Unsupervised learning universal critical behavior via the intrinsic dimension

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XVth Quark Confinement and the Hadron Spectrum Conference

2022 - University of Stavanger

Universität Augsburg University

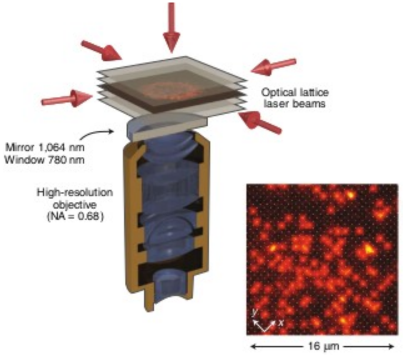
mpipks

ICTP The Abdus Salam International Centre for Theoretical Physics

Large data sets

Handwriting

Physical data sets
[Many-body physics]



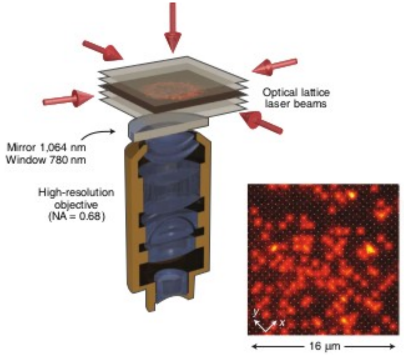
Large **[high-dimensional]** data sets

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

Handwriting

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

Physical data sets
[Many-body physics]

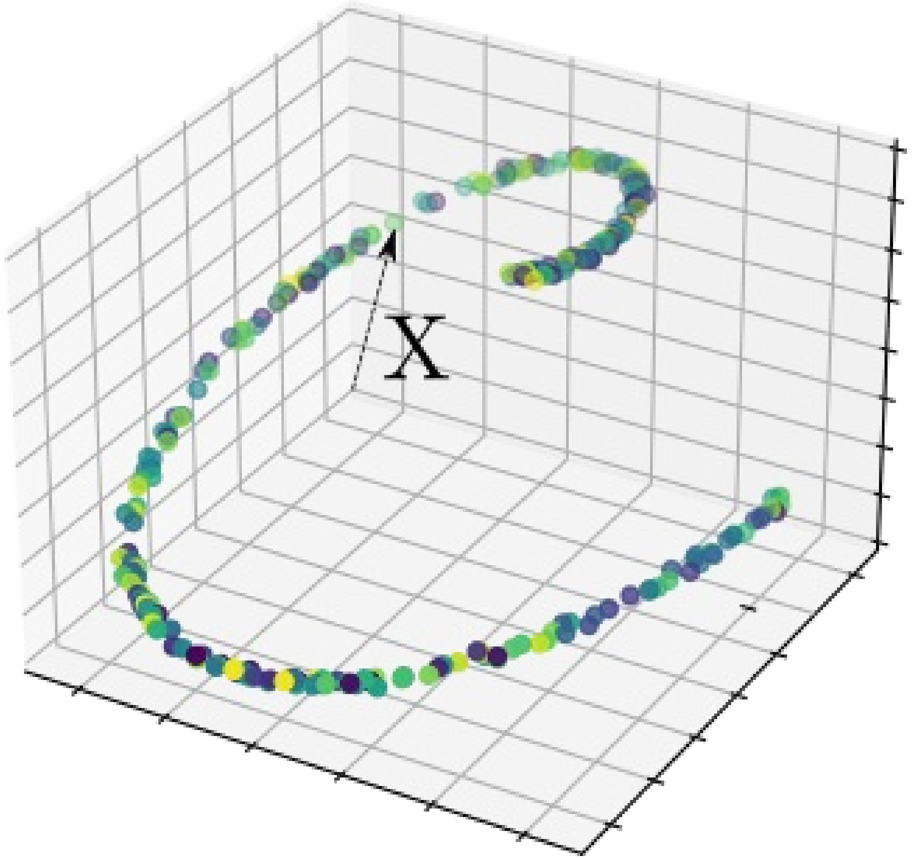


Intrinsic dimension (ID)

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



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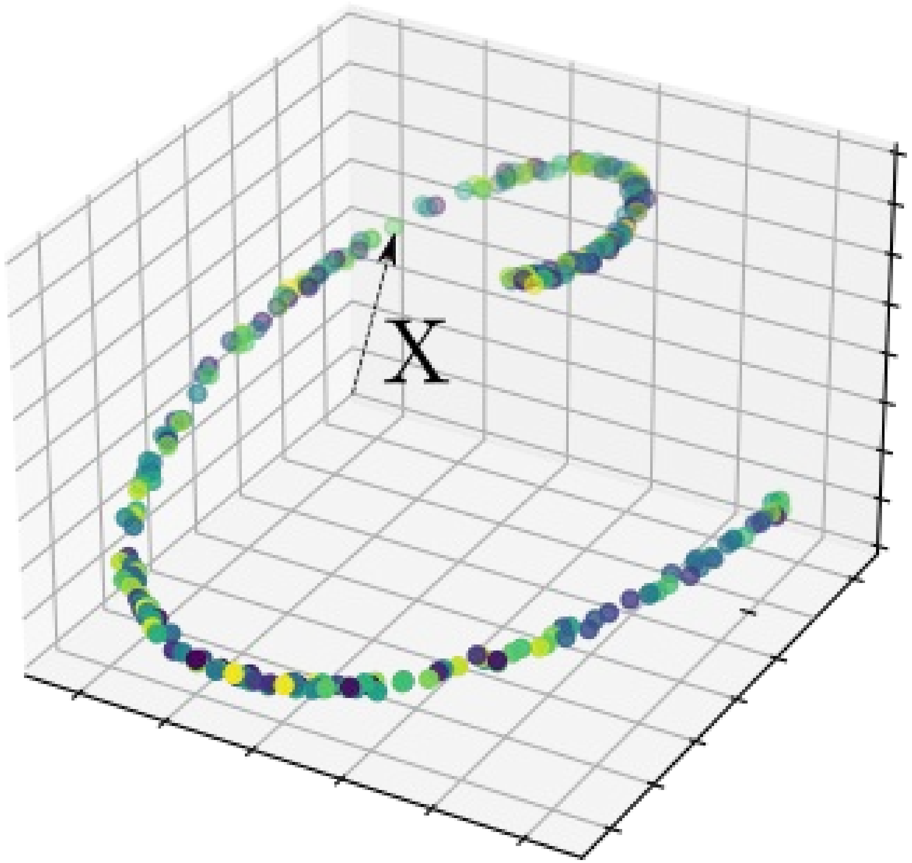


Physical data sets ?

Partition-function data sets

$$\beta = \frac{1}{k_B T}$$

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

$$\vec{X} = (x_1, x_2, ..., x_{N_s})$$

Partition-function data sets

$$\beta = \frac{1}{k_B T}$$

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

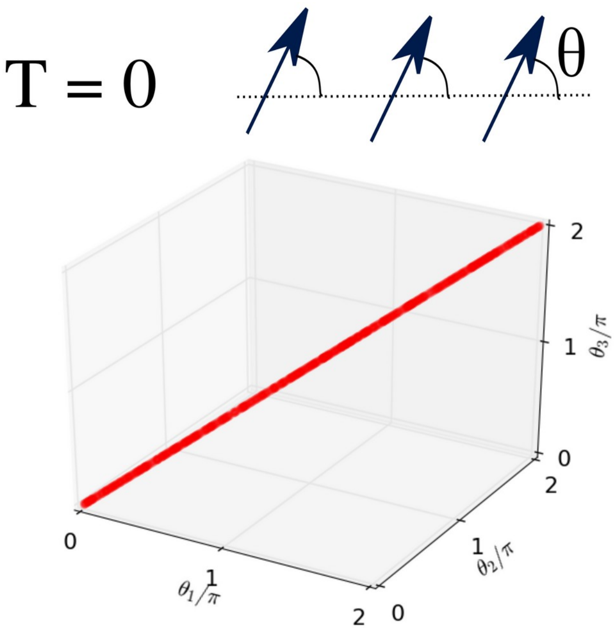
$$\vec{X} = (x_1, x_2, \ldots, x_{N_s})$$

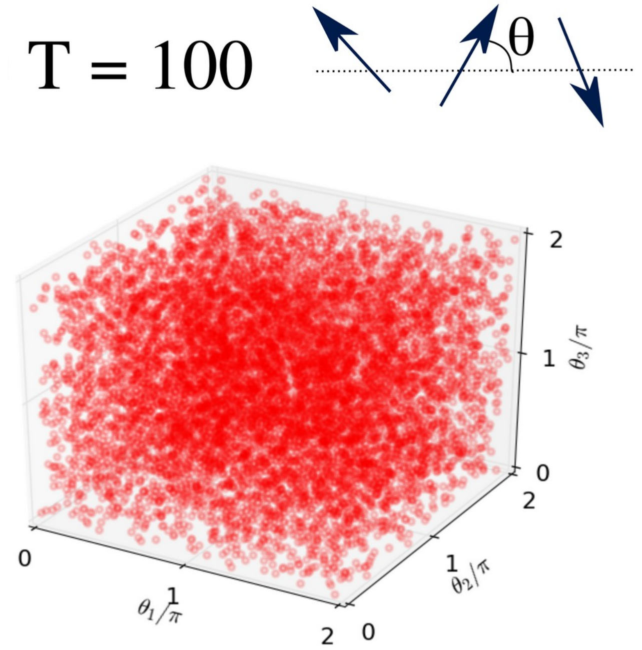
Set of points in a high-dimensional space

Partition-function data sets

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

3-spin XY model



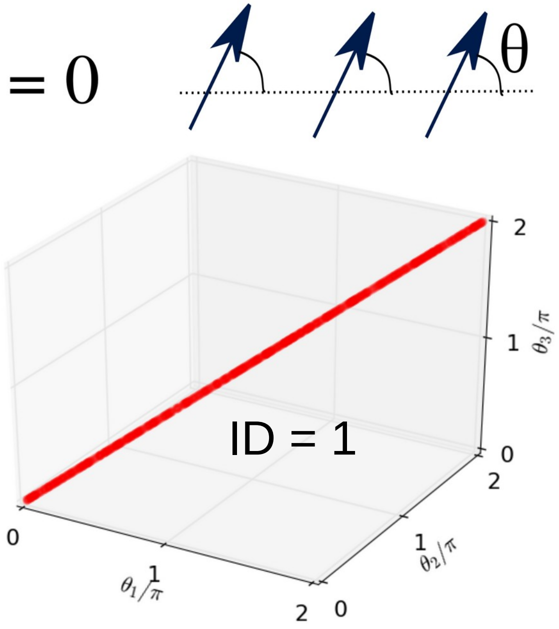


Partition-function data sets

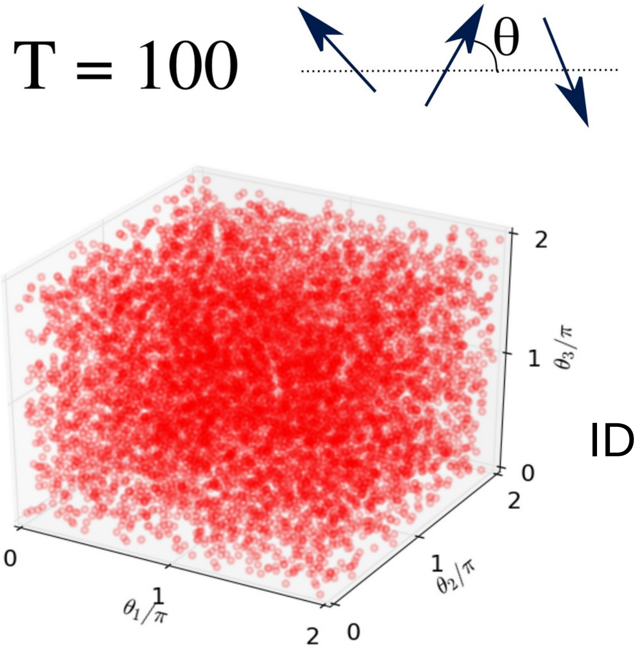
$$Z = \sum_{\vec{X}} e^{-\beta E(\vec{X})}$$

3-spin XY model

T = 0



T = 100

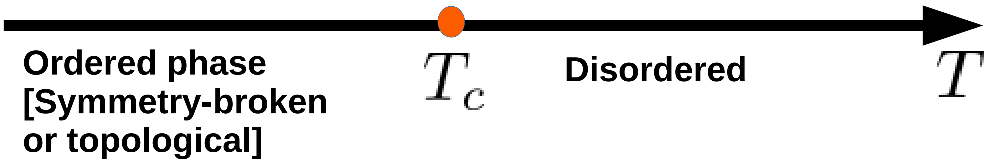


ID = 3

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

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

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




```
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
```

ID of data sets emerging in the vicinity of **phase transitions**

→

Phase transition in configuration space?

Extract information of the system from raw data - **universal properties**?

Outline

→ Machine learning phases of matter and phases transitions [Many-body physics]

→ How to estimate the intrinsic dimension (ID)

→ ID and phase transitions

Machine learning → raw physical data sets

Characterize **phases of matter** and **their transitions**

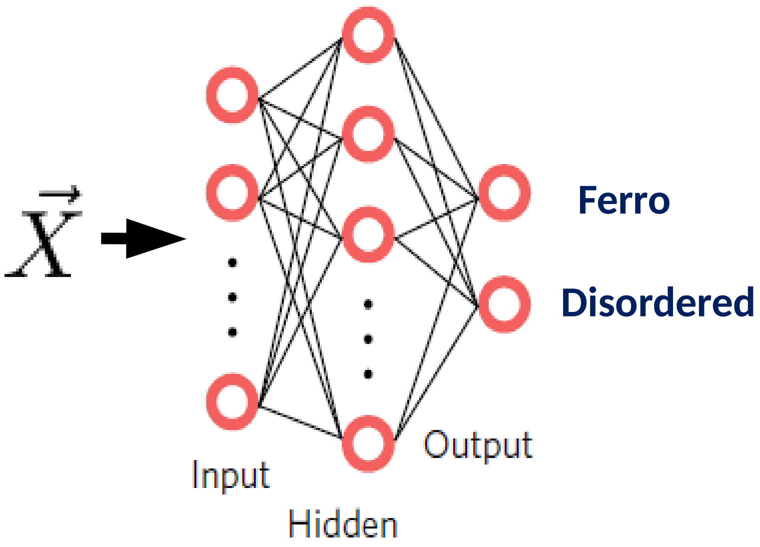
→ Which physical quantity to measure?
Topological transitions, thermal-MBL transitions, …

→ Detect the important degrees of freedom of a system

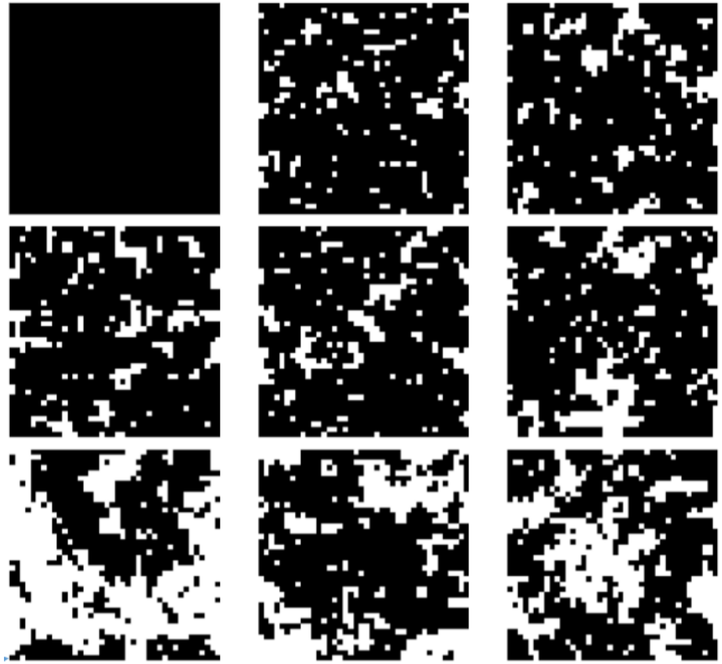
Supervised ML: Labeled configurations

Machine learning phases of matter

Juan Carrasquilla[1*] and Roger G. Melko[1,2] nature physics (2017)



2D-Ising configurations

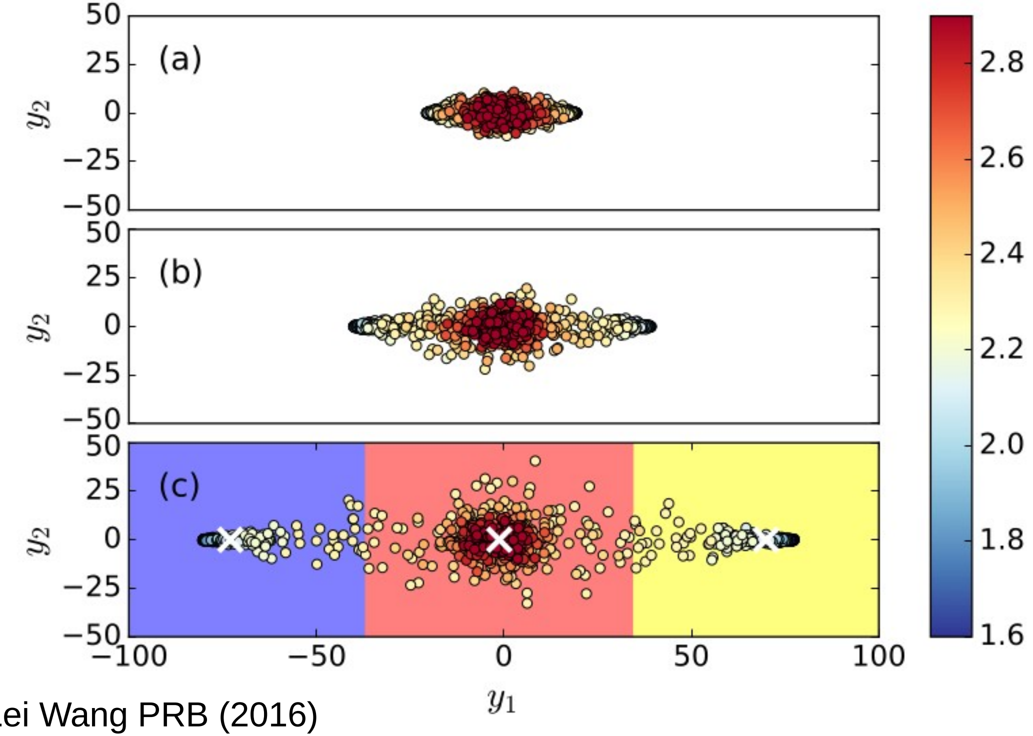


Unsupervised ML:Unlabeled configurations

Dimension reduction

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

2D Ising model



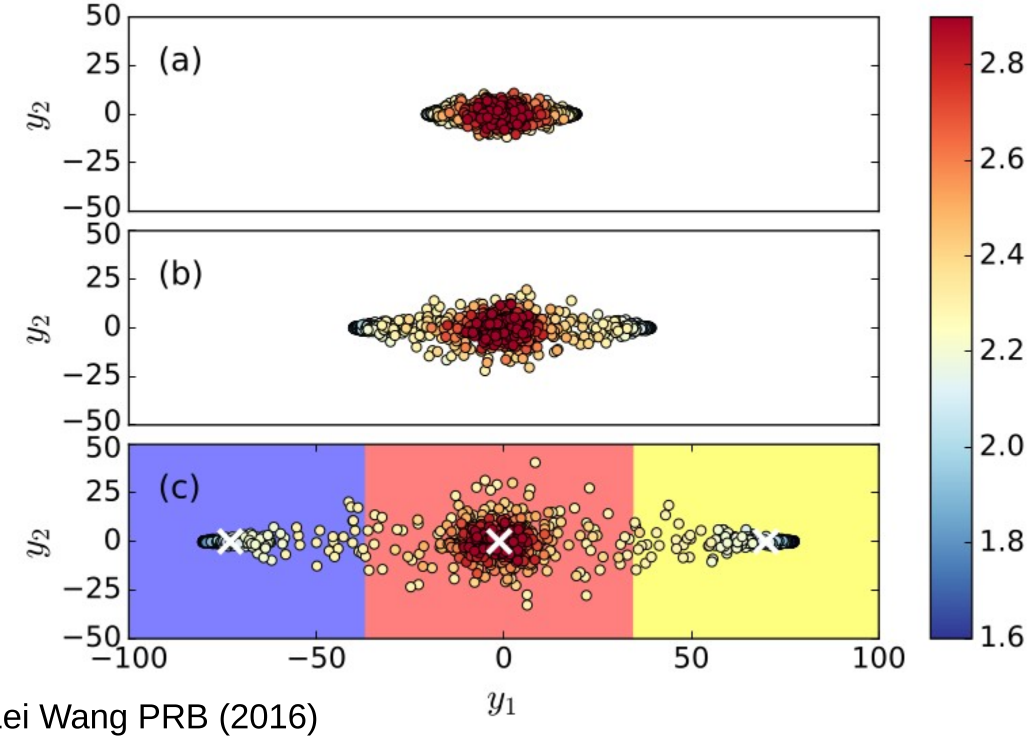
Principal component analysis (PCA)

Lei Wang PRB (2016)

Unsupervised ML:Unlabeled configurations

Dimension reduction

2D Ising model



Lei Wang PRB (2016)

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

➡ **X**

Principal component analysis (PCA)
→ Linear transformation

$$\mathbf{X}^T\mathbf{X}\mathbf{w}_n = \lambda_n \mathbf{w}_n$$

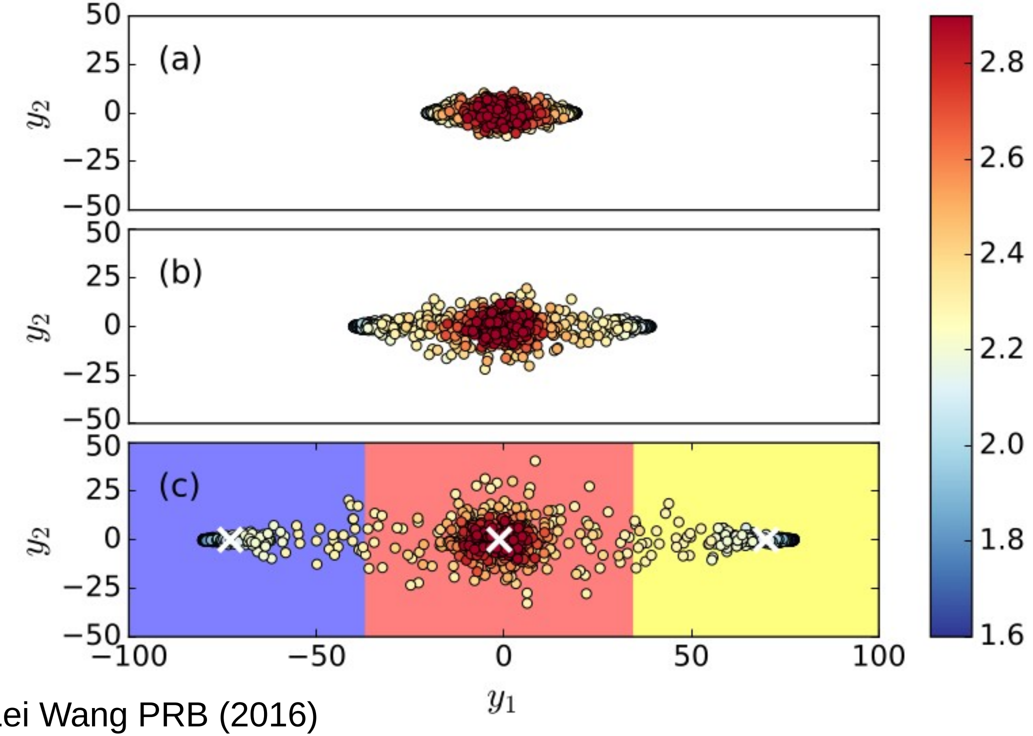
Unsupervised ML:Unlabeled configurations

Dimension reduction

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

$\Rightarrow$ **X**

2D Ising model



Lei Wang PRB (2016)

Principal component analysis (PCA)
→ Linear transformation

$$\mathbf{X}^T\mathbf{X}\mathbf{w}_n = \lambda_n \mathbf{w}_n$$

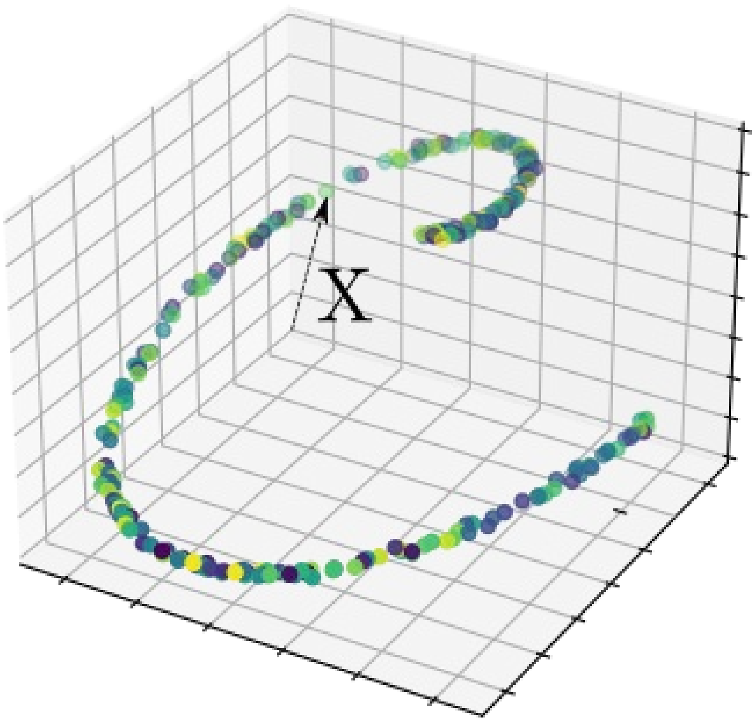
More complicated transitions (e.g., topological transitions, …) are not described by PCA

(I) How to estimate the ID?

(II) ID and phase transitions [classical and quantum]

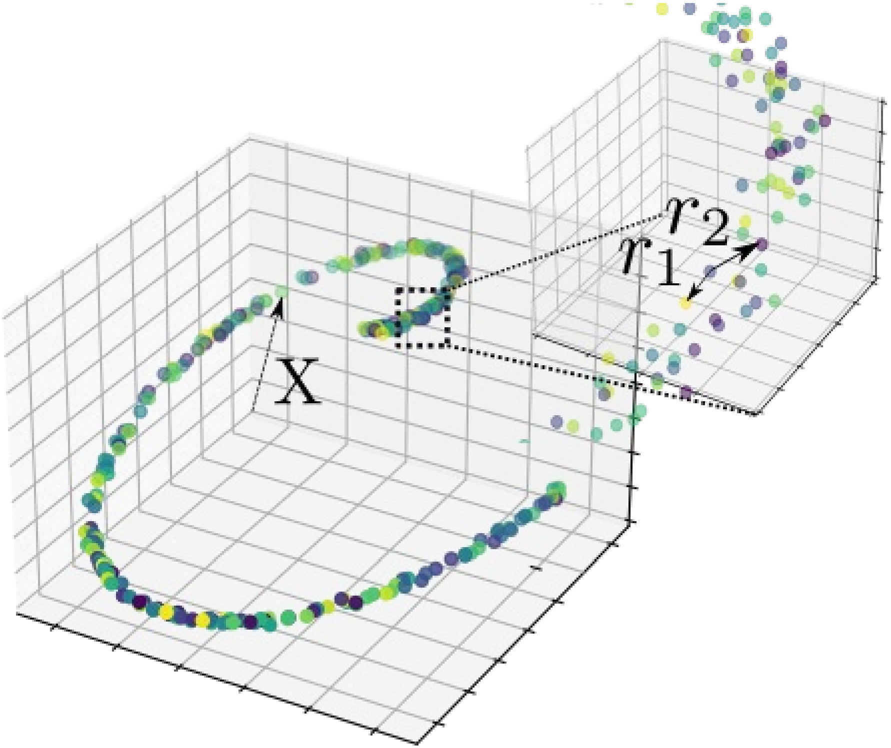
How to estimate the ID?

Different approaches: projection (e.g., **PCA**), fractal, **nearest-neighbors (NN)**

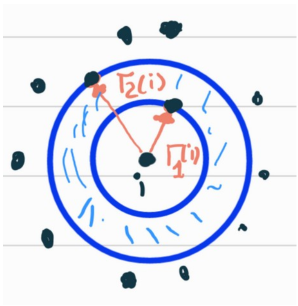


How to estimate the ID?

nearest-neighbors (NN) method
→ geometrical approach



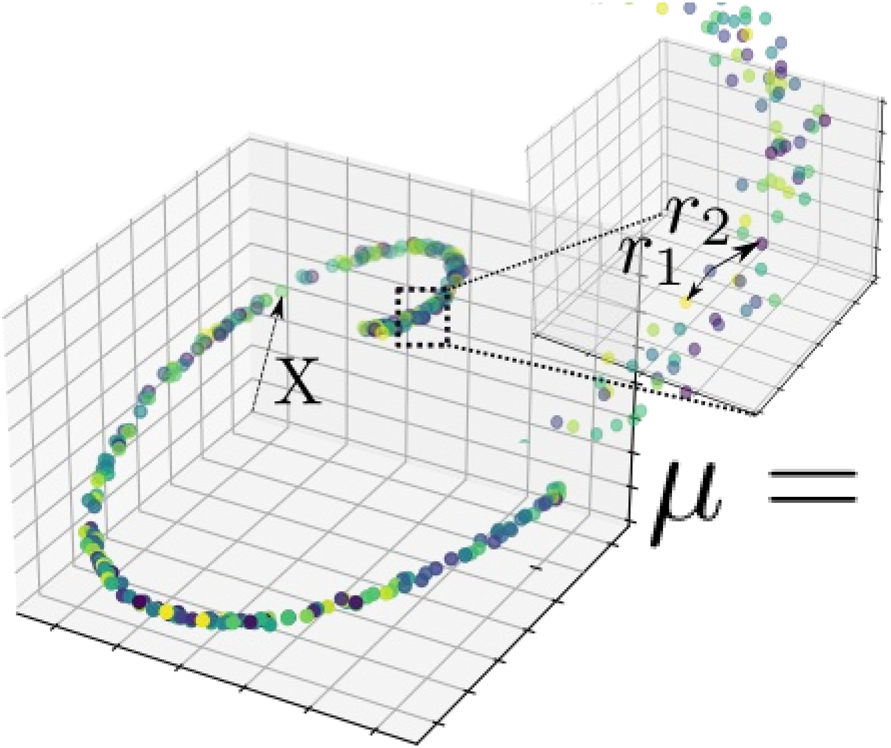
Statistics of NN distances
[e.g., Euclidian, Hamming, etc]



$$v(i) \sim (r_2(i)^{I_d} - r_1(i)^{I_d})$$

How to estimate the ID?

Nearest neighbors(NN)-based estimator [**TWO-NN** method]



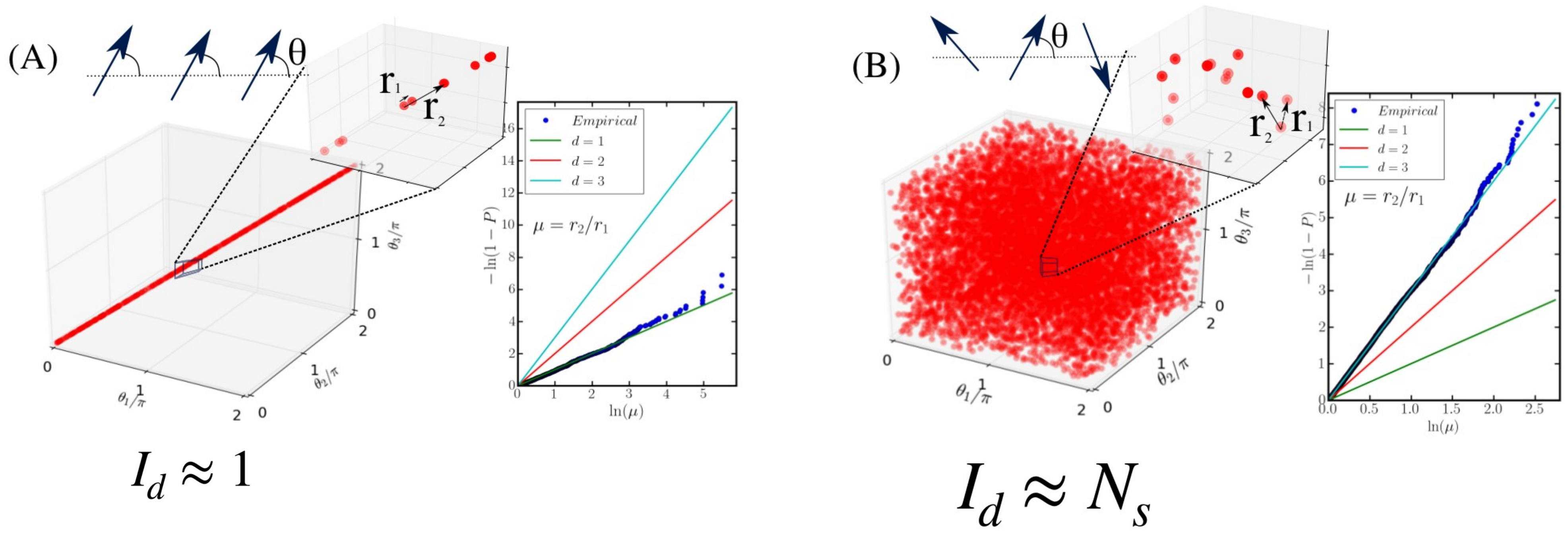
$$\mu = \frac{r_2}{r_1}$$

Probability distribution function

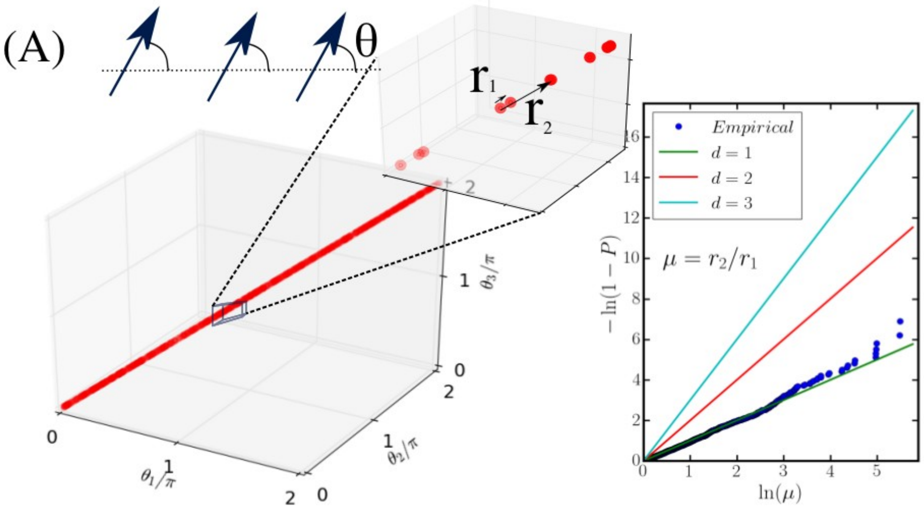
$$\boxed{f(\mu) = I_d \mu^{-1-I_d}}$$

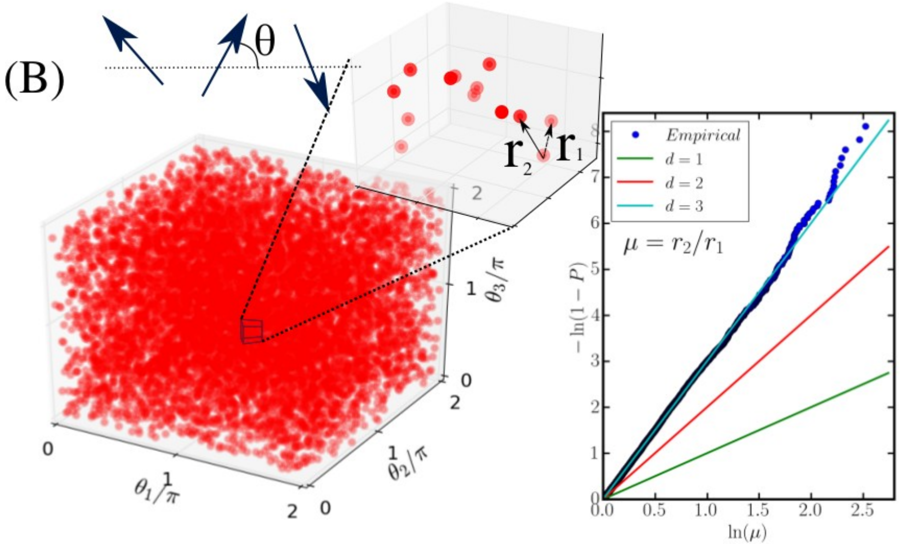
Elena Facco et. al. Scientific Reports (2017)

Assumption: data set is locally uniform in density



(A)
θ
$\mathbf{r}_1$
$\mathbf{r}_2$
θ_1/π
θ_2/π
θ_3/π
Empirical
$d=1$
$d=2$
$d=3$
$\mu = r_2/r_1$
$-\ln(1-P)$
$\ln(\mu)$
$I_d \approx 1$
(B)
θ
$\mathbf{r}_2$
$\mathbf{r}_1$
θ_1/π
θ_2/π
θ_3/π
Empirical
$d=1$
$d=2$
$d=3$
$\mu = r_2/r_1$
$-\ln(1-P)$
$\ln(\mu)$
$I_d \approx N_s$





$$I_d \approx 1$$

$$I_d \approx N_s$$

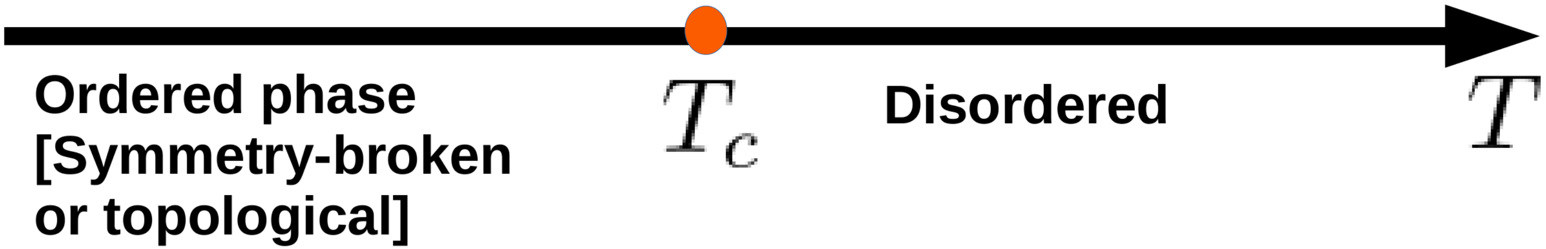
ID (TWO-NN)

→ Local feature of configuration space

→ Depends on the typical value of distances [scale-dependent quantity]

N_r → Number of points in the data set

ID of partition-function data sets
→ Vicinity of phase transitions (Classical and Quantum)



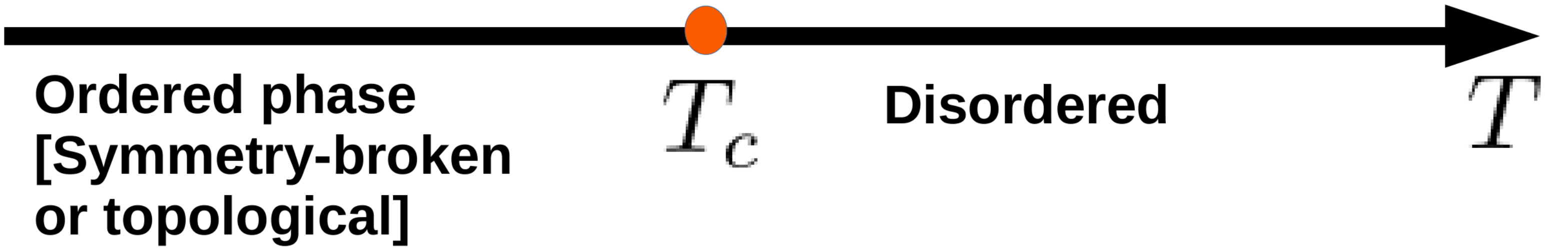
TMS, X. Turkeshi, M. Dalmonte, A. Rodriguez, PRX 11, 011040 (2021)

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

ID of partition-function data sets
→ Vicinity of phase transitions (Classical and Quantum)

(1) Second-order PT
(2) Berezinskii-Kosterlitz-Thouless (BKT)
(3) First-order PT

Data sets generated by Monte Carlo simulations



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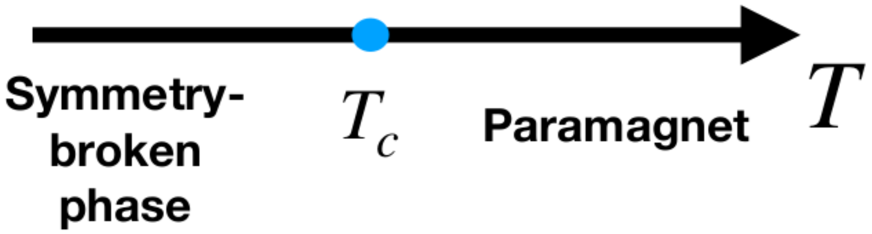
1. Second-order phase transition

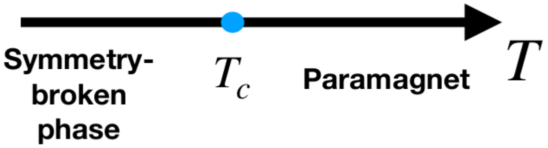


$$\xi \sim (T - T_c)^{-\nu}$$

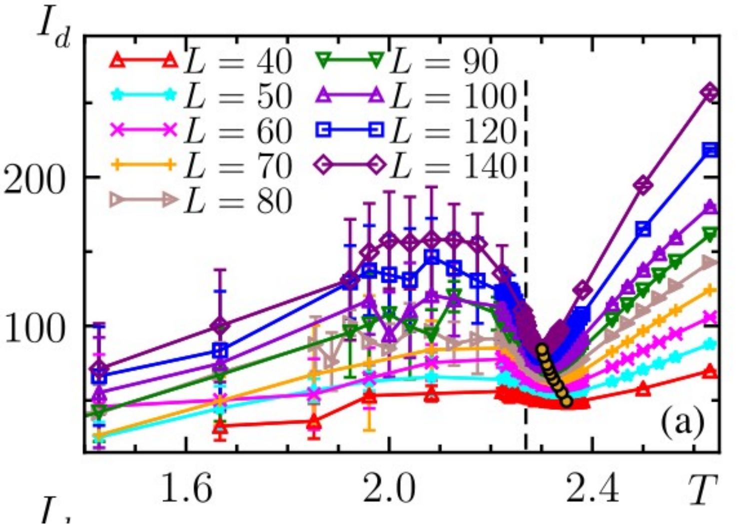
Finite size scaling

$$\boxed{Q(t, L) = L^{\sigma} f(\xi / L)}$$

2D Ising model

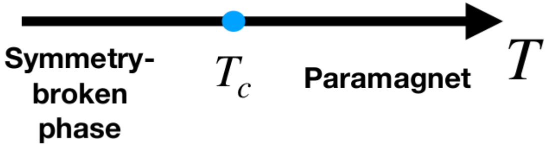


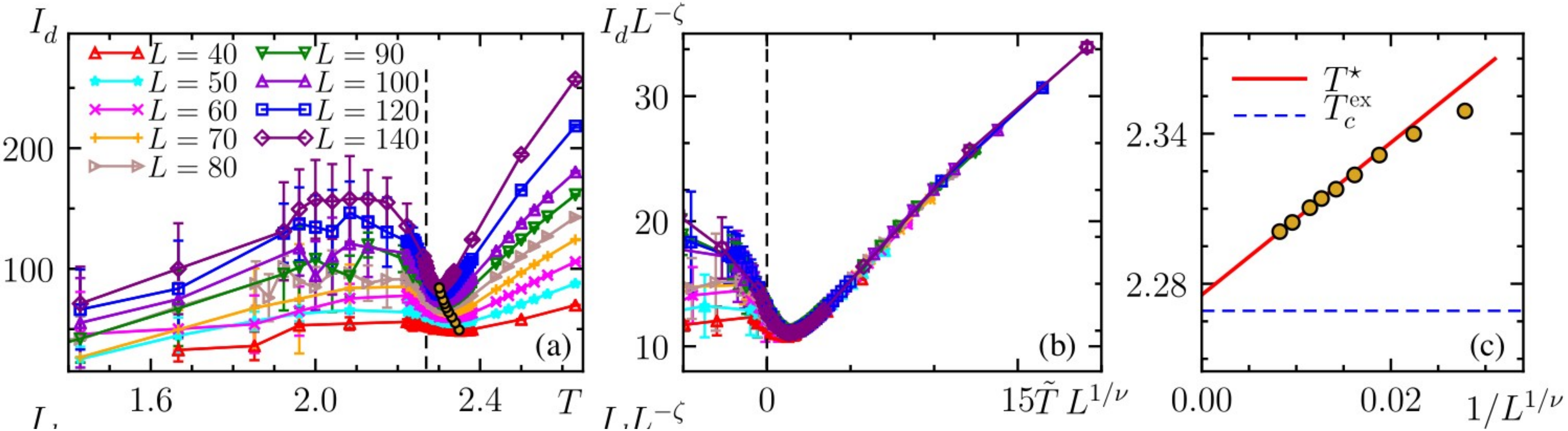
$$E_\sigma = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$



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

2D Ising model

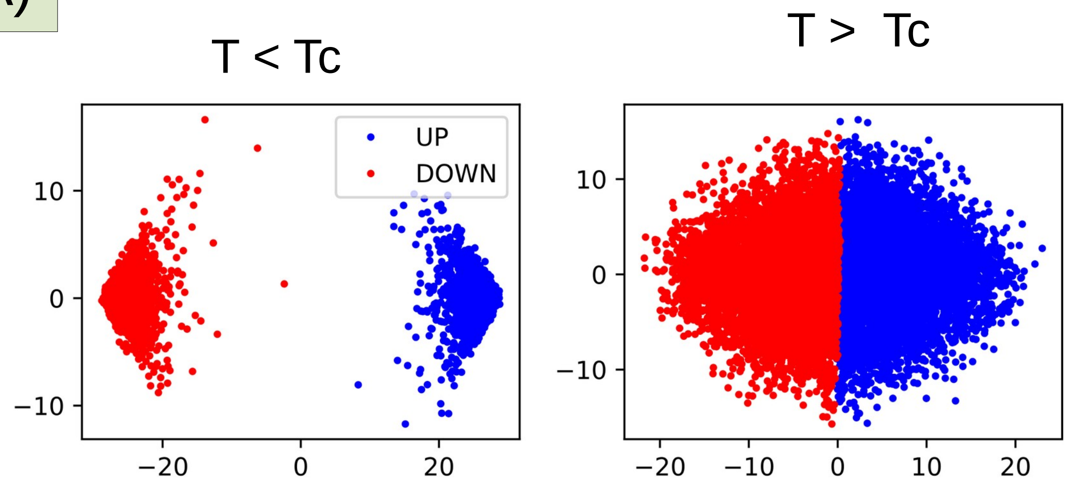




$$T_c = 2.283(2),\ \nu = 1.02(2).$$

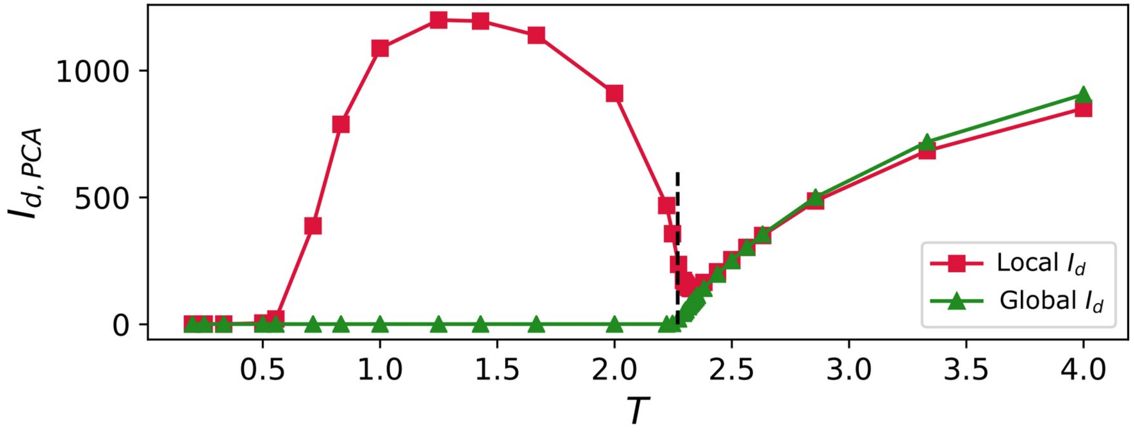
Principal component analysis (PCA)

Projection of the Ising data set in the two leading PC



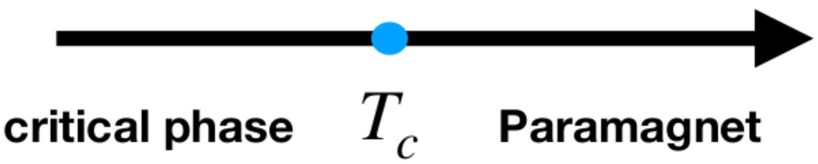
ID obtained with PCA

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



2. BKT phase transition

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



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

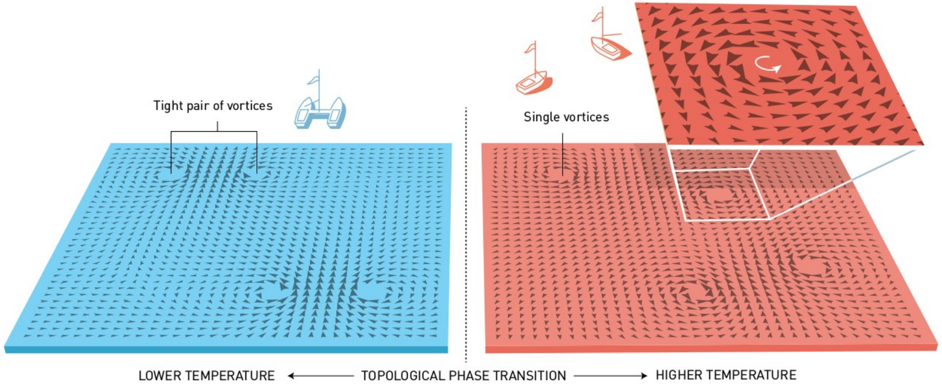
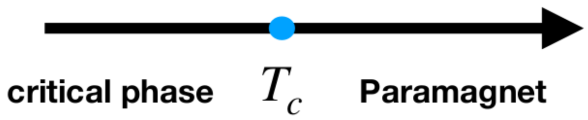
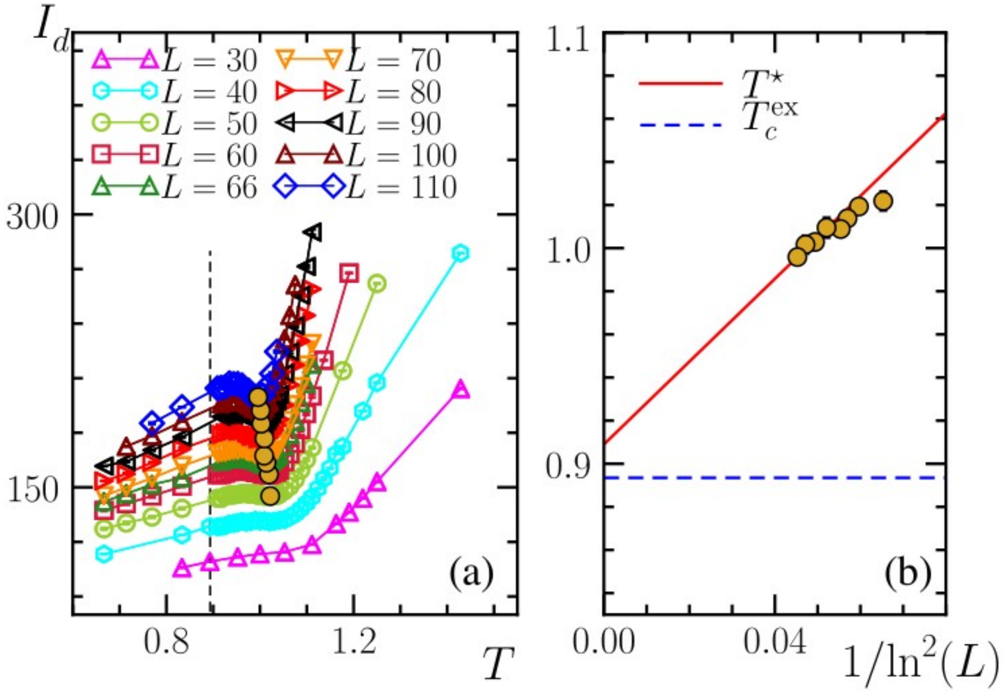
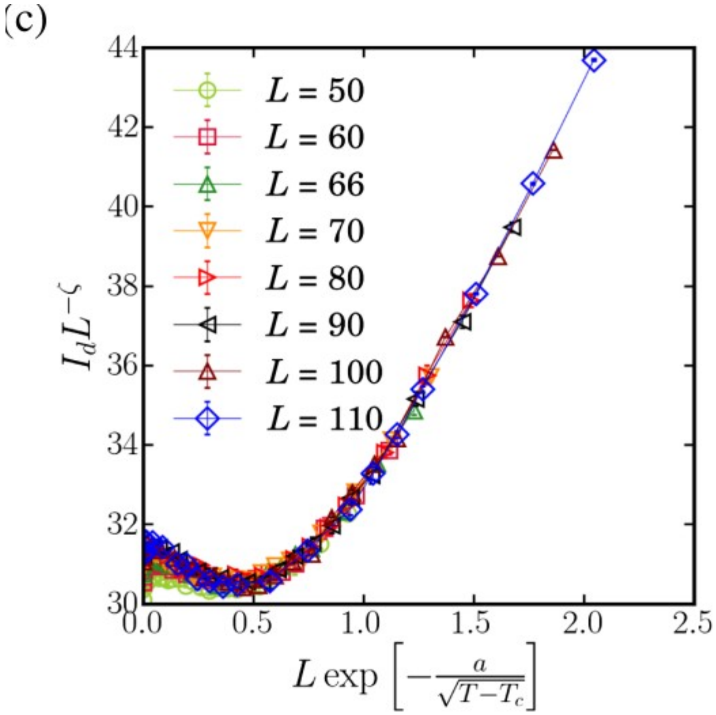


Illustration: ©Johan Jarnestad/The Royal Swedish Academy of Sciences

2D XY model







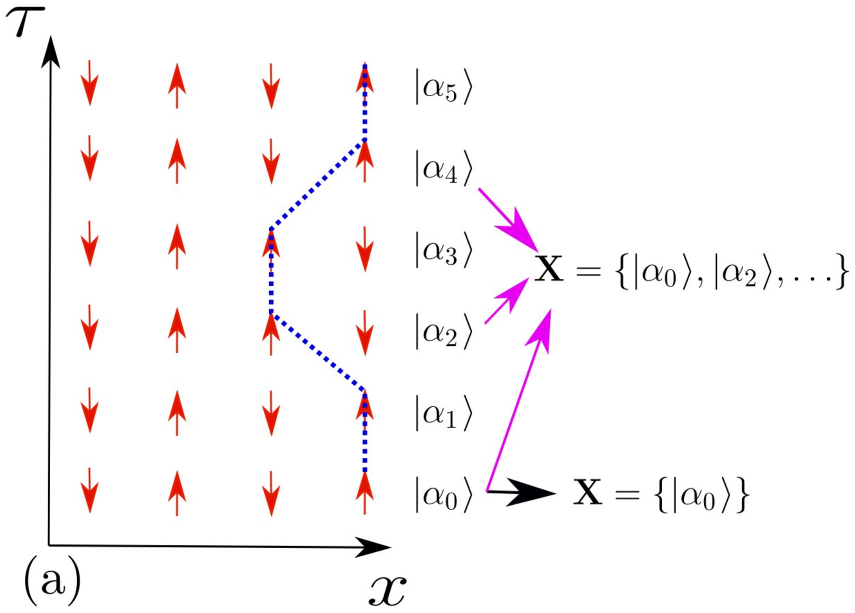
Id exhibit **a local minimum at T***

Finite size scaling

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

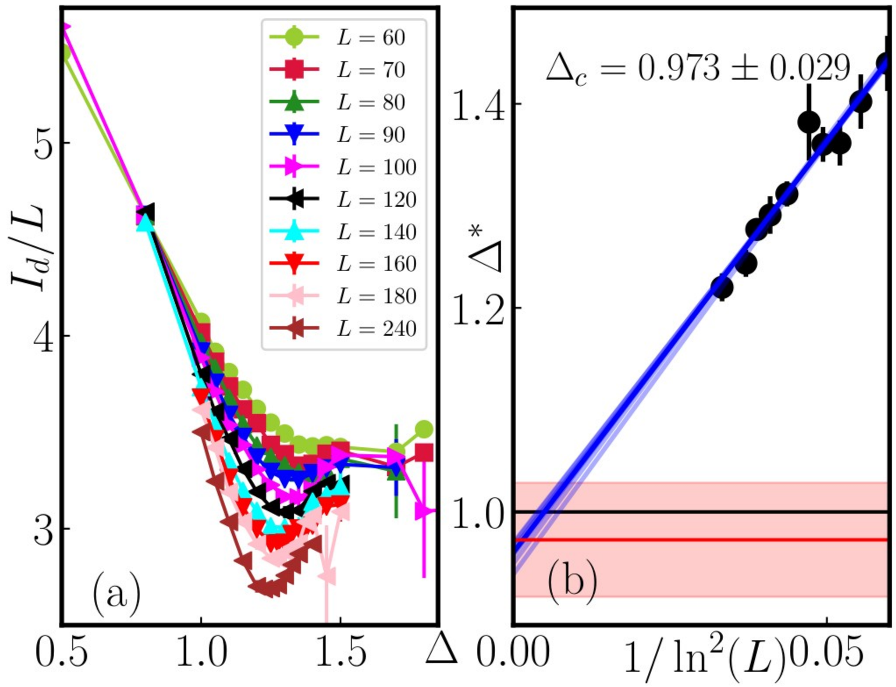
Quantum phase transitions

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

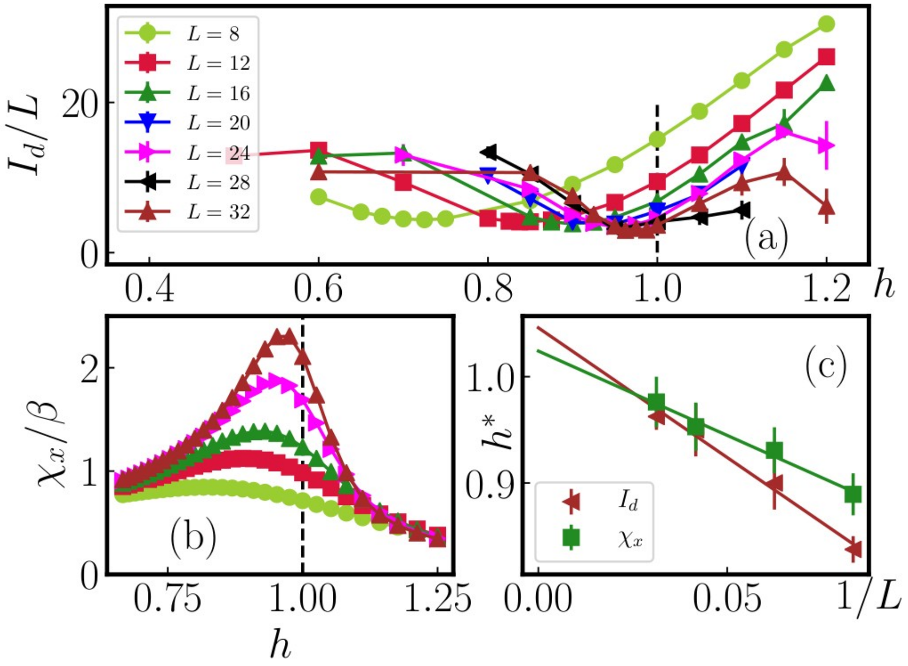


Quantum models

1d XXZ model
BKT transition



1d Quantum Ising model
Sec. order transition



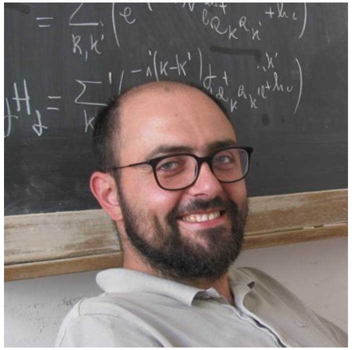
Conclusion

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

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)

Thank you!



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PRX 11, 011040 (2021)

PRX Quantum 2, 030332 (2021)

Supplemental material

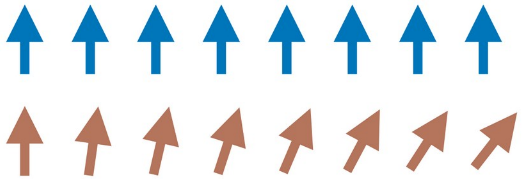
Why the ID exhibit universal scaling behavior?

Distances are related with many-body correlation functions

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

$S_k^i =$

$S_k^j =$



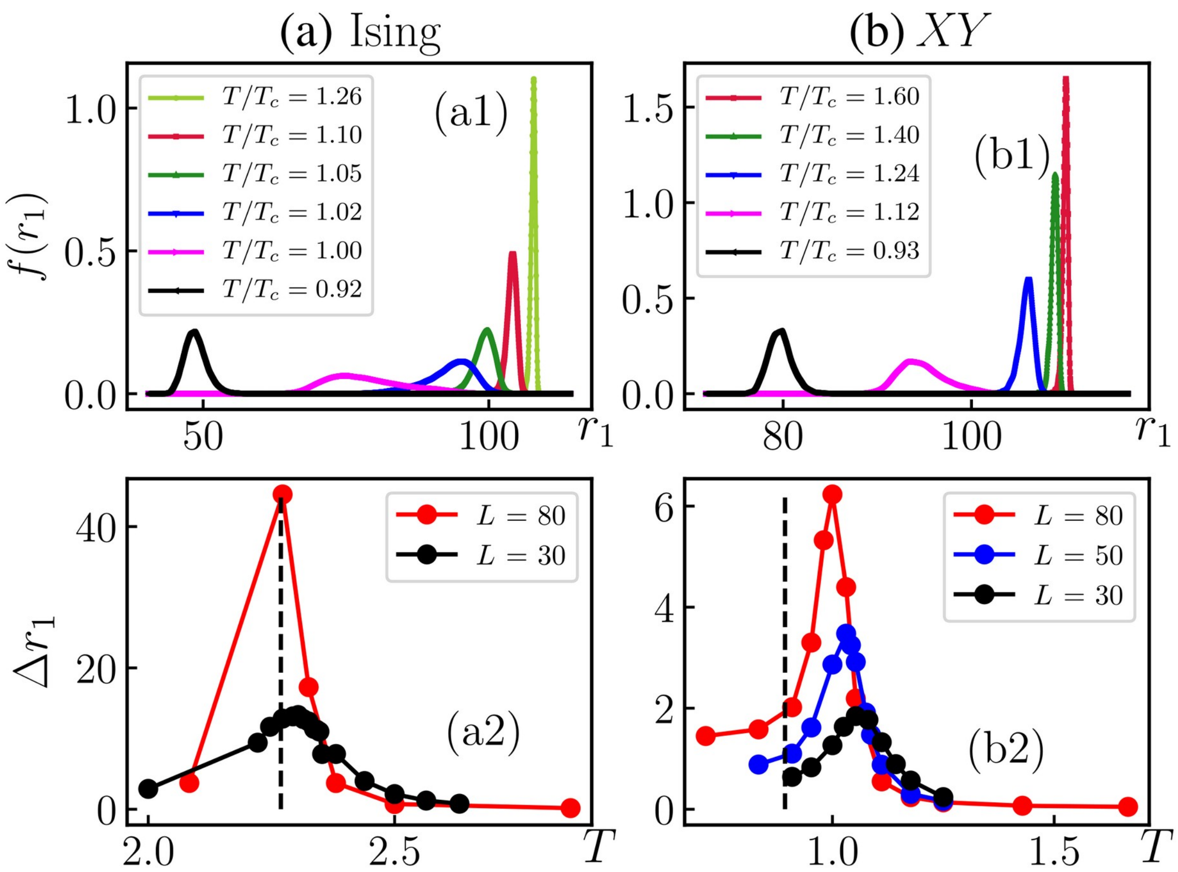
$$\boxed{S_k^i \cdot S_k^j \equiv S_0 \cdot S_k}$$

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

Statistics of first nearest-neighbor distances

Phase transitions

Change of scale in configuration space

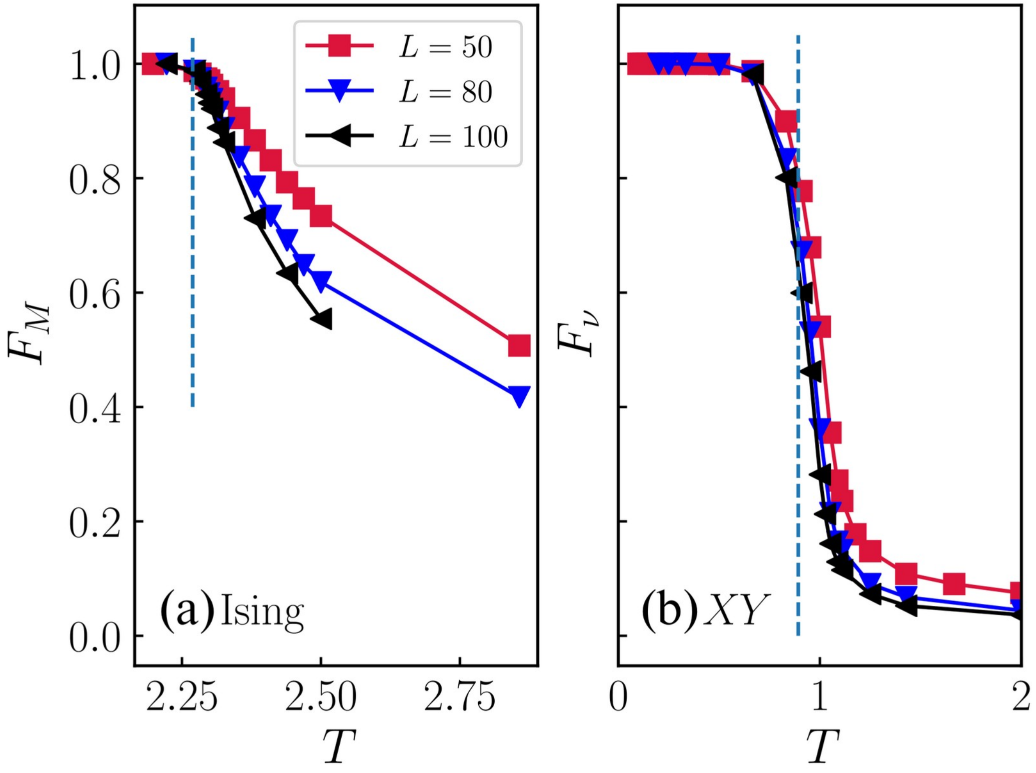


Structural transition in Configuration space

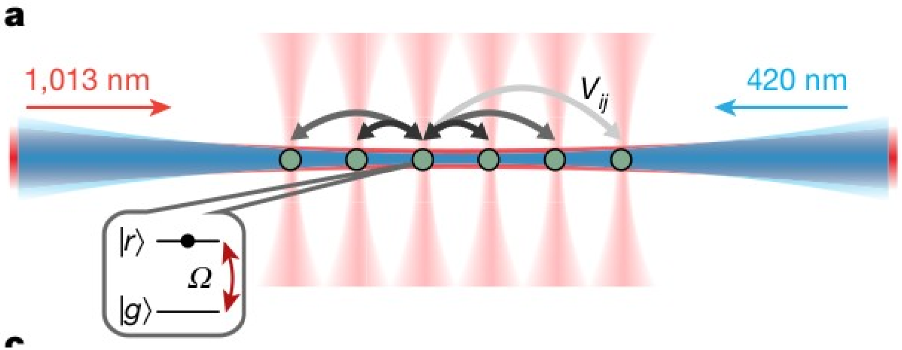
Connectivity between neighboring points in configuration space

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



(1) Rydberg atom arrays

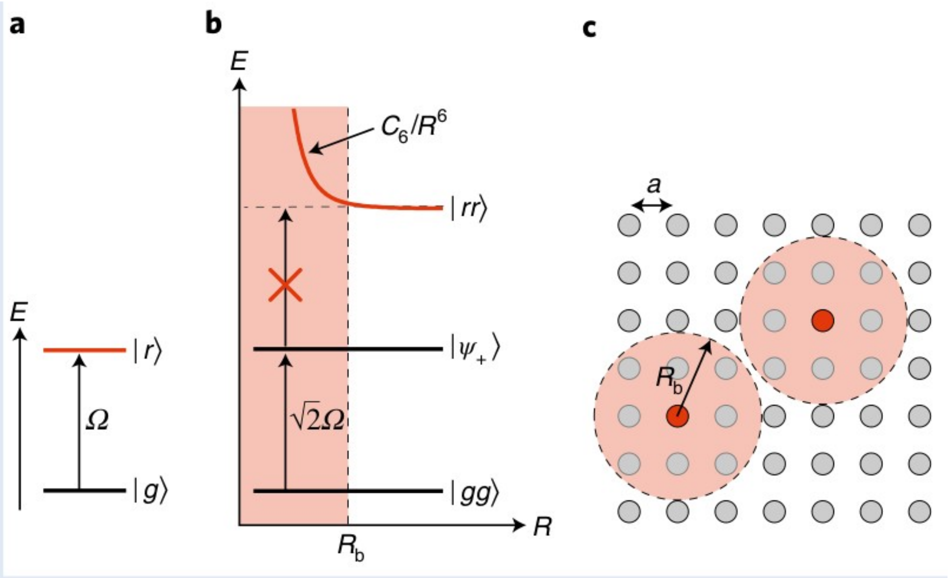


Hard-core bosons (FSS model)

$$\frac{H}{\hbar} = \frac{\Omega(t)}{2}\sum_i \sigma_i^x - \Delta(t)\sum_i n_i + \sum_{i<j} V_{ij} n_i n_j$$

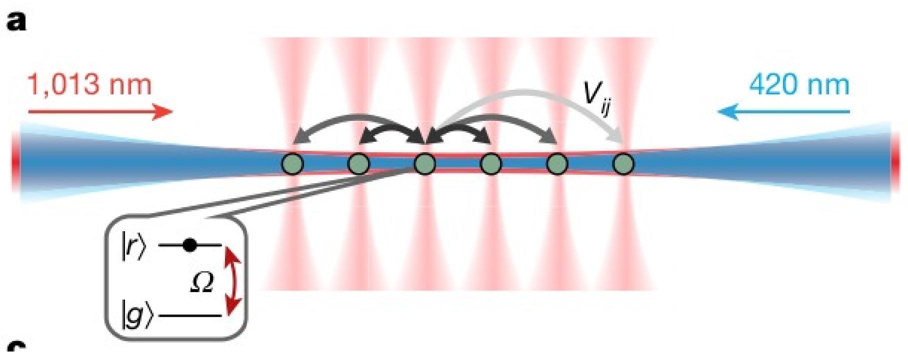
PXP model

$$H = \frac{1}{2}\sum_i \left(\Omega\ P\sigma_i^x P - \delta\ \sigma_i^z\right)$$



Rydberg blockade
→ constraint

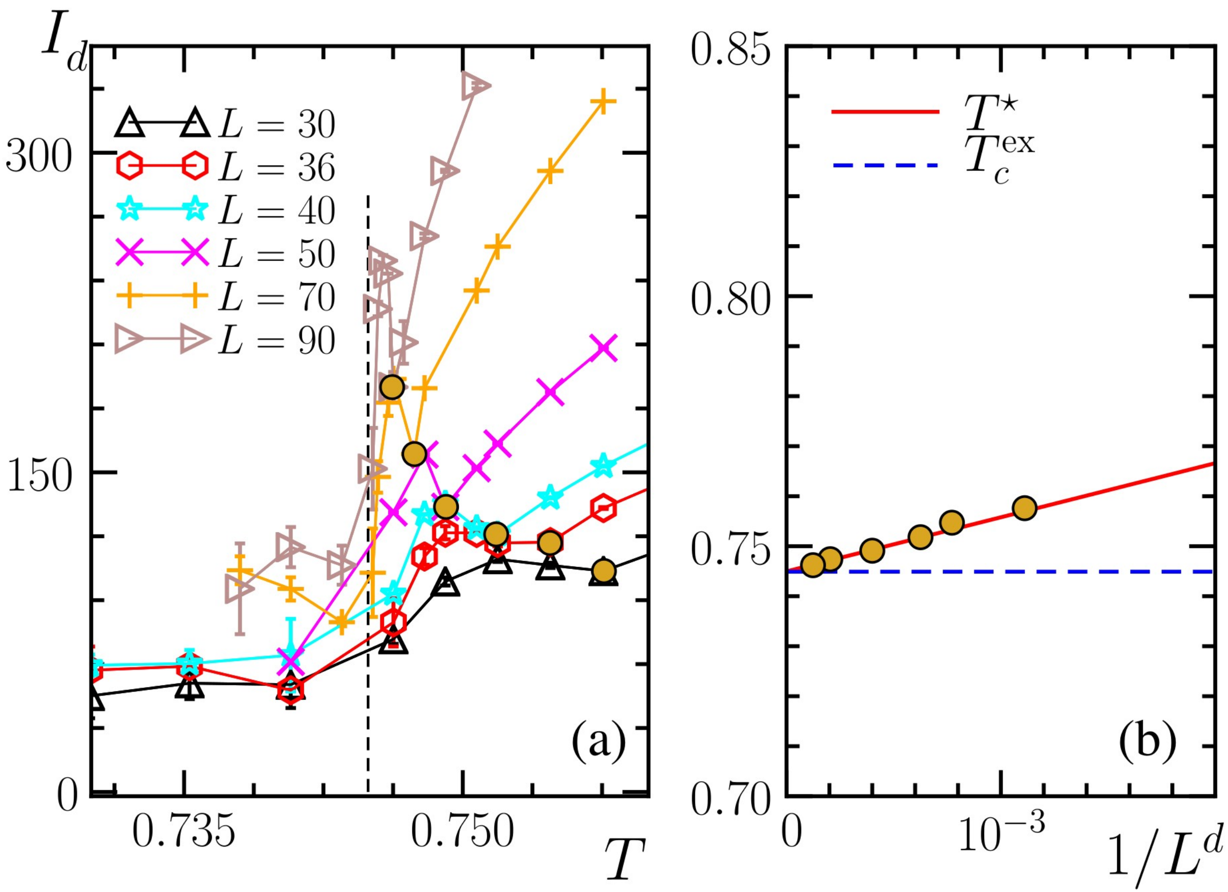
(1) Rydberg atom arrays

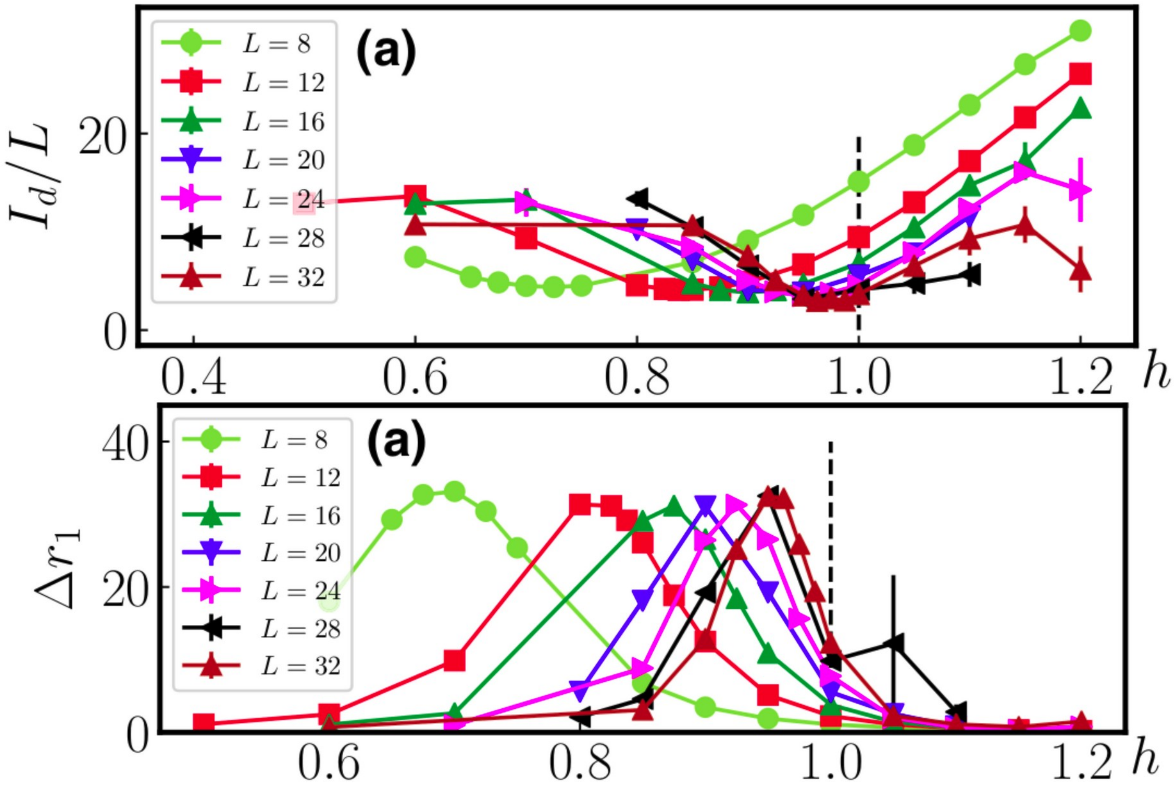


Hard-core bosons (FSS model)

$$\frac{H}{\hbar} = \frac{\Omega(t)}{2} \sum_i \sigma_i^x - \Delta(t) \sum_i n_i + \sum_{i<j} V_{ij} n_i n_j$$

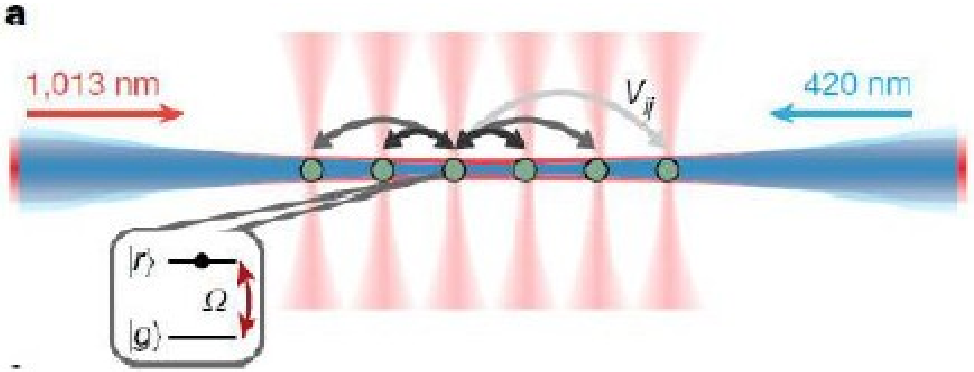
3. First-order phase transition



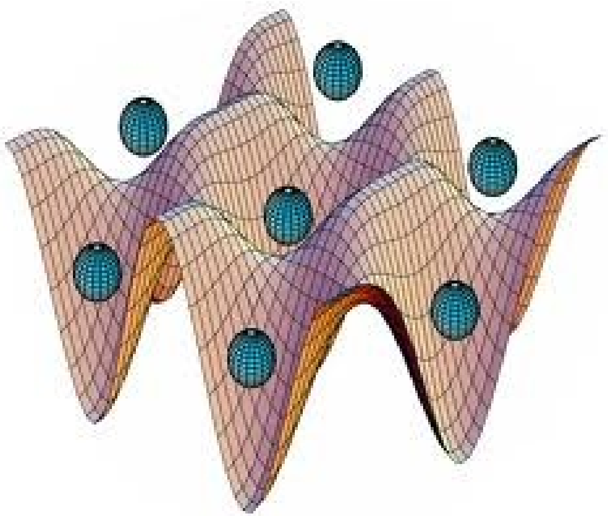


(a)
$L=8$
$L=12$
$L=16$
$L=20$
$L=24$
$L=28$
$L=32$
I_d/L
0
20
0.4
0.6
0.8
1.0
1.2
h
(a)
$L=8$
$L=12$
$L=16$
$L=20$
$L=24$
$L=28$
$L=32$
Δr_1
0
20
40
0.6
0.8
1.0
1.2
h

Synthetic quantum systems



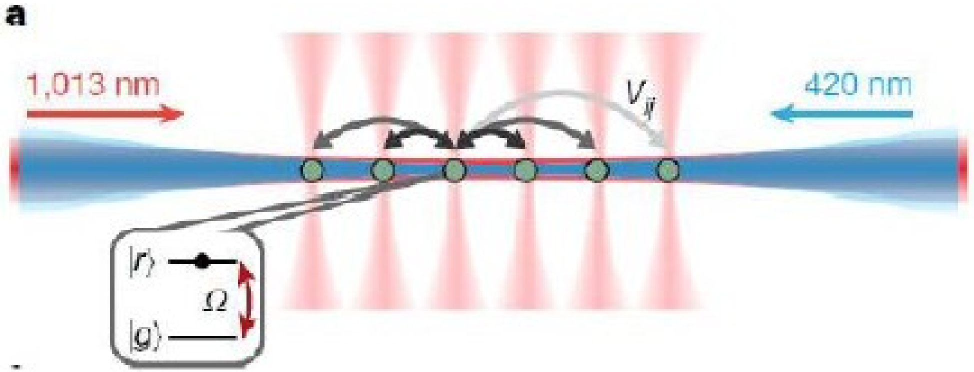
Rydberg atoms in optical tweezers



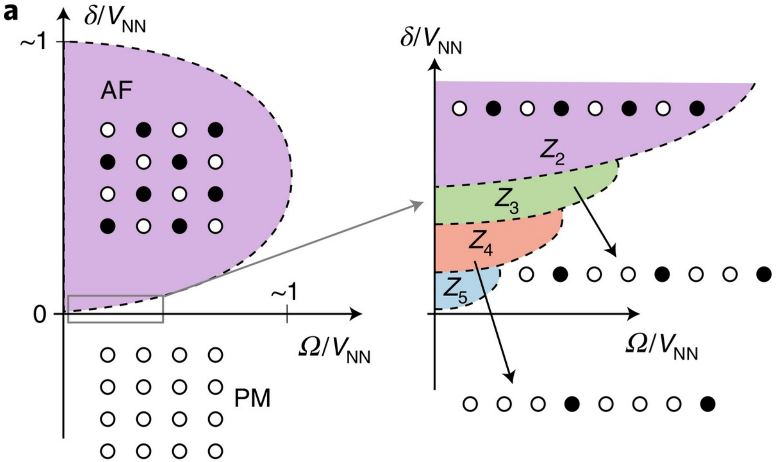
Fermions in optical lattices

Strongly correlated quantum systems

Synthetic quantum systems → Quantum simulators

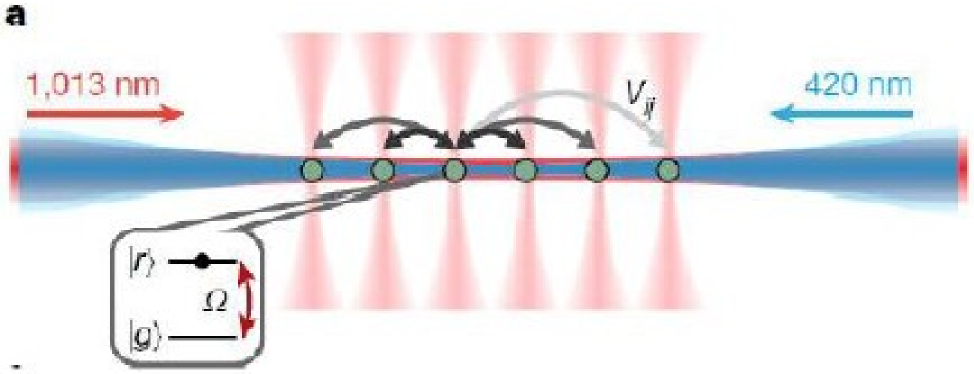


Rydberg atoms in optical tweezers
[Ising-like Hamiltonians]



→ Quantum many-body phases and phase transitions
→ Coherent dynamics

Synthetic quantum systems → Quantum simulators



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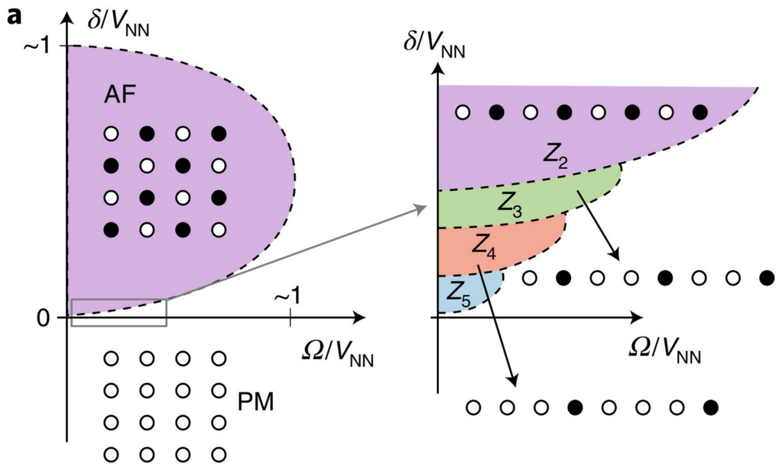


→Tunability
→Probe **local properties** and quantum correlations **[Entanglement]**

Quantum correlations

Entanglement

Probing Rényi entanglement entropy via randomized measurements

Science 2019

Tiff Brydges[1,2]*, Andreas Elben[1,2]*, Petar Jurcevic[1,2], Benoît Vermersch[1,2], Christine Maier[1,2], Ben P. Lanyon[1,2], Peter Zoller[1,2], Rainer Blatt[1,2], Christian F. Roos[1,2]†

Article

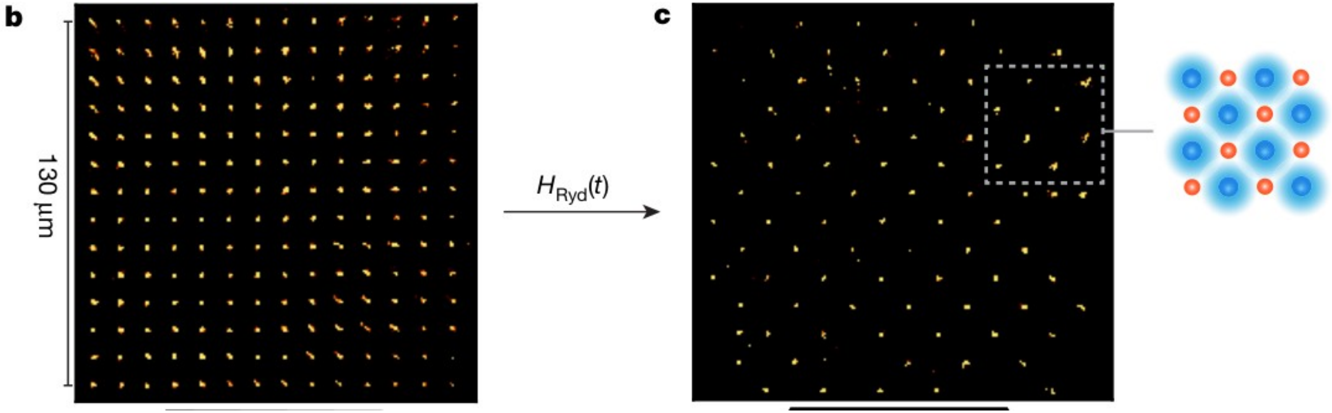
Quantum simulation of 2D antiferromagnets with hundreds of Rydberg atoms

Pascal Scholl et. al. Nature (2021)

Article

Quantum phases of matter on a 256-atom programmable quantum simulator

Sepehr Ebadi et. al. Nature (2021)



Probe MB quantum phases and transitions

Measure wave function snap shots

Article

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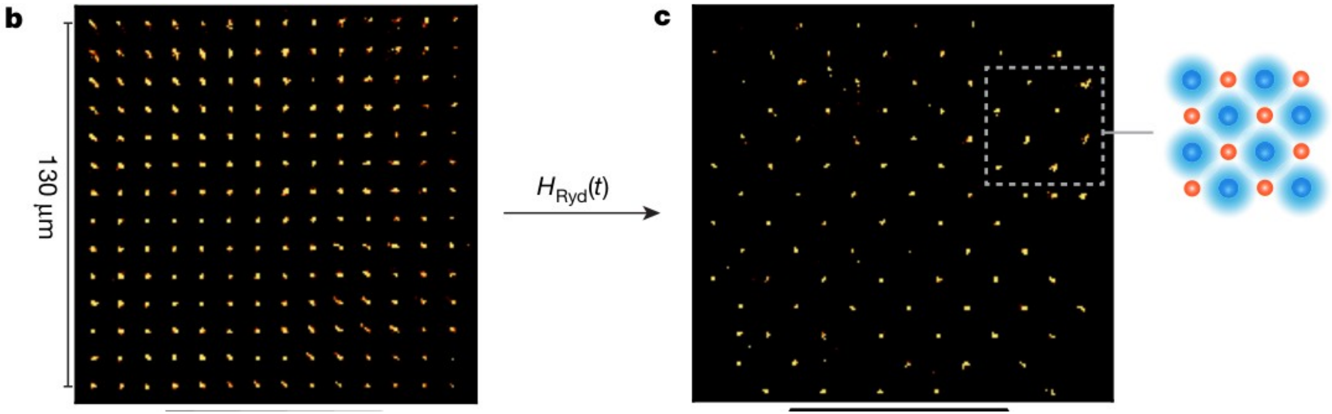


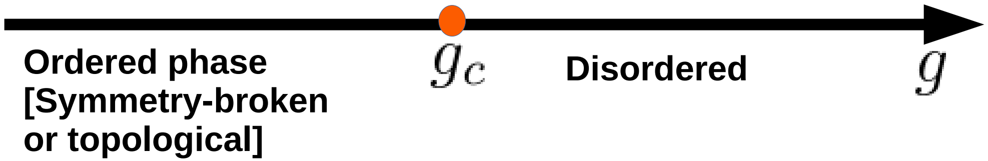
Probe MB quantum phases and transitions

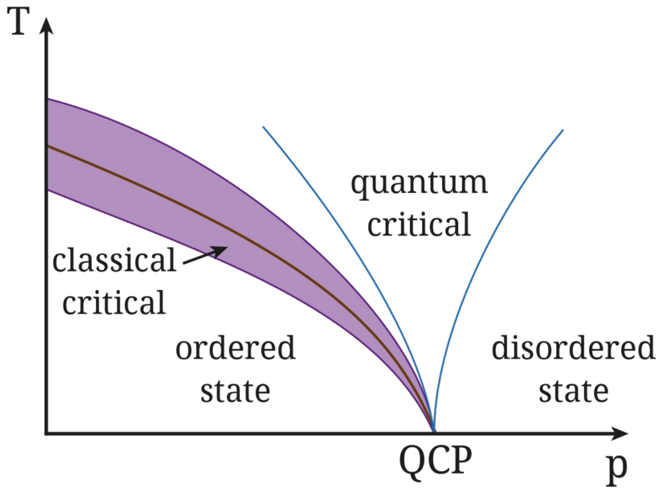
Measure wave function snap shots

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

New tools to characterize quantum correlations in many-body systems?

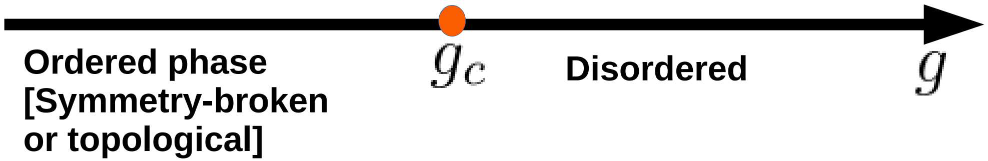
Quantum phase transitions





Quantum spin models
→ 1d quantum Ising model
→ 1d XXZ model
→ 2d Heisenberg bilayer model

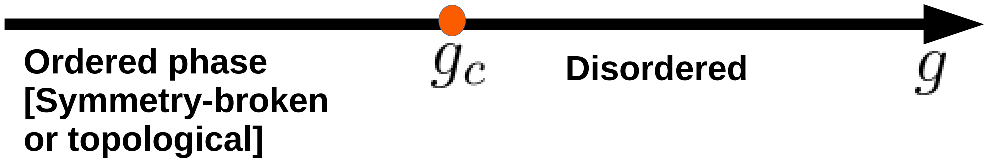
Quantum phase transitions



Defining quantum data sets

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

Quantum phase transitions



Defining quantum data sets

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

Quantum-to-classical mapping
→ path-integral

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

Quantum models

1d Quantum Ising model
Sec. order transition

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