“Data mining investigation of BKT transitions”

Samuele Pedrielli – 29/09/2023 - Nicosia, Cyprus.

Funded by the European Union

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The *AQTIVATE* project receives funding from the European Union’s HORIZON MSCA Doctoral Networks programme, under Grant Agreement No. 101072344.

CONTEXT

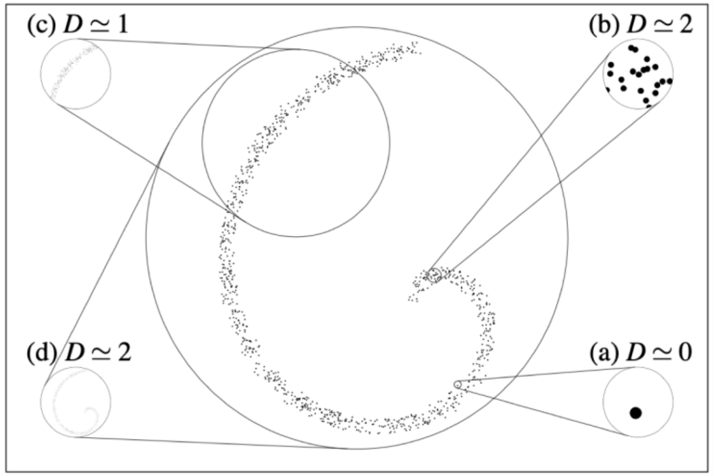
- Using data science tools to study physics problems [1,2]
  - Can these methods improve our understanding?
  - What are their (dis)advantages w.r.t. traditional methods (MC)?

- Young research field still in its testing phase
  - Are these techniques able to reproduce known results?
  - Which tools are best suited to study a given problem?

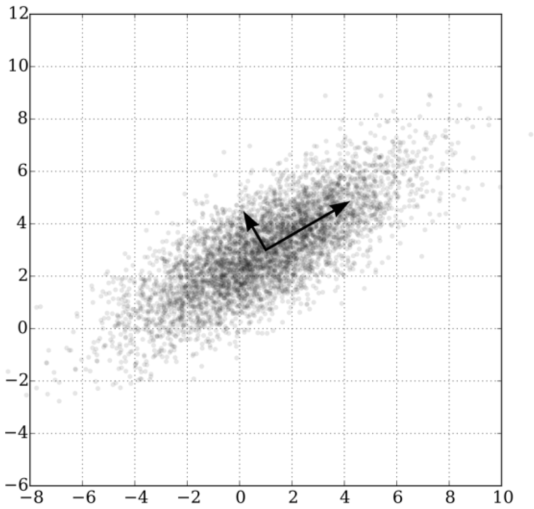
[1] P. Mehta et al., Rep. Prog. Phys., 2019
[2] G. Carleo et al., Rev. Mod. Phys., 2019

CONTEXT

In recent works [3,4], promising results were obtained in the context of phase transitions.



Adapted from K. Balázs., NIPS (2002).



Adapted from https://en.wikipedia.org/wiki/Principal_component_analysis

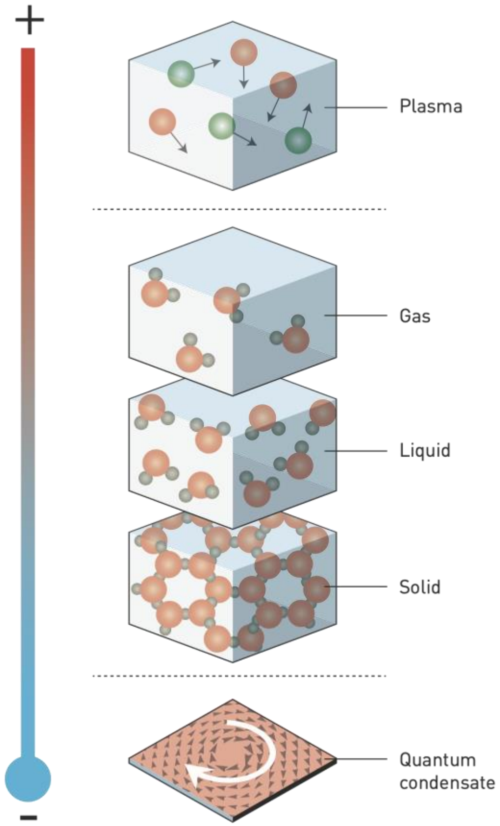


Illustration: ©Johan Jarnestad/The Royal Swedish Academy of Sciences

Adapted from https://www.nobelprize.org/prizes/physics/2016/press-release/

We focus on Berezinskii-Kosterlitz-Thouless [5,6] transitions.

[3] C. Wang et al., Phys. Rev. B, 2017
[4] T. Mendes-Santos et al., Phys. Rev. X, 2021
[5] V. L. Berezinskii, Sov. J. of Exp. and Th. Phys., 1971
[6] J. M. Kosterlitz, D. J. Thouless, J. Phys. C, 1973

OUTLINE

PHASE TRANSITIONS

- Landau-Ginzburg-Wilson paradigm
- BKT transitions
  - XY model
  - 6-clock model

MONTE CARLO SIMULATIONS

- Generating configurations
- Evaluating critical temperatures

DATA MINING

- Intrinsic dimension
  - Application to XY model
  - Application to 6-clock model
- Principal Component Analysis
  - PCA entropy
  - Application to XY model
  - Application to 6-clock model

PHASE TRANSITIONS

PHASE TRANSITIONS

THE LANDAU-GINZBURG-WILSON PARADIGM

- Theoretical framework to describe standard phase transitions
- Based on the notion of spontaneous symmetry breaking
  - *The ground state does not possess the full symmetry of the Hamiltonian*
- Does not explain all possible phase transitions

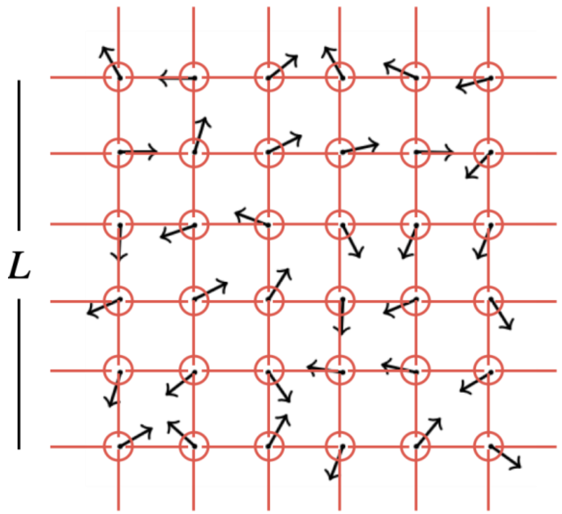
BKT TRANSITIONS

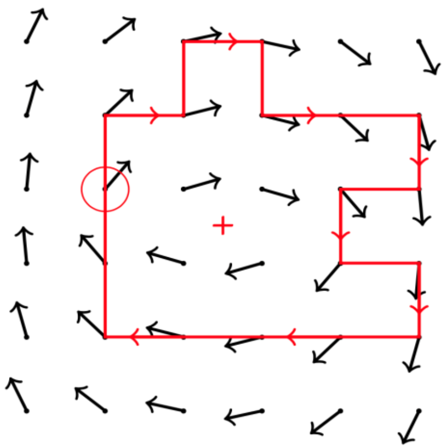
- Phase transitions that are ***not*** the result of s.s.b.
- **Mermin-Wagner-Hohenberg Theorem**
  Continuous symmetries cannot be spontaneously broken at finite temperature in systems of dimensionality $D \leq 2$ *for sufficiently short-ranged interactions*

BKT TRANSITIONS

XY MODEL

- Prototypical example
  - $D = 2$
  - $U(1)$ global symmetry
  - Nearest neighbour interaction
- D*ifferent* kind of transition driven by topological defects
  - $\boldsymbol{T < T^{BKT}}$ - vortices are bound in pairs (QLRO)
  - $\boldsymbol{T > T^{BKT}}$ - vortices unbind and proliferate (DIS)





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BKT TRANSITIONS

6-CLOCK MODEL

- Same Hamiltonian as XY, now 6 discrete spins $\phi = 2\pi q/6,\ q = 0, \ldots, 5$
  - $D = 2$
  - Z_6 global symmetry
  - Nearest neighbour interaction
- MWH Theorem *does not* apply, but 2 BKTs nevertheless

GOALS

- Understand if we can use **PCA Entropy** to obtain the critical points of
  - XY model
  - 6C model
- If so, obtain estimates of the critical points with
  - PCA Entropy
  - **Intrinsic dimension**

  and compare them to those obtained with Monte Carlo techniques.
- Compare PCA Entropy and Intrinsic dimension with each other.

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MONTE CARLO SIMULATIONS

MONTE CARLO SIMULATIONS

GENERATING CONFIGURATIONS

Monte Carlo simulation - numerical technique that simulates the thermal evolution of a system

- Start from a configuration $\{\sigma\}_{i=1}^{N}$
- Propose a new configuration $\{\bar{\sigma}\}_{i=1}^{N}$
- Decide whether to transform $\{\sigma\}_{i=1}^{N}$ into $\{\bar{\sigma}\}_{i=1}^{N}$

At each MC step, a *new configuration* of the system is generated and averages of observables can be computed from it

MONTE CARLO SIMULATIONS

EVALUATING CRITICAL TEMPERATURES

- Find T^* at a given L from observables[8]
- Finite size scaling[9]: $T^* - T^{BKT} \sim ln^{-2}(L)$

System	Average
XY: (L=24,32,64)	$0.910(5) \leftarrow T^{BKT}_{MC}$
6C: (L=24,48,64,80)	$0.91(1) \leftarrow T^{BKT}_{MC,2}$

[8] D. R. Nelson, J. M. Kosterlitz, Phys. Rev. Lett., 1977.
[9] A. W. Sandvik, AIP Conf. Proc., 2010.

DATA MINING

DATA MINING

- How do we get the data set associated with a physical system?
    - Experimental measurements
    - Output configurations of Monte Carlo simulations

$$\mathcal{Z}[K] \xrightarrow{\text{MARKOV CHAIN MONTE CARLO}} \begin{cases} \vec{x}_1 = (x_1^1, x_1^2, \ldots, x_1^N) \\ \vec{x}_2 = (x_2^1, x_2^2, \ldots, x_2^N) \\ \vdots \\ \vec{x}_{N_c} = (x_{N_c}^1, x_{N_c}^2, \ldots, x_{N_c}^N) \end{cases} \xrightarrow{\text{DATA SET}} X = (\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_{N_c})$$

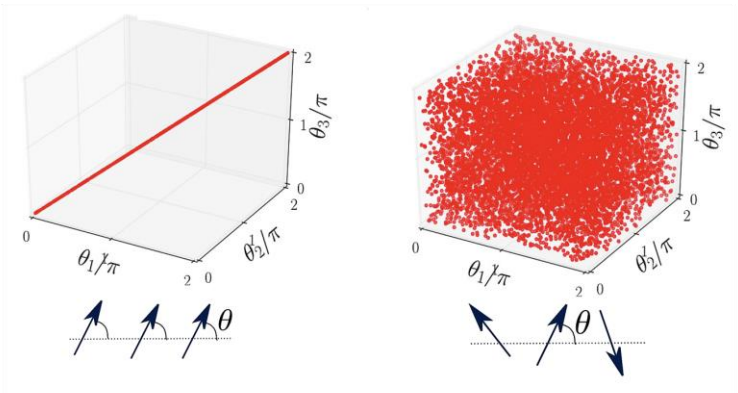
- Once the data set is at hand, we apply our data mining techniques
- The power of the approach resides in its agnostic spirit

DATA MINING

INTRINSIC DIMENSION

Minimum number of variables that describe a data set $\boldsymbol{X}$ embedded in an $\boldsymbol{ND}$ space

Example: 3 sites XY model

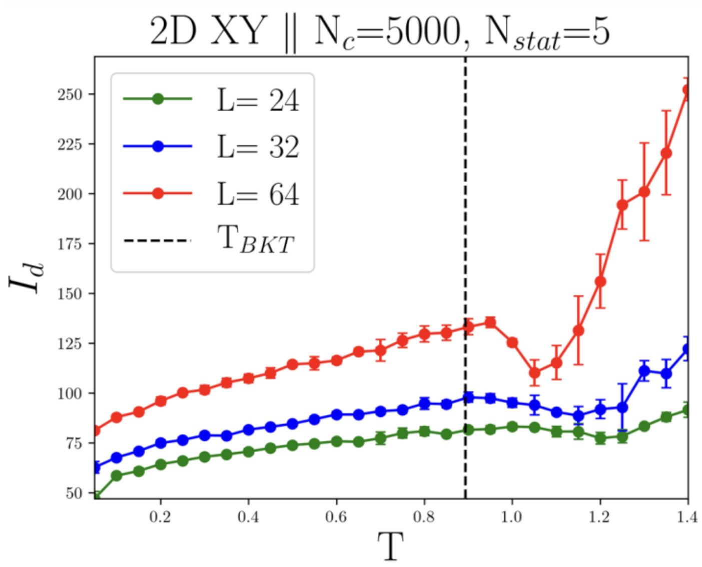


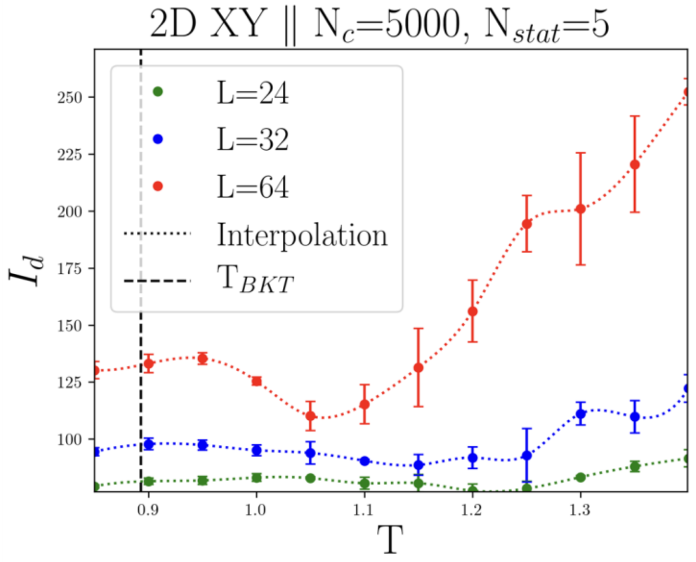
- $T = 0$) spins aligned
  configurations live on a line: $I_d = 1$
- $T = \infty$) random spins
  configurations fill the space: $I_d = N = 3$
- I_d able to distinguish different phases

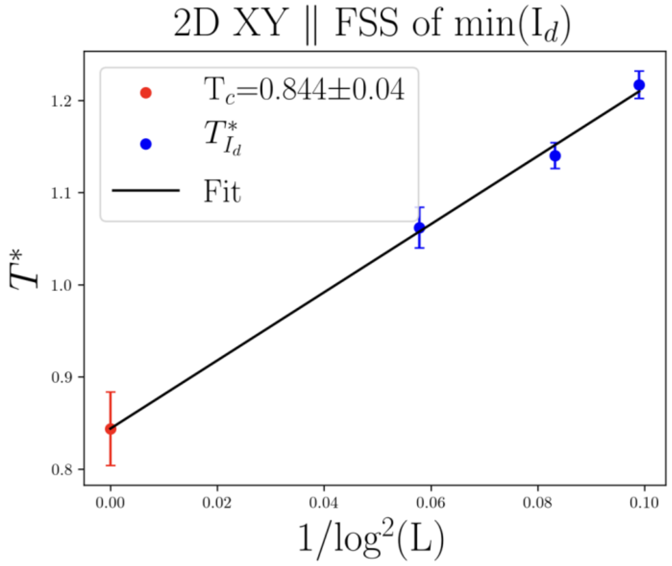
- How do we compute it? *Two nearest neighbour method*
- What happens at intermediate temperatures?
- Can we identify a signal that scales properly? Can we find $\boldsymbol{T^{BKT}}$ from it?

INTRINSIC DIMENSION

APPLICATION TO XY MODEL







- I_d displays a minimum
- Does it scale as expected?

- Interpolation of the data to determine T^*

- Plot T^* against $ln^{-2}(L)$
- Scaling is satisfied

Result: $T_{I_d}^{BKT} = 0.84(4)$, 3% away from agreeing with T_{MC}^{BKT}

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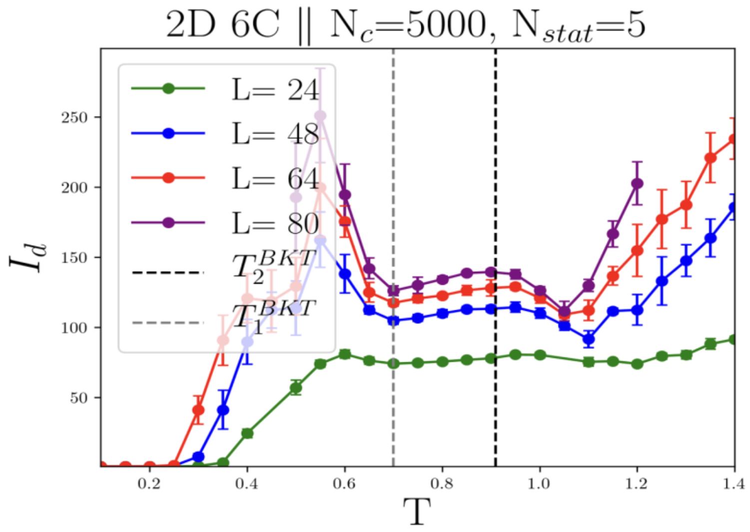
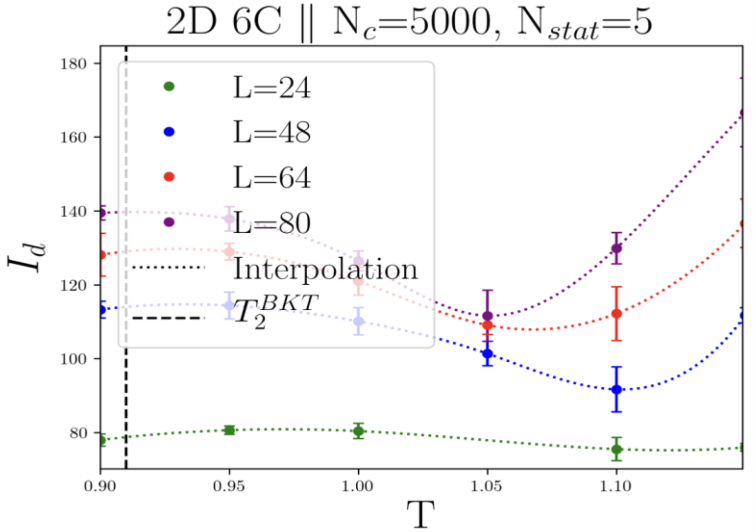
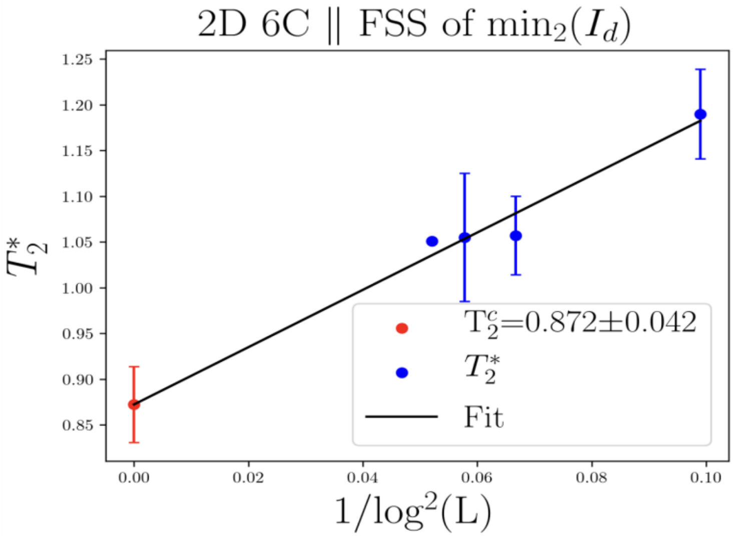
INTRINSIC DIMENSION

APPLICATION TO 6-CLOCK





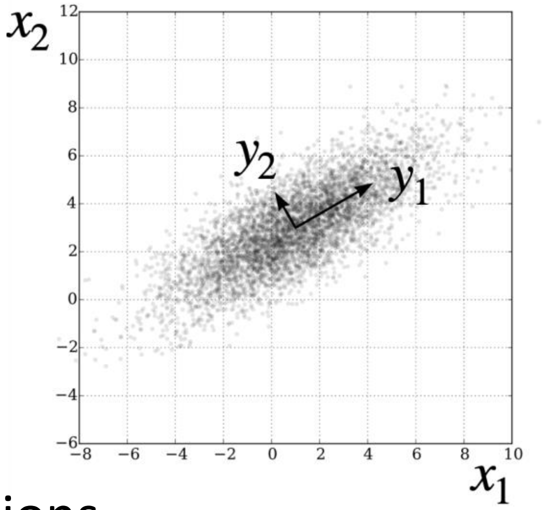


- I_d displays two minima
- Do they scale as expected?
- Interpolation of the data to determine T_2^*
- Plot T^* against $ln^{-2}(L)$
- Scaling is satisfied

$T^{BKT}_{I_d,2} = 0.87(4)$, agrees with T^{BKT}_{MC}; $T^{BKT}_{I_d,1} = 0.87(4)$, agrees with $T^{BKT}_1 = 0.6901(4)$[10]

PRINCIPAL COMPONENT ANALYSIS

Dimensionality reduction technique based on a linear transformation of the data set



- **Idea:** relevant information in the directions of maximum variance
- **Figure:** we want to reduce the dimensionality from 2 to 1
  - Linear transformation $(x_1, x_2) \rightarrow (y_1, y_2)$ eigenvectors of $C(\boldsymbol{X})$
  - Discard eigenvectors with lower eigenvalues (y_2)
- **General case:** $C(\boldsymbol{X})$ has N eigenvectors: systematic way of eliminating directions
  - Set a threshold for the ***fidelity***: $[0,1] \ni F \equiv Tr[C(\boldsymbol{Y})]/Tr[C(\boldsymbol{X})]$
  - Keep all eigenvalues in decreasing order until the threshold is met

PRINCIPAL COMPONENT ANALYSIS

PCA ENTROPY

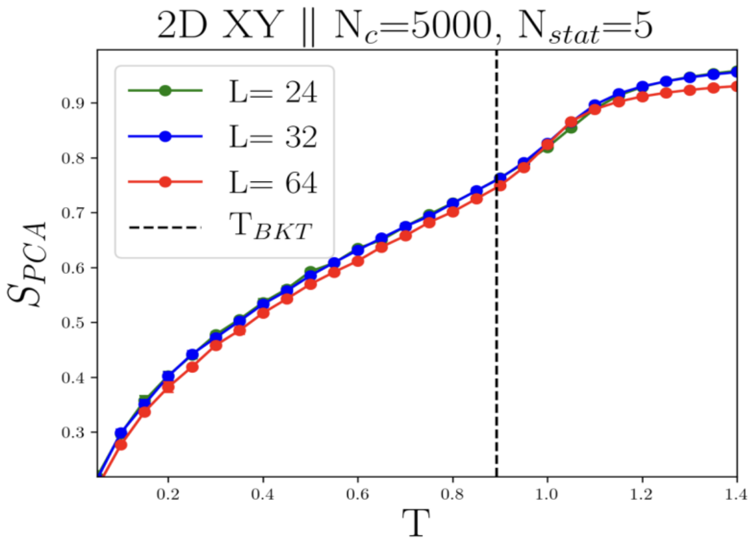
- Problems with PCA
  - Arbitrary threshold
  - By only looking at eigenvalues/vectors is not possible to get T_{PCA}^{BKT} [4]
- Define a new quantity using **all** the eigenvalues

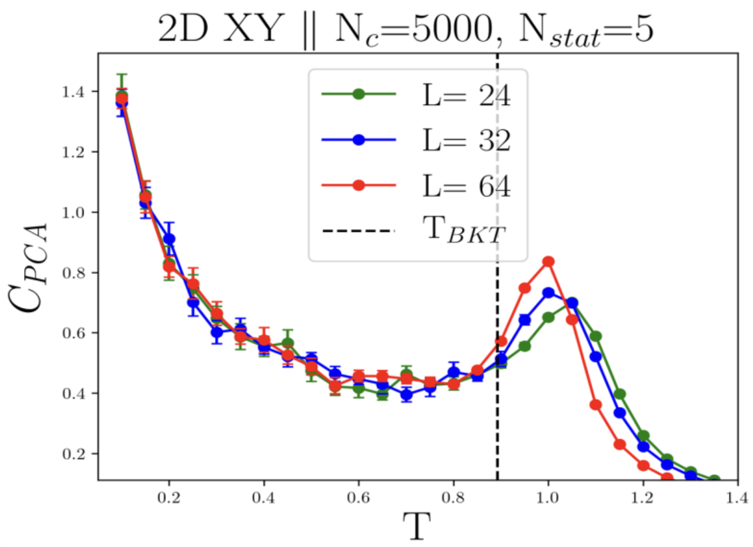
$$S_{PCA} := \frac{1}{lnR} \sum_{i=1}^{R} \tilde{\lambda}_i ln \tilde{\lambda}_i, \qquad \tilde{\lambda}_i = \lambda_i^2 / \sum_j \lambda_j$$

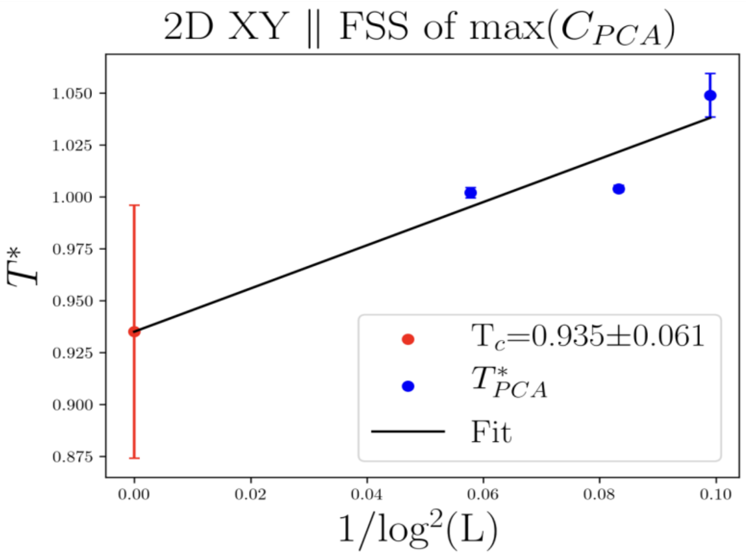
$\tilde{\lambda}_i$ are now positive and sum up to 1, like probabilities: S_{PCA} is an entropy.

PCA ENTROPY

APPLICATION TO XY MODEL







- Agrees with interpretation
- Shows a kink close to T^{BKT}

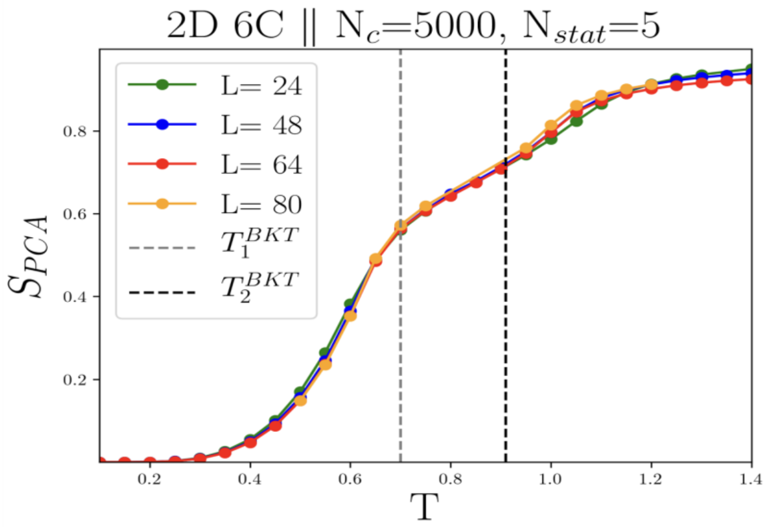
- Derivative has a maximum
- Does it scale properly?

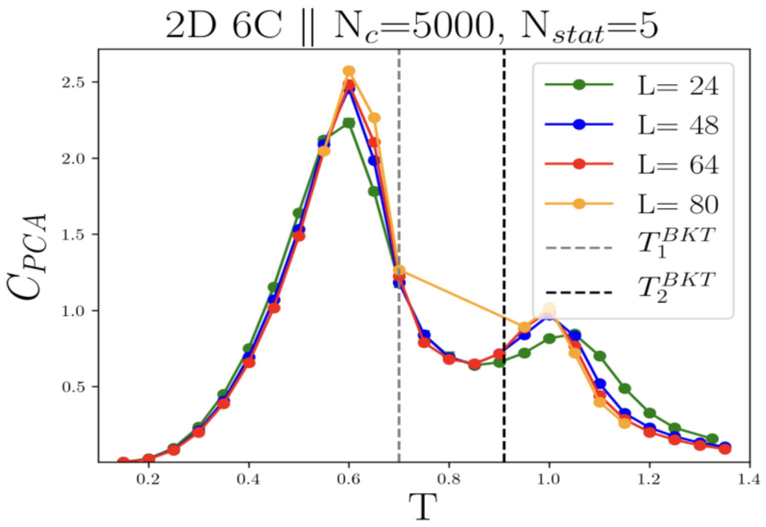
- Small error bars
- The fit gives $T^{BKT}_{PCA} = 0.93(6)$

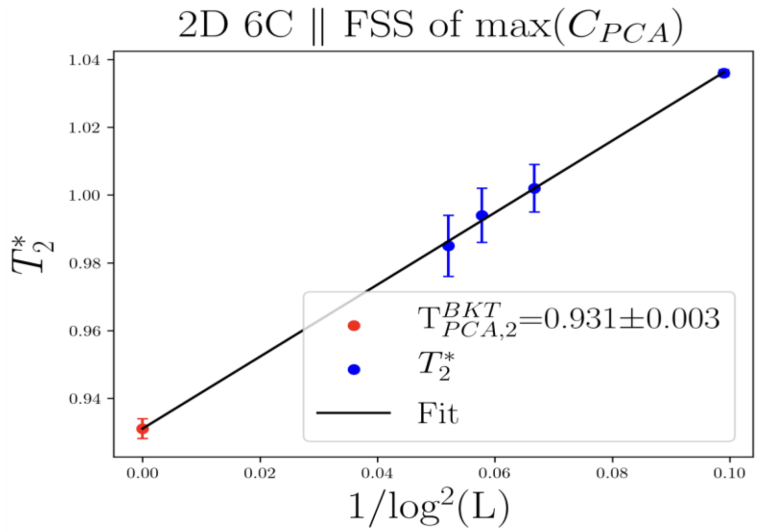
This result is in agreement with T^{BKT}_{MC}

PCA ENTROPY

APPLICATION TO XY MODEL







- Fast growth in LRO
- Kink close to T_2^{BKT}

- Two maxima
- Biggest signal at T_1^{BKT}

- Scaling is satisfied
- Fit gives $T_{PCA,2}^{BKT} = 0.93(3)$

$T_{PCA,2}^{BKT}$ agrees with T_{MC}^{BKT}, while $T_{PCA,1}^{BKT} = 0.627(2)$ does not for a 9%

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SUMMARY OF THE RESULTS

- PCA entropy compatible results with Monte Carlo methods in both models for the estimation of T^{BKT} for QLRO→DIS
  - T_1^{BKT} does not give satisfying results
    - Looking at bigger system sizes
    - More sophisticated techniques for evaluating the error on T^*
- I_d does not give compatible results with T_{MC}^{BKT} in the XY model, but this is due to limited system sizes, as supported by other works [4]
- Results obtained with I_d and S_{PCA} are not always compatible, furthermore
  - I_d seems to work better for LRO→QLRO
  - S_{PCA} seems to work better for QLRO→DIS

THANK YOU