(Kolmogorov) complexity and the many-body problem - from classical statistical mechanics to wave functions

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<u>Exp</u>: Augsburg/Julich/Palaiseau/TS and Heidelberg/TS collaborations

Based on: Phys. Rev. X **11**, 011040, Phys. Rev. X Quantum **2**, 030332 (2021), 2301.13216 + 2305.05396

Outline

Complexity warm-up

Sampling states and **intrinsic dimension**

Data mining partition functions / **criticality as minimal complexity**

Many-body / field theory

Data mining *large scale* quantum simulators:

- wave function networks
- **certification and complexity** of Rybderg experiments

Quantum Info

Complexity and topology in many-body systems

Many-body

Theory big picture: “complexity diagram”

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Computational complexity

(“time”)

See Michał’s lecture

- Refers to a task
- Describes a resource count
- Examples: circuit complexity, computational cost of classical algorithms, holographic,..

Theory big picture: “complexity diagram”

Kolmogorov (algorithmic) complexity
(“space”)

- Refers to information content
- Quantifies incapability of compressing information
- NP hard to compute. Related to ‘effective field theory’

Computational complexity
(“time”)

- Refers to a task
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Theory big picture: “complexity diagram”

Given a many-body (quantum) state:
- How are they related?
- Is KC related to *physical phenomena*?
- Can we actually *measure* KC?

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Kolmogorov complexity

Kolmogorov complexity: How long shall my computer code be in order to reproduce the data structure obtained in the experiments?

Meaningful if we fix the ‘programming language’

Ex: bit strings:

111111111111111111111
111111111111111111111
111111111111111111111
111111111111111111

111000111000111000 111000111000111000
111000111000111000 111000111000111000
111000111000111000 111000111000111000

11000101010110011010
10101010101010101011
00101010001111111001
1010000001111111

`“Write 1 N times”`

`“Write 111000 N/6 times”`

`“Write 111000…1111”`

$K = 15$

$K = 22$

$K = 6 + N = 73$

Refs.: Wikipedia page, Li and Vinayi, *An Introduction to Kolmogorov complexity and its applications*

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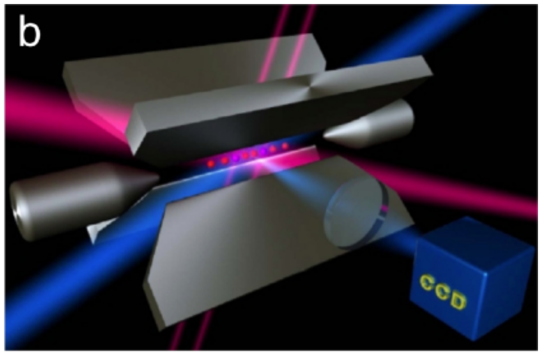
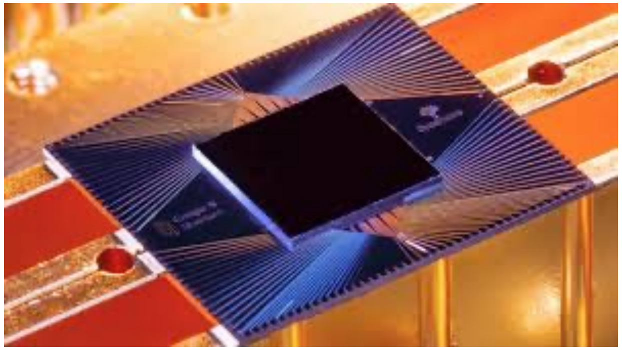
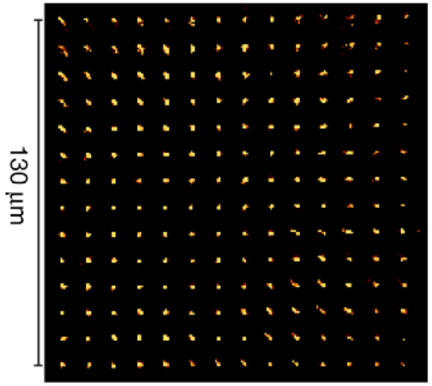
Q: how to adapt to many-body states?

Experimental big picture: complexity of *what?*







See Atsushi's lecture

Pictures credit: Blatt's group, Google, Bloch's group, Browaeys's group

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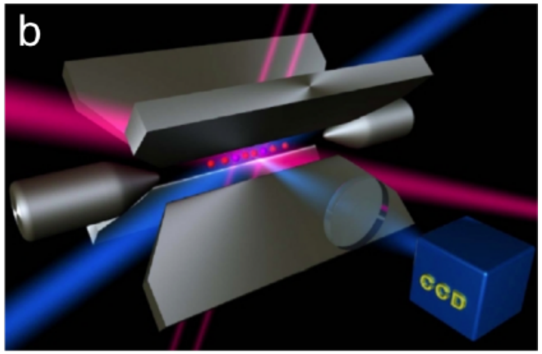
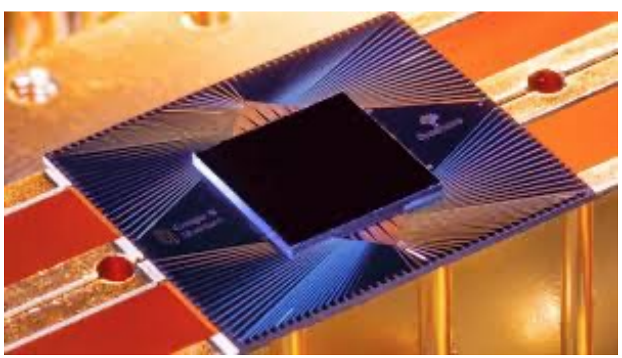
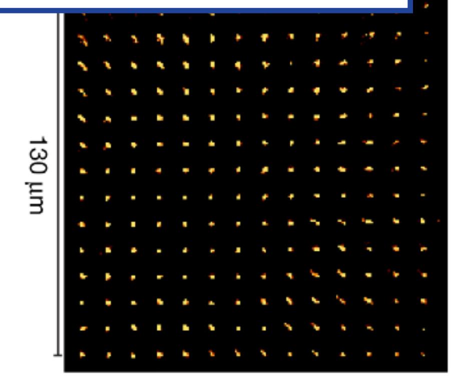


One can now take *photos* of many-body wave functions!





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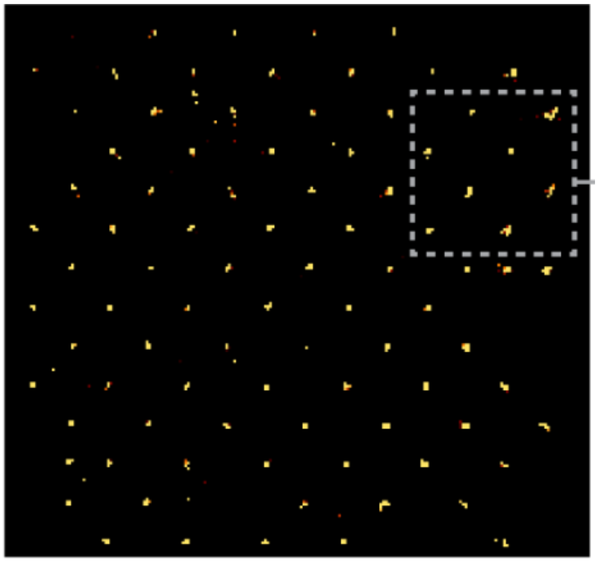
What are we talking about: what is a (many-body) wave function snapshot?



$X_1 =$ 10001001010101…

Scholl et al., Nature 2021

So far: trash most of the information content, and extract **low-order** (site resolved) **correlation functions**

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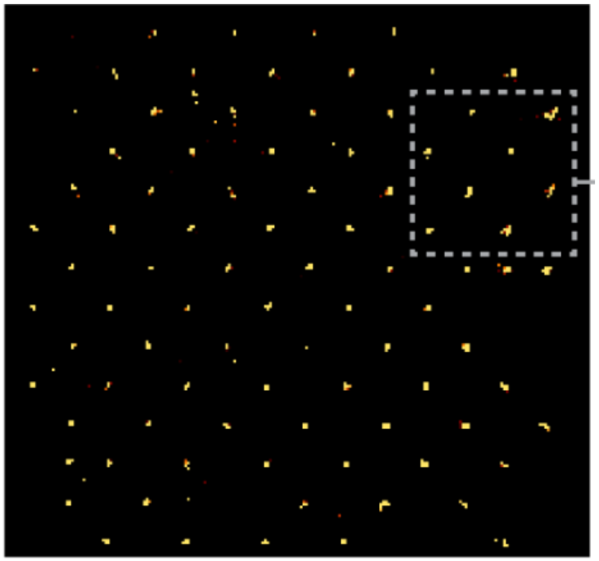

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Similar goals (different methods) in HEP: Berges's, Lucini's groups, 2020, 2022

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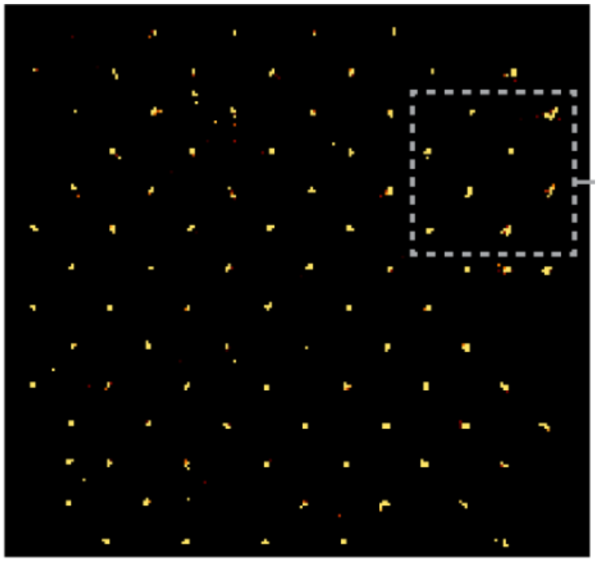

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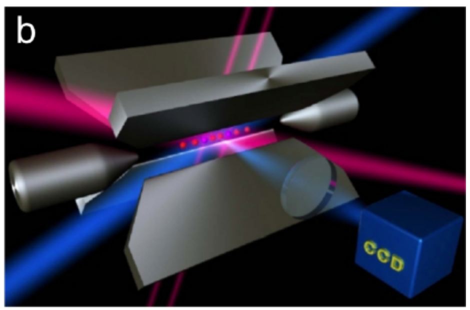
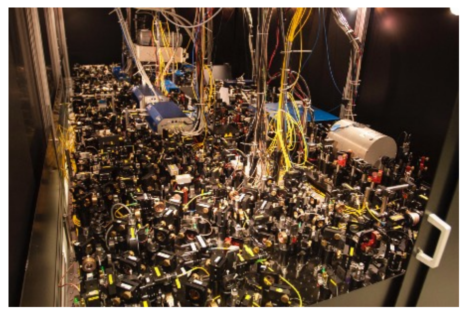
NB: At the conceptual level, complexity of information <u>shall not rely</u> on low-lying correlation functions

Why aren't we happy with just low-order correlations?

Quantum information viewpoint: new tools





Can we trust the outcome of quantum computers/simulators?

Cirac & Zoller, Nat. Phys. 2012;
Buluta and Nori, Science 2014

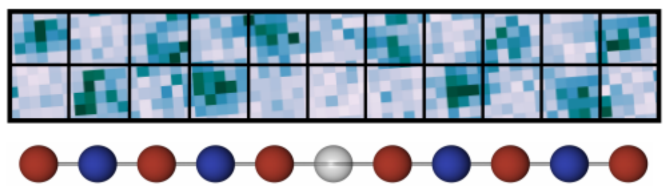
- Cross-platform **verification** of wave functions
- Noise 'tomography'
- Robustness of information

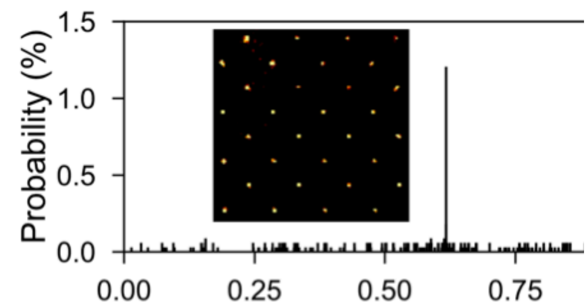
Complementary to microscopic approaches:
randomized benchmarking, optimal control / calibration

Why aren't we happy with just low-order correlations?

Quantum many-body viewpoint: new concepts

B





- How complex is this wave function?
- Can we detect non-local (topological) correlations?
- …

Same reasoning applicable to numerical experiments - and other platforms as well

Theory: outcome of numerical experiments

$$Z = e^{-\beta H}$$

Example:
- Monte Carlo simulations (CM, HEP, etc.)
- Importance / direct sampling of tensor networks

$$X = \{X_1, X_2, ...X_N\}$$

Elements of a Markov chain

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- Monte Carlo simulations (CM, HEP, etc.)
- Importance / direct sampling of tensor networks

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Elements of a Markov chain

Data-wise, classical simulations are "equivalent" to the outcome of a quantum machine

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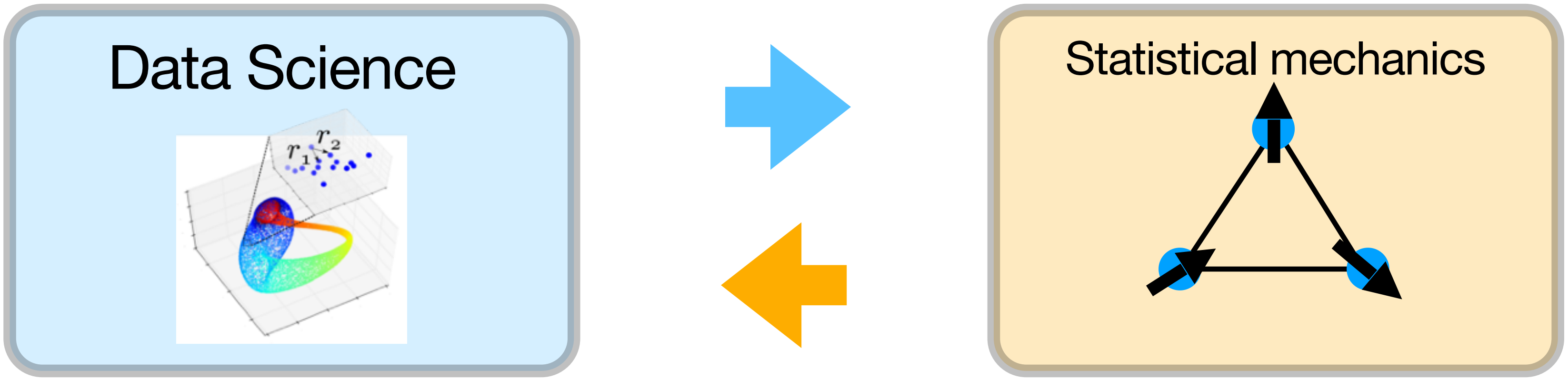
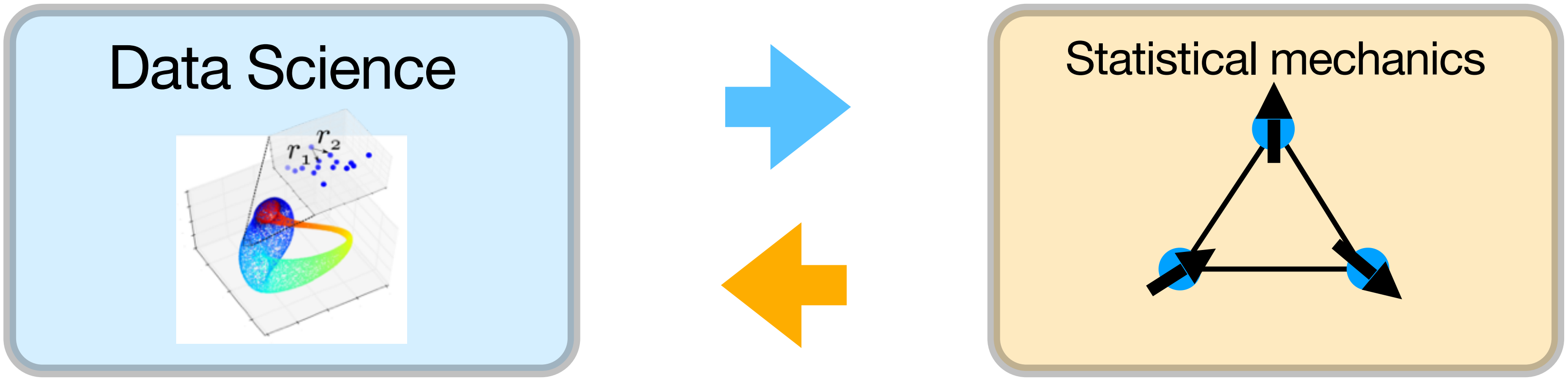
Main idea: combined statistical mechanics with non-parametric learning methods



Guiding principle: identify (and model) the **most elementary amount of information/degrees of freedom** describing a physical system

Main idea: combined statistical mechanics with non-parametric learning methods



Guiding principle: identify (and model) the **most elementary amount of information/degrees of freedom** describing a physical system

In modern AI language, we are interested in manifold characterization - **unsupervised (non-parametric) learning**

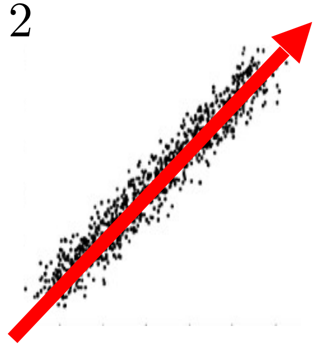
The intrinsic dimension

The intrinsic dimension

the minimal number of variables required to describe a dataset

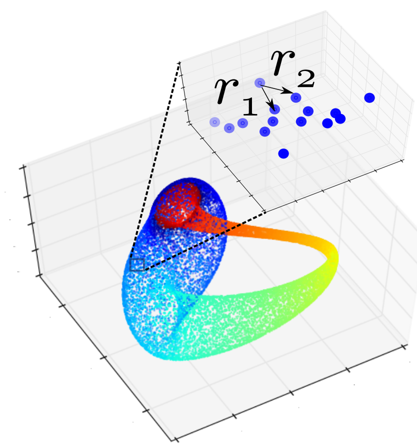
Widely applied in ab initio molecular dynamics (Laio, Rodriguez, etc.).

$D = 2$



$I_d = 1$

$D = 3$



$I_d = 2$

Operational meaning: one just needs a single variable to properly describe the object of interest

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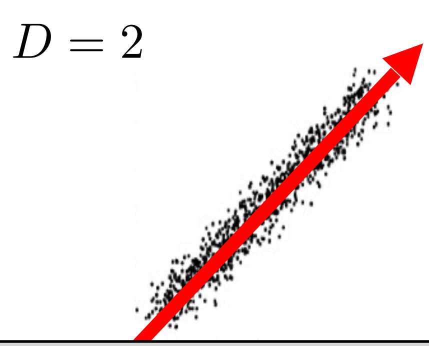
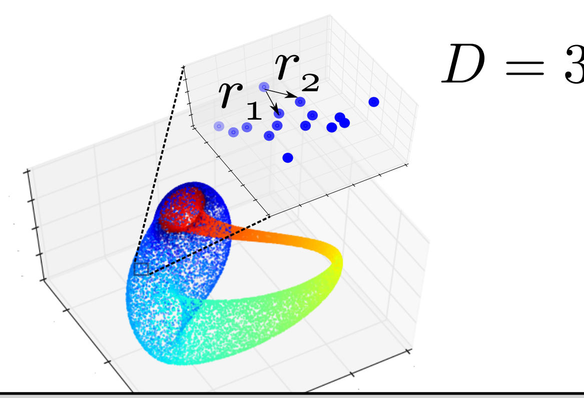




Op
ne
de

Intuition: the intrinsic dimension is informative about

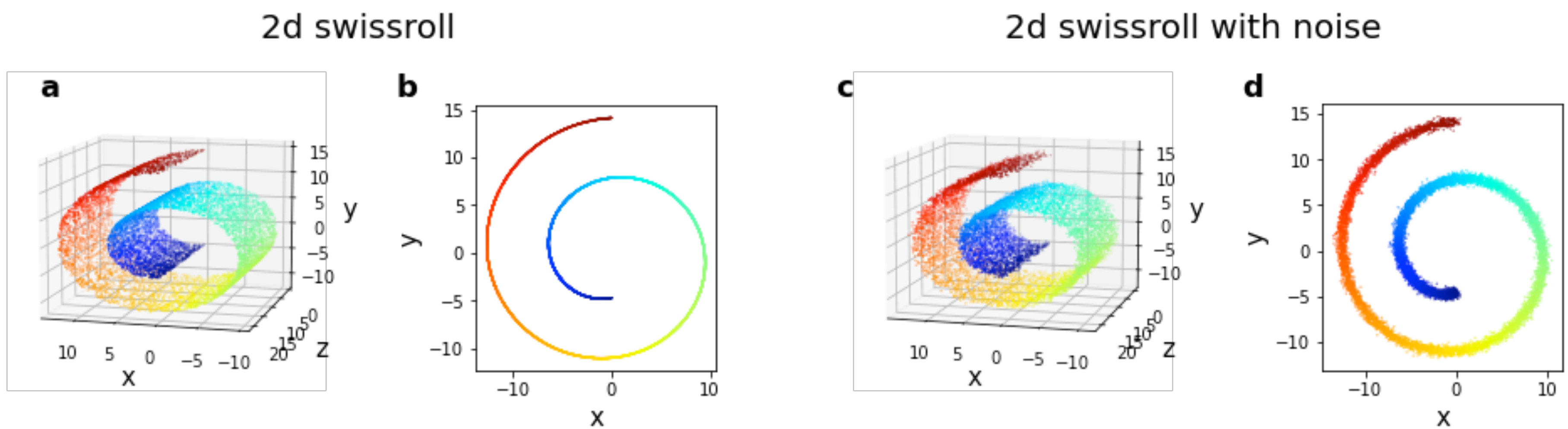
(1) number of relevant degrees of freedom, and

(2) **complexity** of a manifold (qualitative so far)

The intrinsic dimension: how to

Won’t be discussed here - for a reference, see DaDapy, tutorial “Intrinsic dimension”

arXiv:2205.03373



Correct value: Id=2

ID = 1.98	*r = 0.27*
ID_noisy = 2.93	*r_noisy = 0.40*

Sensitive to local details - so must be handled with care!

The intrinsic dimension: properties and estimators

- Used as a preamble to dimensional reduction (e.g., in clustering analysis) to estimate the 'correct' dimensionality.
- lower bound complexity of a data set

Example: relation with bottleneck in autoencoders, Zoncolan at al. 2019

- Traditional estimators (PCA, box counting) rely on **assumptions** that are typically not met for the data sets we are interested in

- Modern estimators based on distances have **only very mild assumptions**: we will use **2-NN** (Facci et al., 2017)
  A. Arbitrary curvatures, clustering etc.
  B. Very strict sanity checks can be applied

Glielmo et al. Chem Rev. 2021; Facco et al., Sci. Rep. 2017, 7, 12140.

The intrinsic dimension

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Physics?

A basic example: a 3 site model

Simple example: sampling a 3-site Heisenberg model

$$N_r \simeq 10^4/10^5$$

1) States / data space (D=3)

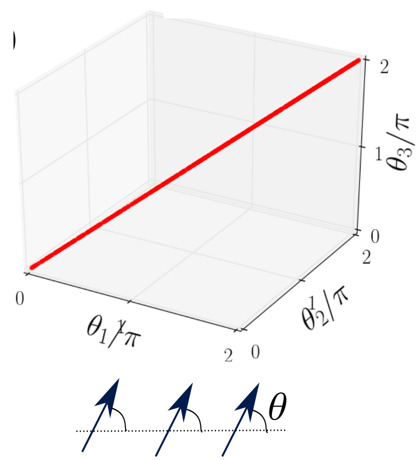
$$\vec{x} = (\vartheta_1, \vartheta_2, \vartheta_3)$$

2) Equilibrium weight:

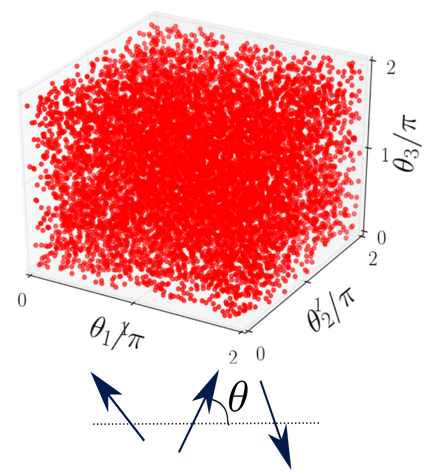
$$\rho(E) \sim e^{-E(\vec{x})/T}$$

3) Hamiltonian:

$$E(\vec{\theta}) = -\sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j,$$



$$I_d = 1$$



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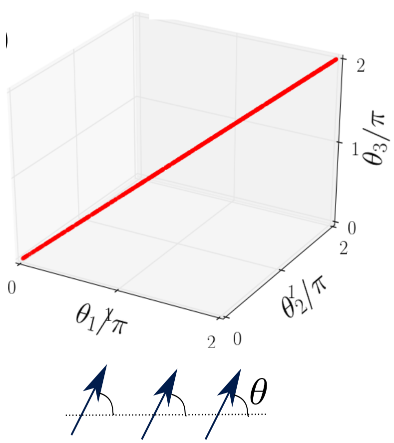

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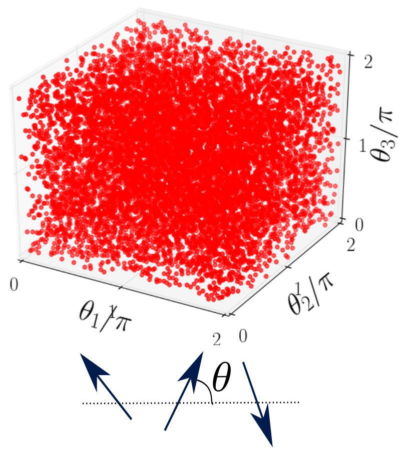

$$I_d = 3$$

Remember!
I_d ***minimal number of variables*** *required to describe a dataset*

Message 1: Intrinsic dimension:
(1) very low in ordered phases
(2) as high as it can get at high temperature

All of this makes sense! but what about transitions?

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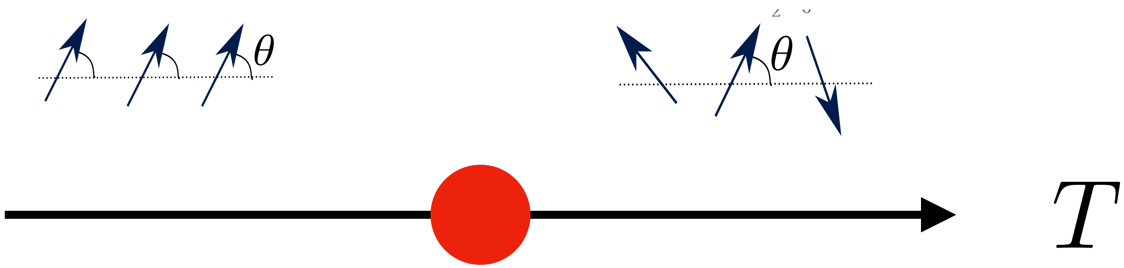
How does complexity behave at criticality?



<u>Intuition 1</u> [real space]: at critical points, correlations diverge!

$$\xi \to \infty$$

very correlated manifold, so maximal intrinsic dimension

<u>Intuition 2</u> [RG]: at critical points, physics is universal

$$\langle O(r) \rangle = f(r, \nu, z..)$$

manifold is very constrained, so minimal intrinsic dimension

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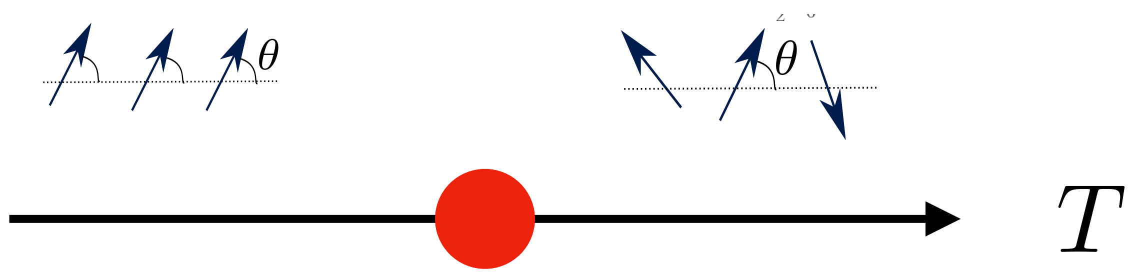

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Strategy
(1) numerical tests on classical statistical mechanics models
(2) Theory [only sketched here]

Many-body: the Ising model in 2D

Hamiltonian

$$E(\vec{s}) = -\sum_{\langle i,j \rangle} s_i s_j ,$$

Data configurations

$$\vec{s} = (s_1, s_2, ..., s_{N_s})$$

Second order (conformal) phase transition at

$$T_c = 2/\ln(1+\sqrt{2}) \simeq 2.26...$$

$$\nu = 1$$

Data structure: $s_1 = (s_{11}, s_{12}, ..) = (0, 1, 0, 1, 1, 1, 0, ...)$

Data space of the Ising model in 2D

Data configurations

$$\vec{s} = (s_1, s_2, ..., s_{N_s}) \qquad s_1 = (s_{11}, s_{12}, ..) = (0, 1, 0, 1, 1, 1, 0, ...)$$

Distance between points:
Hamming distance

$$r(\vec{s^i}, \vec{s^j}) = \sum_p |s_p^i - s_p^j|$$

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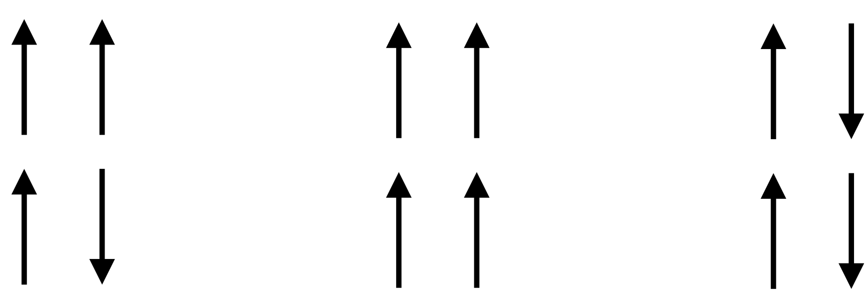
Example: N=4

s_1 $\qquad$ s_2 $\qquad$ s_3



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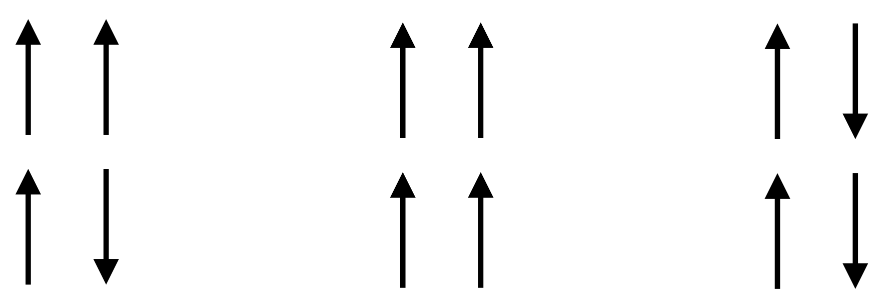
s_1 $\quad s_2$ $\quad s_3$



$r(s_1, s_2)$

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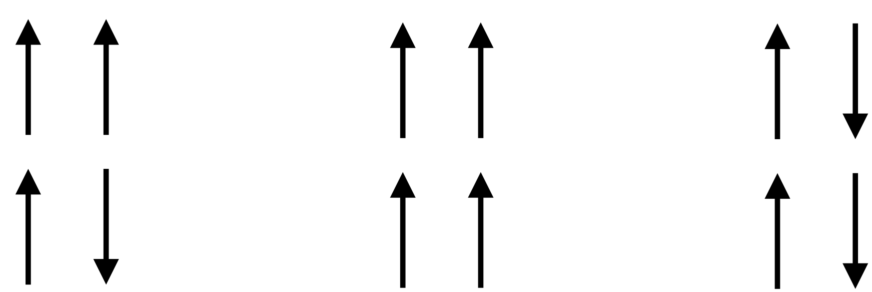

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$r(s_2, s_3)$

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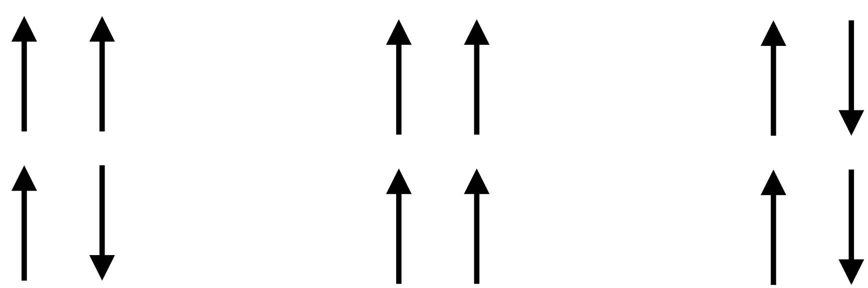

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$$r(s_2, s_3) = 4$$

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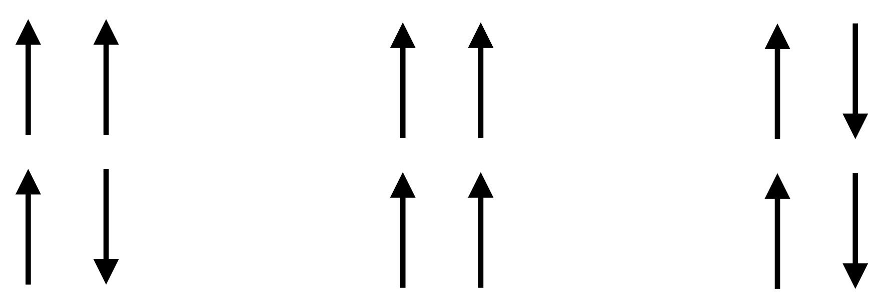

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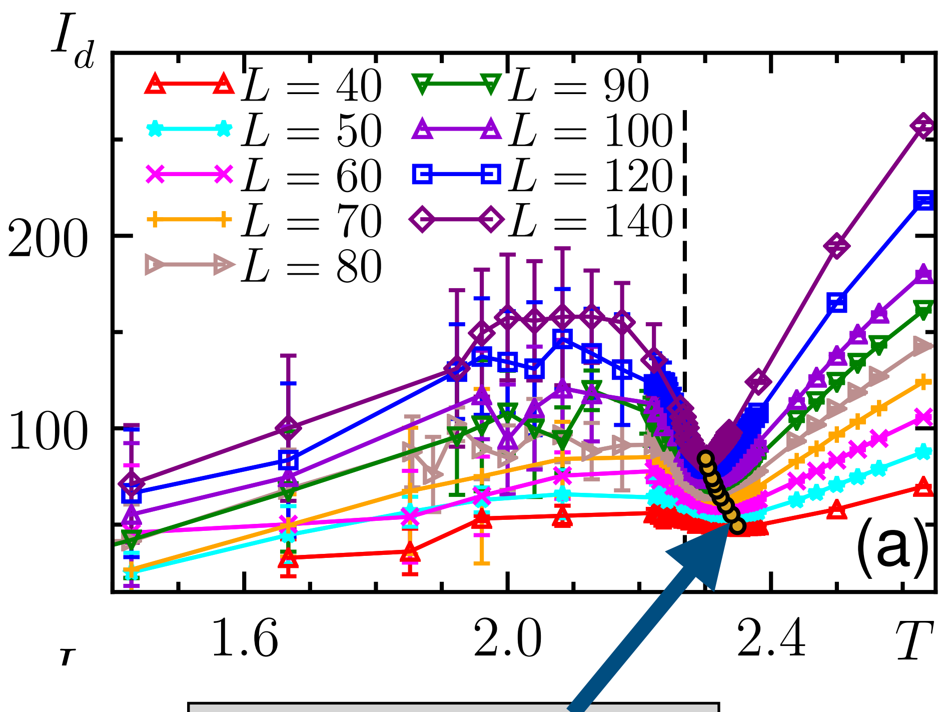
Intrinsic dimension: emergent simplicity



emergent simplicity: manifold simplifies at transition points!

Second order (conformal) phase transition at

$$T_c = 2/\ln(1+\sqrt{2}) \simeq 2.26...$$

$$\nu = 1$$

Intrinsic dimension: universal behavior

Universal collapse
scaling from
renormalization group

Scaling function

$$I_d = L^{\zeta} f(\xi/L)$$

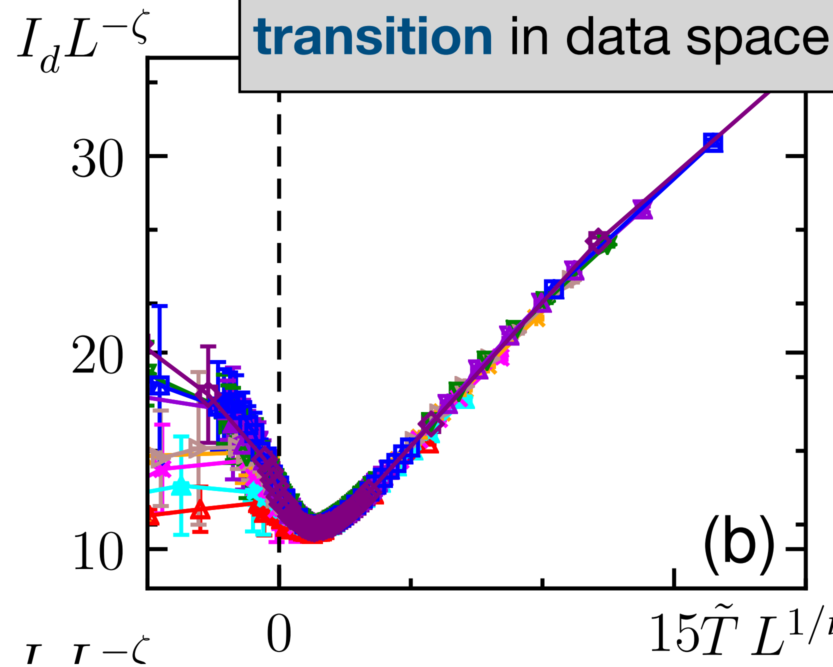
$$\xi \sim (T - T_c)^{-\nu}$$

Second order (conformal) phase transition at

$$T_c = 2/\ln(1+\sqrt{2}) \simeq 2.26...$$

$$\nu = 1$$

Universality of data structure: **structural transition** in data space



Free parameters: T_c, ν, ζ

$T_c = 2.283(2), \nu = 1.02(2), \zeta = 0.410(5)$

Review: A Pelissetto & E Vicari, Physics Reports (2002)

Intrinsic dimension: quantitative predictions

Universal collapse scaling from renormalization group

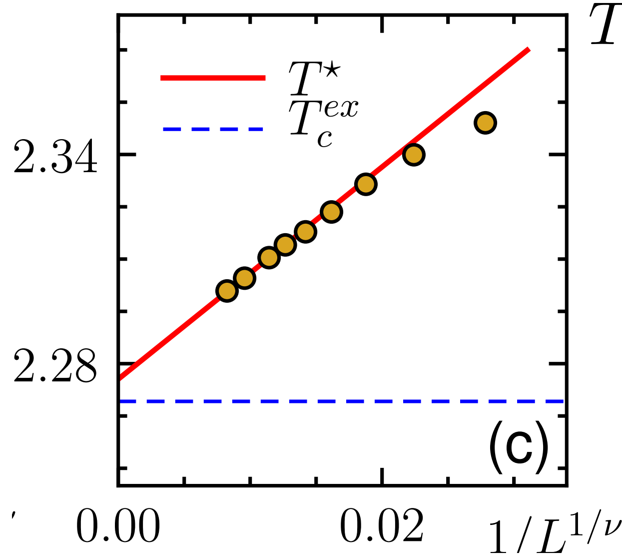
$$T^*(L) - T_c \sim \frac{1}{L^{1/\nu}}$$

Second order (conformal) phase transition at

$$T_c = 2/\ln(1+\sqrt{2}) \simeq 2.26...$$

$$\nu = 1$$

Useful to find **critical temperature and exponents** *without* any assumption on order parameters!



$$T_c = 2.2784(2)$$

Why is complexity minimal at transition points?

Rationale: complexity of the manifold dominated by the most significant correlation function (generically, *not* few-body)

Math: cumulant expansions (+more)

$$I_d = -\frac{\ln(1 - 1/N_r)}{\ln[r_2(1)] - \ln[r_1(1)]}$$

$$\ln[r_2(1)] - \ln[r_1(1)] = \mathcal{F}_2 + \mathcal{F}_4 + \ldots$$

$\mathcal{F}_p$ p-point correlation functions between configurations

$$I_d \simeq \frac{1}{\ln(\langle S_i S_j \rangle)} = \frac{1}{\xi}$$

Origin of **universality of data structures**!

Statements

For classical stat mech sampling,

Kolmogorov complexity <—> intrinsic dimension

$$I_d \simeq \frac{1}{\xi}$$

Complexity is minimal for field theories / critical points

—> **Emergent simplicity**

see also:
data compression: O. Melchert and A. K. Hartmann, Phys. Rev. E 91, 023306 (2014);
local complexity: Schmitt and Lenarcic, Phys. Rev. B 106, L041110 (2022);
out of eq.: Martirani et al. PRX 9, 011031 (2019).

Outline

Complexity warm-up

Sampling states and **intrinsic dimension**

Data mining partition functions / **criticality as minimal complexity**

Many-body / field theory

Data mining *large scale* quantum simulators:

- wave function networks
- **certification and complexity** of Rybderg experiments

Quantum Info

Complexity and topology in many-body systems

Many-body

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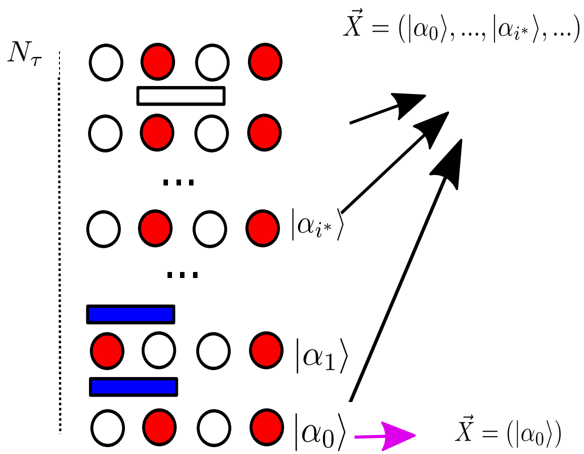
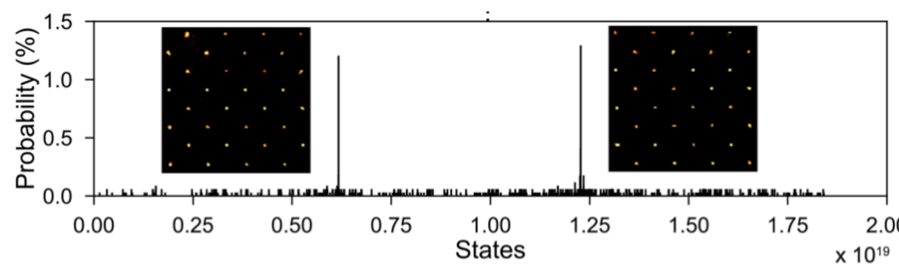
Many-body

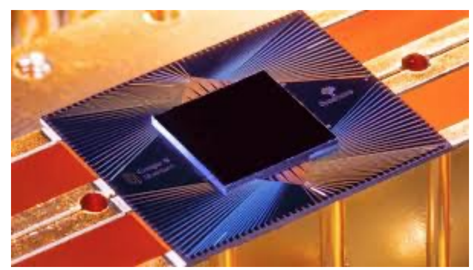
What about quantum?

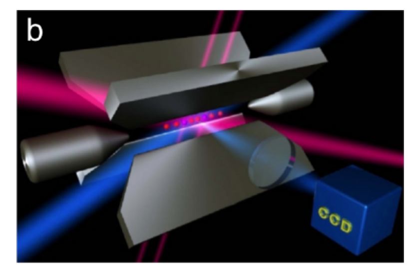
Application to quantum mechanics: wave function **snapshots**

Path integrals:
quantum MC





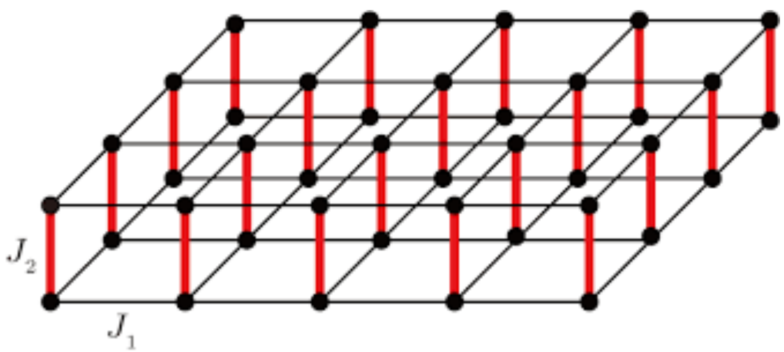




Q: Are quantum systems also described by universal data structures?

Step 0: study path integrals

$$H = \sum_{a=1,2} \sum_{\langle i,j \rangle} \boldsymbol{S}_{i,a} \cdot \boldsymbol{S}_{j,a} + g \sum_{i=1}^{N_s} \boldsymbol{S}_{i,1} \cdot \boldsymbol{S}_{i,2}$$

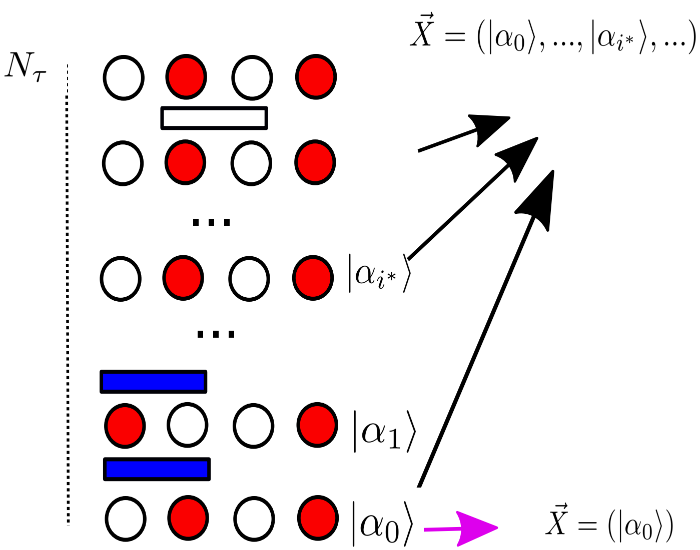


$$g_c \simeq 2.52$$

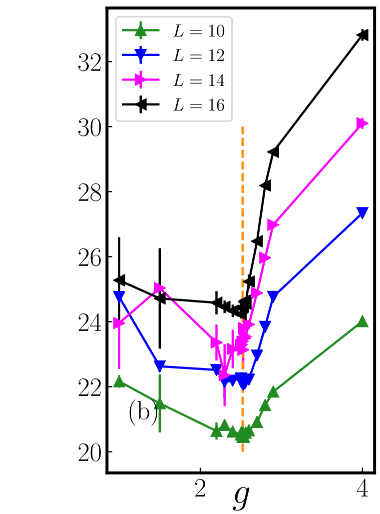
$$g = J_2/J_1$$

L. Wang, K. S. D. Beach, and A. W. Sandvik, Phys. Rev. B 73, 014431 (2006).

Example: the bilayer-Heisenberg model

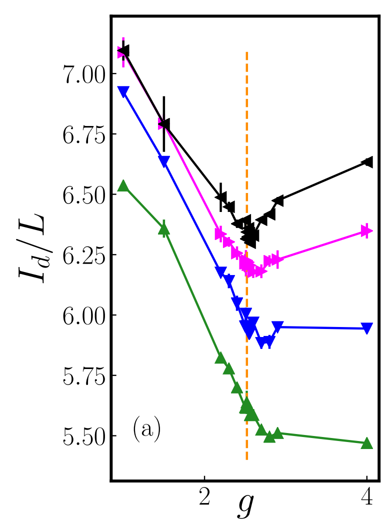


$$\beta = L$$



Full path integral

Both single slice and full path integral show emergent simplicity!



Single slice

Now change of gear

So far: theory. Quite idealized conditions (no noise, huge sampling, etc.)

Now change of gear

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What about *experiments*?

Now change of gear

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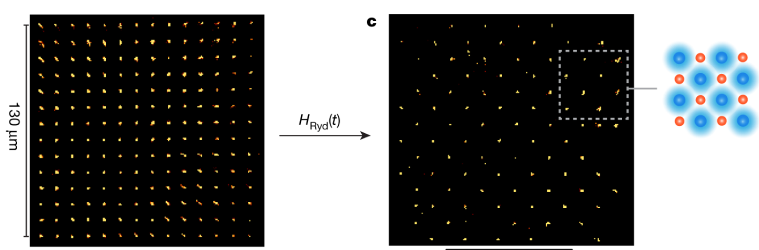
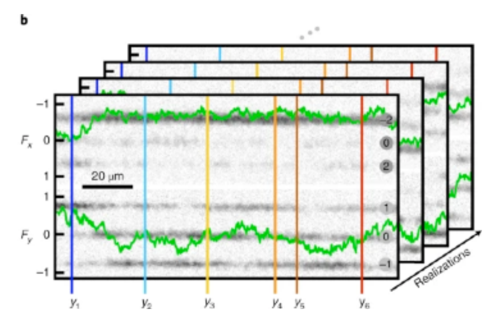
What about *experiments*?



Rydberg atoms in optical tweezers

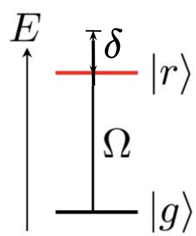
Scholl et al., Nature 2021

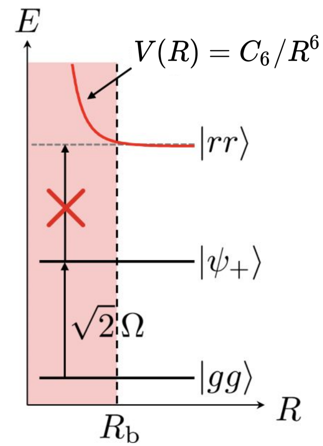


Spinor Bose gases

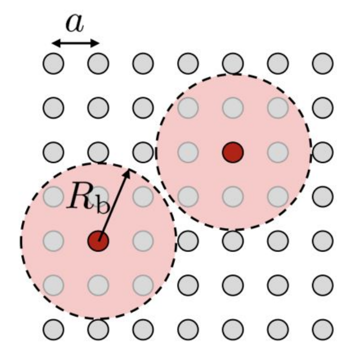
Prüfer et al., Nat. Phys. 2020

Rydberg atom arrays: quick intro





Rydberg blockade potential



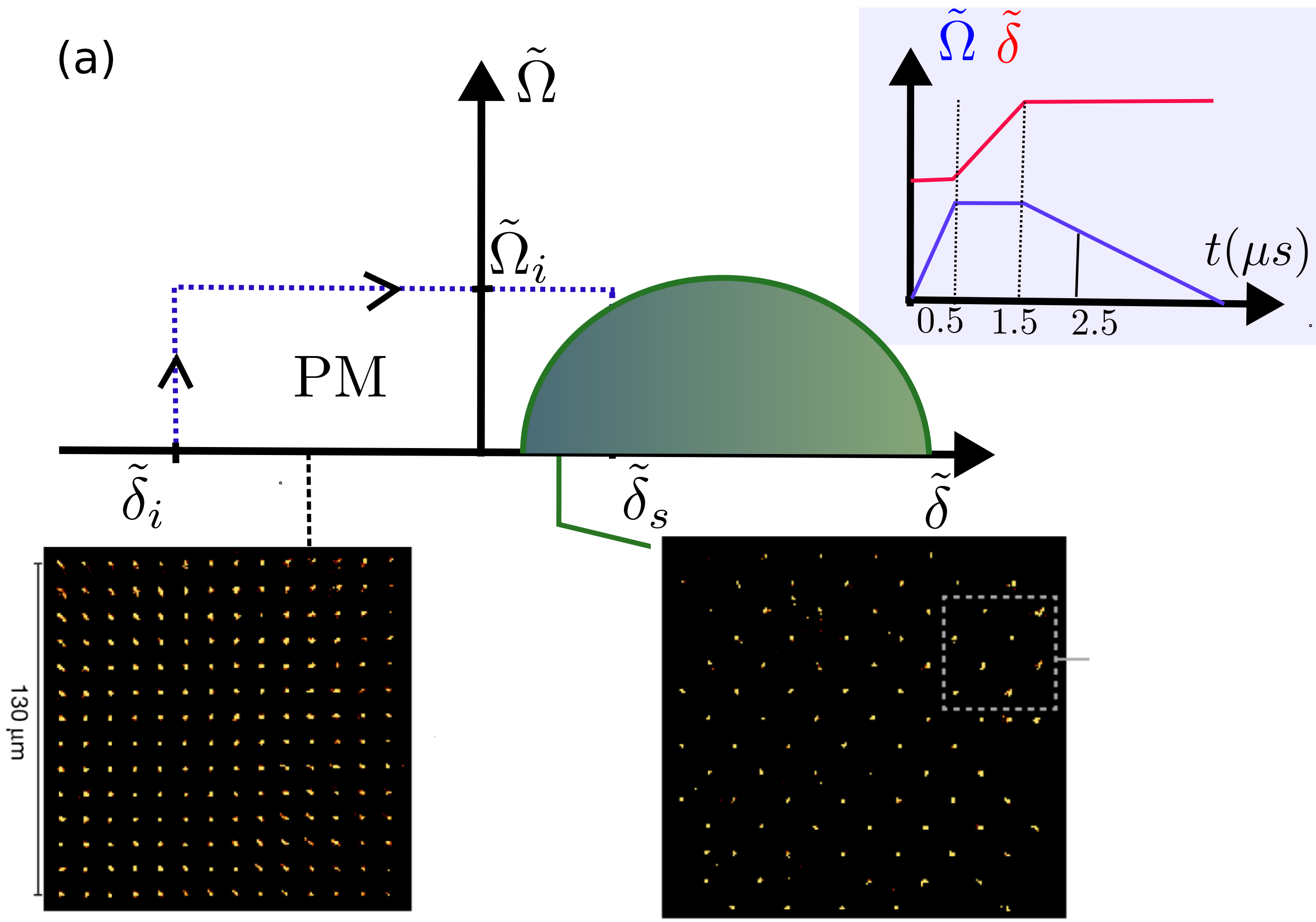
$V(R_b) := \Omega$

Blockade radius

Effective Hamiltonian:

$$\hat{H}_{\text{FSS}} = \sum_j \left(\Omega\, \hat{\sigma}_j^x + \delta\, \hat{n}_j\right) + \sum_{j<l} V_{j,l}\, \hat{n}_j \hat{n}_l$$

Data mining Rydberg atom arrays: crossing a phase transition



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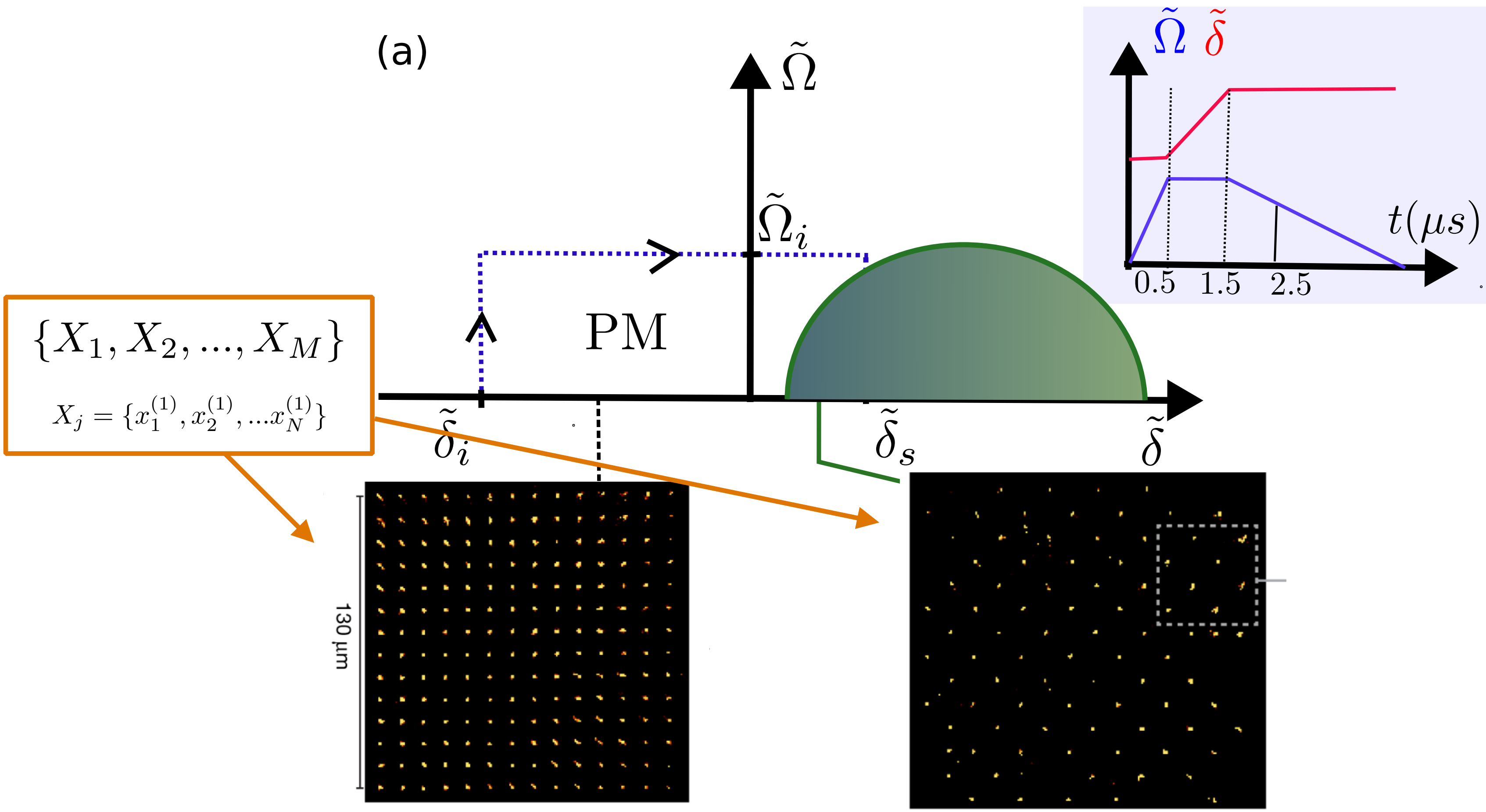
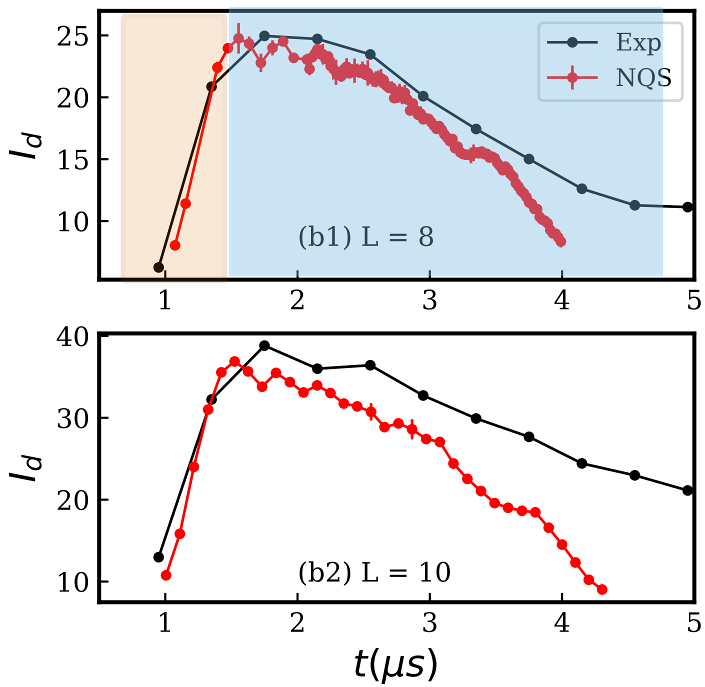


Physics: emergent simplicity across Kibble-Zurek



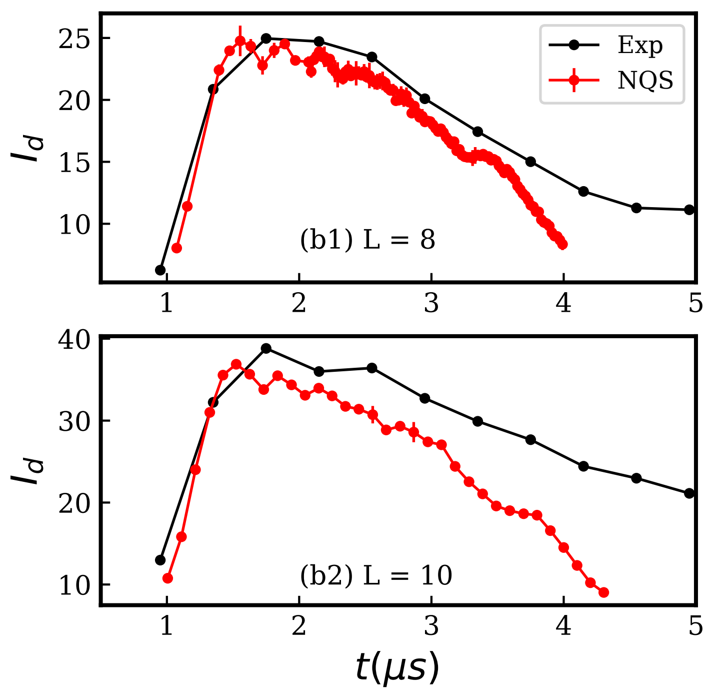
Crossing a quantum phase transition (Kibble-Zurek-like regime)

Short times: random network, Id not really informative

KZ-like regime: scale-free network, Id corresponds to Kolmogorov complexity

Observation of **emergent simplicity**, a consequence of universal behavior on information propagation

Physics: emergent simplicity



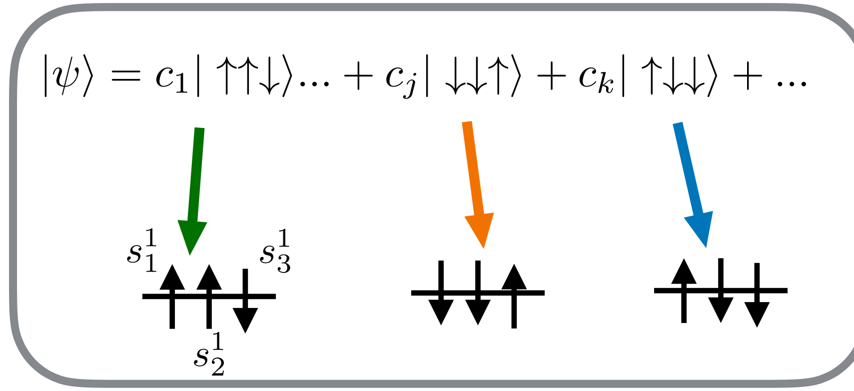
Q: Why is Kolmogorov complexity informative about experiments?

Our approach: full stochastic wave function characterization

New tool: wave function networks

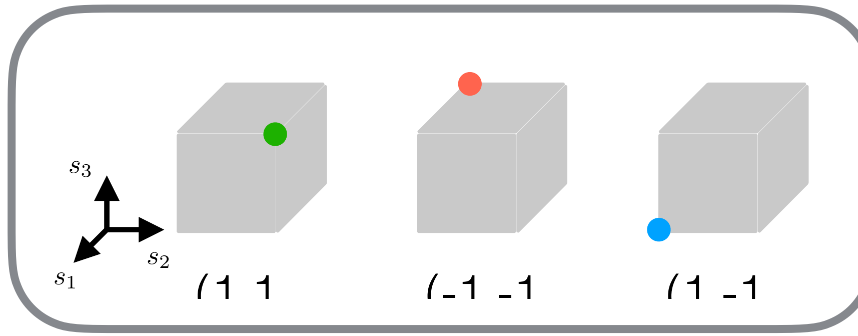
Collection of **wave function snapshots**

(Stochastic sampling of a wave function)



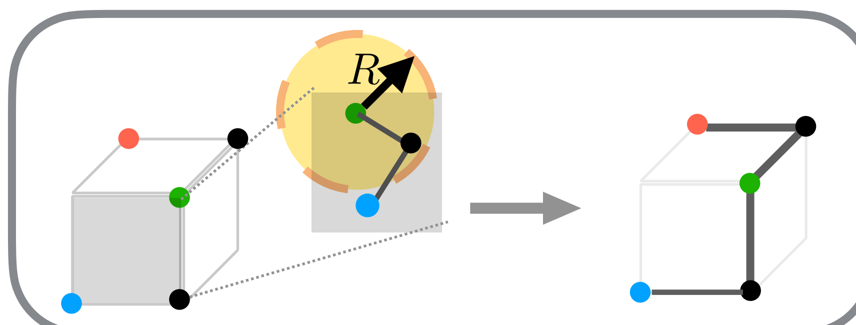
Interpretation of those in data space

(e.g.: Fock space)

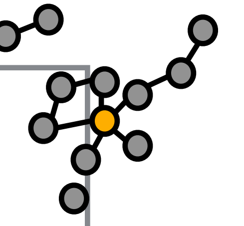


Mapping to **networks**

Definition of a metric and ‘cut-off’ scale in data space



Scale-free network conjecture

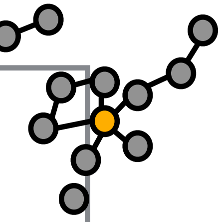


The wave function snapshots of strongly correlated quantum matter are described by **scale-free networks**

Quantum Computers/
simulators:

- Spin systems
- Hubbard models
- Lattice gauge theories
- All architectures alike (cQED, atoms, ions, etc.)

Scale-free network conjecture



The wave function snapshots of strongly correlated quantum matter are described by **scale-free networks**

Barabasi, *Network Science*

Quantum Computers/ simulators:

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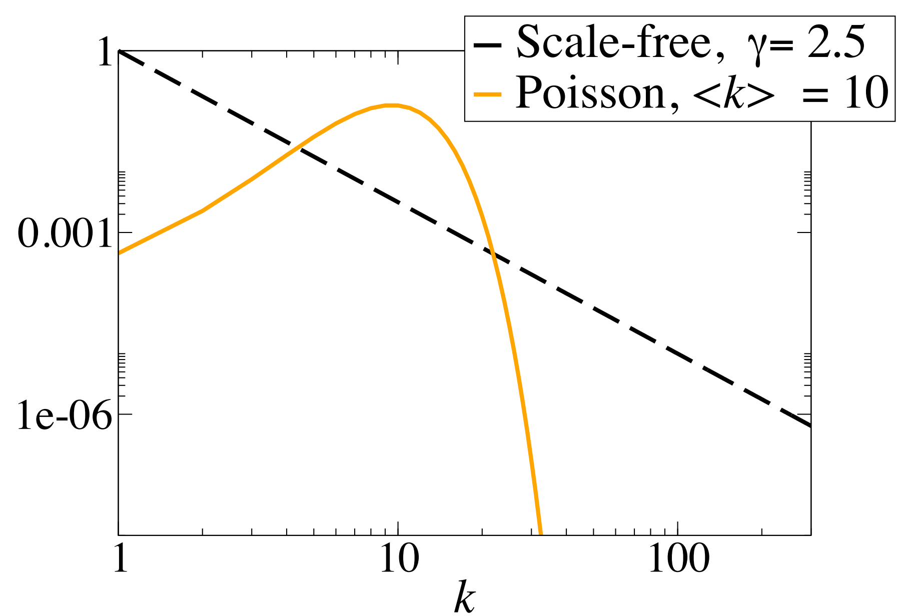
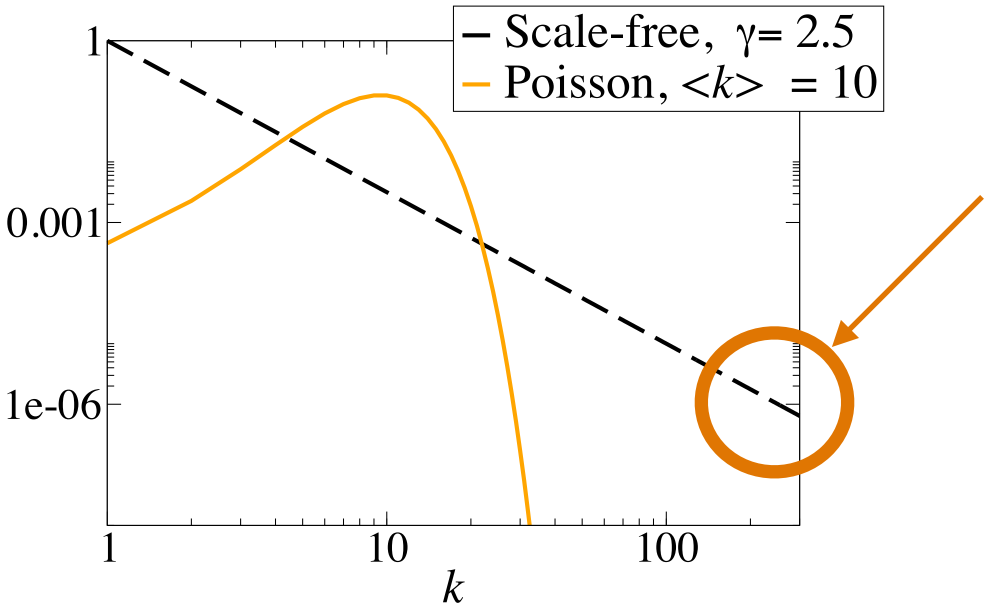
Fraction of nodes with k neighbors



What is a scale free network?

Fraction of nodes with *k* neighbors



(1) Large number of hubs!

(2) Strong fluctuations

$$\sigma^2 / \langle k \rangle \gg 1$$

(Example: friends on Facebook)

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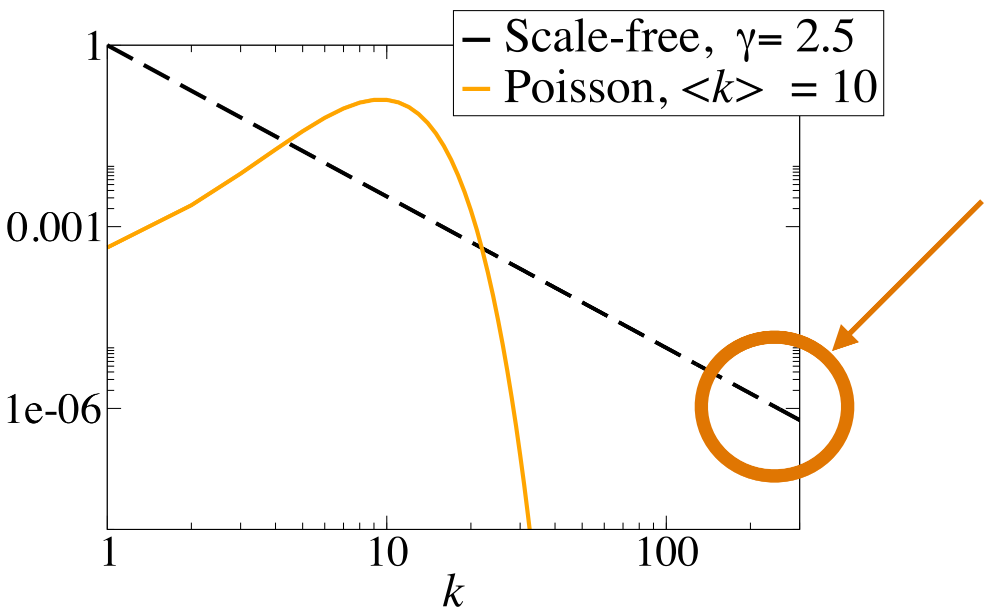

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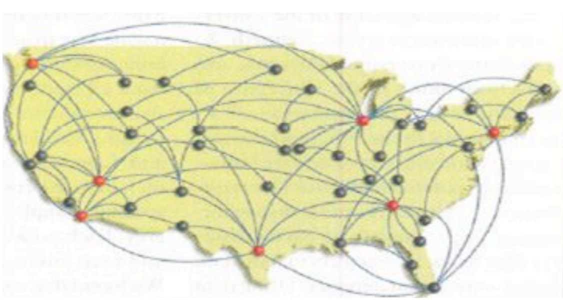

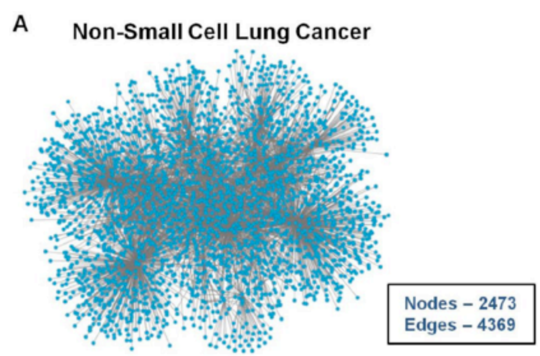

Known examples:

- Social networks
- Power grids
- Airports
- Ecological systems
- Cell dynamics…

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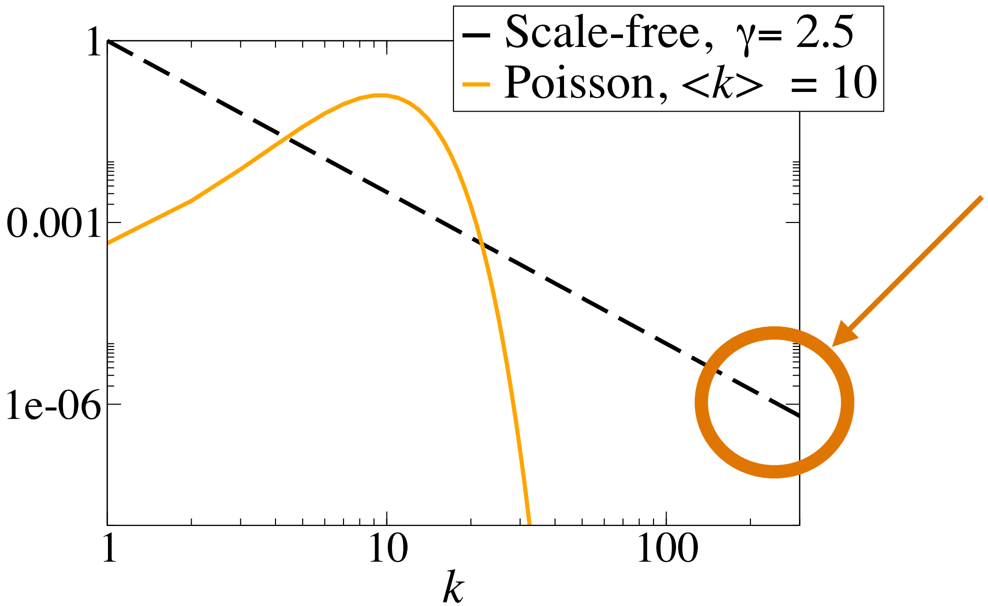

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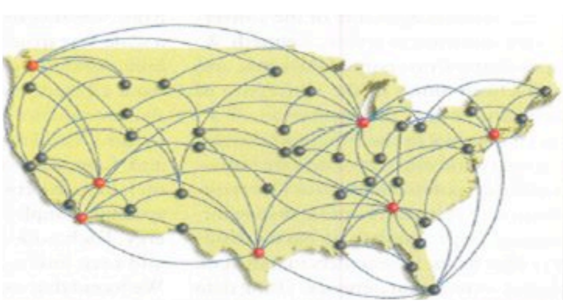

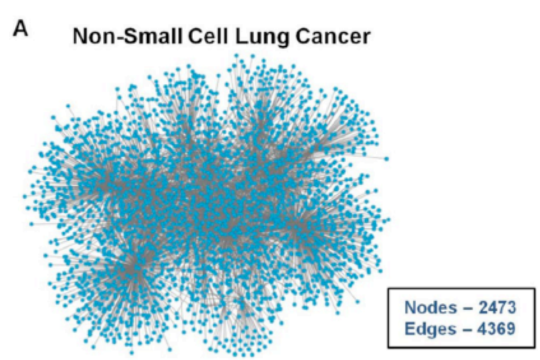

Known examples:

- Social networks
- Power grids
- Airports
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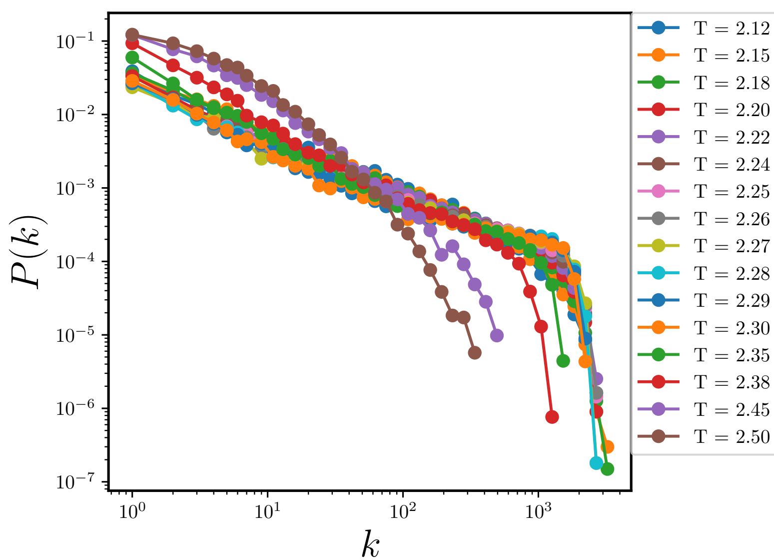
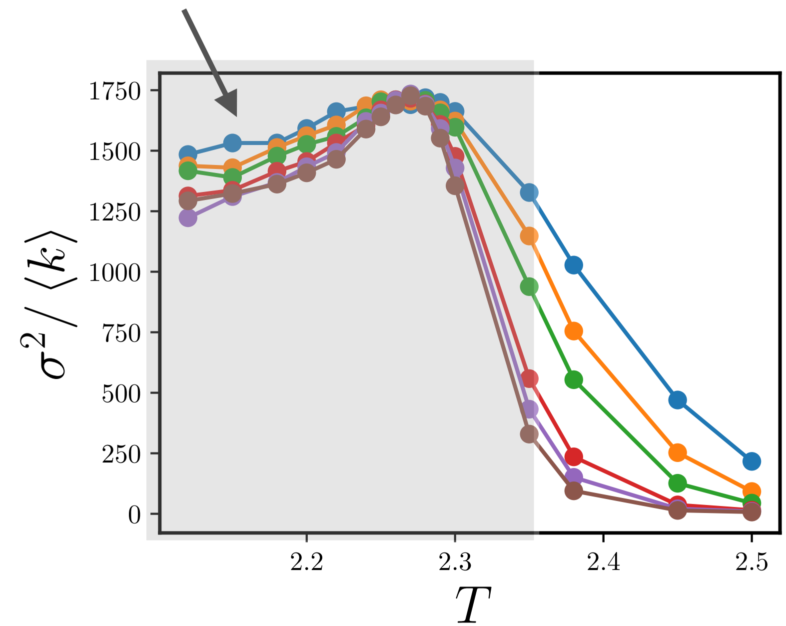
- Cell dynamics…
- **Quantum computers and simulators!**

Emergence of scale-free networks: classical sanity checks

Classical statmech / 2D Ising



Both critical and ordered regimes are scale free!



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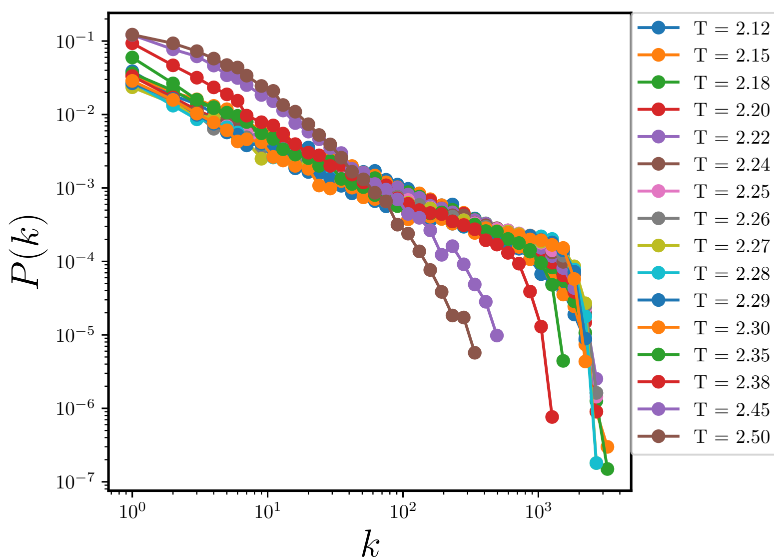

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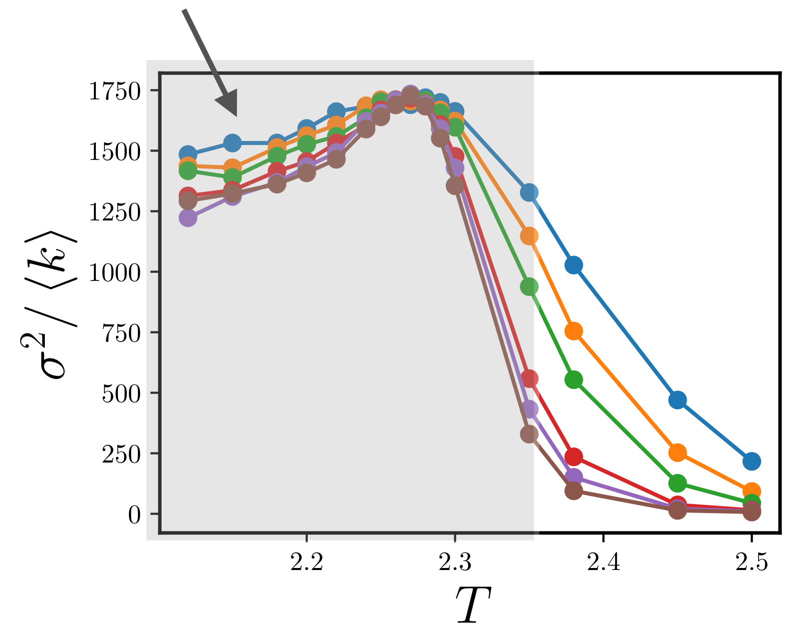
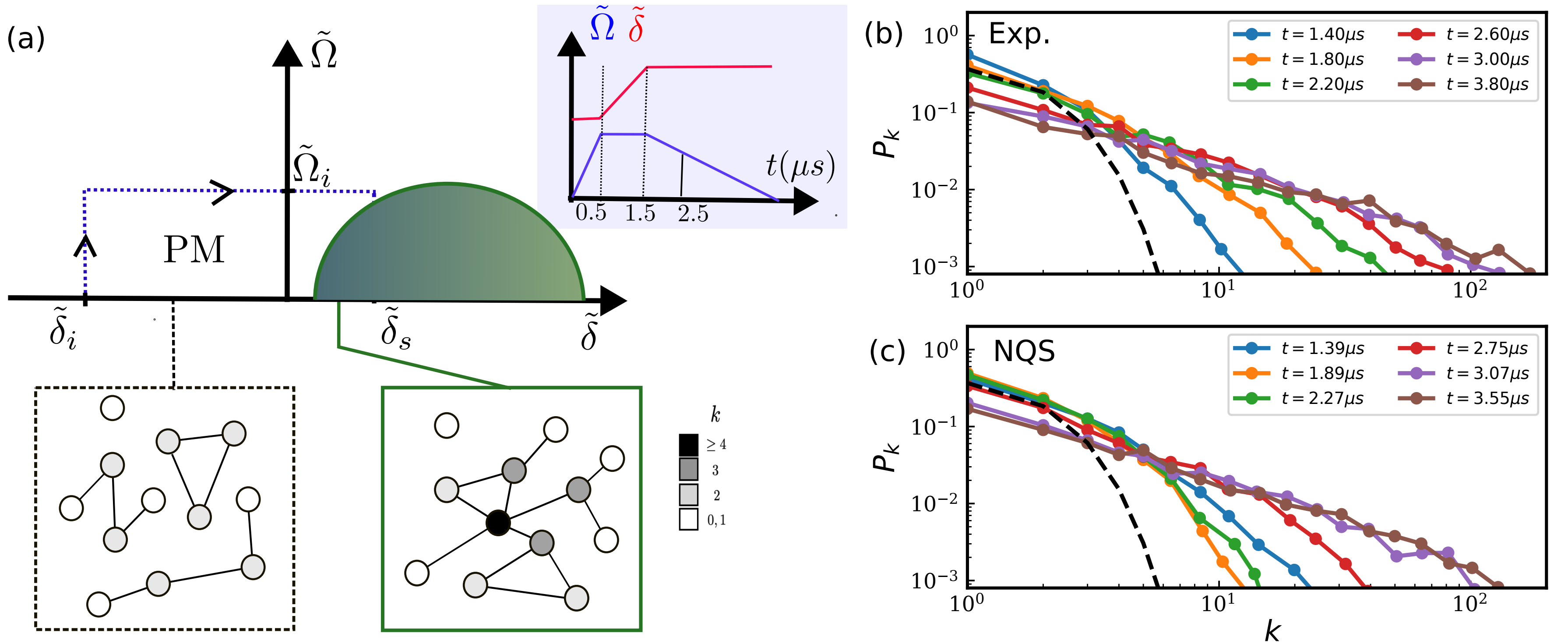


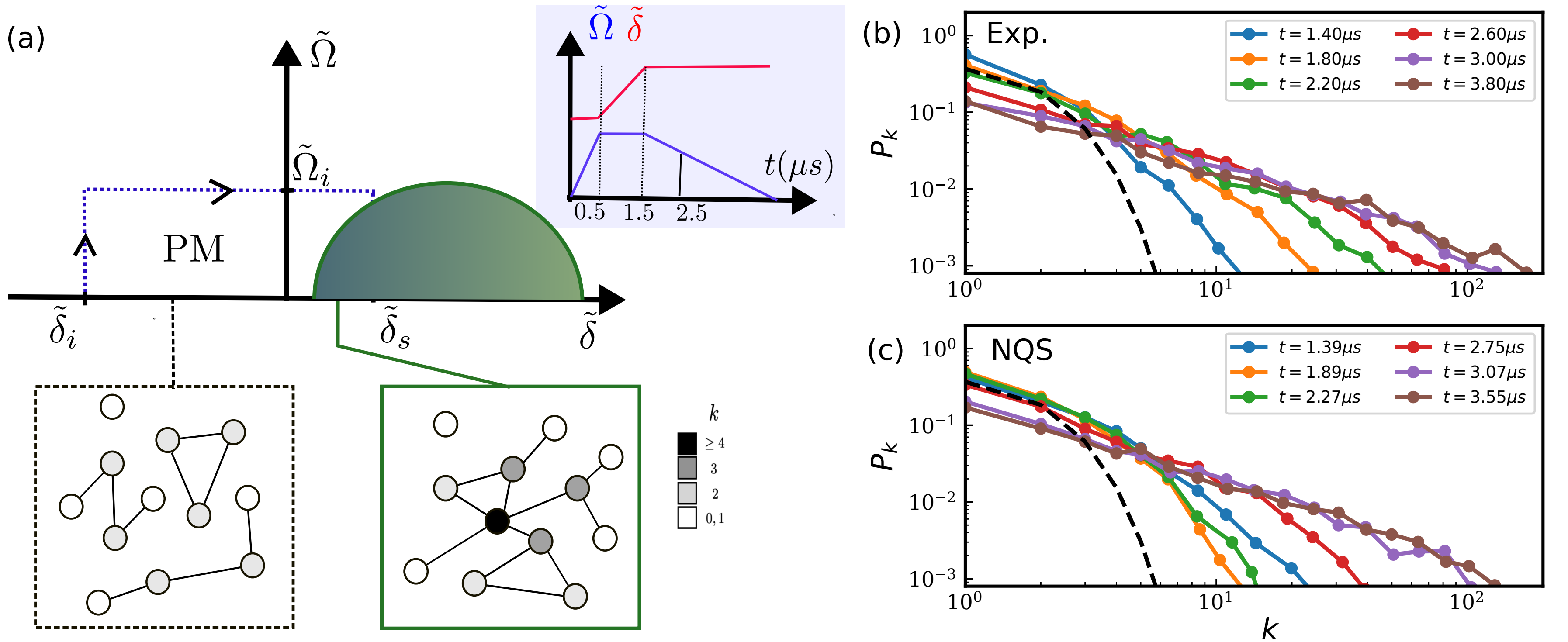
Strongly correlated regimes indeed described by **scale-free networks!**

Situation is ubiquitous - quantum Ising, classical 3D, etc. . However, exact applicability regime yet to be determined

Emergence of scale-free networks: experiments

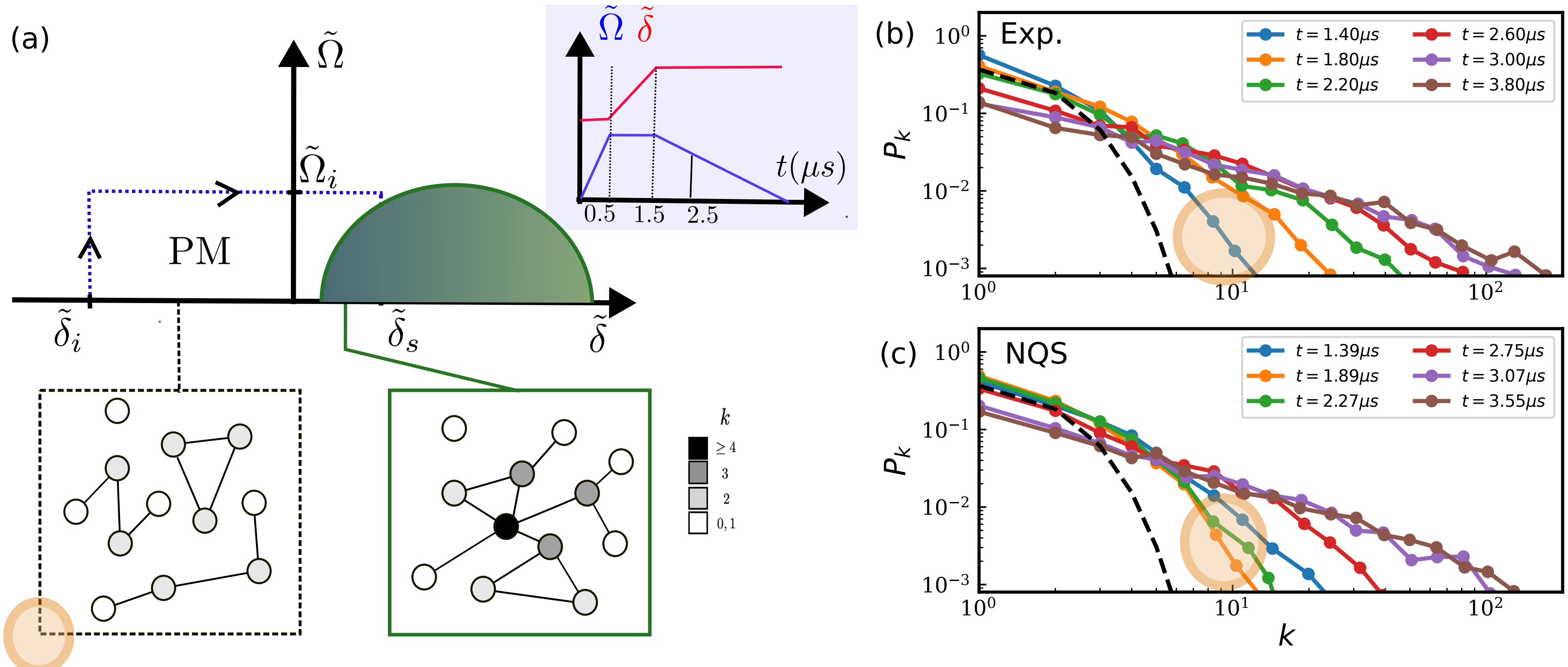


Emergence of scale-free networks: experiments



Short times: random network
After that: emergent scale-free network

Emergence of scale-free networks: experiments



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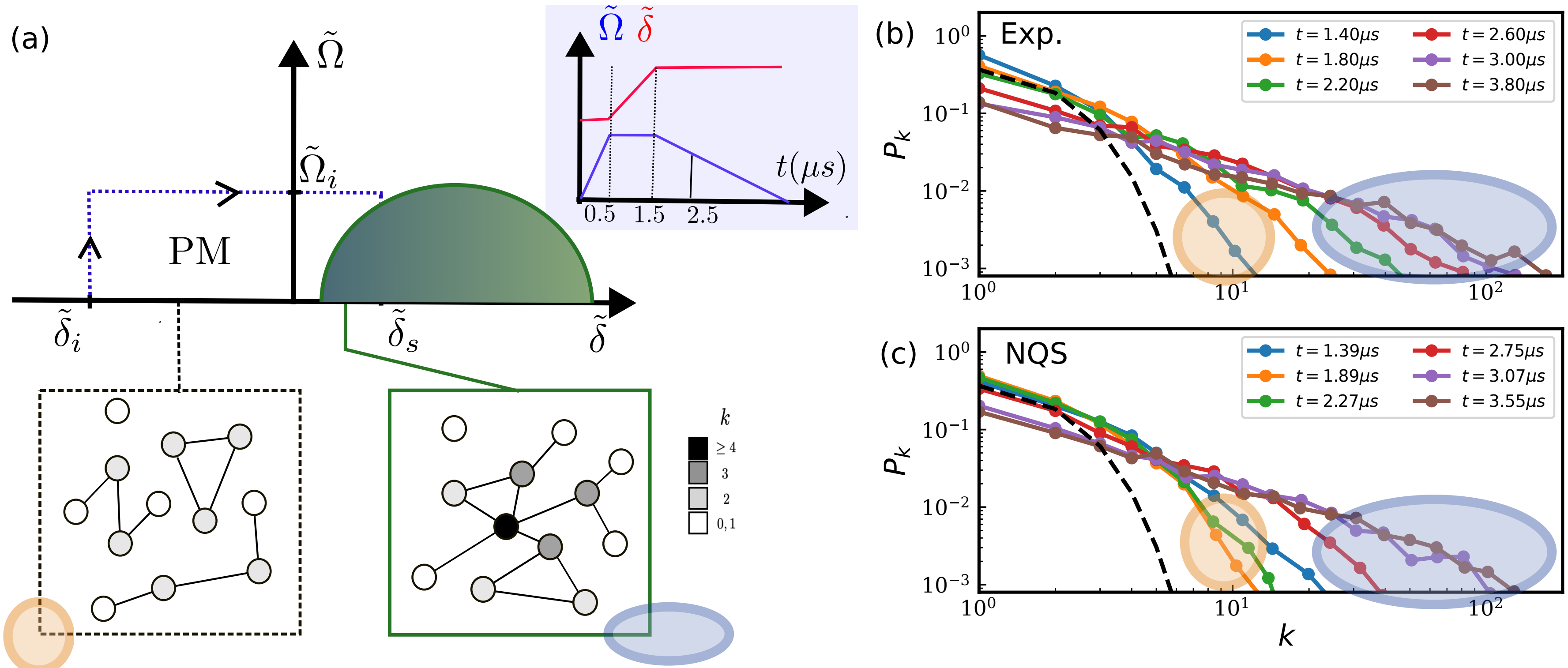

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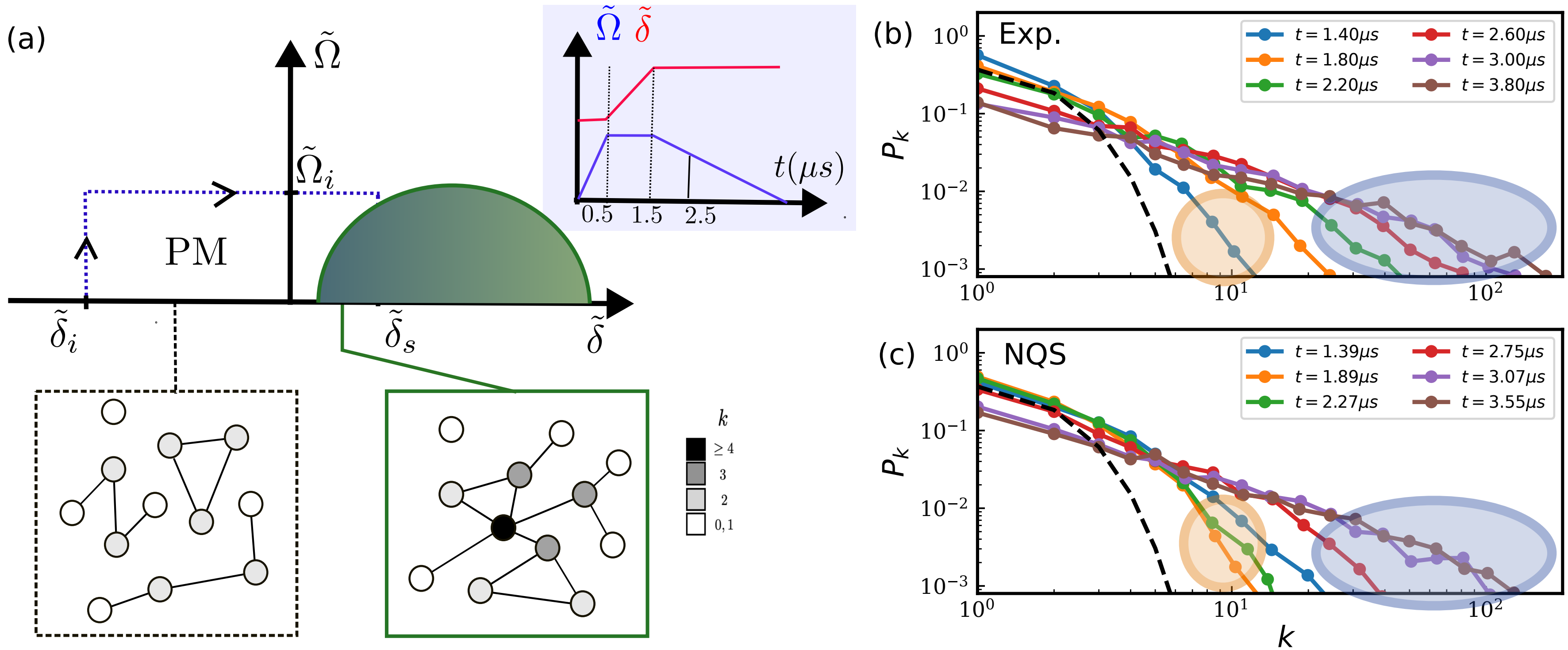
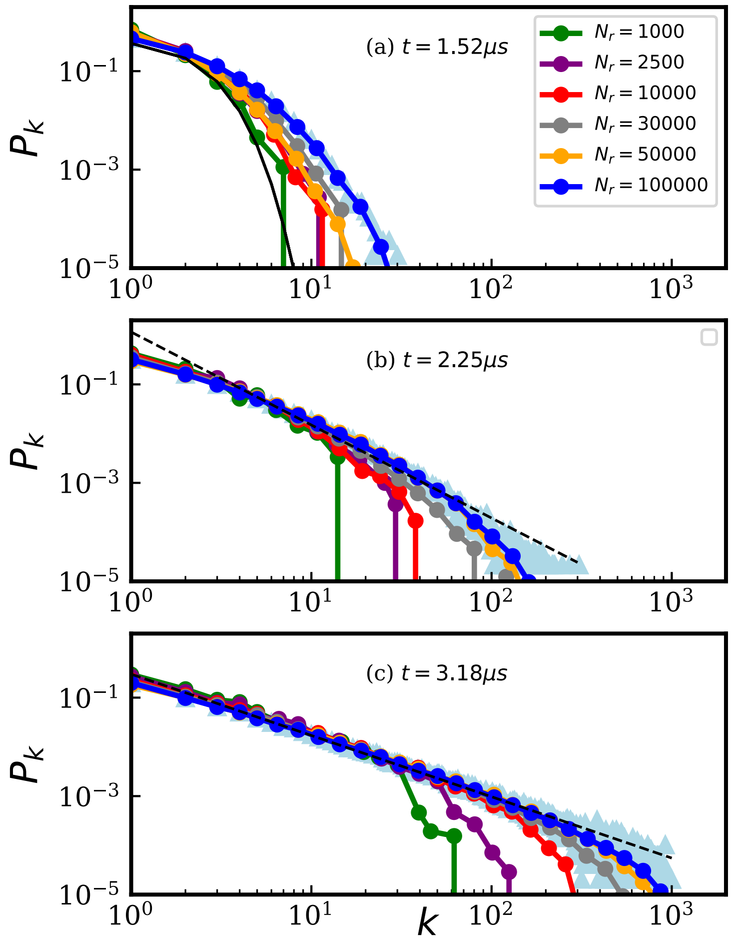


Short times: random network

After that: emergent scale-free network

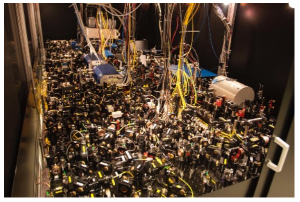
Is this an effect of finite sampling?

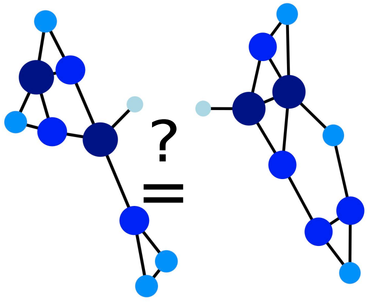


Scale-free is a robust feature, at least according to our simulations based on Neural network states

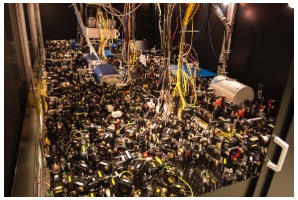
Markus Schmitt

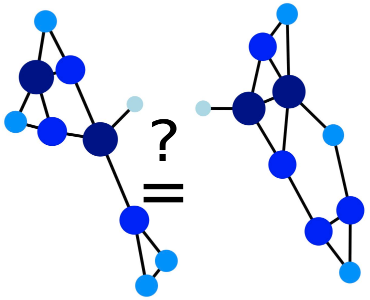
Quantum information tools: cross-platform verification





Quantum information tools: cross-platform verification

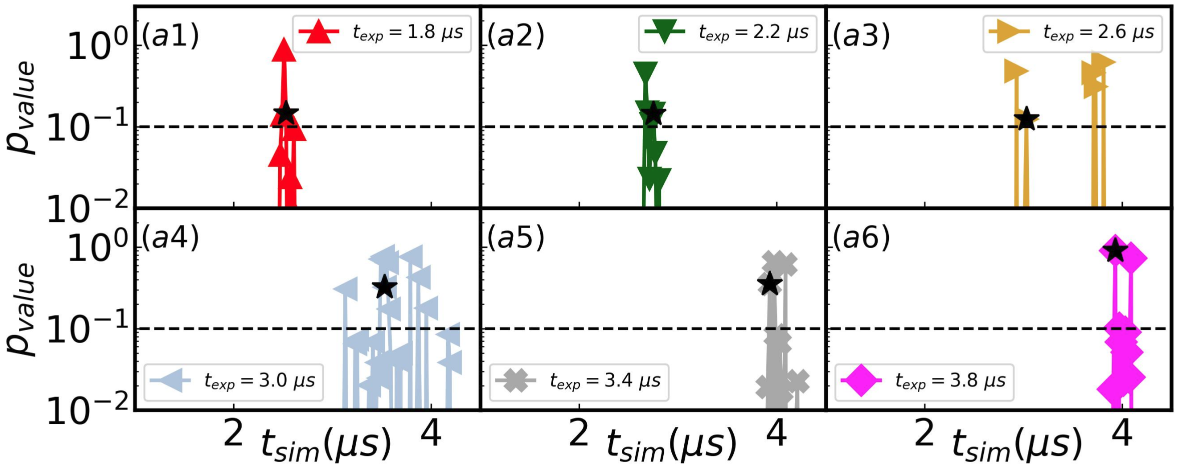




Epps-Singleton test of compatibility between probability distributions

$p_v > 0.1$

Compatible



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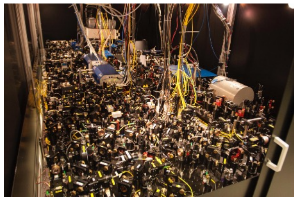
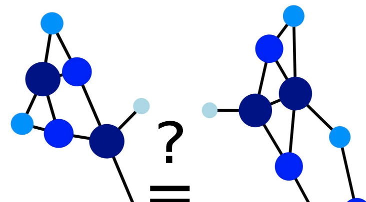


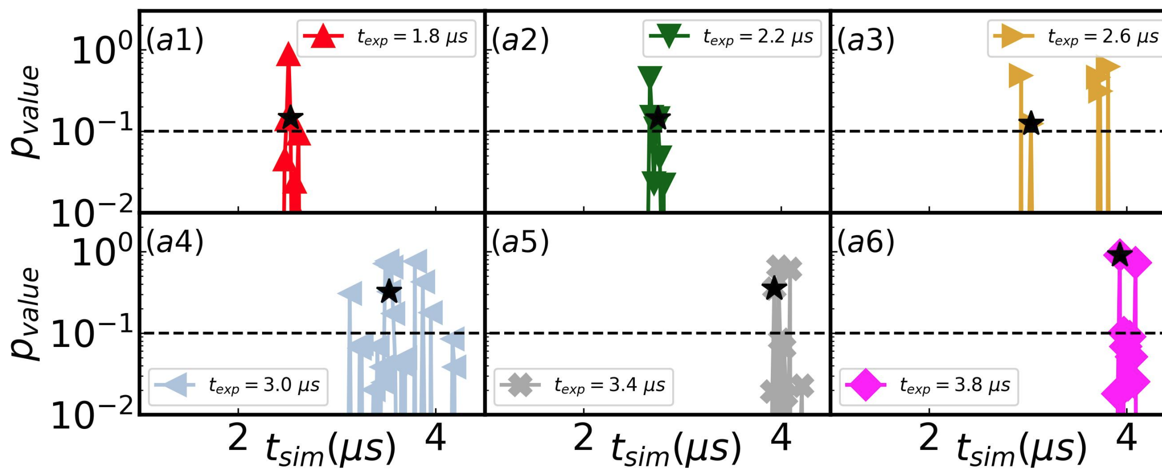


Cross-platform verification up to timescales where simulations become not fully reliable

Epps-Singleton test of compatibility between probability distributions

$p_v > 0.1$

★ ⇩ Compatible



Statements

For classical stat mech sampling,

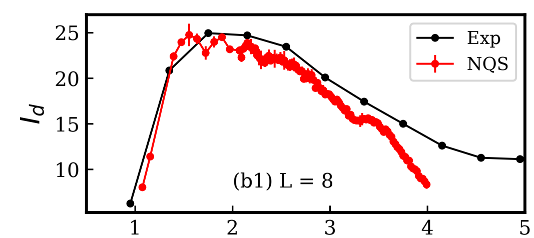
Kolmogorov complexity <—> intrinsic dimension

$$I_d \simeq \frac{1}{\xi}$$

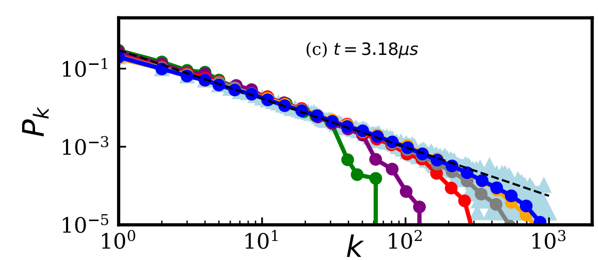
Complexity is minimal for field theories / critical points

—> **Emergent simplicity**

Emergent simplicity for quantum stat mech (only numerics so far)



Observation of decreasing complexity in quantum simulators (Kibble-Zurek)



New math to understand wave function stochastically: **wave function networks**

Outline

Complexity warm-up

Sampling states and **intrinsic dimension**

Data mining partition functions / **criticality as minimal complexity**

Many-body / field theory

Data mining *large scale* quantum simulators:

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Quantum Info

Complexity and topology in many-body systems

Many-body

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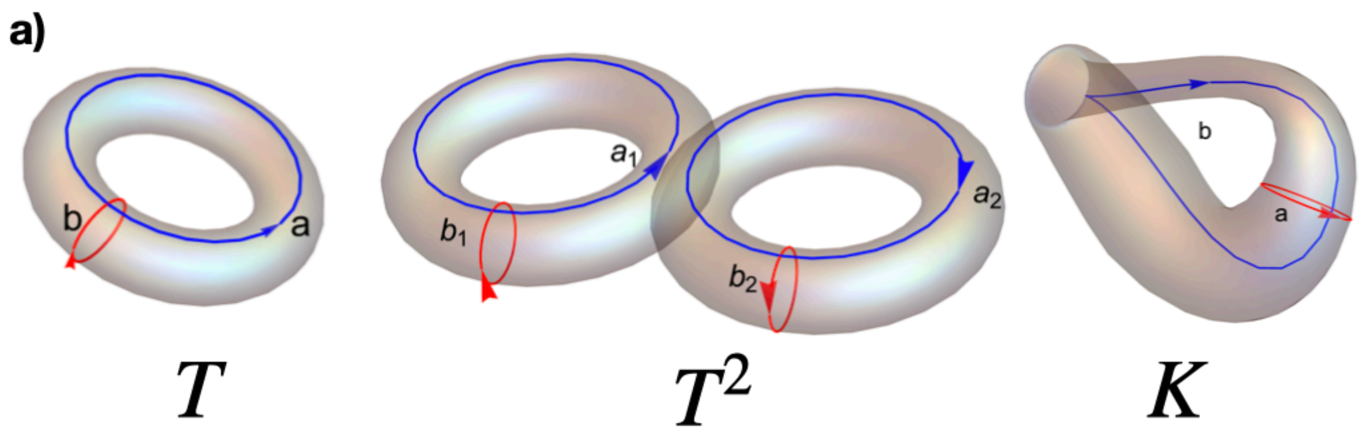
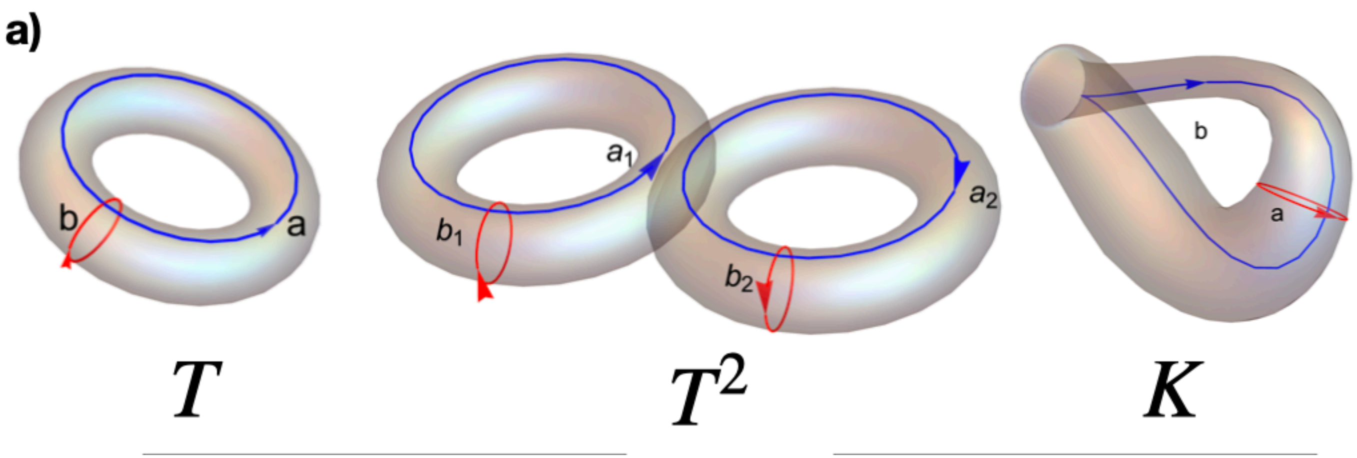
Many-body

A glimpse of on-going work: complexity and topology

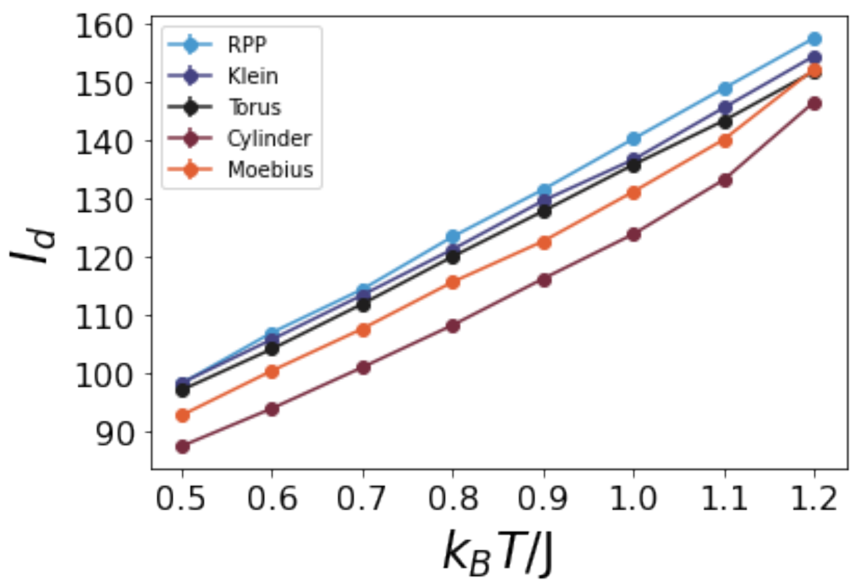


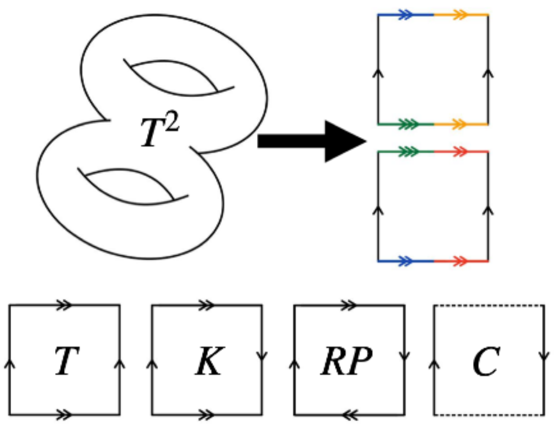
A glimpse of on-going work: complexity and topology



Can we determine whether the **complexity of physical phenomena** is dictated by **topological properties**?

Example: Berezinskii-Kosterlitz-Thouless mechanism in the 2D XY model





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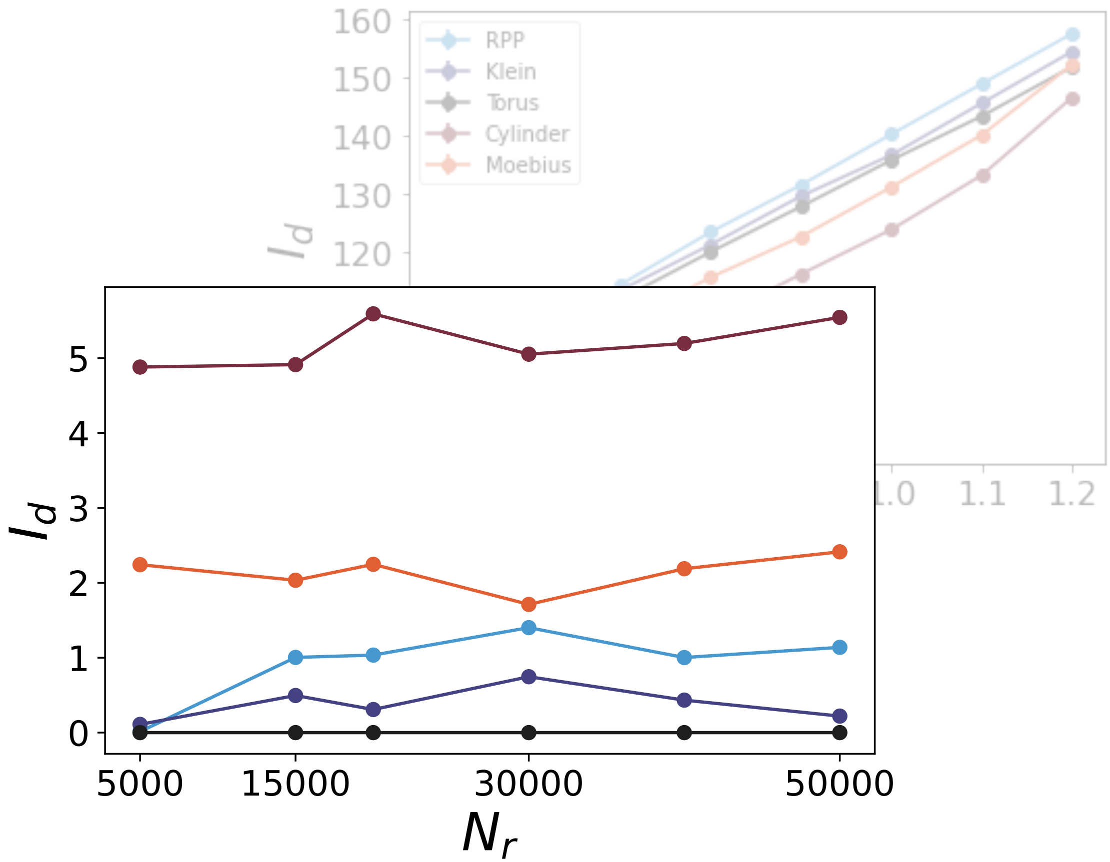

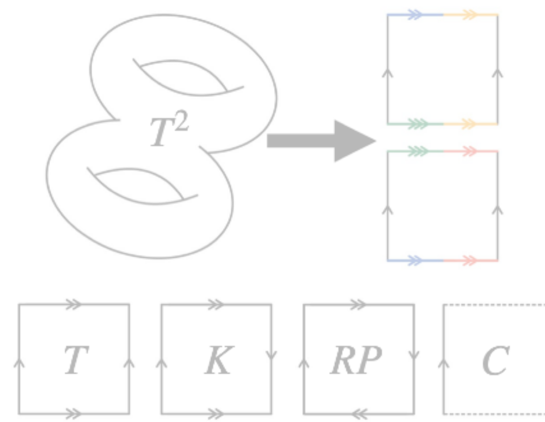

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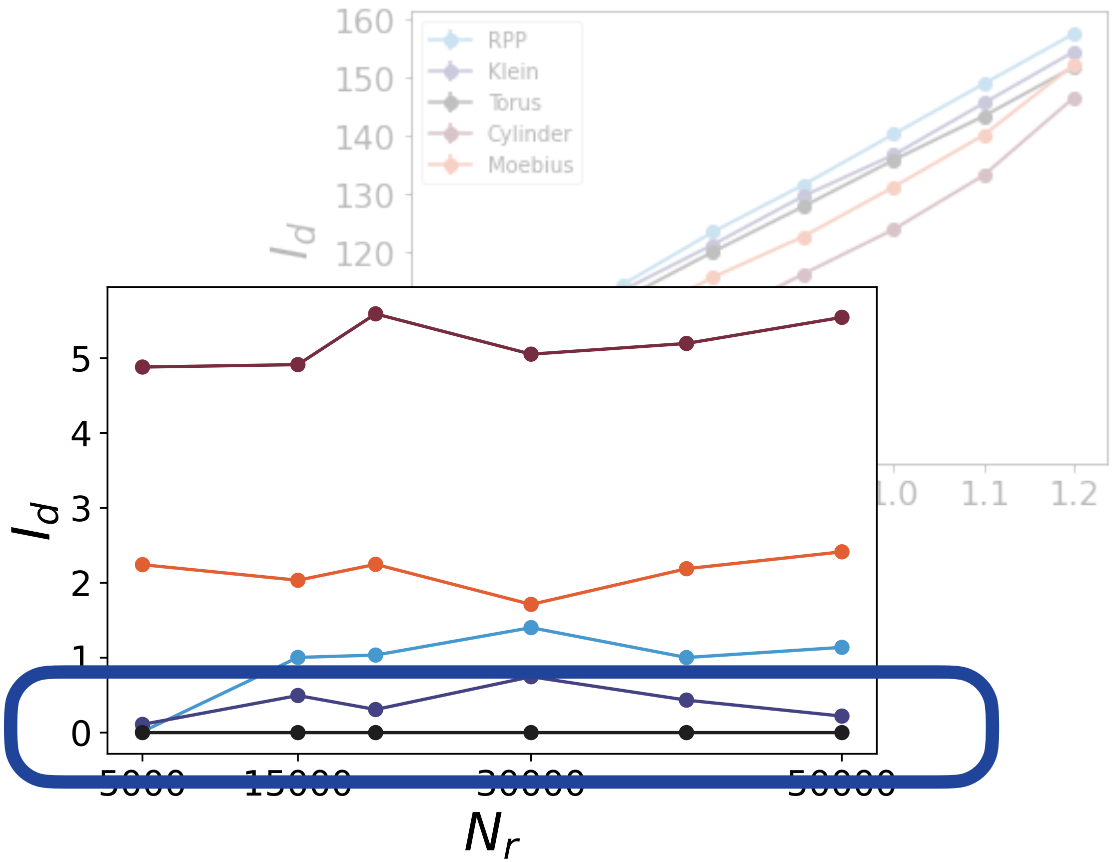
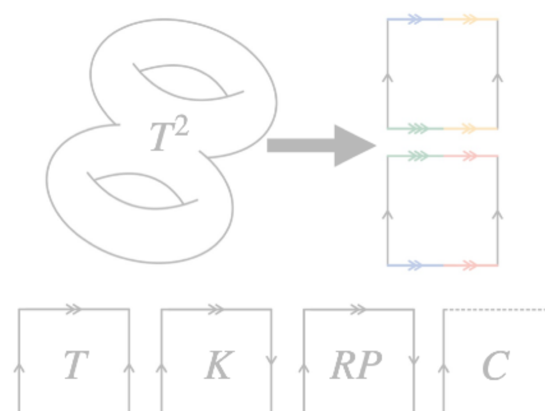
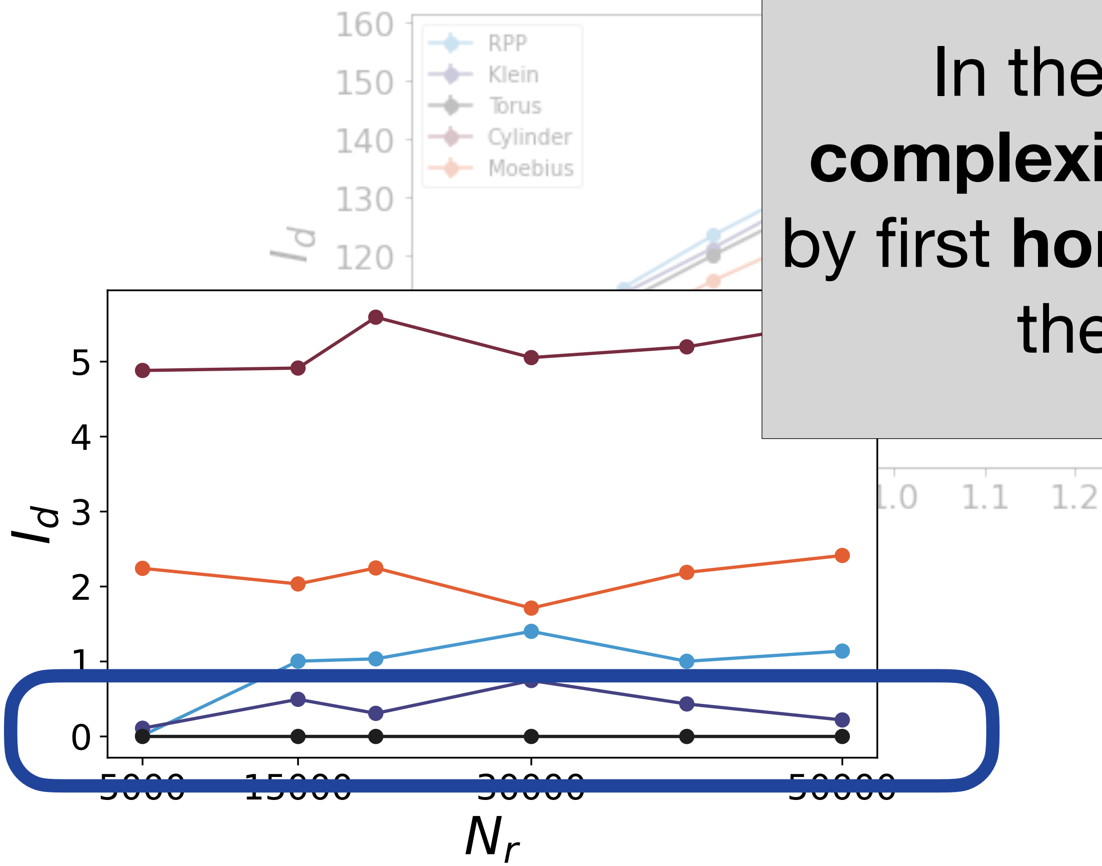




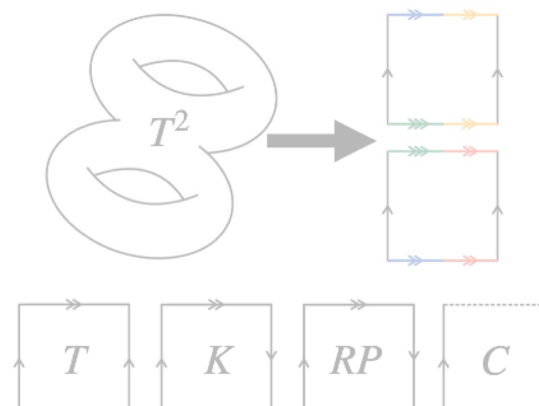
$$\mathrm{Id}_T = \mathrm{Id}_K \neq \mathrm{Id}_{T^2}$$

Example: Berezinskii-Kosterlitz-Thouless mechanism in the 2D XY model



In the BKT phase, **complexity** is determined by first **homotopy group** of the manifold

$$\mathrm{Id}_T = \mathrm{Id}_K \neq \mathrm{Id}_{T^2}$$



Statements

For classical stat mech sampling,

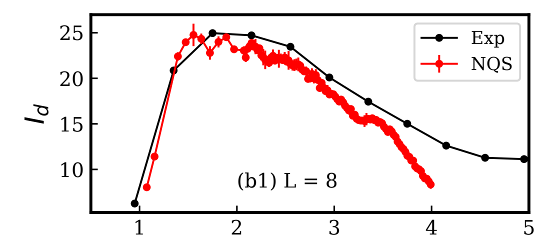
Kolmogorov complexity <—> intrinsic dimension

$$I_d \simeq \frac{1}{\xi}$$

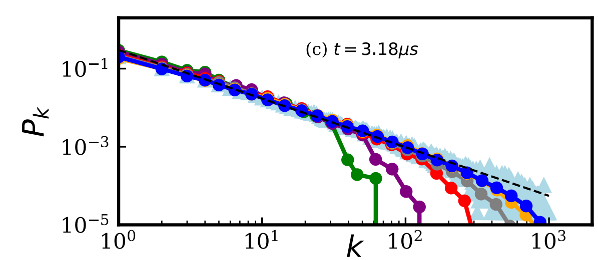
Complexity is minimal for field theories / critical points

—> **Emergent simplicity**

Emergent simplicity for quantum stat mech (only numerics so far)



Observation of decreasing complexity in quantum simulators (Kibble-Zurek)



New math to understand wave function stochastically: **wave function networks**

KC and topology intertwined (example: BKT)

Outlook

- Are computational and Kolmogorov complexity connected?
- Are states of matter classified by their Kolmogorov complexity and/or network structure? Or are they not?
- Does complexity bound correlations (entanglement/discord/magic)?
- Is KC related to general / universal properties of a field theory (beyond CFTs)?

ICTP and SISSA

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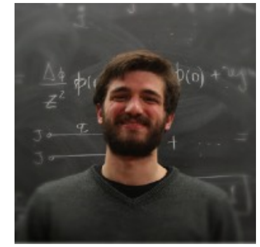
Alex Rodriguez



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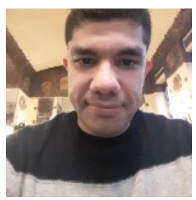
e)

Markus Schmitt (Julich)

Thank you!

Vittorio Vitale (-> Grenoble)



Tiago Mendes-Santos (-> Augsburg)

Rajat Panda

Roberto Verdel Aranda

Markus Heyl (Augsburg)

<u>Key collaborations</u> with Browayes's and Oberthaler's groups

Classical stat mech: Phys. Rev. X 11, 011040 (2021) and unpublished
Quantum stat mech: Phys. Rev. X Quantum 2, 030332 (2021)
Topology and data spaces: 2305.05396
Rydberg experiments: 2301.13216 (Augsubrg-Julich-Palaiseau-Trieste)
Cold atom experiments - 2307.10040