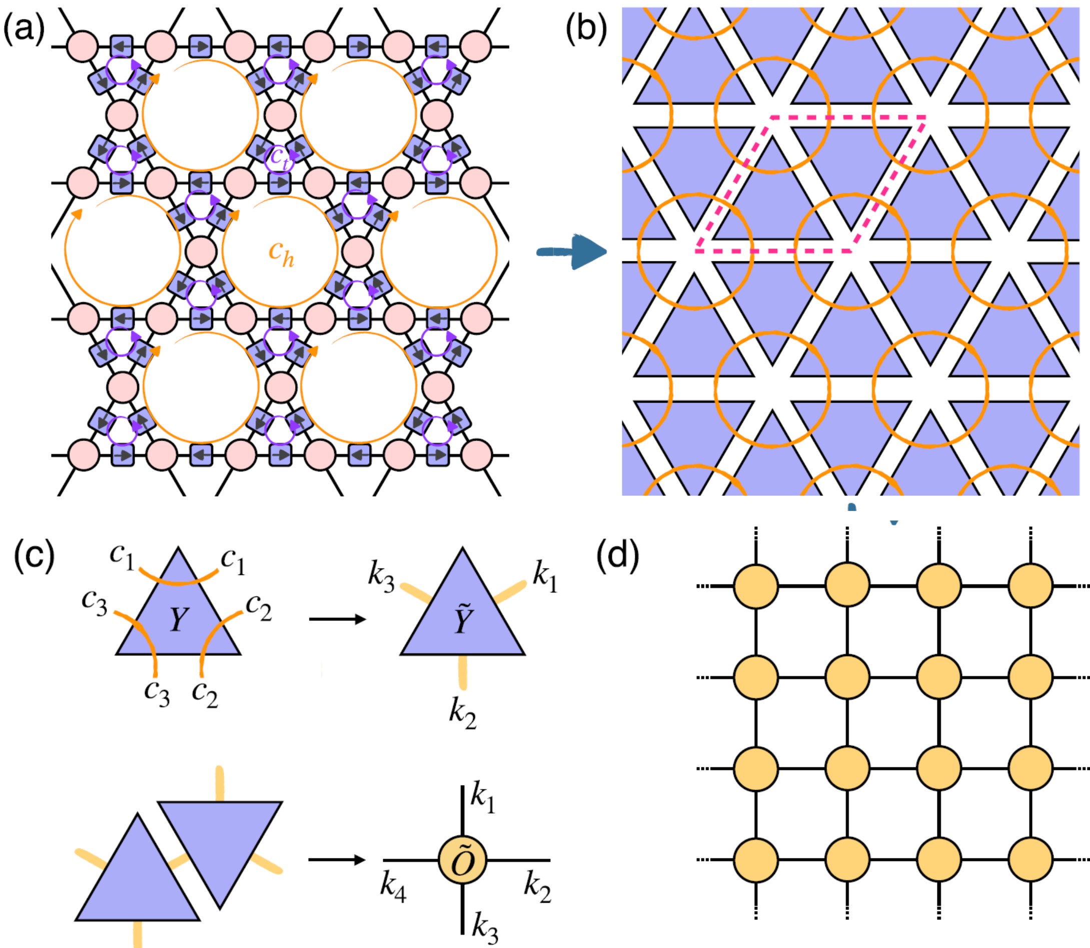
The free energy density strongly depends on the cutoff of the Fourier transformation *d.*



Tensor network representation of the partition function

$$Z = \prod_i \int \frac{\mathrm{d}\theta_i}{2\pi} \prod_{\langle i,j\rangle} W(\theta_i, \theta_j),$$

$$W(\theta_i, \theta_j) = \mathrm{e}^{-\beta J_1 \cos(\theta_i - \theta_j)} = \sum_{n_l} I_{n_l}(-\beta) \mathrm{e}^{i n_l (\theta_i - \theta_j)},$$



Duality transformation

$$n_l = c_h + c_t,$$

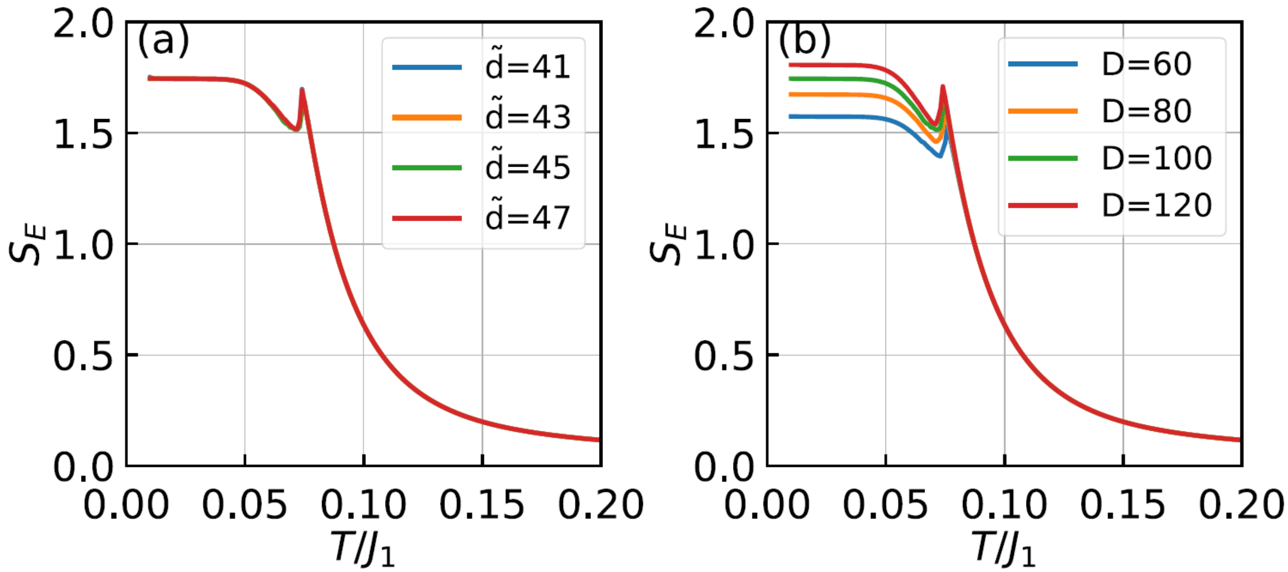
$$Z = \sum_{\{c_h\}} \prod_t \sum_{c_t=-\infty}^{\infty} \prod_{h_t=1}^{3} I_{c_{h_t}+c_t}(-\beta),$$

$$k_1 = c_1 - c_2, \quad k_2 = c_2 - c_3,$$

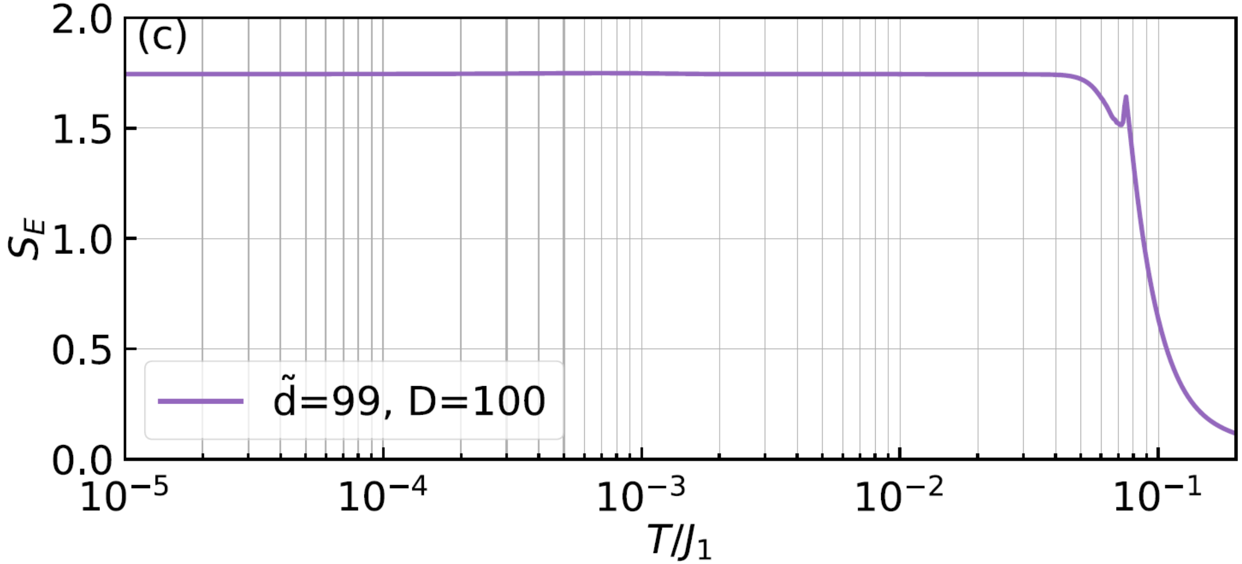
$$k_3 = c_3 - c_1,$$

$$Z = \mathrm{tTr} \prod_s \tilde{O}^{k_3,k_4}_{k_1,k_2}(s).$$

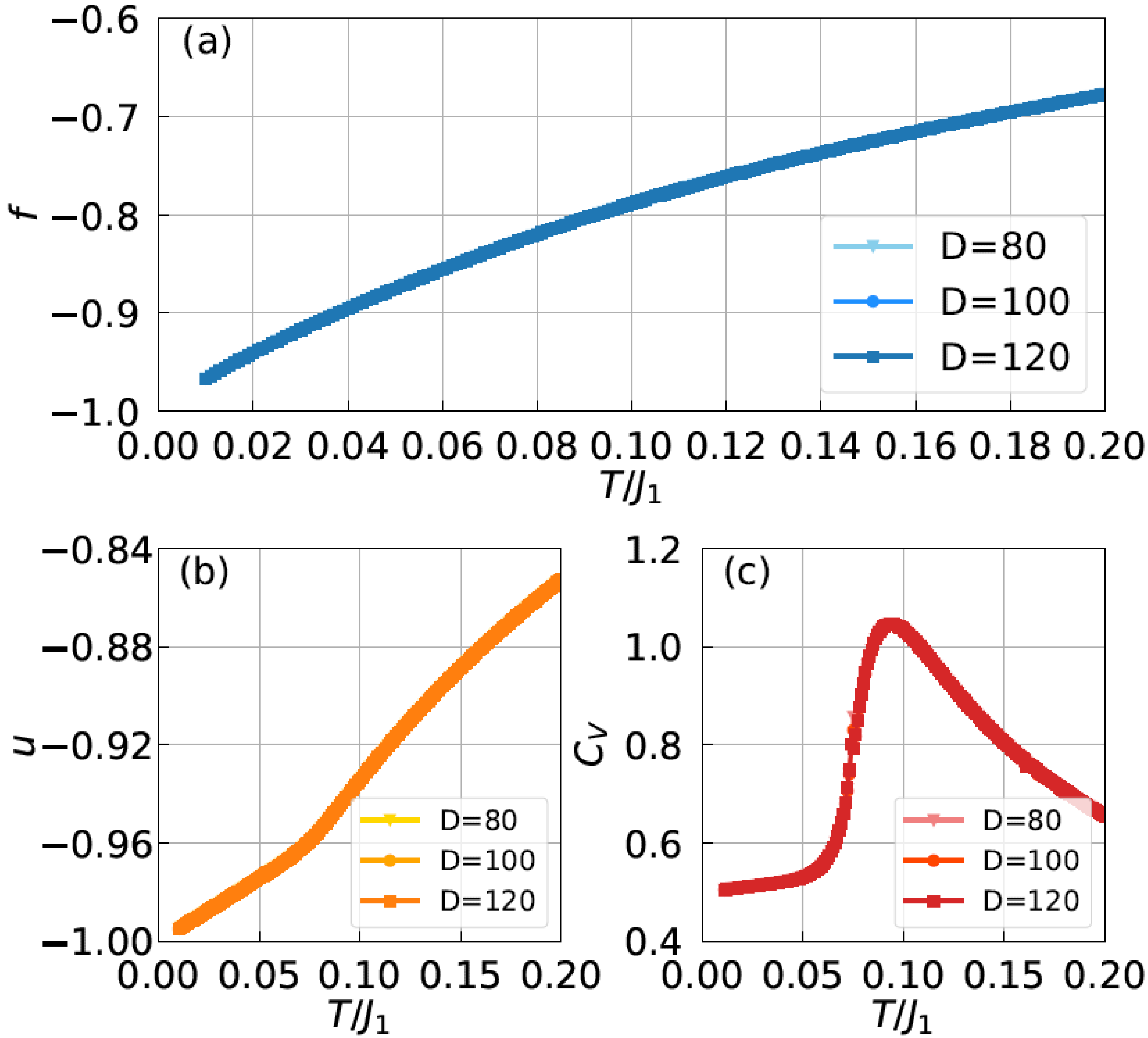
Numerical results of the entanglement entropy



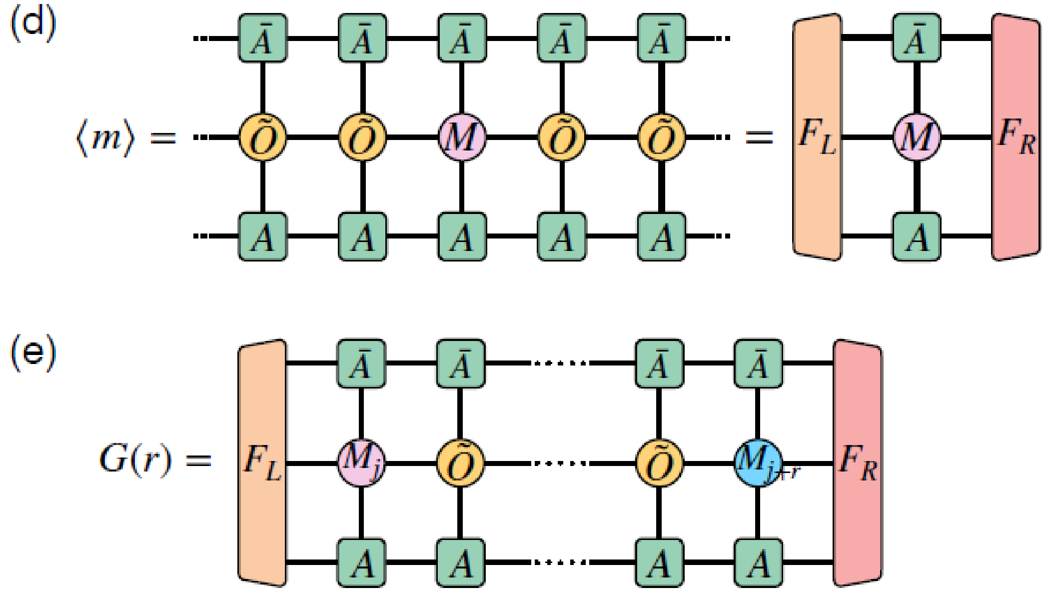
$$T_c \approx \frac{\pi\sqrt{3}}{72} J_1 \approx 0.075 J_1$$



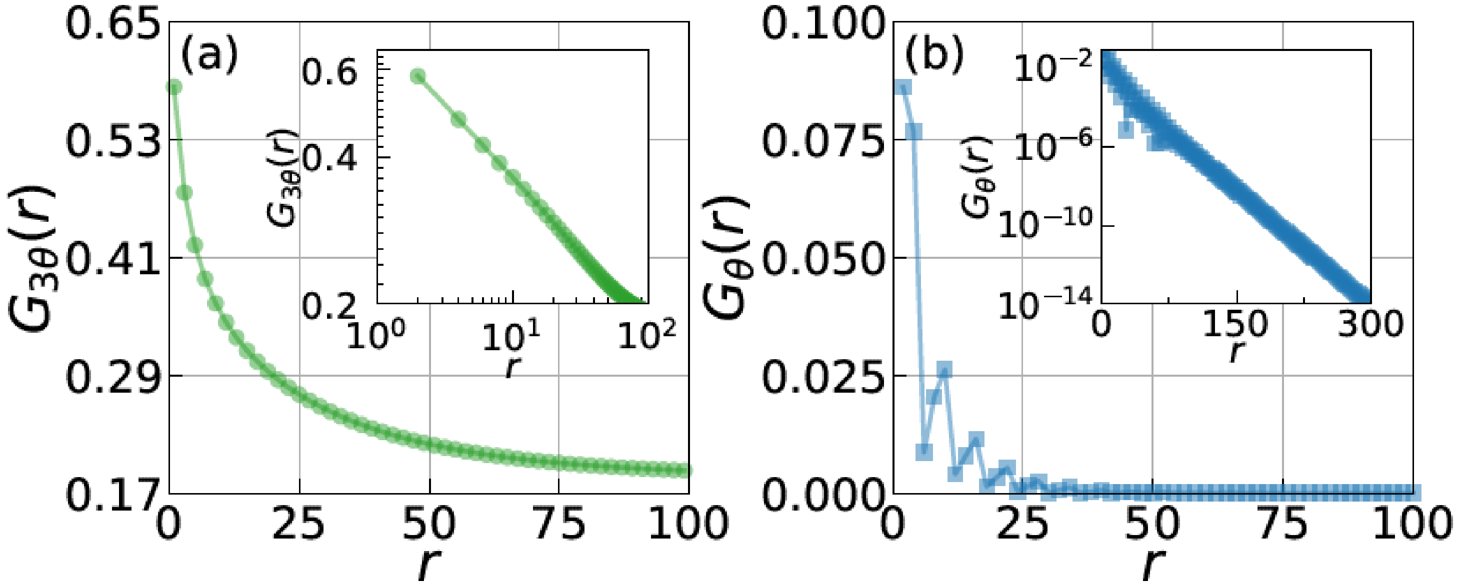
Numerical results of free energy, internal energy, specific heat



Correlation functions & numerical results at low T phase



$$G_{3\theta}(r) = \langle \cos(3\theta_j - 3\theta_{j+r}) \rangle \qquad G_{\theta}(r) = \langle \cos(\theta_j - \theta_{j+r}) \rangle$$



Conclusion

- A tensor network approach is established for the 2D fully frustrated classical XY spin Kagome lattice model, and the partition function is written as a product of 1D transfer matrix operators.

- The eigen-equation of 1D quantum operator can be solved by the uniform variational matrix product state algorithm. The singularity of the entanglement entropy provides a stringent criterion for various phase transitions.

- In the thermodynamic limit, we proved that the Kagome model exhibits a single BKT phase transition only, which is driven by the unbinding of 1/3 fractional vortex-antivortex pairs determined.

Thanks for your attention!

Fully frustrated XY spin model on a square lattice

F. F. Song & G. M. Zhang, Phys. Rev. B **105**, 134516 (2022).

Fully frustrated 2D XY spin model

From the Ginsburg-Landau free energy density of superconductivity in the external gauge field,

$$\mathcal{F}_{GL} = a|\psi|^2 + \frac{b}{2}|\psi|^4 + \frac{1}{2m^*}\left|\left(\frac{\hbar}{i}\nabla - \frac{e^*}{c}\vec{A}\right)\psi\right|^2,$$

where $\psi(\vec{r}) = \langle c^\dagger_\uparrow(\vec{r}) c^\dagger_\downarrow(\vec{r})\rangle$ $\qquad \psi(\vec{r}) = |\psi(\vec{r})|e^{i\theta(\vec{r})}$

When the magnitude of the local order parameter field is frozen and the external gauge field makes half quantum flux per triangular plaquette, $\sum_{\langle i,j\rangle\in\triangle} A_{ij} \equiv \pi \pmod{2\pi}$,

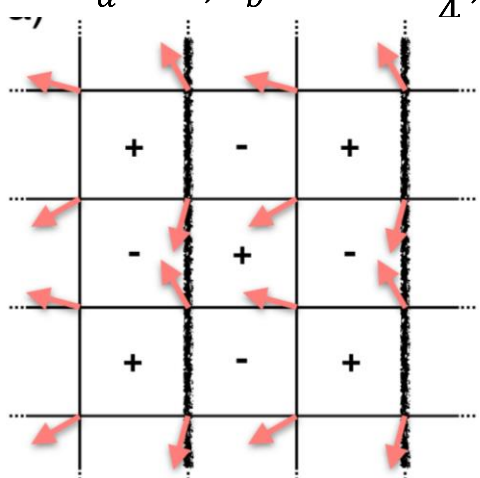
$$H = -J\sum_{\langle ij\rangle}\cos(\theta_j - \theta_i + A_{ij})$$

As a result of minimization of local interaction, new degrees of freedom are formed:

$$\max[\sum\cos(\theta_j - \theta_i + A_{ij})] \longrightarrow \theta_a = \theta, \theta_b = \theta + \tau\frac{\pi}{4}, \theta_c = \theta + \tau\frac{\pi}{2}, \theta_d = \theta - \tau\frac{\pi}{4}$$

chirality $\quad \tau = \pm 1$

topological charge $\quad q_i = \pm\frac{1}{2}$

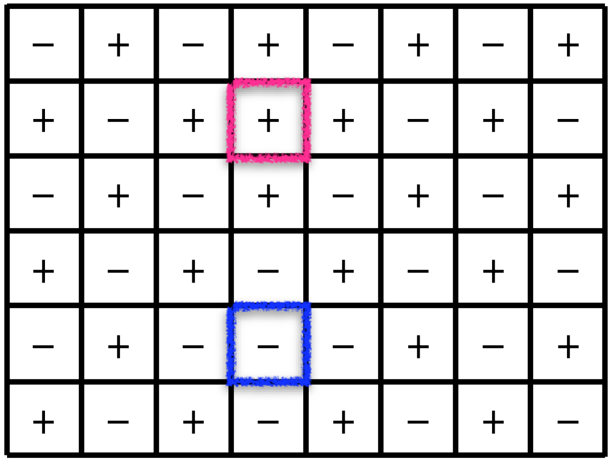


checkerboard pattern like AFM Ising model

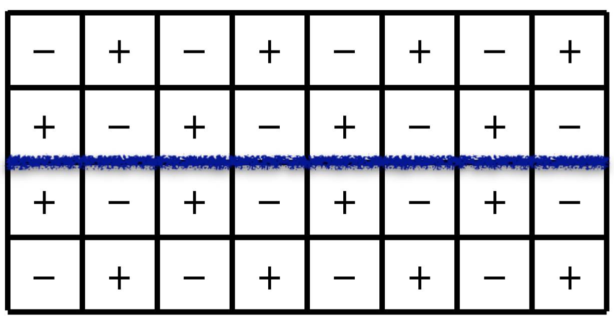
Z_2 degenerate ground state

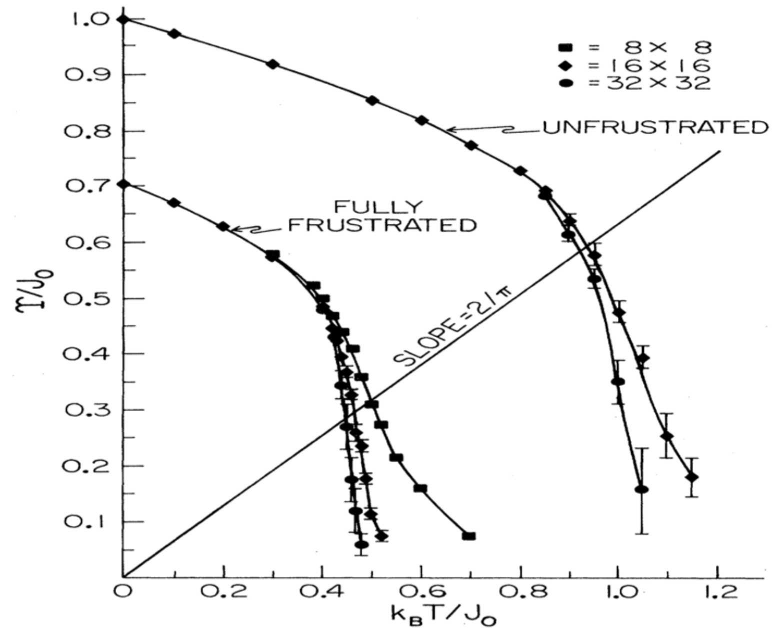
Phase transitions with two different topological excitations

vortices



domain walls





S. Teitel and C. Jayaprakash, Phys. Rev. B 27, 598 (1983).

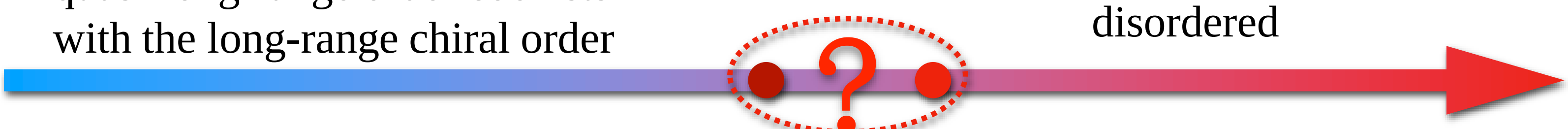
finite energy per length

S. E. Korshunov, Phys. Rev. Lett. **88**, 167007(2002).

controversial phase transitions

quasi-long-range order coexists
with the long-range chiral order

disordered



$T_{BKT} \leq T_{Ising}$

differ by at most 1-2%

Controversial phase transitions

There is not yet a general consensus on the critical behavior of the FFXY model.

	Model	Method	Transitions	Chiral exponents
(1983)	$FFXY_{sq}$	MC ($L \leq 32$)		Consistent with Ising
(1984)	$FFXY_{tr}$	MC ($L \leq 32$)	2tr	
(1984)	$FFXY_{sq}$	MC ($L \leq 45$)	2tr, $\delta \approx 0.02$	
(1985)	$FFXY_{sq}$		$\delta \geq 0$	
(1985)	$FFXY_{sq}$, CG	RG	1tr	
(1985)	2cXY	RG	1tr	
(1986)	$FFXY_{tr}$	MC ($L \leq 72$)	1–2tr, $\delta \lesssim 0.01$	Consistent with Ising
(1986)	$FFXY_{tr}$	MC ($L \leq 72$)	1tr	
(1986)	$FFXY_{sq}$	MC ($L \leq 100$)	1tr	
(1986)	2cXY	Real-space RG	1tr	
(1988)	CG	MC ($L \leq 30$)	1tr	
(1989)	CG	MC ($L \leq 50$)	2tr, $\delta \approx 0.03$	
(1989)	CG	MC ($L \leq 48$)	1tr	
(1990)	$FFXY_{sq}$	TM MC ($L \leq 12$)	1tr	$\nu \approx 1$, $\eta = 0.40(2)$
27] (1991)	$FFXY_{sq}$	MC ($L \leq 40$)	1tr	$\nu = 0.85(3)$, $\eta = 0.31(3)$
27] (1991)	$FFXY_{tr}$	MC ($L \leq 40$)	1tr	$\nu = 0.83(4)$, $\eta = 0.28(4)$
(1991)	$FFXY_{sq}$	MC ($L \leq 128$)	1–2tr	$\nu = 1.009(26)$
(1991)	IsXY ($C = -0.2885$)	MC ($L \leq 32$)	1–2tr	$\nu = 0.84(3)$
(1991)	FXY_{J_1,J_2}	MC ($L \leq 150$)	1tr	$\nu = 0.9(2)$, $\eta = 0.4(1)$
(1992)	SOS-Is	TM ($L \leq 7$)	1tr	$\nu = 1.0(1)$, $\eta = 0.26(1)$
(1992)	$FFXY_{sq}$	MC ($L \leq 240$)	1–2tr, $\delta \gtrsim -0.07$	$\nu = 0.875(35)$
45] (1992)	QLJJ ($E_x/E_y = 1$)	TM QMC		$\nu = 0.81(4)$, $\eta = 0.47(4)$
45] (1992)	QLJJ ($E_x/E_y = 3$)	TM QMC		$\nu = 1.05(6)$, $\eta = 0.27(3)$
(1993)	$FFXY_{sq}$	TM MC ($L \leq 14$)	1tr	$\nu = 0.80(5)$, $\eta = 0.38(2)$
(1994)	CG	MC ($L \leq 30$)	2tr, $\delta \approx 0.04$	$\nu = 0.84(3)$, $\eta = 0.26(4)$
(1994)	$FFXY_{sq}$	MC ($L \leq 48$)	2tr, $\delta \approx 0.03$	$\nu = 0.813(5)$, $\beta = 0.089(8)$
(1994)	19-vertex model	TM ($L \leq 15$)	1tr	$\nu = 0.81(3)$, $\eta = 0.28(2)$

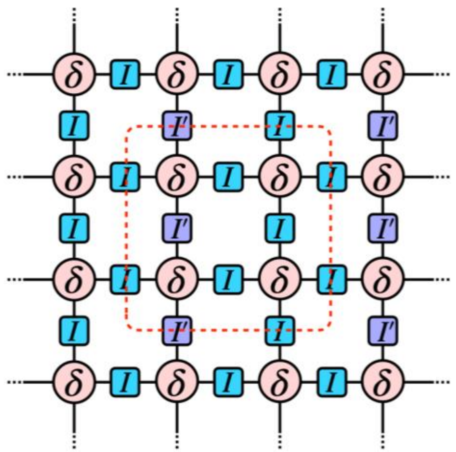
	Model	Method	Transitions	Chiral exponen
(1995)	$FFXY_{sq}$	MC ($L \leq 128$)	2tr, $\delta \approx 0.013$	Consistent with Ising
45] (1995)	IsXY ($C = -0.2885$)	TM MC ($L \leq 30$)	1tr	$\nu = 0.79$, $\eta = 0.40$
(1996)	$FFXY_{sq}$	MC ($L \leq 128$)		$\nu = 0.898(3)$
(1996)	$FFXY_{tr}$	MC ($L \leq 144$)	2tr, $\delta \approx 0.02$	$\gamma = 1.6(3)$, $\beta = 0.11(3)$
(1997)	Villain $FFXY_{sq}$	MC ($L \leq 256$)	2tr, $\delta \approx 0.014$	Consistent with Ising
(1997)	Villain $FFXY_{sq}$	Spin waves, LT phase	1tr	
(1997)	FXY_{zz} ($\rho = 0.7$)	MC ($L \leq 36$)	1tr	$\nu = 0.78(2)$, $\eta = 0.32(4)$
(1997)	FXY_{zz} ($\rho = 1.5$)	MC ($L \leq 36$)	1tr	$\nu = 0.80(1)$, $\eta = 0.29(2)$
(1997)	FFXY, 2cXY, CG	Position-space RG	2tr, $\delta \approx 0.0005$	Different from Ising
(1997)	SOS-Is	MC ($L \leq 22$)	2tr	Consistent with Ising
(1997)	FXY_{J_1,J_2}, CG	RG	1tr	
(1998)	$FFXY_{sq}$	NER_{std} MC ($L \leq 256$)		$\nu = 0.81(2)$, $\eta = 0.261(5)$
(1998)	$FFXY_{tr}$	MC ($L \leq 60$)	2tr, $\delta \approx 0.012$	$\nu = 0.833(7)$, $\eta = 0.25(2)$
(1998)	$FFXXZ_{tr}$	MC ($L \leq 120$)	2tr, $\delta \lesssim 0.01$	Consistent with Ising
(1998)	$FFXY_{sq}$	MC ($L \leq 140$)	1tr	$\nu = 0.852(2)$, $\eta = 0.203(6)$
(2000)	FXY_{J_1,J_2}	MC ($L \leq 150$)	2tr, $\delta \approx 0.003$	$\nu = 0.795(20)$, $\eta = 0.25(1)$
(2000)	FXY_{nn+nnn}	MC ($L \leq 72$)	2tr, $\delta \lesssim 0.01$	$\nu = 1.0(1)$
(2001)	$FFXY_{sq}$	NER_{std} MC ($L \leq 256$)		$\nu = 0.80(2)$, $\eta = 0.276(7)$
(2001)	FXY_{nn+nnn}	NER_{std} MC ($L \leq 256$)		$\nu = 0.80(3)$, $\eta = 0.282(8)$
(2002)	FA6SC	MC ($L \leq 192$)	2tr, $\delta \approx 0.003$	Consistent with Ising
(2002)	FFXY		2tr, $\delta > 0$	
35] (2003)	LGW ϕ^4	Five-loop FT	Stable FP	
(2003)	$FFXY_{sq}$	NER MC ($L \leq 2000$)	2tr, $\delta \approx 0.010$	$\nu = 0.82(2)$, $\eta = 0.272(15)$
(2003)	$FFXY_{tr}$	NER MC ($L \leq 2000$)	2tr, $\delta \approx 0.008$	$\nu = 0.84(2)$, $\eta = 0.250(10)$
(2005)	$FFXY_{sq}$	MC ($L \leq 180$)	1tr	$\nu = 0.9(1)$
(2005)	$FFXY_{sq}$	MC ($L \leq 128$)	2tr, $\delta > 0$	
(2011)	FFXYsq	MC ($L \sim O(10^3)$)	2tr, $\delta \approx 0.025$	$\eta = 0.20(1)$
(2019)	FFXYsq	energy probability distribution zeros	1tr	$\nu = 0.824(30)$

Hasenbusch, et al., J. Stat. Mech. Theory Exp.(2005); Soichirou Okumura, et al, Phys. Rev. B 83, 094429 (2011); A. B. Lima, et al, J Stat Phys 175, 960–971 (2019).

Tensor network approach

standard contraction algorithms fail to converge (e.g. VUMPS, CTMRG)

$$Z = \mathrm{Tr}e^{-\beta H} = \prod_i \int \frac{\mathrm{d}\theta_i}{2\pi} \prod_{\langle ij\rangle} \mathrm{e}^{J_{ij}\beta\cos(\theta_j-\theta_i)} = \sum_{n_l}\prod_{\langle ij\rangle}(-1)^{n_l} I_{n_l}(\beta)\delta_{n_1+n_3}^{n_2+n_4}(i)$$

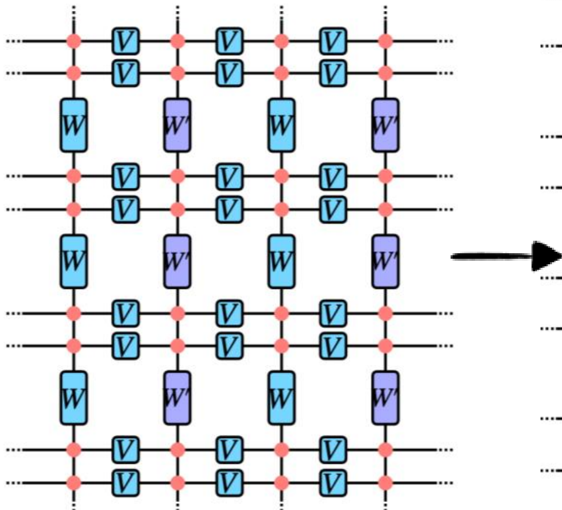


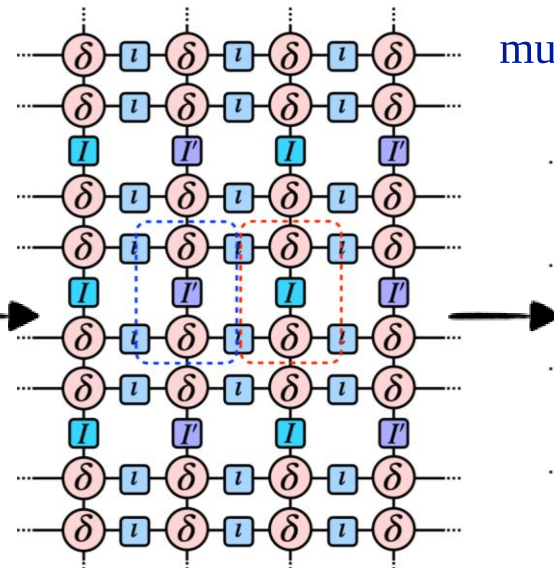
Direct expansion on the original lattice

(i) constrains only imposed within a cluster

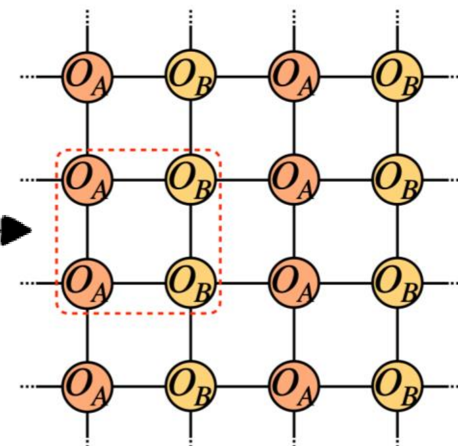
(ii) non-Hermitian transfer matrix

Splitting of $U(1)$ spins



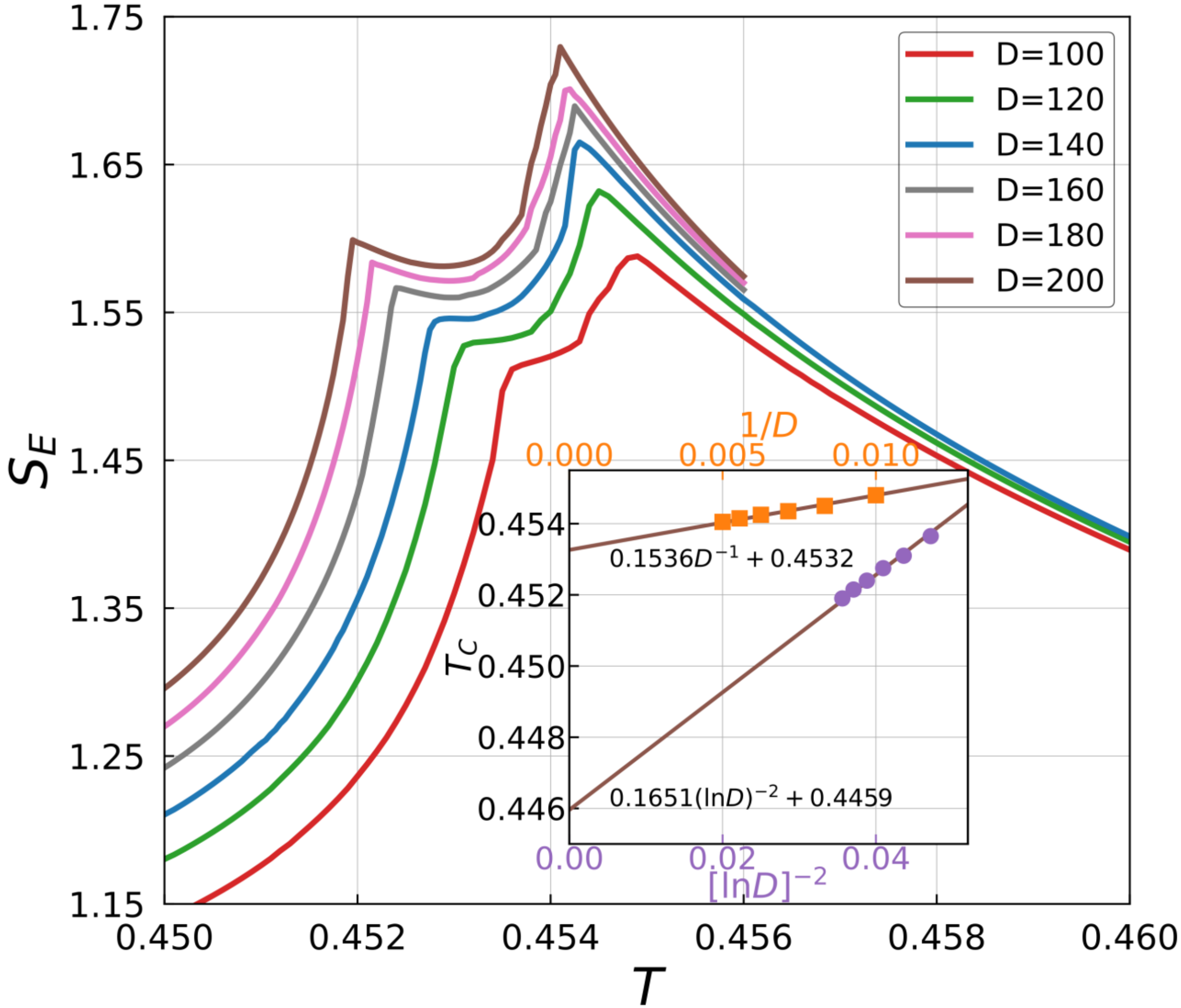


multisite VUMPS algorithm



Numerical results [Phys. Rev. B 105, 134516(2022)]

entanglement entropy



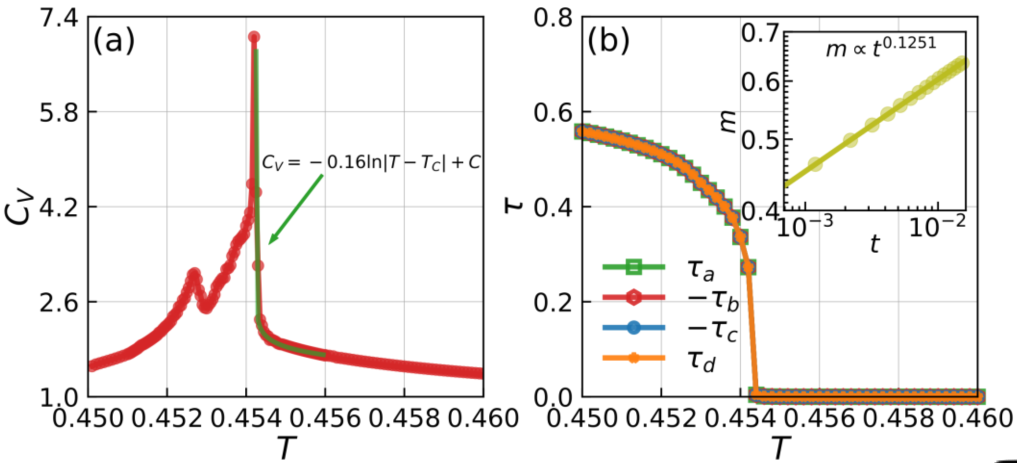
finite bond scaling consistent with BKT and Ising transition

$$\xi_{Ising} \propto \frac{1}{|T - T_C|} \qquad \xi_{BKT} \propto \exp\left(\frac{b}{\sqrt{T - T_C}}\right)$$

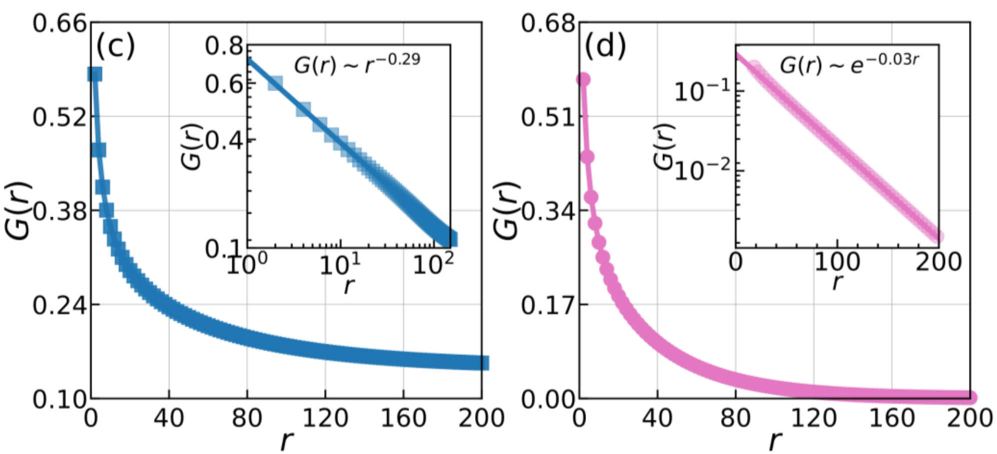
Numerical results

Phys. Rev. B 105, 134516 (2022).

Specific heat & chiral order parameter



correlation functions: $G(r) = \langle \cos(\theta_r - \theta_0) \rangle$



$T < T_{c1}$ $\quad$ $T_{c1} < T < T_{c2}$

phase diagram