Intrinsic Dimension of quantum data sets: Data-Mining criticality and emergent simplicity

Tiago Mendes Santos

Universität Augsburg University

mpipks

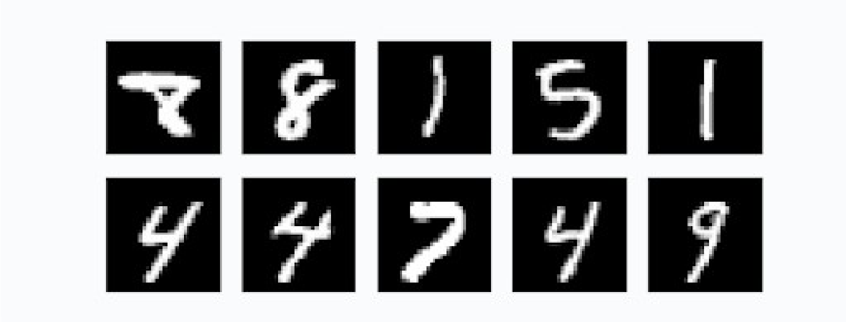
The Abdus Salam International Centre for Theoretical Physics (ICTP)

TMS, X. Turkeshi, M. Dalmonte, A. Rodriguez, PRX 11, 011040 (2021)

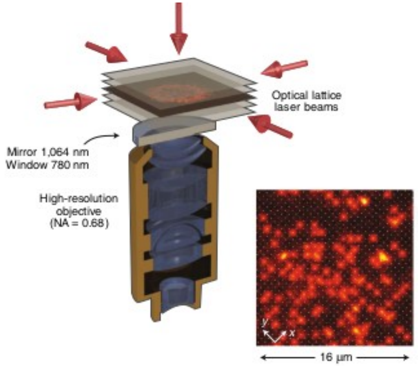
TMS, A. Angelone, A. Rodriguez, R. Fazio, M Dalmonte, PRX Quantum 2, 030332 (2021)

Large data sets → Extract information

Handwriting



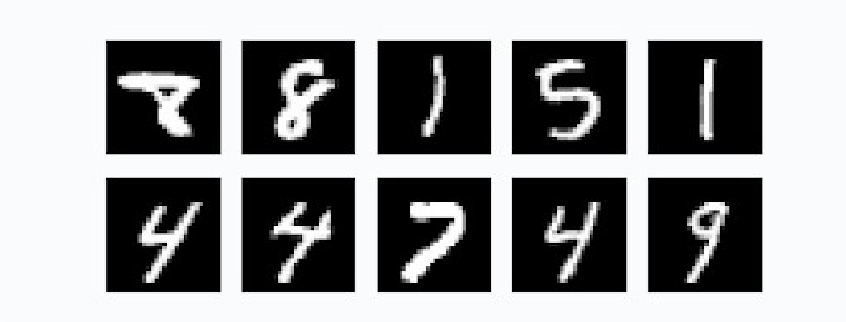
Physical data sets



Large **[high-dimensional]** data sets

Extract information
[Characterize phases of matter and **their transitions**]

Handwriting



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0 0 0 1 0 1 1 0
0 1 1 1 0 1 0 1
0 1 0 0 1 0 0 1
       ...
0 0 0 0 1 0 1 1
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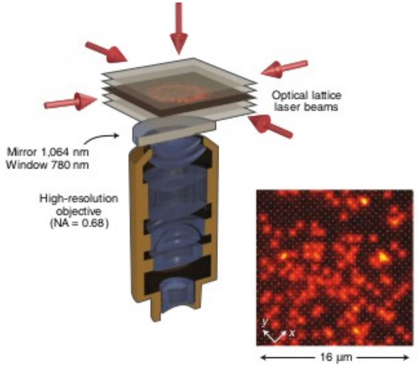
Physical data sets
[Many-body physics]



Characterize phases of matter and their transitions

Machine learning phases of matter

Juan Carrasquilla[1*] and Roger G. Melko[1,2]

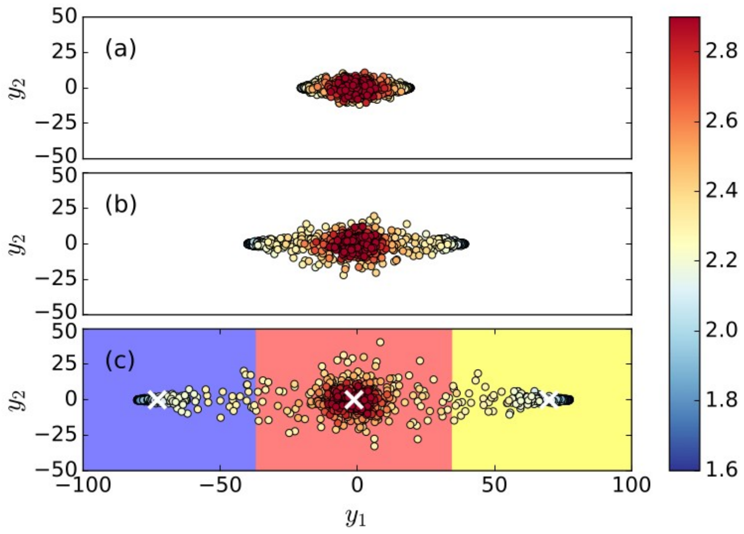
nature physics (2017)

Labeled configurations
[Supervised ML]

Learning phase transitions by confusion

Evert P. L. van Nieuwenburg*, Ye-Hua Liu and Sebastian D. Huber

nature physics (2017)



Lei Wang PRB (2016)

Unlabeled configurations
[Unsupervised ML]

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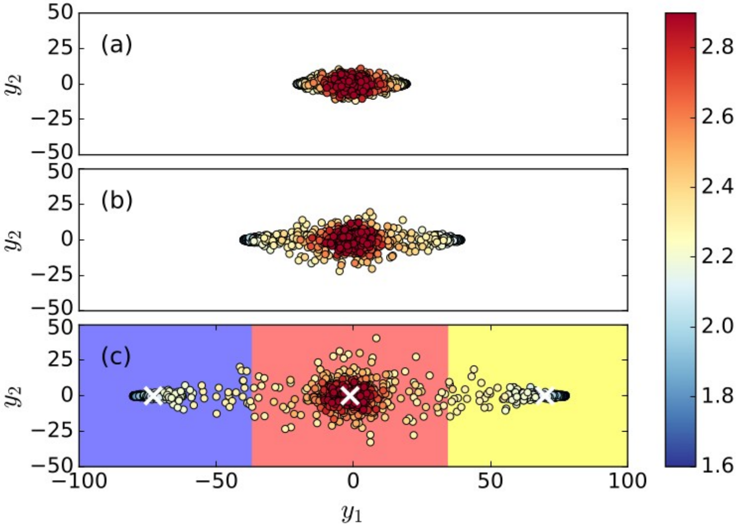


Lei Wang PRB (2016)

Unlabeled configurations
[Unsupervised ML]

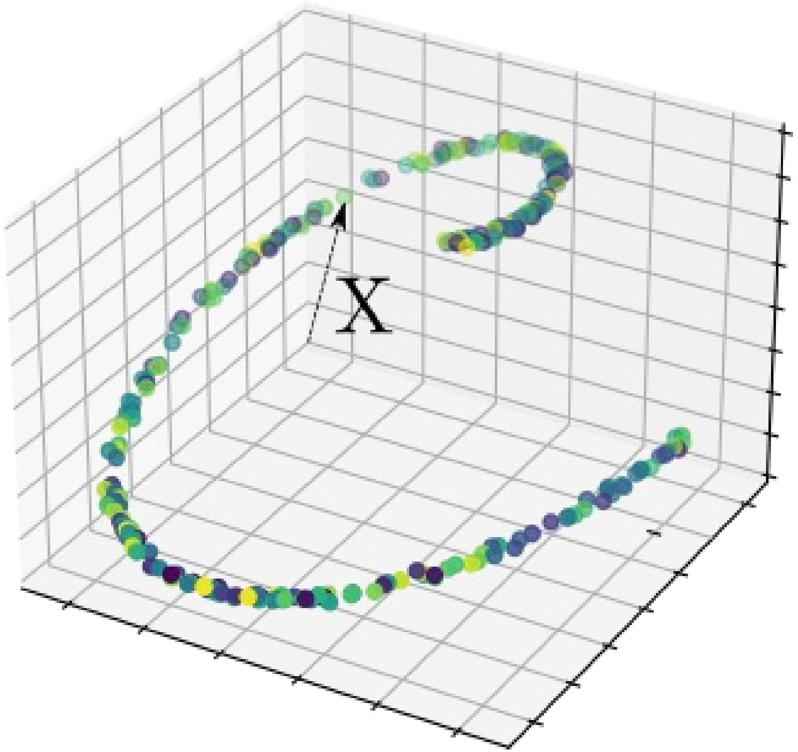
Unsupervised learning without dimension reduction?

Intrinsic dimension (ID)

Data set lies in a manifold whose ID is lower than the number of coordinates

$$\vec{X} = (x_1, x_2, x_3)$$

ID = 1

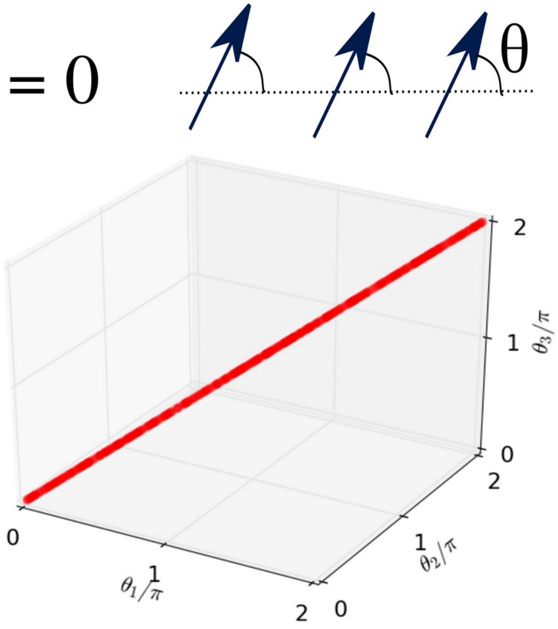


Partition-function data sets

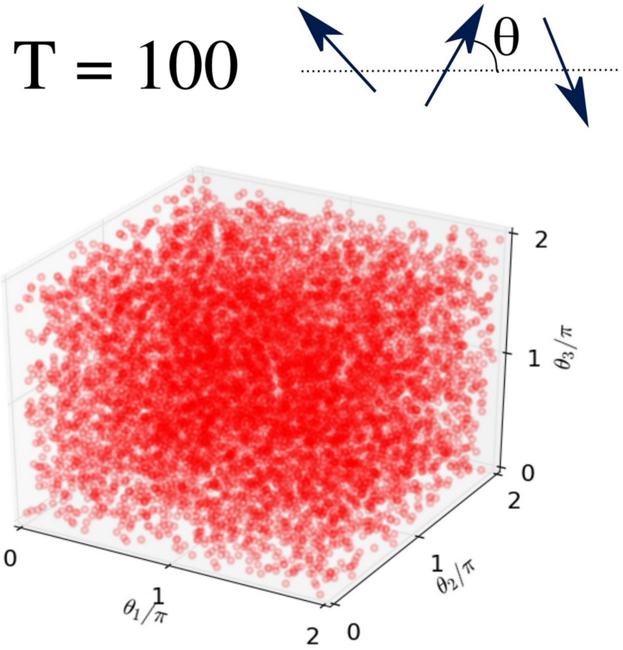
$$Z = \sum_{\vec{X}} e^{-\beta E(\vec{X})}$$

3-spin XY model

T = 0



T = 100



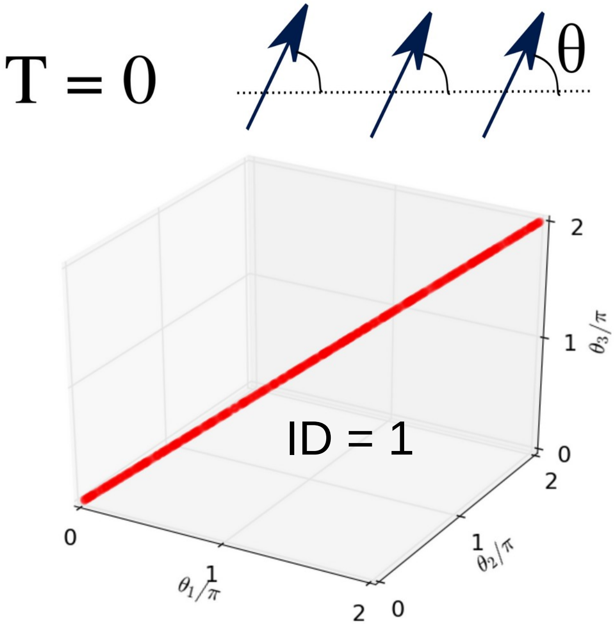
$$E(\{\vec{\theta}\}) = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)$$

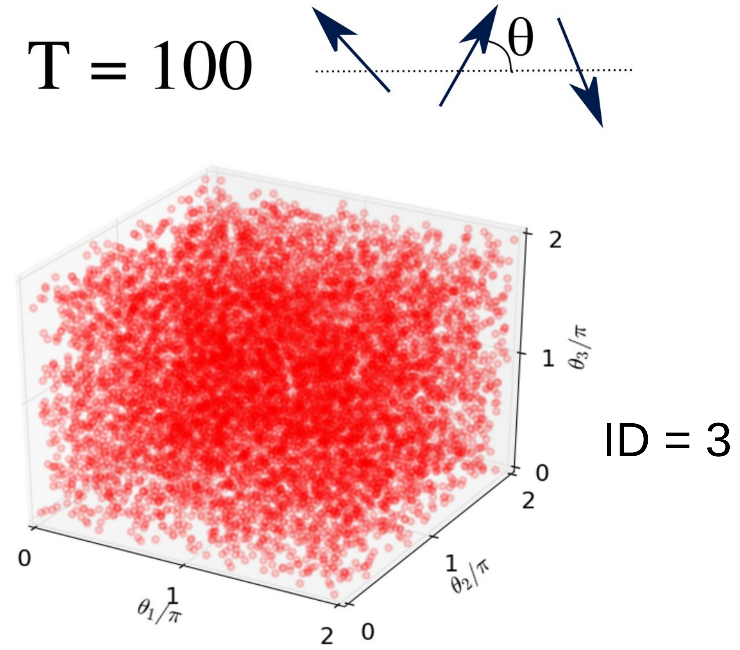
$$\vec{\theta} = (\theta_1, \theta_2, \theta_3)$$

Partition-function data sets

$$Z = \sum_{\vec{X}} e^{-\beta E(\vec{X})}$$

3-spin XY model





Outline

→ How to estimate the ID

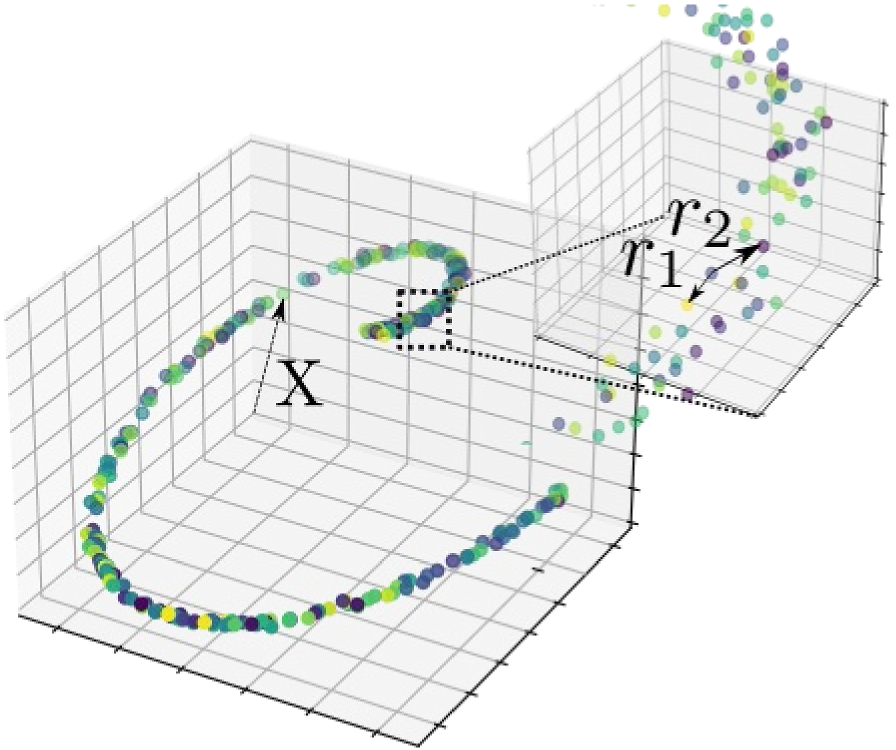
→ Quantum data sets
[Quantum Monte Carlo]

→ ID and quantum phase transitions (QPTs)

Intrinsic dimension (ID)

ID → Nearest neighbors(NN)-based estimator

Statistics of NN distances
[e.g., Euclidian, Hamming]



Intrinsic dimension (ID)

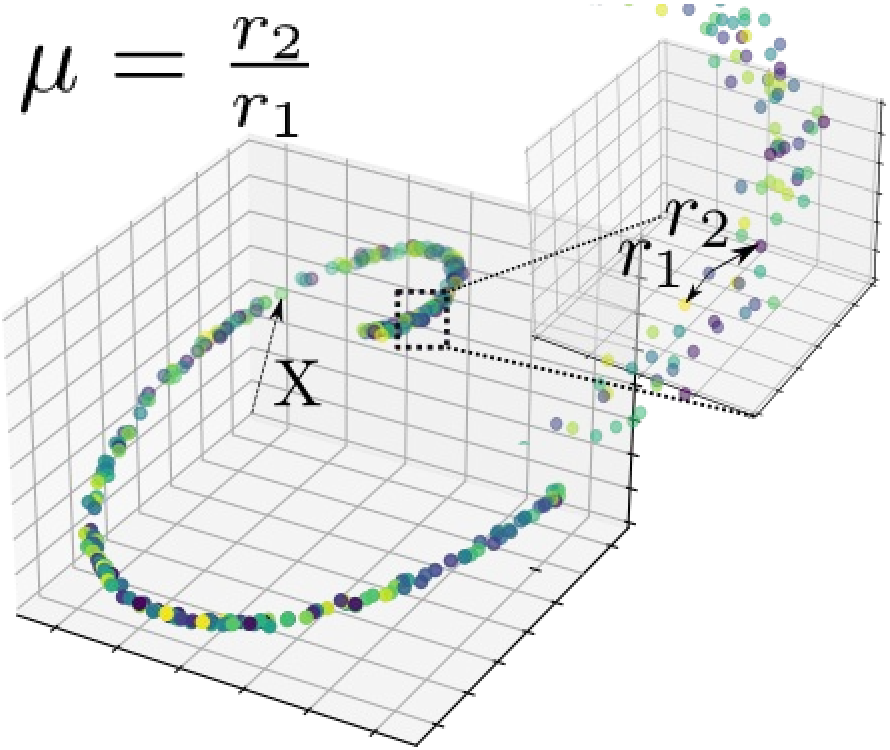
ID → Nearest neighbors(NN)-based estimator

Statistics of NN distances
[e.g., Euclidian, Hamming]

Probability distribution function

$$f(\mu) = I_d \mu^{-1-I_d}$$

Elena Facco et. al. Scientific Reports (2017)

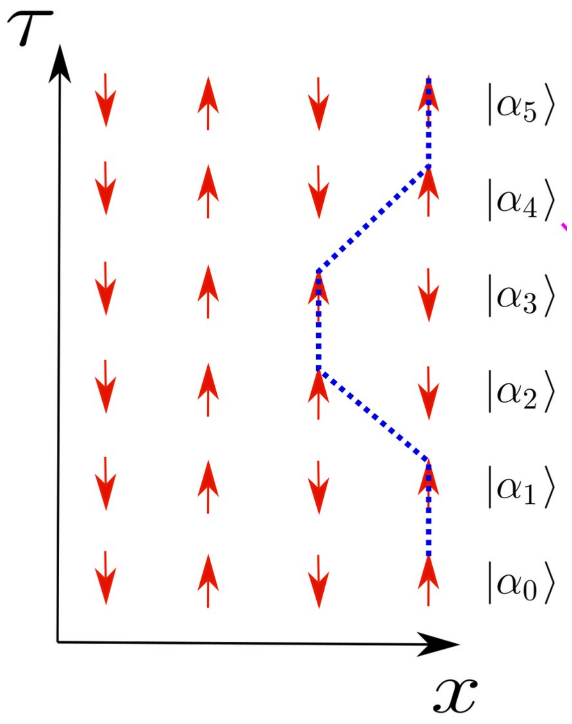


Quantum data sets

$$Z = \sum_\alpha \langle\alpha|\, e^{-\beta\hat{H}}\, |\alpha\rangle$$

Quantum data sets

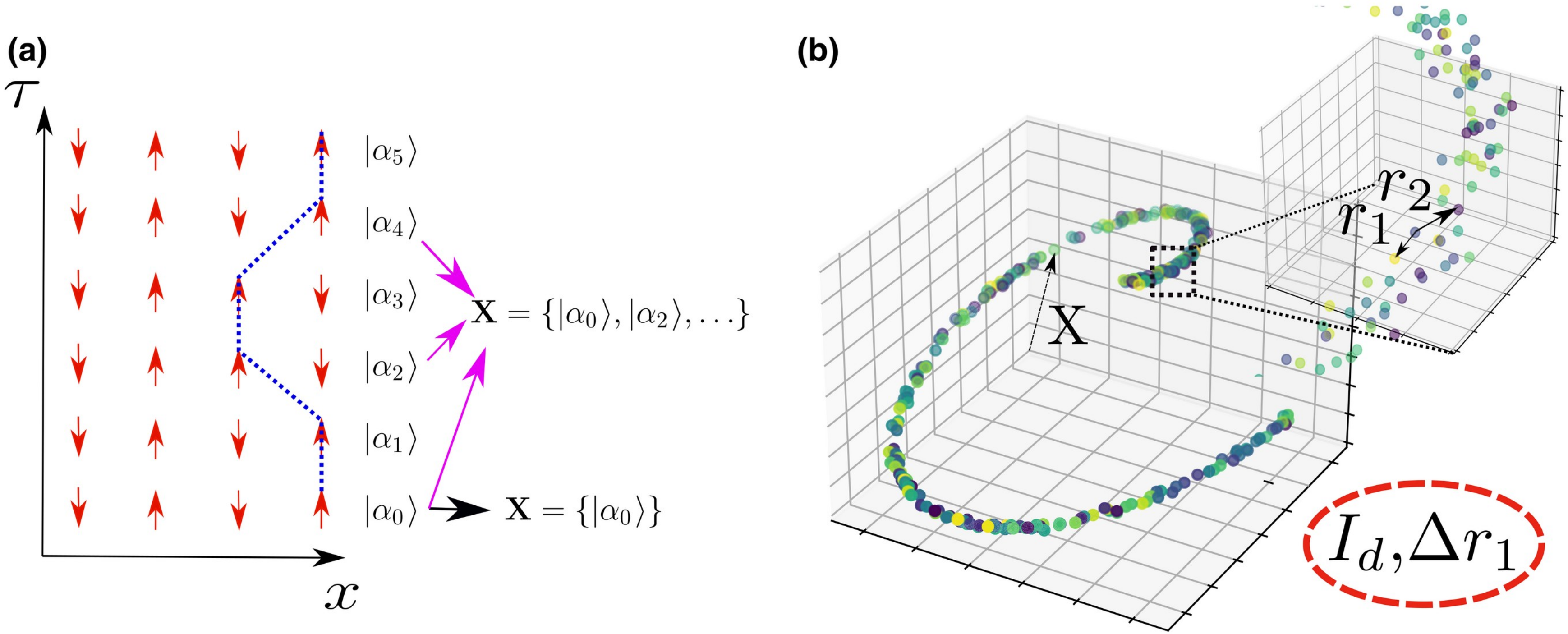
$$Z = \sum_\alpha \langle \alpha | e^{-\beta \hat{H}} | \alpha \rangle$$



Quantum-to-classical mapping
→ path-integral and stochastic series expansion

$$Z = \sum_{\alpha_0} \sum_{\alpha_1} \cdots \sum_{\alpha_L - 1} \langle \alpha_0 | \mathrm{e}^{-\Delta_\tau H} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | \mathrm{e}^{-\Delta_\tau H} | \alpha_1 \rangle \langle \alpha_1 | \mathrm{e}^{-\Delta_\tau H} | \alpha_0 \rangle$$

Quantum data sets and generic features of data sets

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0 0 0 1 0 1 1 0
0 1 1 1 0 1 0 1
0 1 0 0 1 0 0 1
...
0 0 0 0 1 0 1 1
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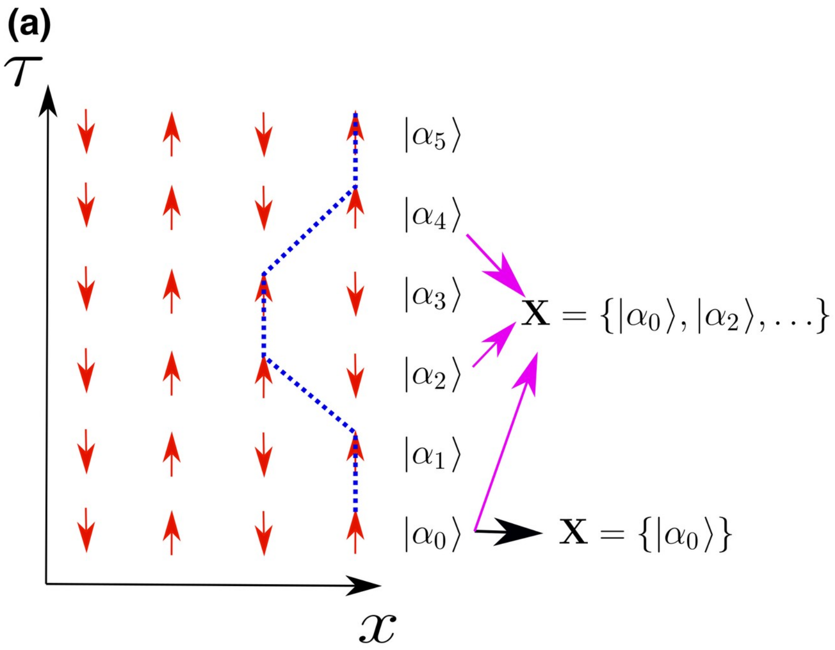
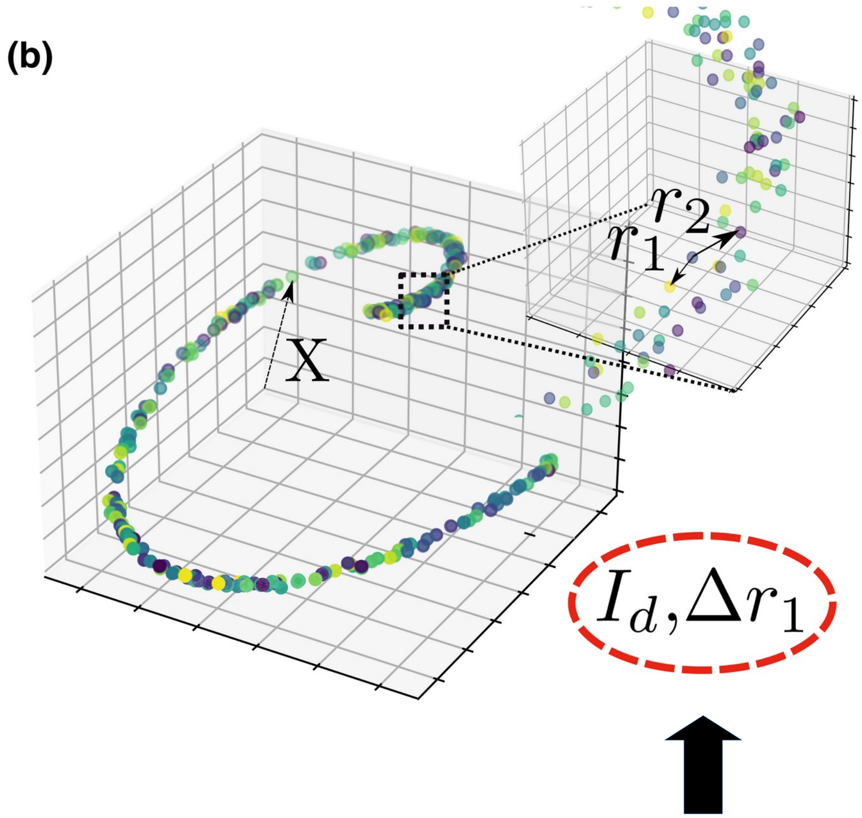
Quantum data sets and generic features of data sets



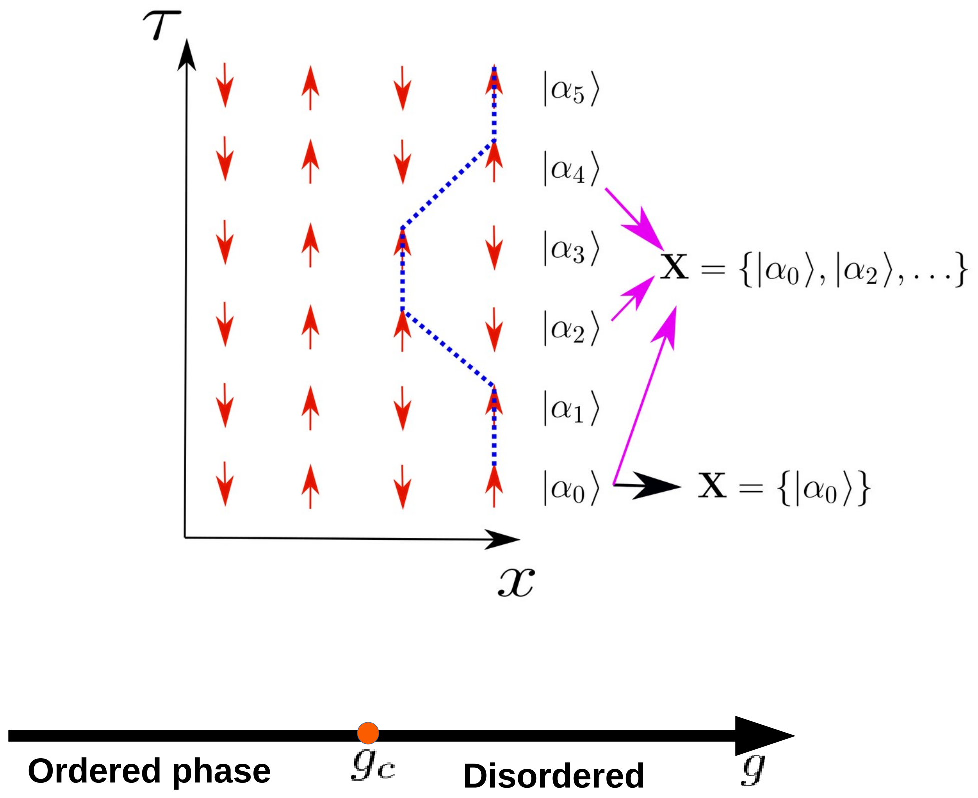


Data sets with a **single** slice or **multiple** slices

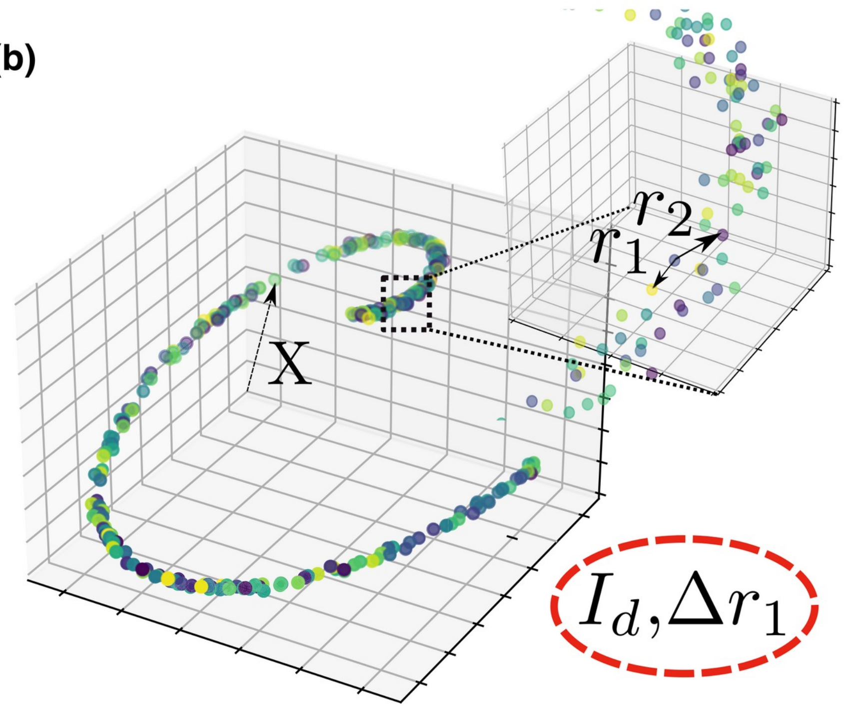
Quantities related to nn distances

Quantum data sets and generic features of data sets

(a)

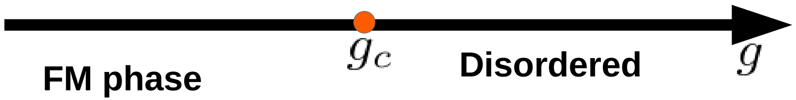


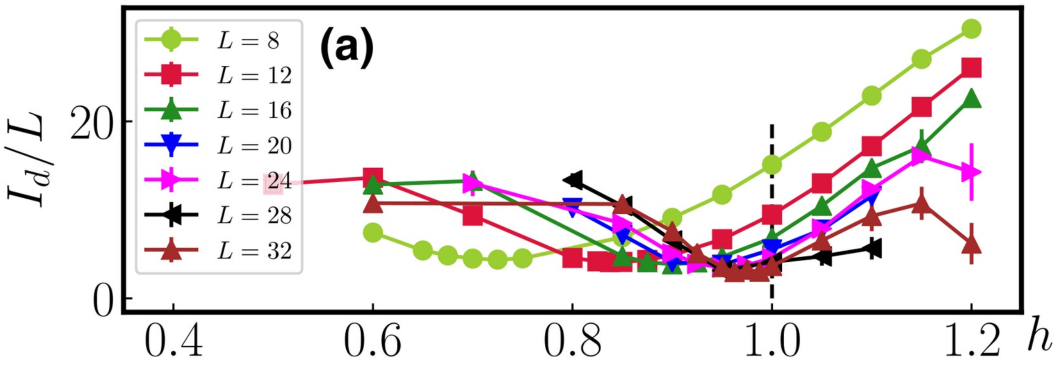
(b)



Second order transitions
(1) Quantum Ising chain
(2) 2d dimerized Heisenberg models
BKT transitions
(3) XXZ chain

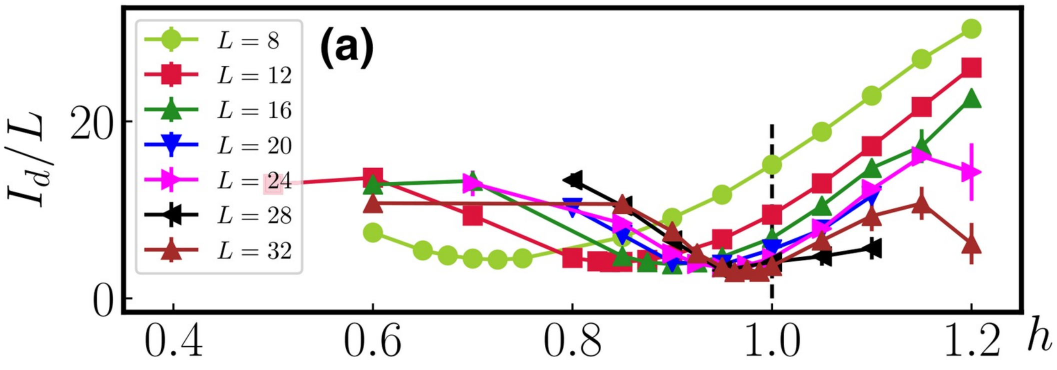
Second order QPT [1d quantum Ising model]



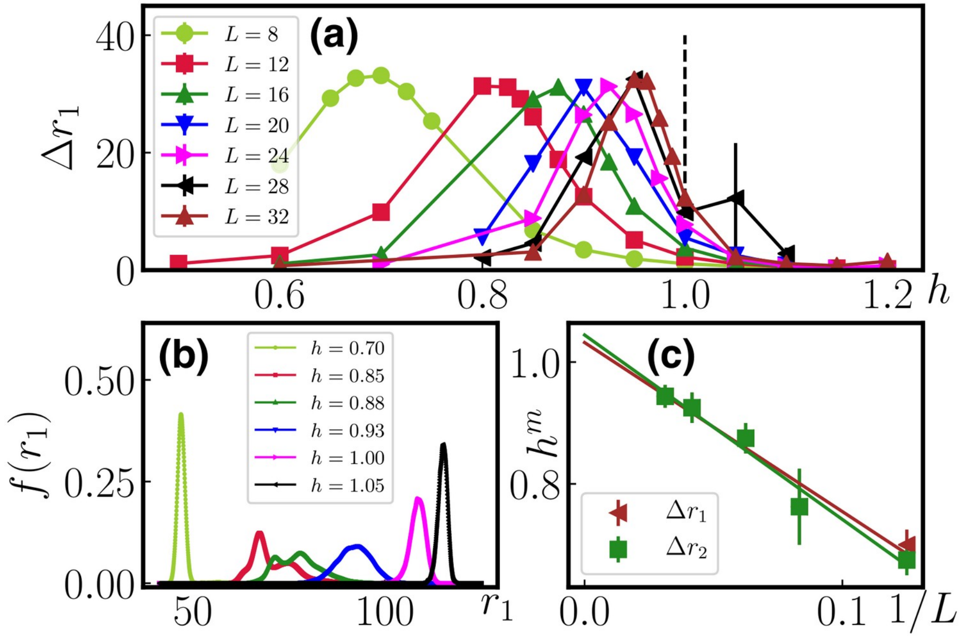


Id exhibits **a minimum** in the vicinity of $\mathbf{h_c}$

Second order QPT [1d quantum Ising model]

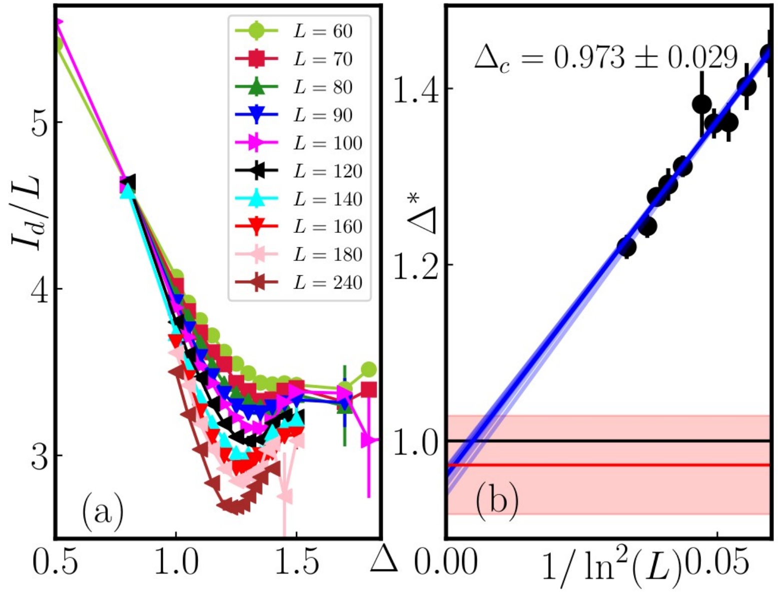


Id exhibits **a minimum** in the vicinity of **h_c**



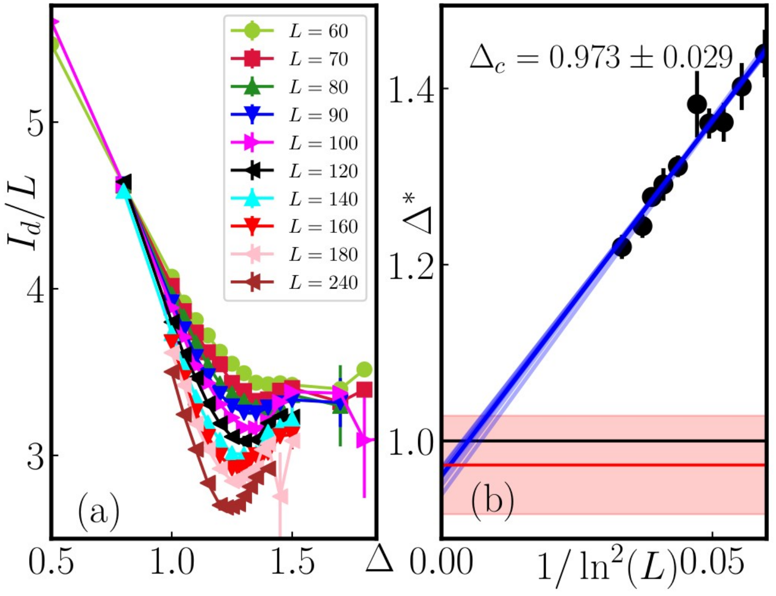
Statistics of first nn distances also reveal quantum criticality

BKT transition [1d XXZ model]

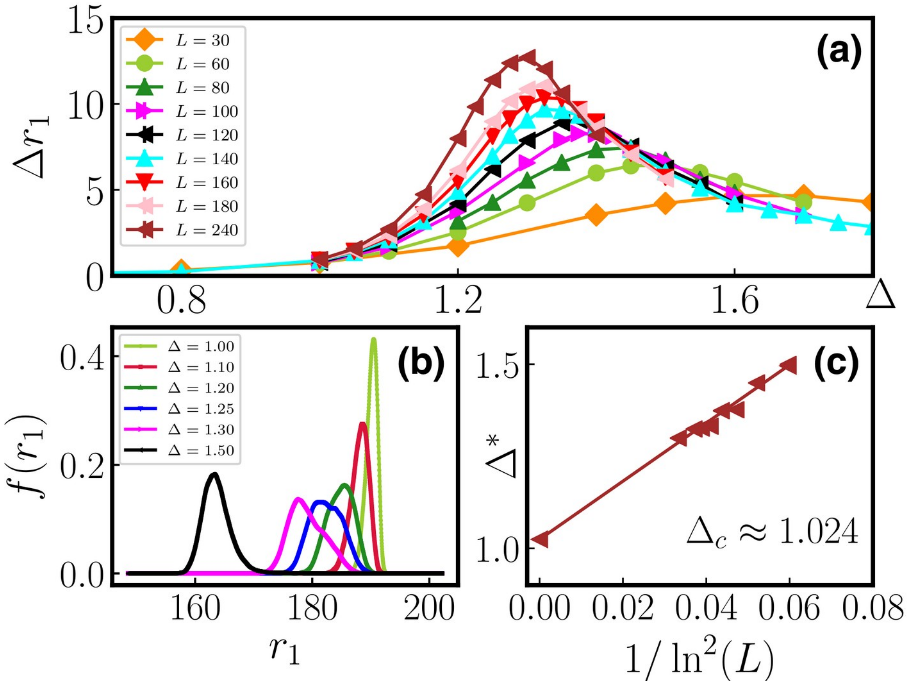


Id exhibits **a minimum**
in the vicinity of Δ_c

BKT transition [1d XXZ model]

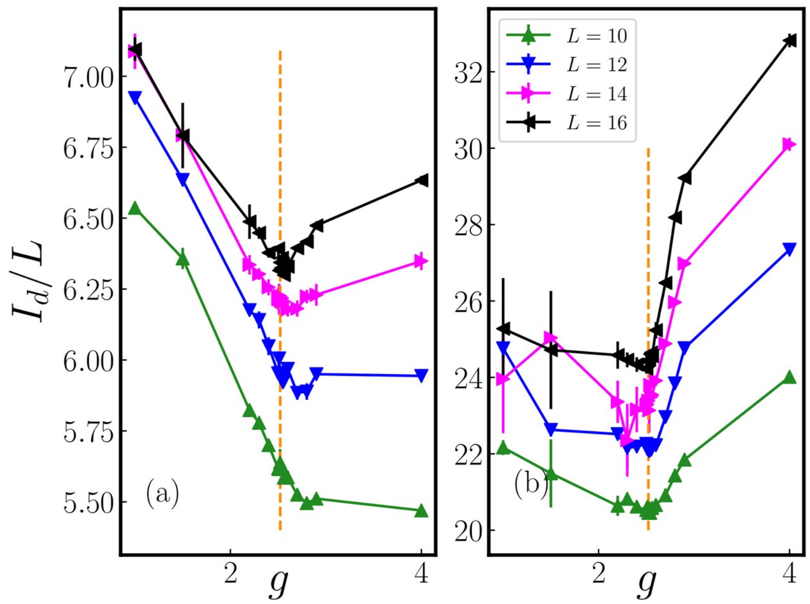


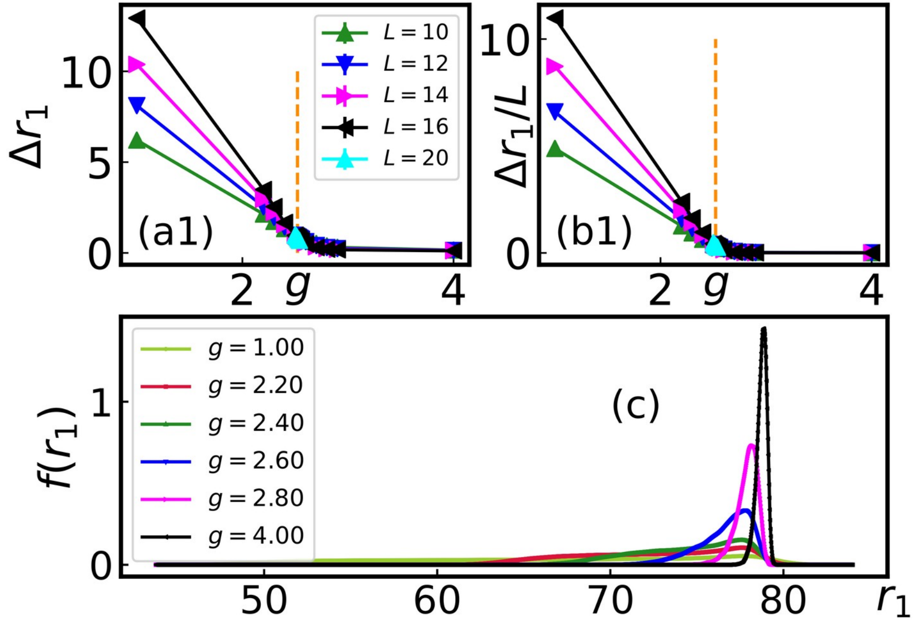
Id exhibits **a minimum** in the vicinity of Δ_c



Statistics of first nn distances also reveal quantum criticality

2d QPT [dimerized Heisenberg model]





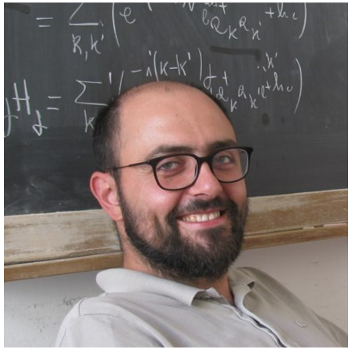
Id exhibits **a minimum** in the vicinity of g_c

Extensive behavior of Δr_1 in the SU(2) AFM phase

Conclusion

Generic features of raw quantum data sets [e.g., Id and Δr_1] exhibit scaling behavior in the vicinity of quantum critical points
→Unsupervised learning quantum phase transitions

Thank you!



Marcello Dalmonte (ICTP/SISSA)

Xhek Turkeshi (ICTP/SISSA)

Alex Rodriguez (ICTP)

Adriano Angelone
(LPTMC,Sorbonne Université)

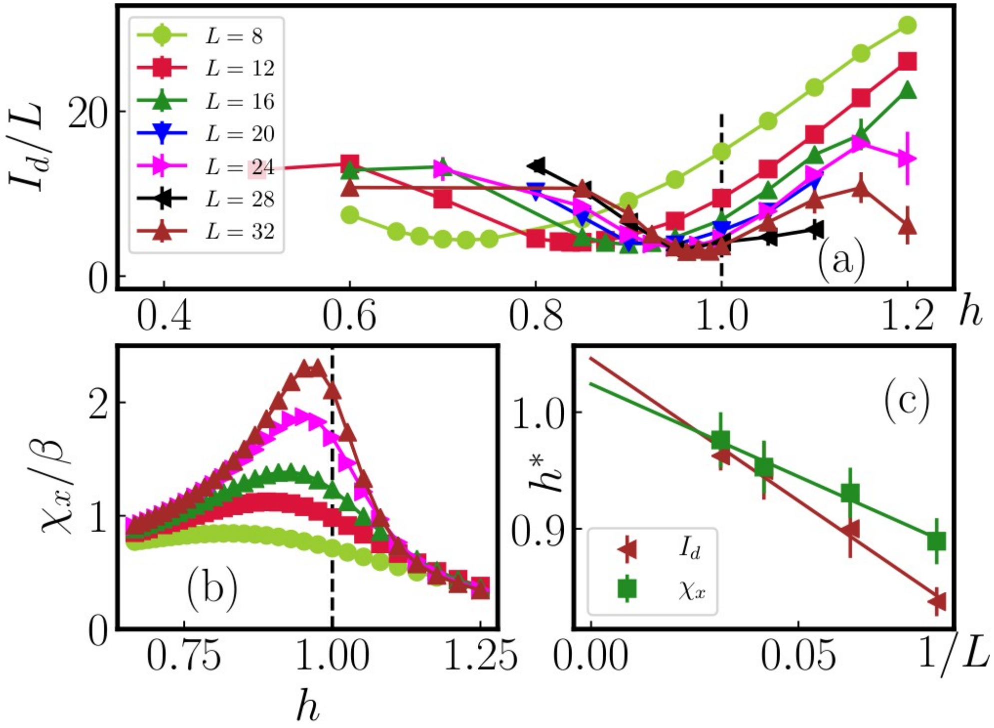
Rosario Fazio (ICTP)

PRX 11, 011040 (2021)

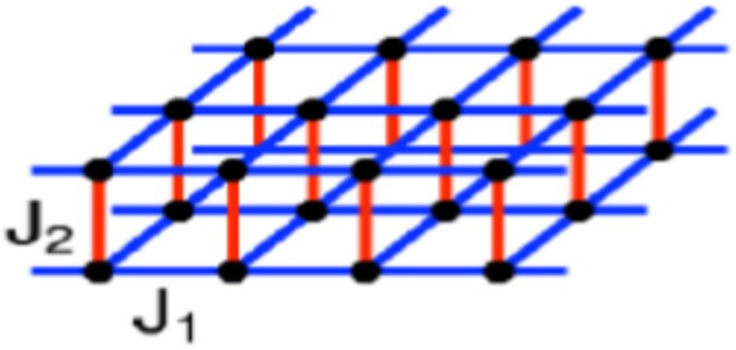
PRX Quantum 2, 030332 (2021)

Supplemental Material

Second order QPT [1d quantum Ising model]

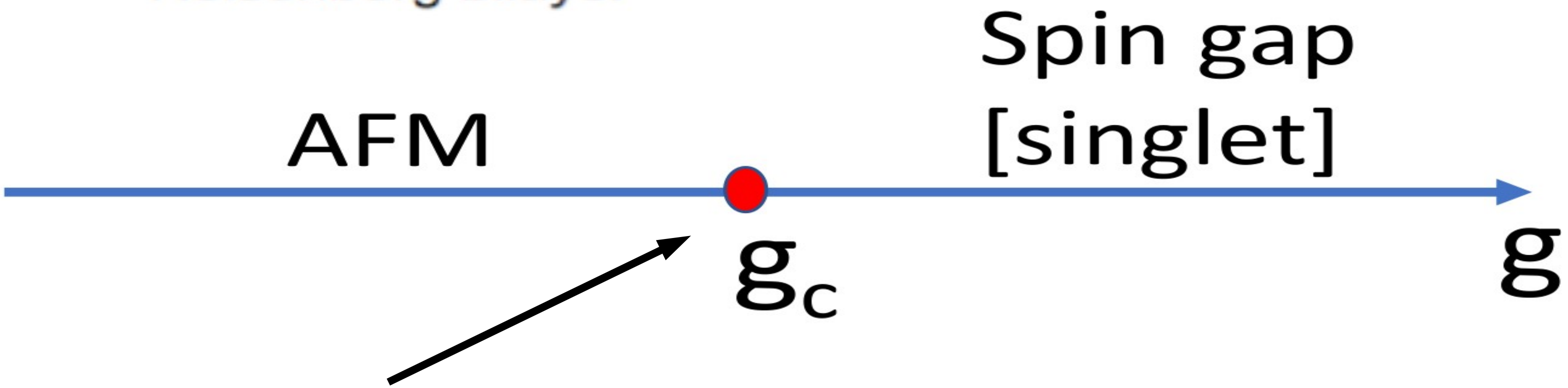


Two-dimensional quantum critical point



Heisenberg bilayer

$$g = J_2 / J_1$$

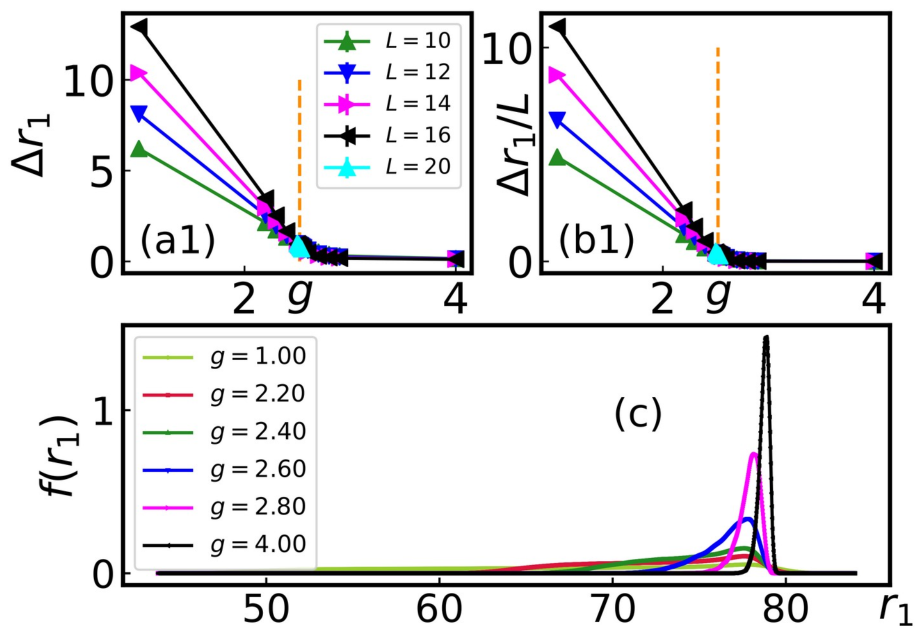


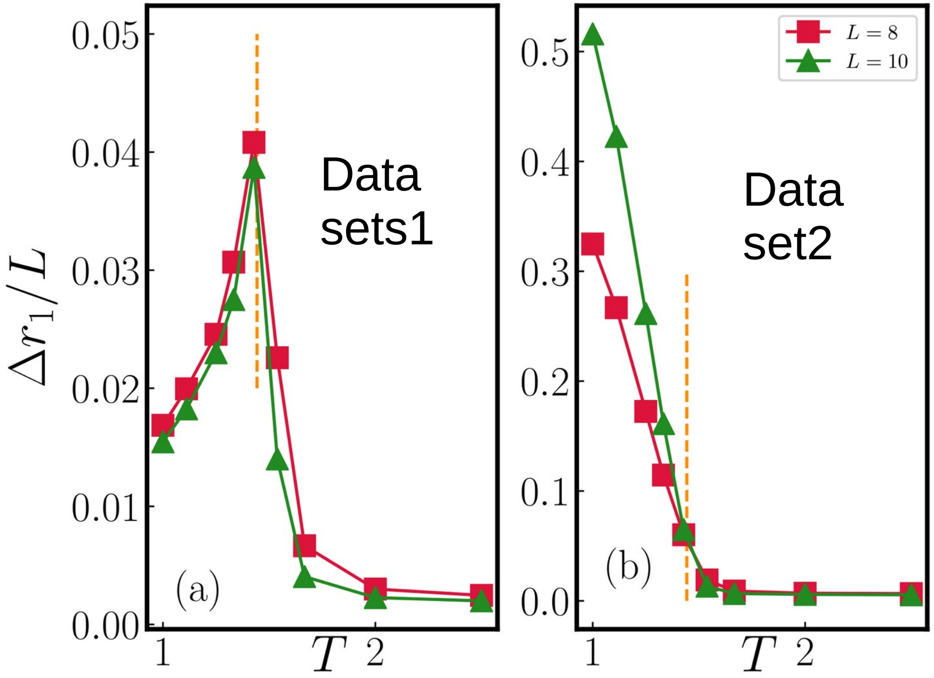
Universality class:
3D Classical
Heisenberg model

$$H_{\rm bilayer} = \sum_{l=1,2} \sum_{\langle \vec{i},\vec{j} \rangle} S_{\vec{i},l} S_{\vec{j},l} + g \sum_{\vec{i}} S_{\vec{i},1} S_{\vec{i},2},$$

Extensive behavior inside the SU(2) AFM phase

3D Classical Heisenberg model





Symmetry is no fully resolved

Data set1

$$\vec{X} = (\vec{S}_1, ..., \vec{S}_{N_s}), \text{ where, } \vec{S}_i = (S_i^x, S_i^y, S_i^z),$$

Data set2

$$\vec{X} = (S_1^z, ..., S_{N_s}^z)$$

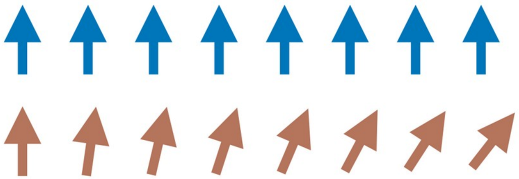
Why the ID exhibit universal scaling behavior?

Distances are related with many-body correlation functions

$$r(\vec{\theta}^i, \vec{\theta}^j) = \sqrt{2 \sum_{k=1}^{N_s} \left(1 - \vec{S}_k^i \vec{S}_k^j\right)}.$$

$S_k^i =$

$S_k^j =$



$$S_k^i \cdot S_k^j \equiv S_0 \cdot S_k$$

$$I_d \sim -\frac{1}{\ln(r_2^* / r_1^*)}$$

Detect and characterize phase transitions?

Which physical quantity to measure?
Topological transitions, thermal-MBL transitions, ...

Machine learning → raw physical data sets

Our unsupervised approach …

Does not rely on **dimension reduction**

Intrinsic dimension (ID)
of partition-function data sets

→

$$Z = \sum_{\vec{X}} e^{-\beta E(\vec{X})}$$

ID of partition-function data sets

$$Z = \sum_{\vec{X}} e^{-\beta E(\vec{X})}$$

Data sets emerging in the vicinity of phase transitions

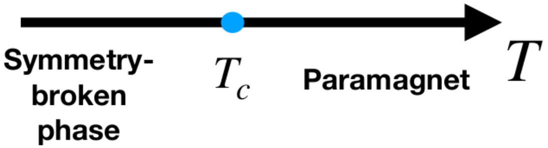
- Second-order PT
- First-order PT
- Berezinskii-Kosterlitz-Thouless (BKT) [topological PT]

$\vec{X}$ →

Spin configurations
Generated with Monte Carlo simulations

Technical details
Number of configurations [Nr = 50000]
Distance [Hamming (Ising and Potts) and Euclidean (XY)]

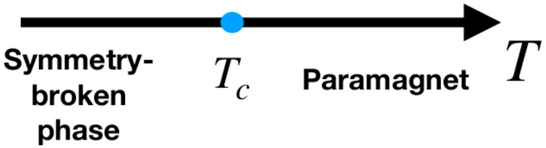
2D Ising model



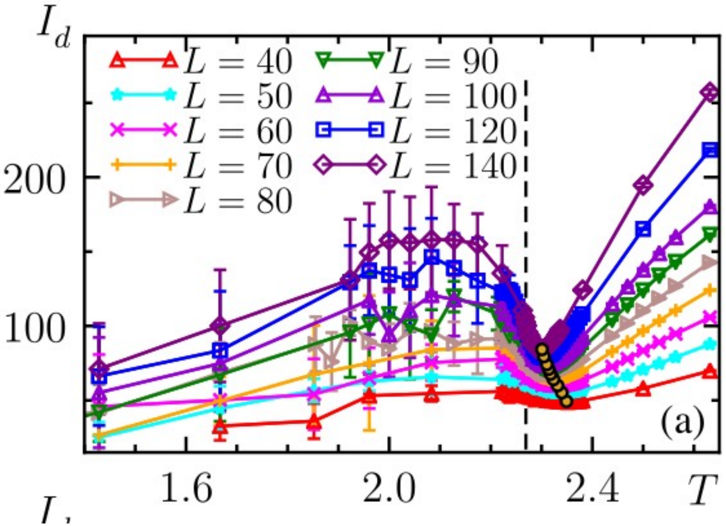
$$E_\sigma = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

$$\xi \sim (T - T_c)^{-\nu}$$

2D Ising model

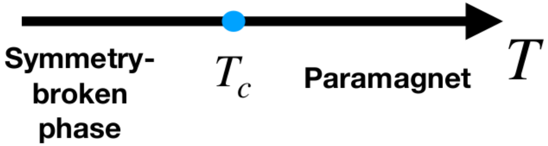


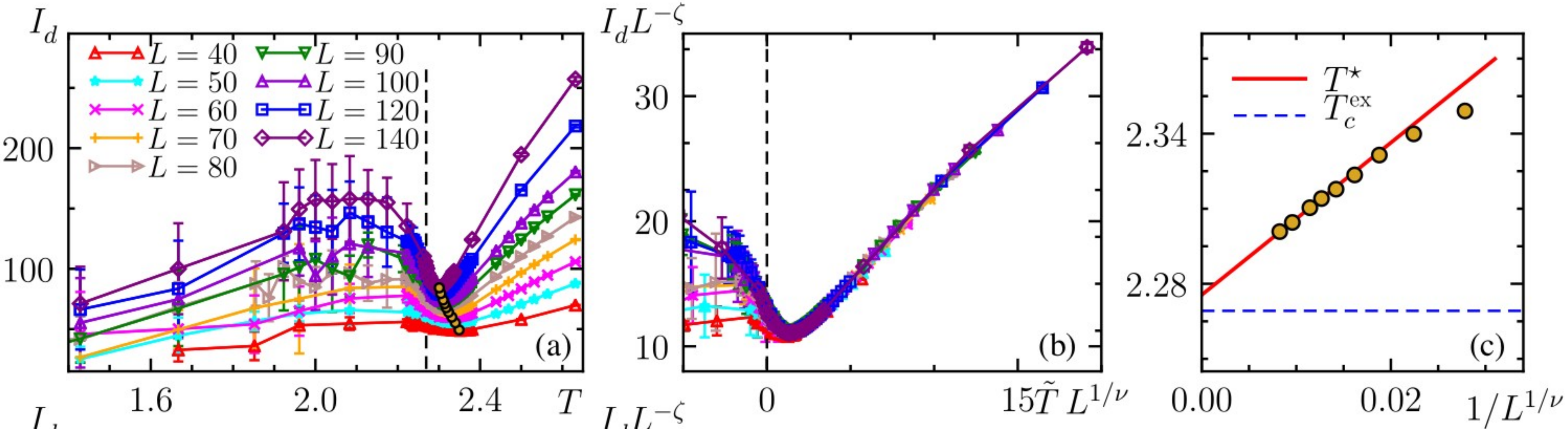
$$E_\sigma = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$



Id exhibit **a local minimum at T***

1. Second-order phase transition

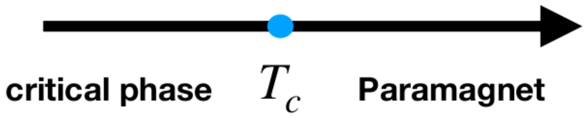




Finite size scaling $\xi \sim (T - T_c)^{-\nu}$

$$T_c = 2.283(2),\ \nu = 1.02(2).$$

2D XY model



$$E(\{\vec{\theta}\}) = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)$$

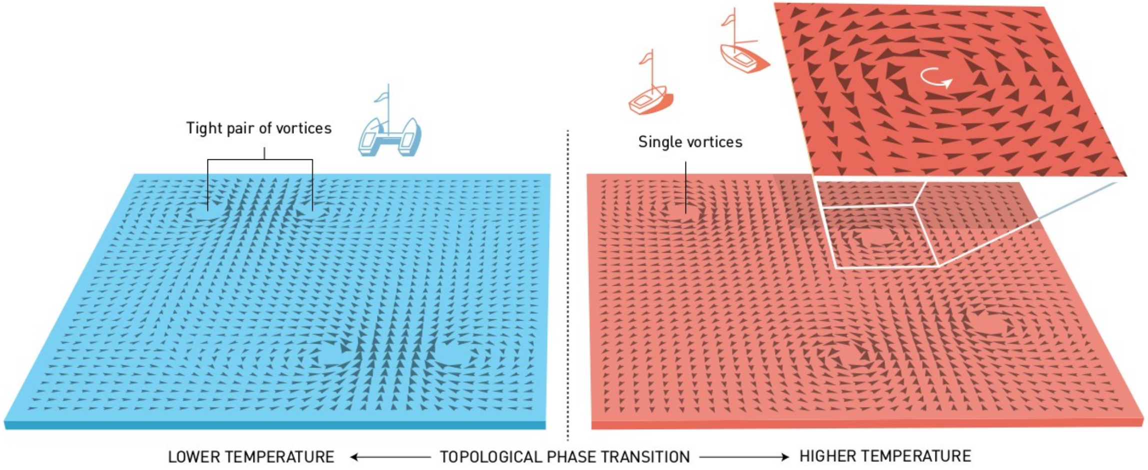
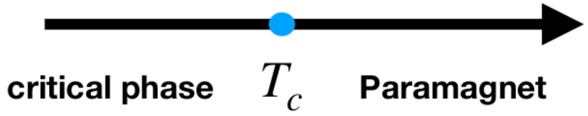
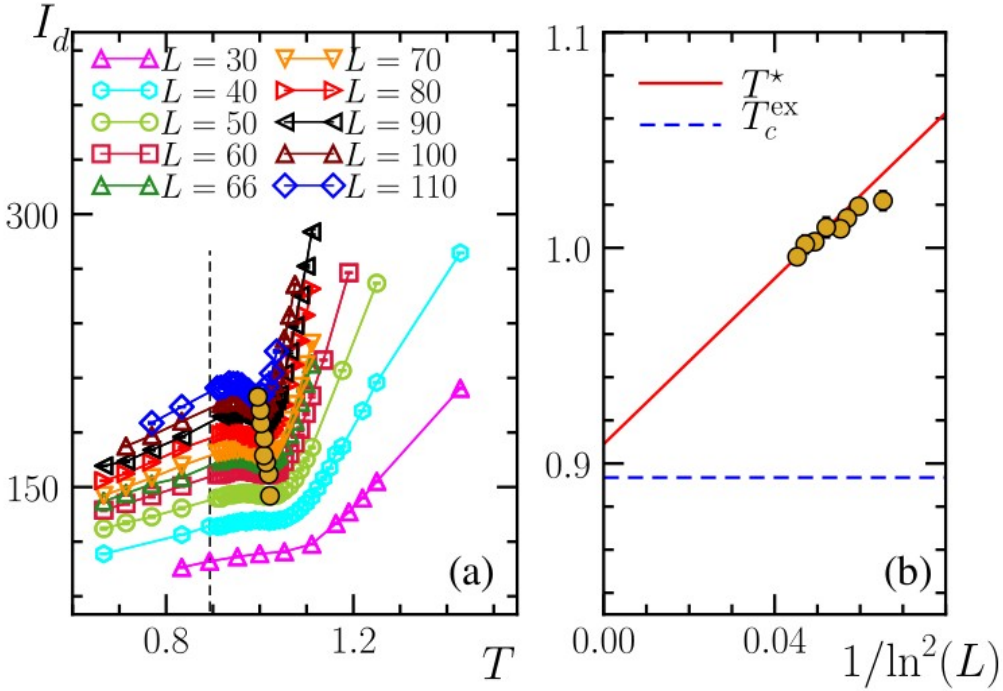
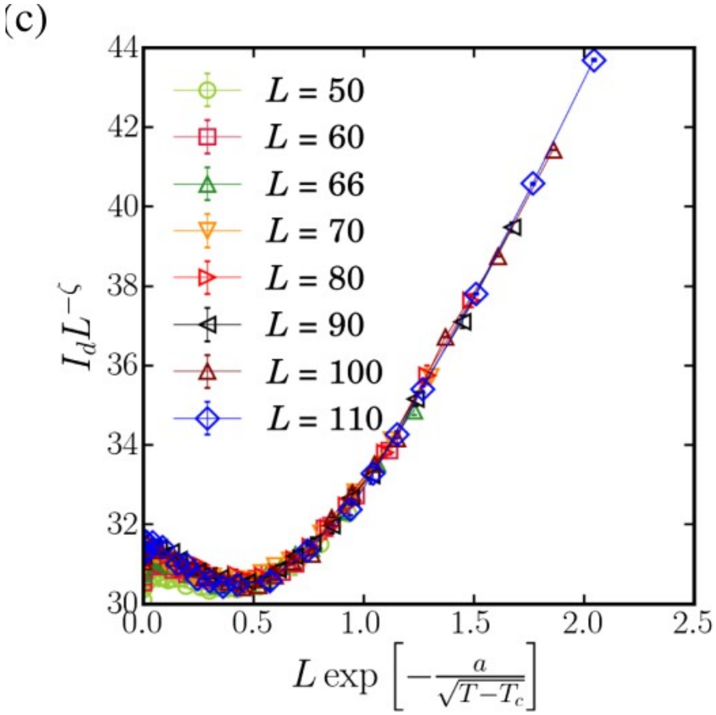


Illustration: ©Johan Jarnestad/The Royal Swedish Academy of Sciences

2. BKT phase transition







Id exhibit **a local minimum at T***

Finite size scaling

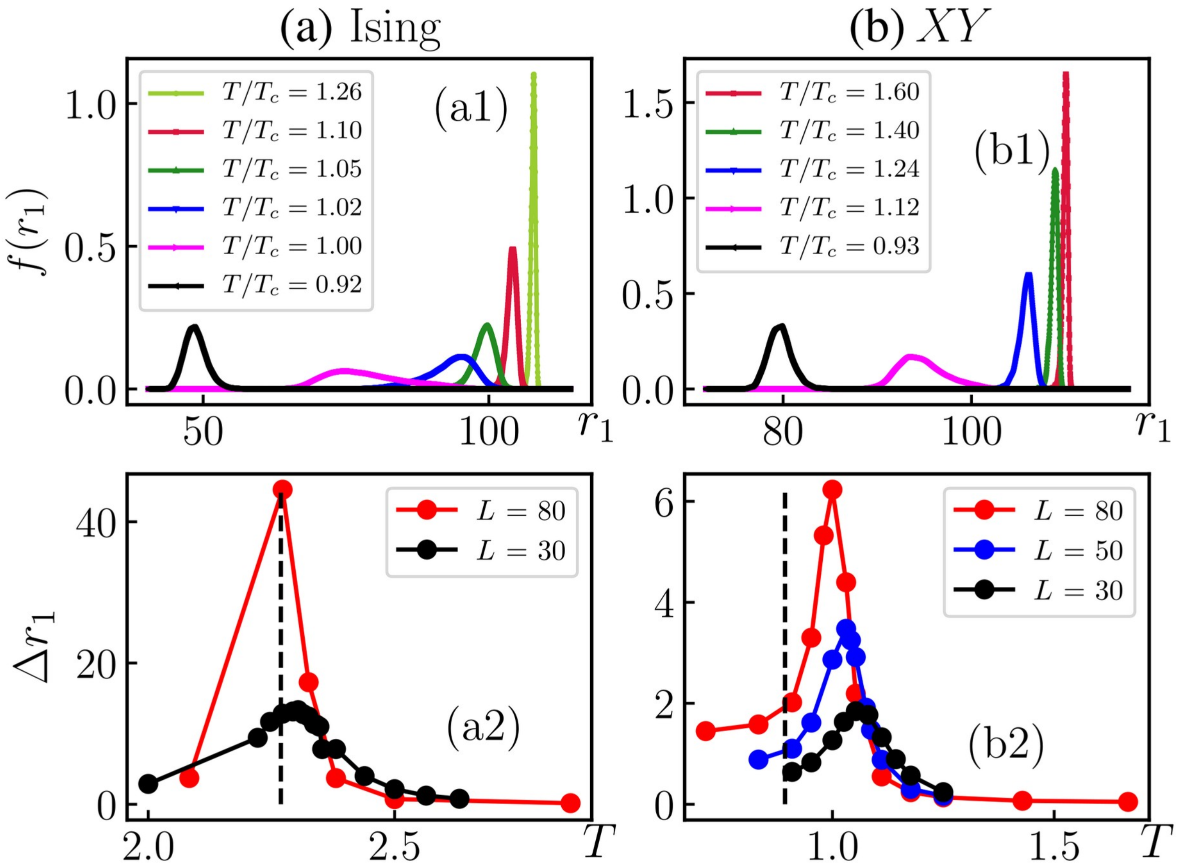
$$\xi \sim \exp\left(\frac{a}{\sqrt{T-T_c}}\right)$$

Statistics of first nearest-neighbor distances

Phase transitions

↓

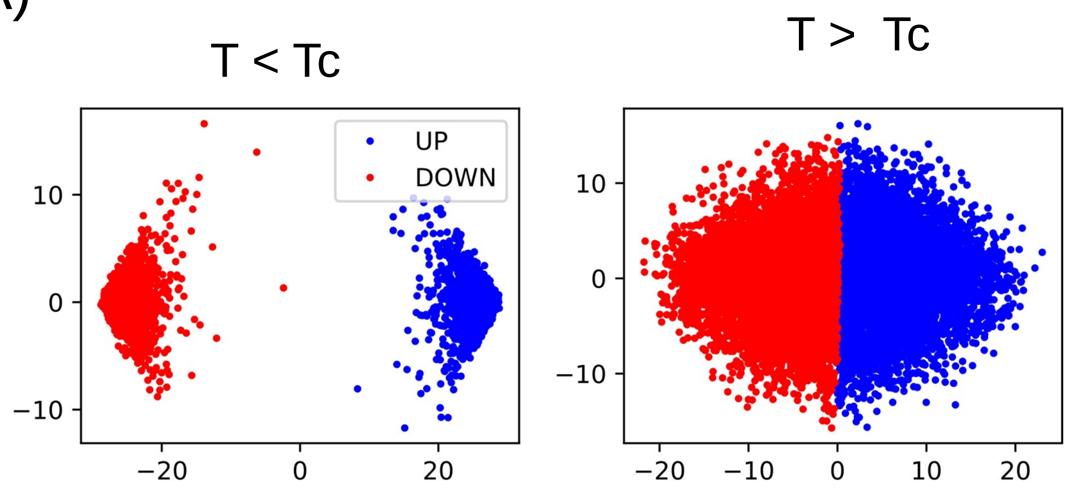
Change of scale in configuration space



Structural transition in Configuration space

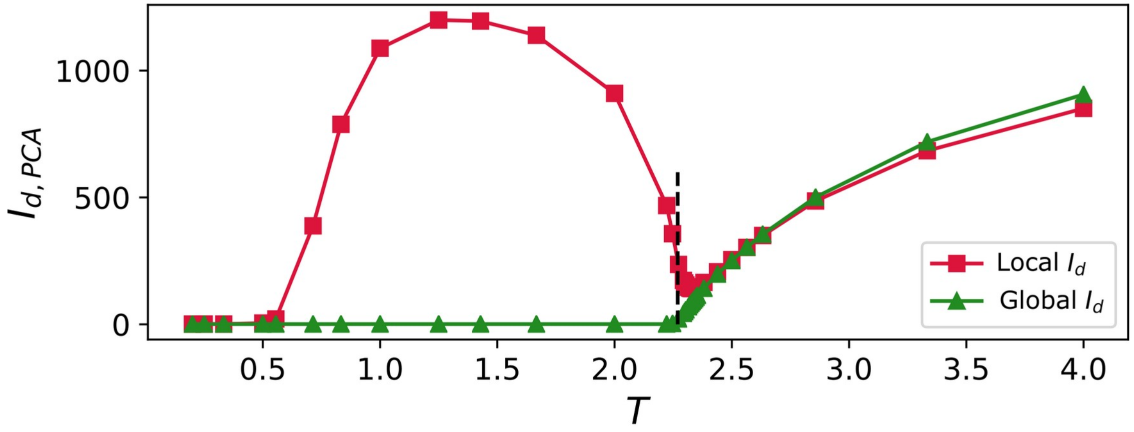
Principal component analysis (PCA)

Projection of the Ising data set in the two leading PC

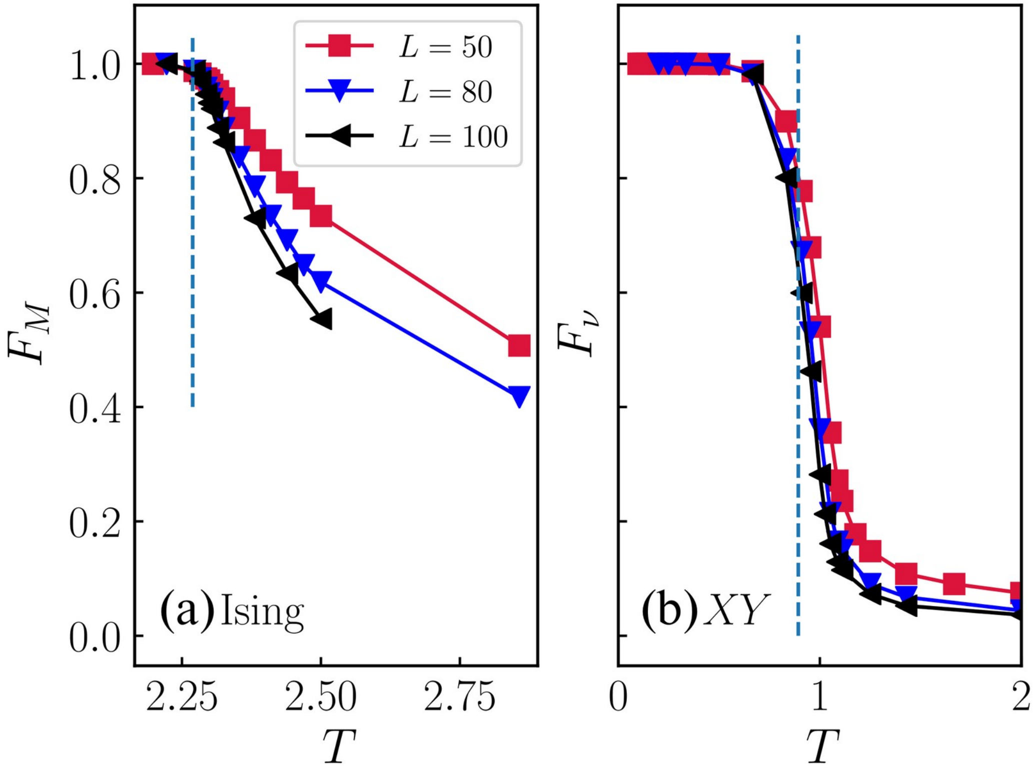


ID obtained with PCA

$$\sum_{n=1}^{I_{d,\mathrm{PCA}}} \tilde{\lambda}_n \approx f,$$



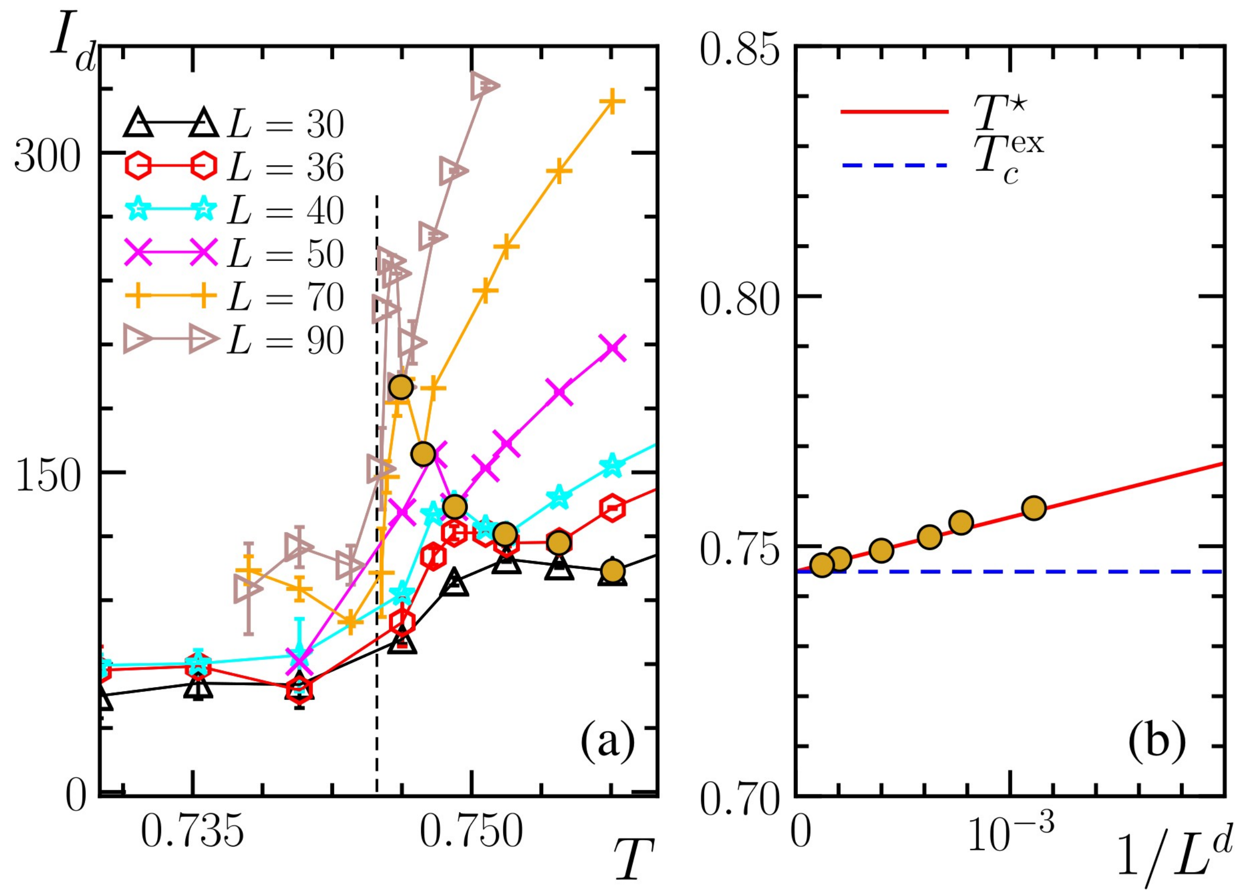
Connectivity between neighboring points in configuration space

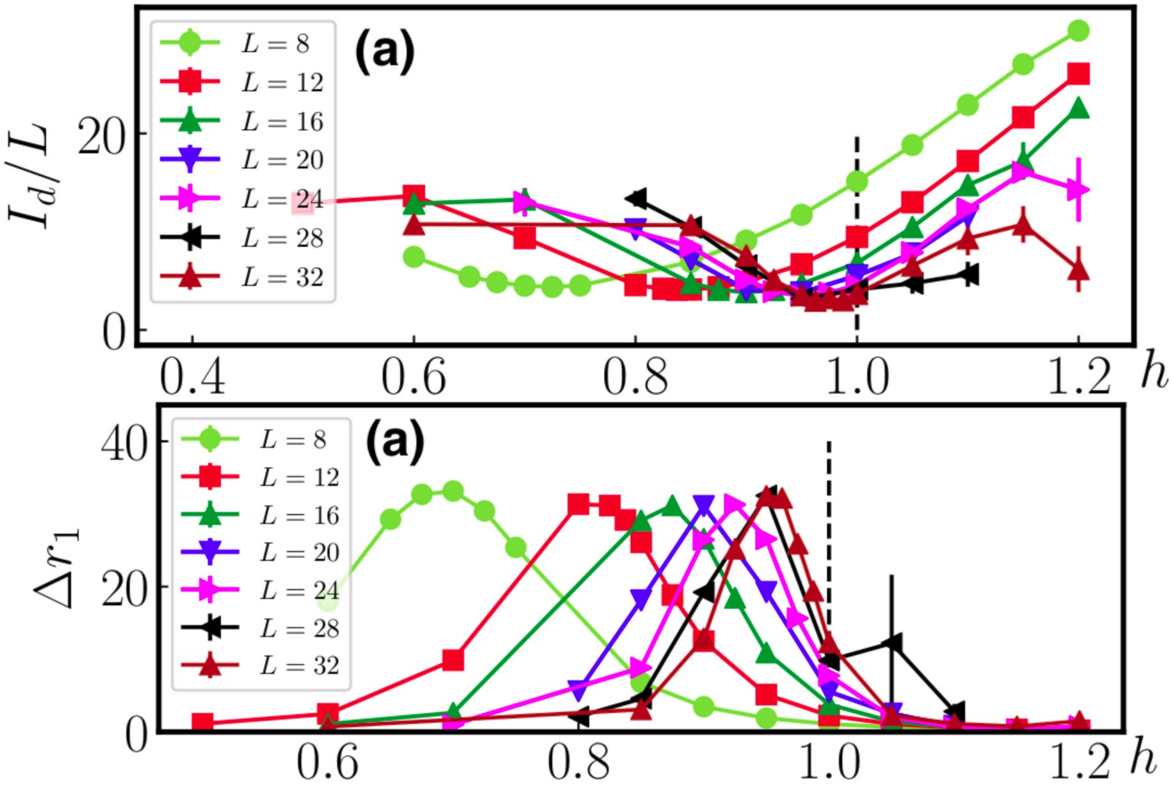


Fm → fraction of points in the data set whose first two neighbors have same magnetization sign

Fnu → fraction of points in the data set whose first two neighbors have same winding number

3. First-order phase transition





(a)
$L = 8$
$L = 12$
$L = 16$
$L = 20$
$L = 24$
$L = 28$
$L = 32$
I_d/L
20
0
0.4
0.6
0.8
1.0
1.2
h
(a)
Δr_1
40
20
0