Poisson-Dirichlet distributions and weakly first-order spin-nematic phase transitions

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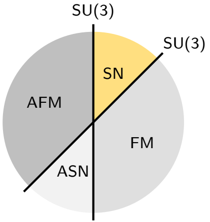
Model & Approaches



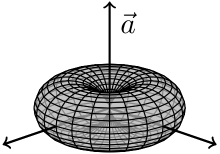
Generic SU(2) symmetric S=1 Hamiltonian on simple cubic lattice Λ

$$H = -J \sum_{\langle i,j \rangle \in \mathcal{B}_\Lambda} \left[\underset{\cos(\phi)}{u} \, \vec{S}_i \cdot \vec{S}_j + \underset{\sin(\phi)}{v} \left(\vec{S}_i \cdot \vec{S}_j \right)^2 \right]$$

A. Läuchli et al.,**PRL**97(2006). D. Ueltschi,**PRE**91(2015).

Planar spin-nematic:

Fluctuations constrained to plane perpendicular to director $\vec{a} \in P\mathbb{S}^2$.
Planar nematic characterized by *minimization* of fluctuations in plane.



Earlier works report thermal melting of nematic state to be continuous with new critical exponents. K. Harada et al., **PRB**65(2002). Growing interest in weakly first-order transitions recently

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Stochastic series expansion (QMC) + Loops & Poisson-Dirichlet distributions $\rightarrow$ Accurate quantitative description

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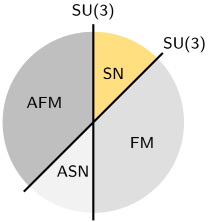

Generic SU(2) symmetric S=1 Hamiltonian on simple cubic lattice Λ

$$H = -J \sum_{\langle i,j\rangle \in \mathcal{B}_\Lambda} \left[\underset{\in [0,1]}{u}\, \vec{S}_i \cdot \vec{S}_j + \underset{=1}{v} \left(\vec{S}_i \cdot \vec{S}_j \right)^2 \right]$$

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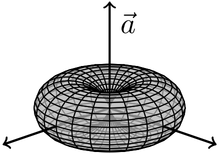

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Stochastic series expansion (QMC) + Loops & Poisson-Dirichlet distributions → Accurate quantitative description

Stochastic series expansion

A. W. Sandvik et al., **PRB**43(1991).

High temperature expansion of quantum partition function

$$\boxed{Z = \mathrm{Tr}\left(e^{-\beta H}\right) = \sum_{\alpha \in \{|\alpha\rangle\}} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle\alpha| \left(-H\right)^n |\alpha\rangle}$$

How to evaluate matrix elements $\langle\alpha| \left(-H\right)^n |\alpha\rangle$?

- Decompose H into sum of bond-operators $H = -\sum_b H_b$ such that

$$H_b |\alpha\rangle \propto |\alpha'\rangle\ , \quad \text{with} \quad |\alpha\rangle, |\alpha'\rangle \in \{|\alpha\rangle\}$$

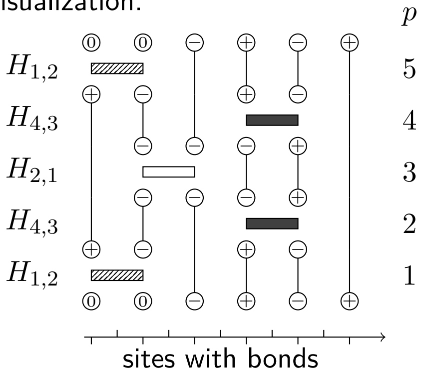
- $(-H)^n$ yields product of bond operators $H_{b_1} H_{b_2} \cdots H_{b_n}$
- Introduce operator sequence $S_n = \left\{b_1, \ldots, b_n\right\}$

Stochastic series expansion

Using bond decomposition and operator string gives

$$Z = \underbrace{\sum_{\{|\alpha\rangle\}} \sum_{n=0}^{\infty} \sum_{\{S_n\}}}_{:=\sum_{\{X\}}} \underbrace{\frac{\beta^n}{n!} \langle\alpha| \prod_{p=1}^{n} H_{b_p} |\alpha\rangle}_{:=W(X)}$$

Visualization:



→ There exist very efficient global updates

O. Syljuåsen and A. Sandvik, **PRE**66(2002)., F. Alet et al., **PRE**71(2005).

→ Method scales linearly in system size (but also linearly in β)

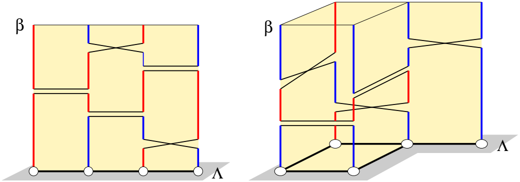
↯ Suffers from sign problem for frustrated models

$\boxed{\text{Unbiased and quantitative approach to study large-scale quantum systems!}}$

Loop representation & PD distributions

B. Tóth, **LMP** 28(1993)., D. Ueltschi, **J. Math. Phys.** 54(2013).
M. Aizenman & B. Nachtergaele, **Comm. Math. Phys.** 164(1994).

Loop models involve one dimensional objects "living" in d-dimensional space



$$Z = e^{2\beta|\mathcal{B}_\Lambda|} \sum_{k,\ell=0}^{\infty} \frac{(1-u)^k u^\ell}{k!\,\ell!} \times \sum_{\substack{b_1,\dots,b_k \\ c_1,\dots,c_\ell}} \int_0^\beta ds_1 \dots ds_k dt_1 \dots dt_\ell \, 3^{|\mathcal{L}(\omega)|}.$$

Joint distribution of lenghts of long loops displays universal behavior: Always given by PD distribution characterized by real number θ, denoted as PD(θ). (For $u = 0, 1 : \theta = 3$, and for $u \in (0,1) : \theta = 3/2$)

PD conjecture:

C. Goldschmidt et al., **Contemp. Math.** 552(2011). D. Ueltschi, **PRE** 91(2015).

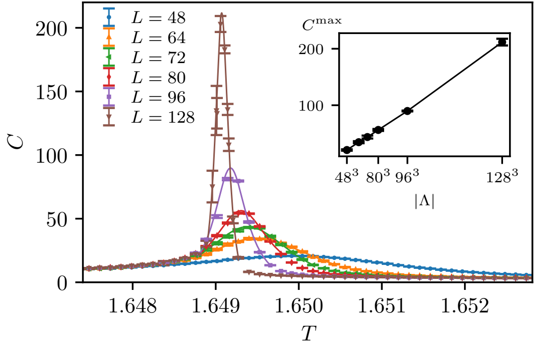
> As $L \to \infty$, we can replace expectation in loop model by expectation with respect to PD(θ), scaled by number $\eta \in [0,1]$ (fraction of long loops at imaginary time 0)

Nature of the phase transition

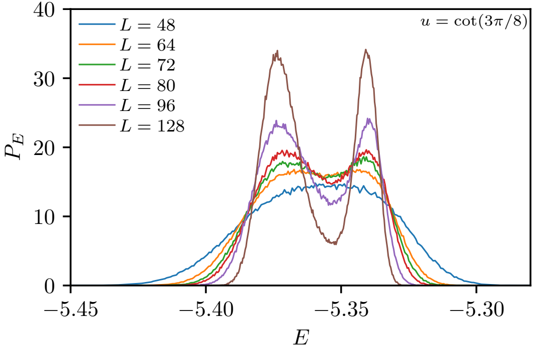
Phase transition was previously reported to be continuous. For large systems there is however genuine first-order behavior identifiable:

J. Lee and J. M. Kosterlitz, **PRL**65(1990).

Specific heat peaks scale as $C_{\max} \propto |\Lambda|$



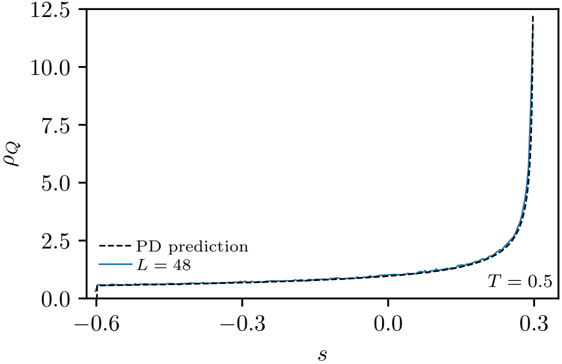
Coexistence in energy histograms



In contrast to earlier claims we identify thermal melting to be (weakly) first-order!

Order parameter distribution

Spin nematic order detectable using $Q = \sum_{i=1}^{N} (S_i^z)^2 - \frac{2}{3}$.From PD calculations we obtain:



Distribution

$$\rho_Q(s) = \begin{cases} \frac{1}{2\sqrt{\eta}\sqrt{\frac{1}{3}\eta - s}} & \text{if } -\frac{2}{3}\eta \le s \le \frac{1}{3}\eta, \\ 0 & \text{otherwise.} \end{cases}$$

Moments

	θ	$\langle Q^2 \rangle_\beta$	$\langle Q^3 \rangle_\beta$	$\langle Q^4 \rangle_\beta$
$u \in (0,1)$	3/2	$\frac{4}{45}\eta^2$	$-\frac{16}{27 \cdot 35}\eta^3$	$\frac{16}{27 \cdot 35}\eta^4$
$u \in \{0,1\}$	3	$\frac{1}{18}\eta^2$	$-\frac{1}{135}\eta^3$	$\frac{1}{135}\eta^4$

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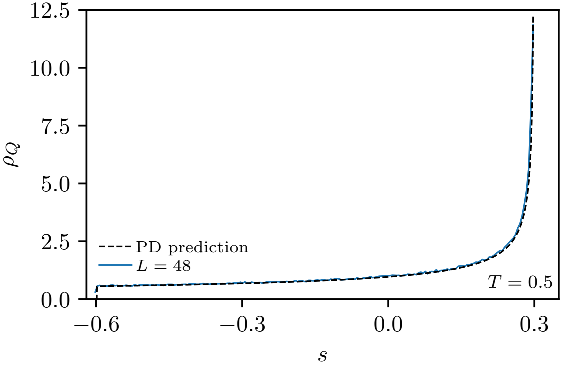

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What happens at T_c?

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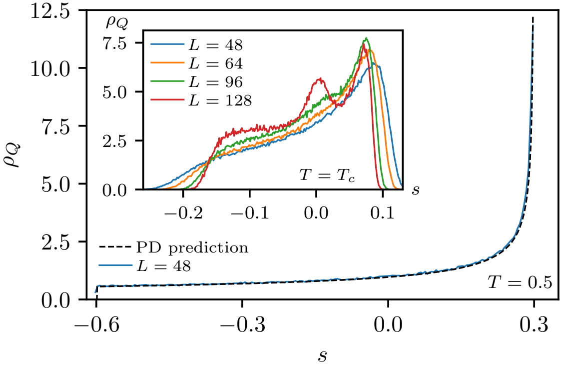

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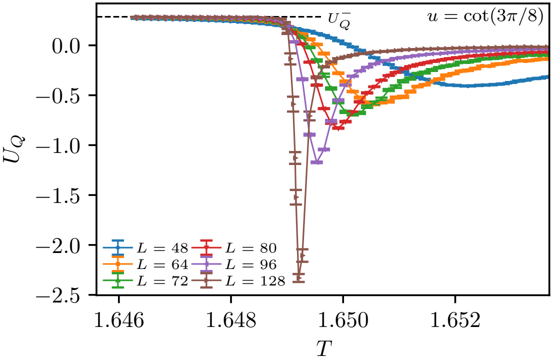
What happens at T_c?$\rightarrow$ Additonal contribution from disordered states observable for $L \gtrsim 100$!

Moment ratios

Moment ratios such as Binder cumulant $U_Q = 1 - \frac{1}{3}\frac{\langle Q^4 \rangle}{\langle Q^2 \rangle^2}$ do not depend on η anymore!



PD predictions:

→ Binder cumulant within spin-nematic phase: $U_Q^- = 2/7$

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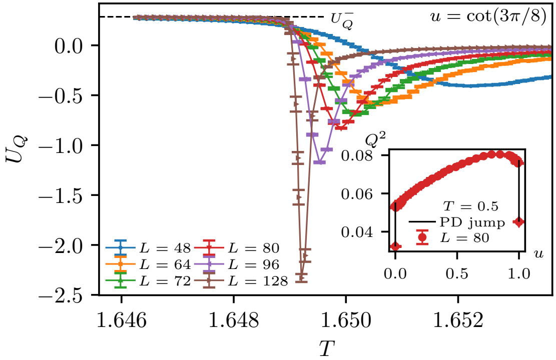

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→ Moment ratios towards SU(3) end points: $\lim_{u\to 0^+} \frac{\langle Q^2\rangle_\beta(u)}{\langle Q^2\rangle_\beta(u=0)} = \lim_{u\to 1^-} \frac{\langle Q^2\rangle_\beta(u)}{\langle Q^2\rangle_\beta(u=1)} = \frac{8}{5}$

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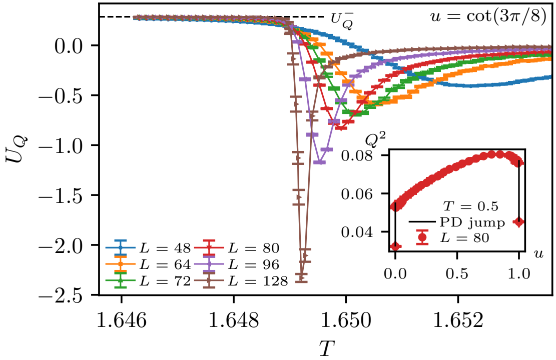

Can we also predict Binder cumulant at T_c?

PD predictions:

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Critical Binder cumulant

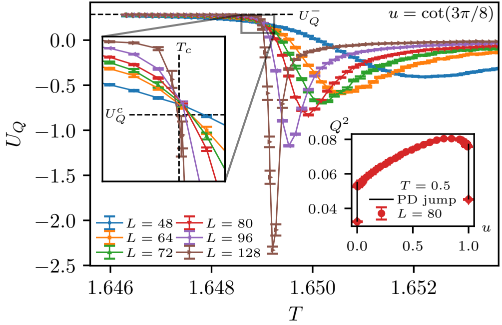
Coexistence of ordered and disordered states (weight of ordered states α):

$$\boxed{\langle \cdot \rangle_{\beta_c} = \alpha \lim_{\beta \to \beta_c^+} \langle \cdot \rangle_\beta + (1-\alpha) \lim_{\beta \to \beta_c^-} \langle \cdot \rangle_\beta}$$

For discrete symmetries in the q-state Potts model one obtains: $\alpha = q/(q+1)$. What is α for continuous symmetries? J. Xu, S.-H. Tsai, D. P. Landau, and K. Binder, **PRE**99(2019).

$\rightarrow$ For continuous case, replace q by integral measure of space of extremal states (here $q = 2\pi$)

$\rightarrow$ This yields $U_Q^c = \frac{2}{7} - \frac{5}{14\pi}$



Conclusion

- Used a combination of QMC and PD calculations based on a loop model formulation
- Uncovered weakly first-order thermal melting transitions of planar spin-nematic states in quantum S=1 systems with SU(2) symmetry
- Demonstrated how generic properties of both low-temperature nematic phase and phase coexistence line can be calculated based on PD conjecture

Open questions:

- Further explain weakness of these first-order transitions using methods such as RG
- Base heuristics for coexistence of phases with continuous symmetries on more rigorous considerations

Thank you for your attention!