Data mining the many-body problem

University of Hong Kong

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Marcello Dalmonte

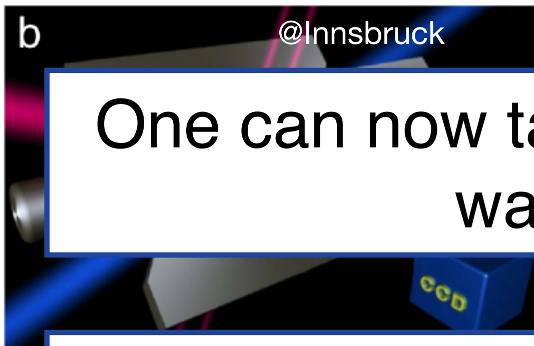
ICTP, Trieste

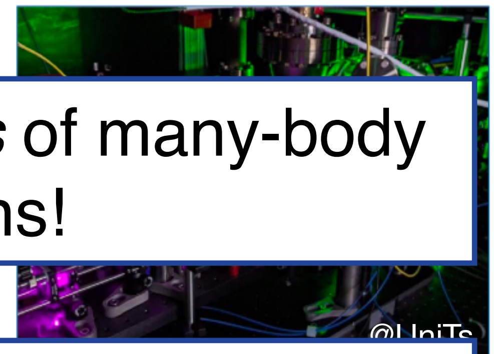
Theory work with: A. Angelone, D. Bhakuni, T. Mendes-Santos, C. Muzzi, R. Panda, A. Rodriguez, X. Turkeshi, R. Verdel Aranda, V. Vitale
Exp: Augsburg/Julich/Palaiseau/TS and Heidelberg/TS collaborations

Based on Th: Phys. Rev. X **11**, 011040, Phys. Rev. X Quantum **2**, 030332 (2021), Phys. Rev. B 110, 144204 (2024) + unpublished
Th/Exp: Phys. Rev. X 14, 021029, Phys. Rev. B 109, 075152 (2024)

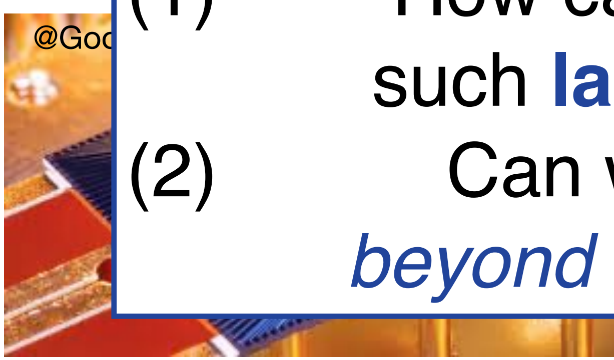
Big picture

Large, “controllable” quantum machines (simulators, computers) are an **experimental reality**





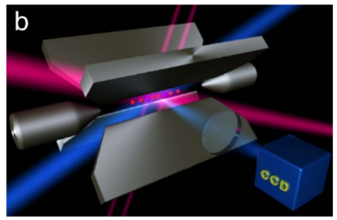
One can now take *photos* of many-body wave functions!

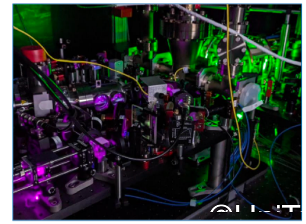


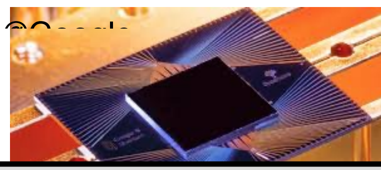
(1) How can we make sense of such **large amount of data**?

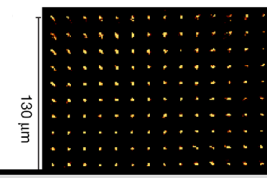
(2) Can we learn something *beyond correlations* we know?

Main message

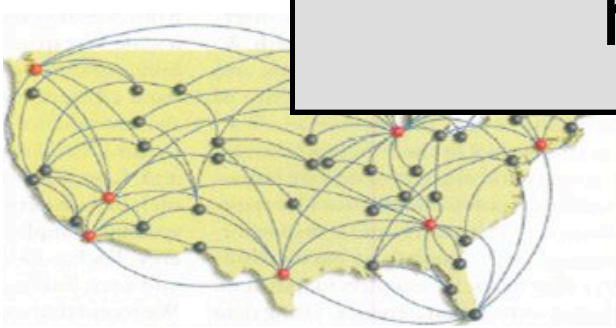


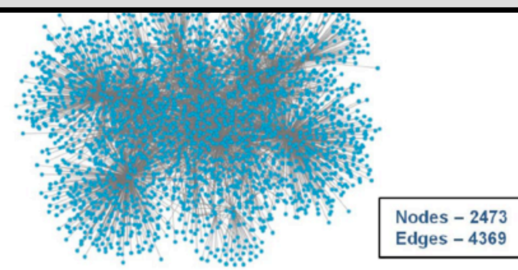




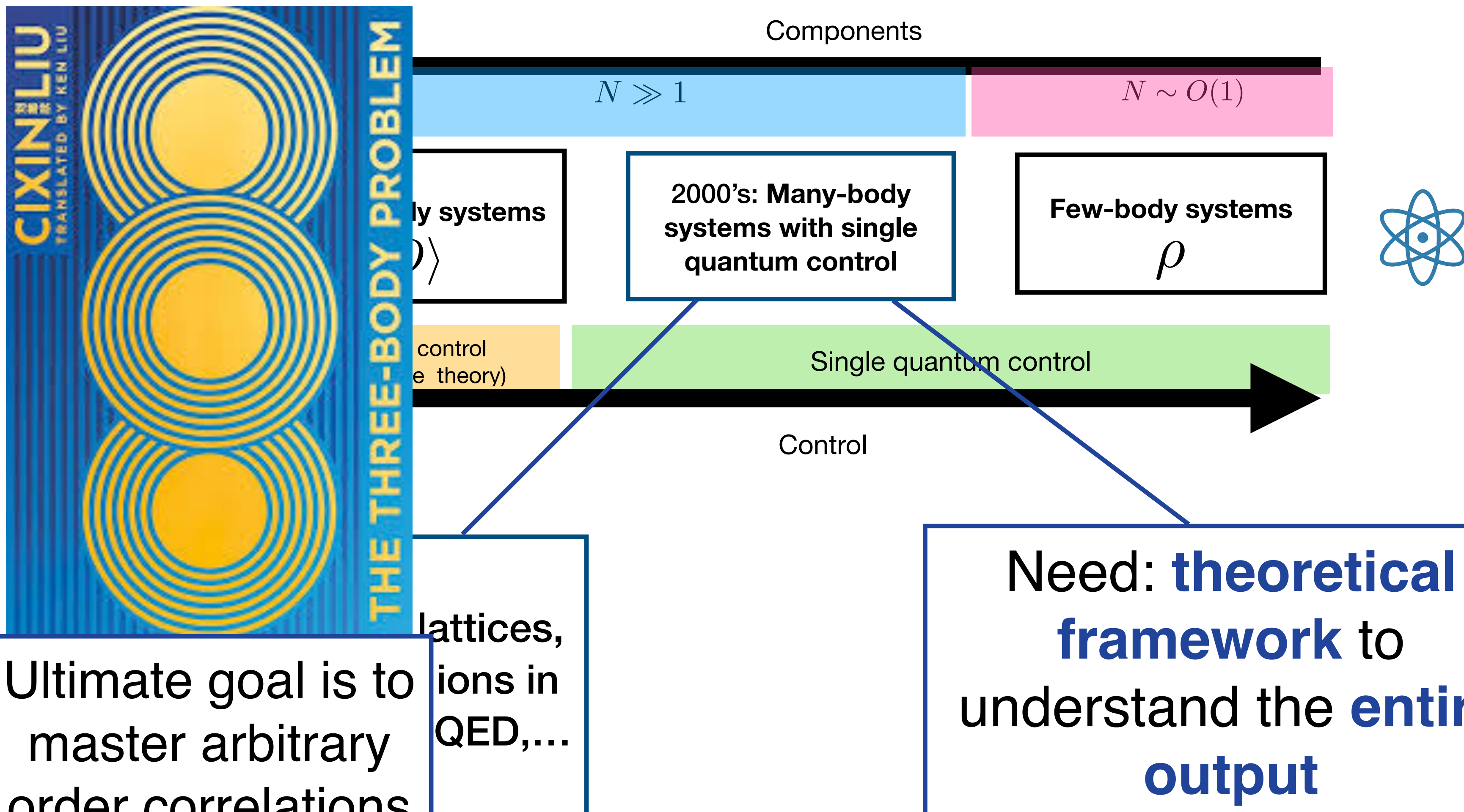


Described by the very same mathematics!





Theorist’s view: Information *conundrum* of quantum computers and simulators



Ultimate goal is to master arbitrary order correlations

Need: **theoretical framework** to understand the **entire output**

Outline

Huge ‘many-body physics’ data sets: what are we talking about? And why?

Unsupervised learning and intrinsic dimension

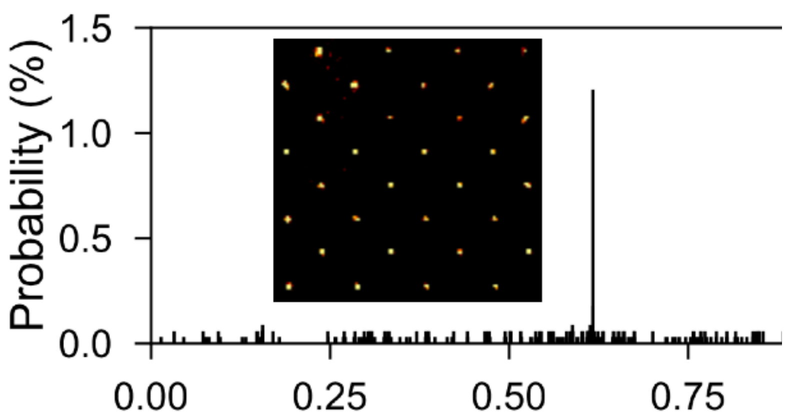
Illustration 1: classical partition functions and complexity - *is a critical point complex?*

Illustration 2: emergence of scale-free networks and *scalable* validation of quantum simulators in lattice models

Illustration 3: *stochastic* classification of matter

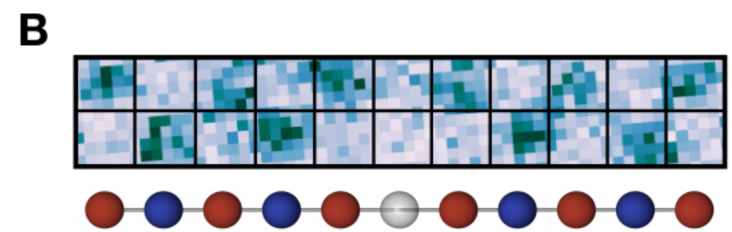
What are our datasets? Quantum simulation and computing

Projective measurements
of a many-body state



$X_1 =$ 10001001010101…

Scholl et al., Nature 2021
(optical tweezers)



$X_1 =$ 1 -1 1 -1 1 0 1 -1 1 -1 1

Gross's and Bloch's group,
Nature 2021 (optical lattices)

Very *generic* capability -
trapped ions, superconducting
circuits, etc..

What are our datasets? Stat mech

Stat mech: sampling a partition function

$$Z = \sum_{\{X\}} e^{-\beta E_X} = \sum_{\{X\}} P(X)$$

X : some configuration

Sampling of a probability distribution (direct, Markov chain, etc.)

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

Example: Ising model, 4 sites

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

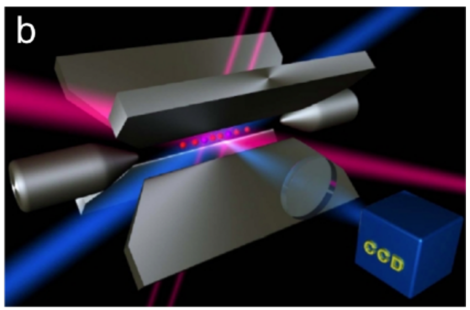
Datasets: spin configurations

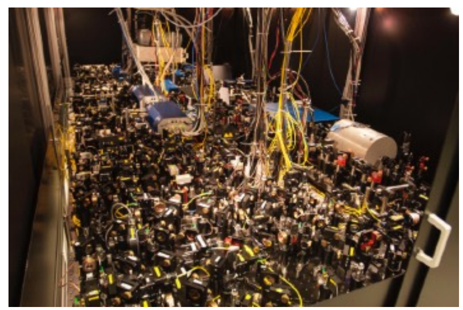
$$\{[0100], [0101], [1111], ...\}$$

Why are we looking at these? Some specific motivations

Motivation 1: quantum sciences

Quantum information viewpoint: new tools





Can we trust the outcome of quantum computers/simulators?

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

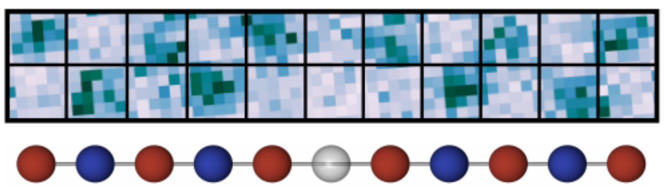
- Cross-platform **verification** of wave functions
- Noise ‘tomography’
- Robustness of information

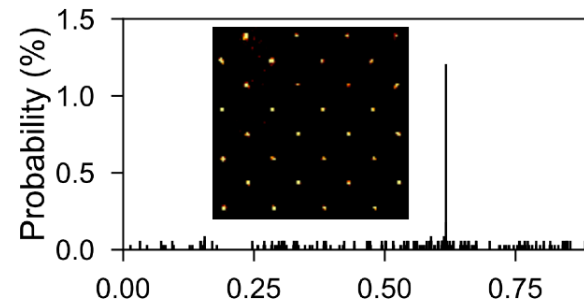
Complementary to microscopic approaches:
randomized benchmarking, optimal control / calibration

Motivation 2: statistical physics

Quantum many-body viewpoint: new concepts

B





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

Note: very same motivations as in neuroscience / soft-matter / molecular science

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’

Given a many-body (quantum) state:

- How are they related?
- Is KC related to *physical phenomena*?
- Can we actually *measure* KC?

Computational complexity
(“time”)

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

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

“Write 1 N times”

$K = 15$

111000111000111000 111000111000111000
111000111000111000 111000111000111000
111000111000111000 111000111000111000

“Write 111000 N/6 times”

$K = 22$

11000101010110011010
10101010101010101011
00101010001111111001
1010000001111111

“Write 111000…1111”

$K = 6 + N = 73$

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

Q: how to adapt to many-body states?

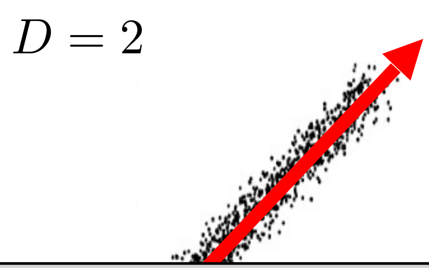
Classical partition functions and complexity - *is a critical point complex?*

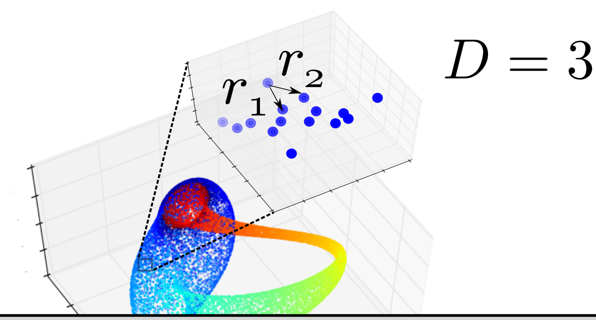
Tool 1: The intrinsic dimension - “geometrical”

The intrinsic dimension

the minimal number of variables required to describe a dataset

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





Intuition: the intrinsic dimension is informative about

(1) number of relevant degrees of freedom, and

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

Op[...] needs a single variable to properly describe the object of interest

Review: Glielmo et al., Chem Rev. 2021

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

11111111
11111111
11111111
11111111

Q: how to adapt to many-body states?
Is this connected to physical phenomena?

"Write 1 N times"

$K = 15$

"Write 111000 N/6 times"

$K = 22$

"Write 111000…1111"

$K = 6 + N = 73$

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

A basic example: a 3 site model

Simple example: sampling a 3-site rotor model

1) States / data space (D=3)

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

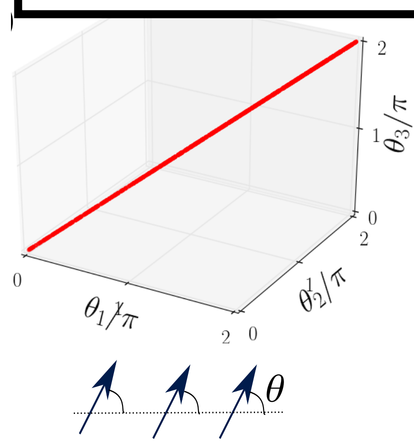
2) Equilibrium weight:

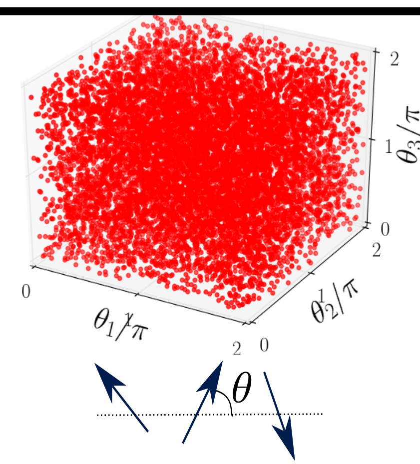
$$\rho(E) \sim e^{-E(\vec{x})/T}$$

3) Hamiltonian:

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

All of this makes sense! but what about transitions?





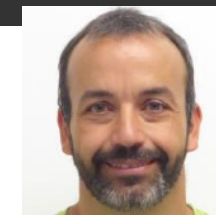
$$I_d = 1$$

$$I_d = 3$$

$$S_{PCA} = 0$$

$$S_{PCA} \simeq d$$

How does complexity behave at criticality?

Is a critical point *complex* or *simple*?

T

Intuition 1 [real space]: at critical points, correlations diverge!

$$\xi \to \infty$$

very correlated manifold, so maximal intrinsic dimension

Intuition 2 [RG]: at critical points, physics is universal

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

manifold is very constrained, so minimal intrinsic dimension

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

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

Example: N=4

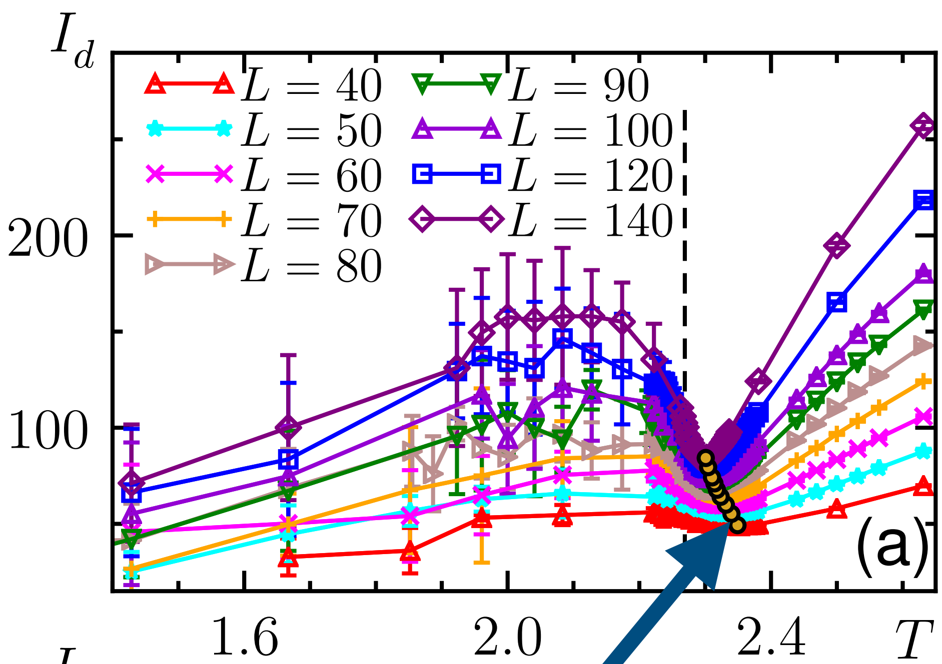
s_1	s_2	s_3
$\uparrow\ \uparrow$	$\uparrow\ \uparrow$	$\uparrow\ \downarrow$
$\uparrow\ \downarrow$	$\uparrow\ \uparrow$	$\uparrow\ \downarrow$

$$r(s_1, s_2) = 2$$

$$r(s_1, s_3) = 2$$

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

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

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

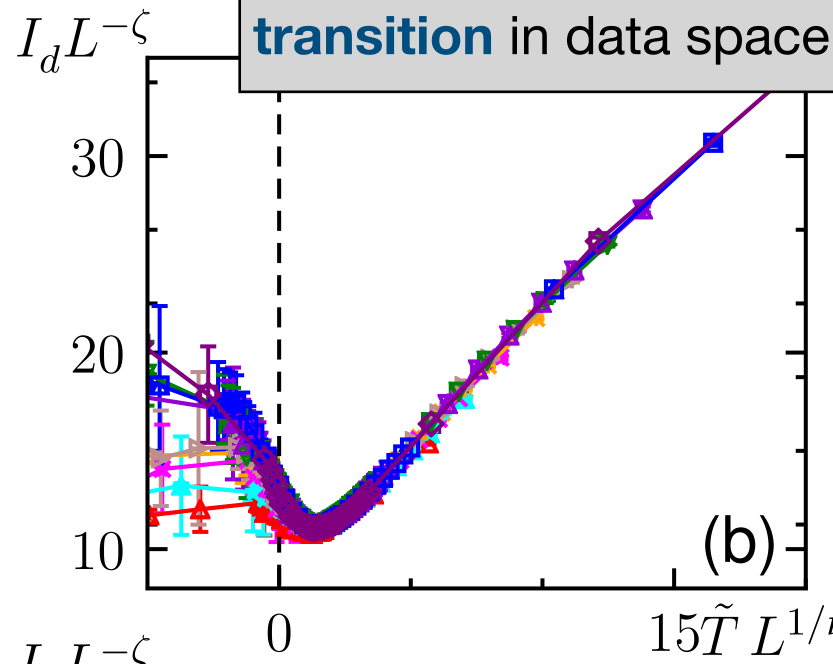
$$\xi \sim (T - T_c)^{-\nu}$$

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)

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

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

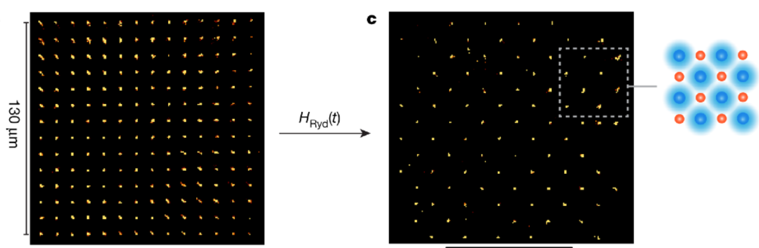
Complexity is minimal for field theories / critical points
—> **Emergent simplicity**

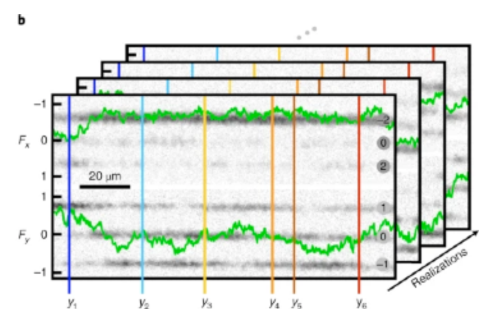
see also:
data compression: O. Melchert and A. K. Hartmann, Phys. Rev. E 91, 023306 (2014);
local complexity: Schmitt and Lenarcic, Phys. Rev. B 106, L041110 (2022);
out of eq.: Martirani et al. PRX 9, 011031 (2019).

Experiments

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

What about *experiments*?





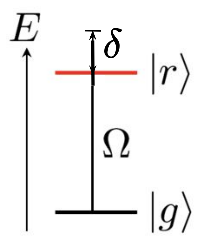
Rydberg atoms in optical tweezers

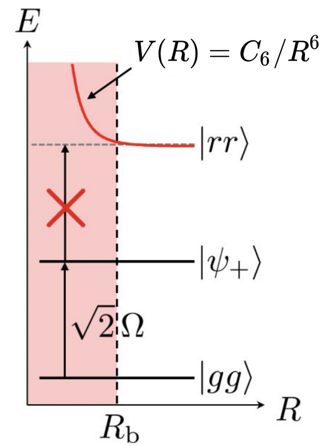
Scholl et al., Nature 2021

Spinor Bose gases

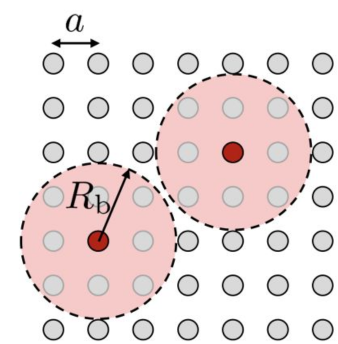
Prüfer et al., Nat. Phys. 2020

Rydberg atom arrays: quick intro





Rydberg blockade potential



$V(R_b) := \Omega$

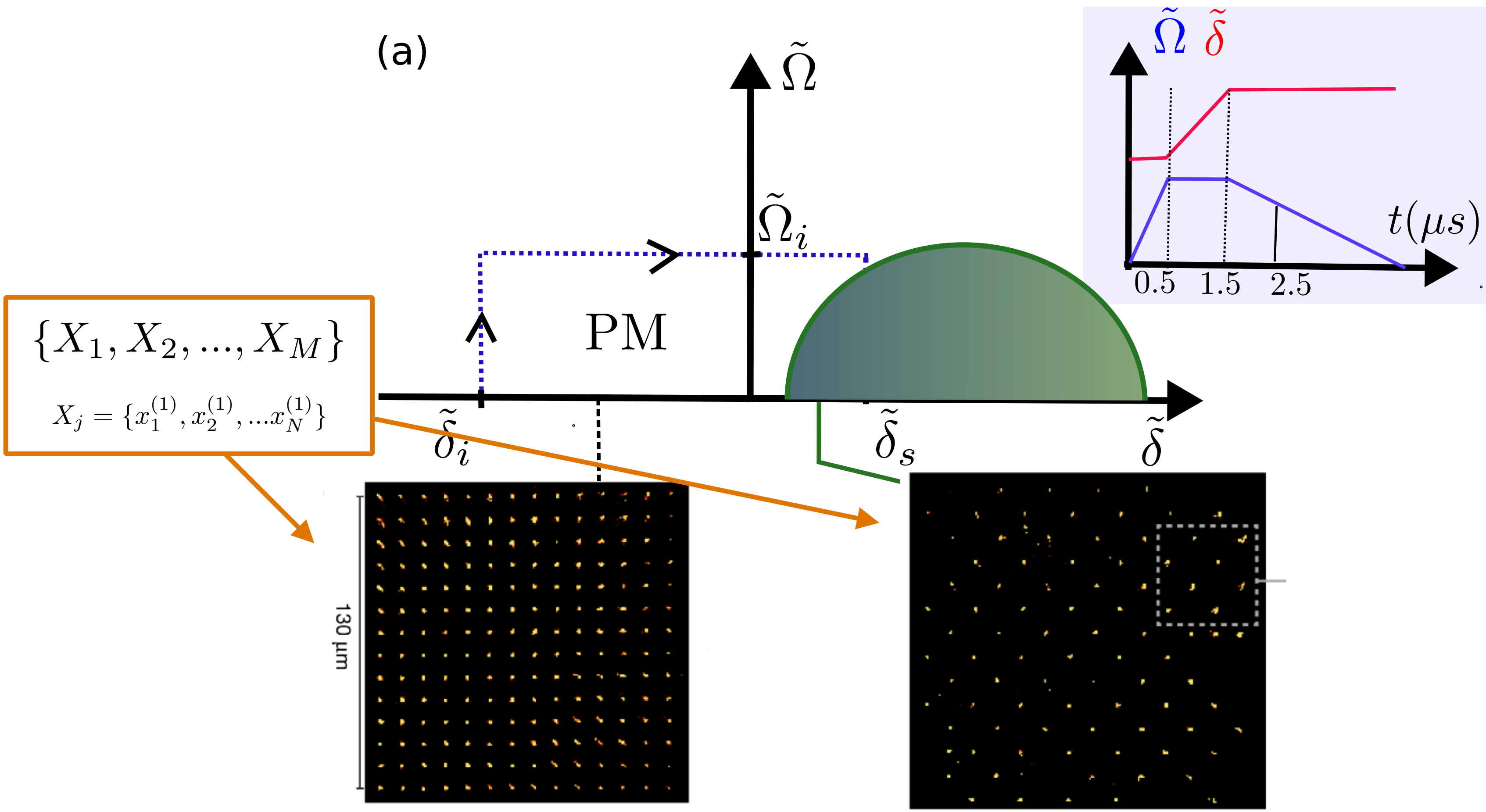
Blockade radius

Effective Hamiltonian:

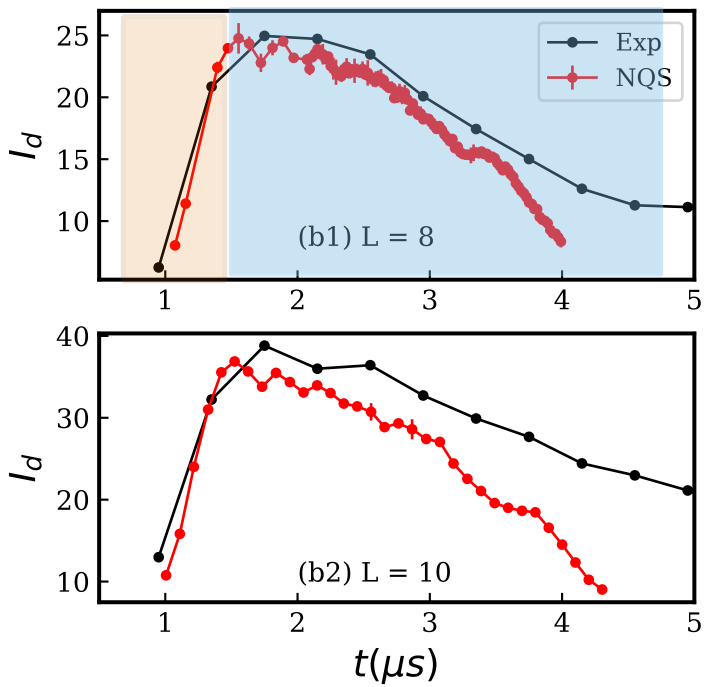
$$\hat{H}_{\mathrm{FSS}} = \sum_j \left(\Omega\, \hat{\sigma}_j^x + \delta\, \hat{n}_j\right) + \sum_{j<l} V_{j,l}\, \hat{n}_j \hat{n}_l$$

See pioneering works in Palaiseau, Wisconsin, Stuttgart, Heidelberg, Munich, Harvard, …

Data mining Rydberg atom arrays: crossing a phase transition



Physics: emergent simplicity across Kibble-Zurek



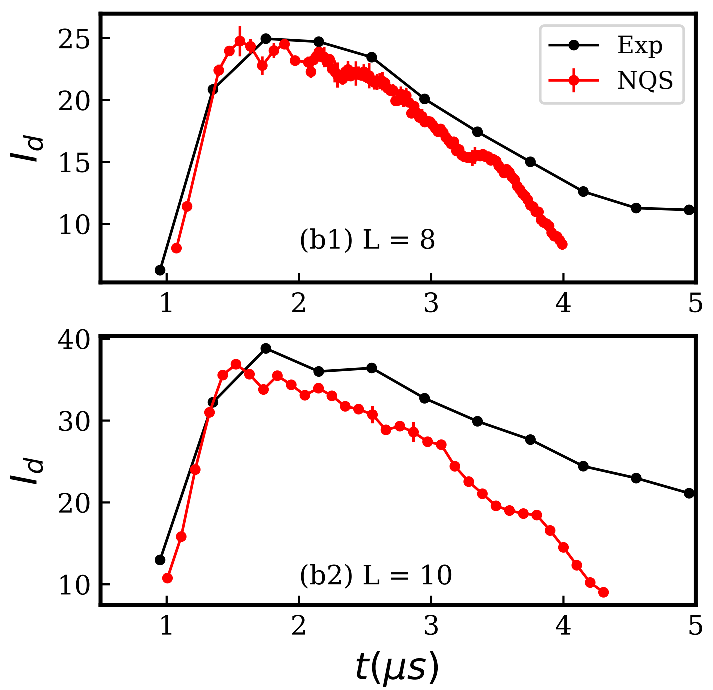
Crossing a quantum phase transition (Kibble-Zurek-like regime)

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

Statements

For classical stat mech sampling,

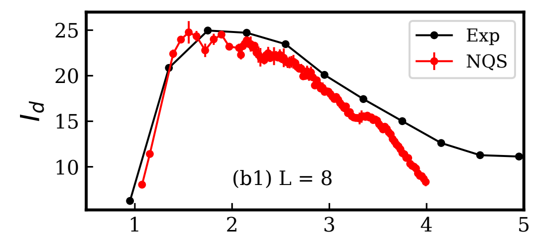
Kolmogorov complexity <—> intrinsic dimension

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

Complexity is minimal for field theories / critical points

—> **Emergent simplicity**

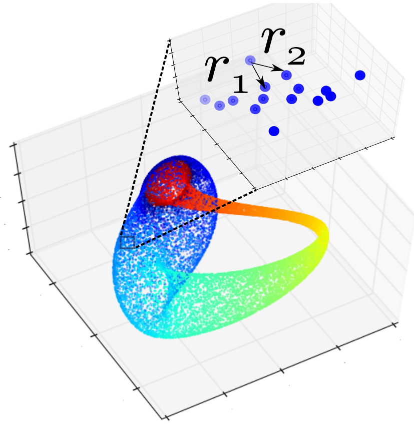
Observation of decreasing complexity in quantum simulators (Kibble-Zurek)



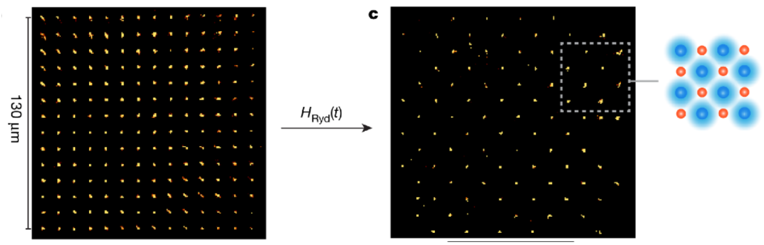
Can we go beyond bare complexity?
How?

Can we go beyond complexity only?

Manifold (math)



Physics (wave function)



Layers of understanding:
dimensionality
curvature
orientability
topological properties
…

Layers of understanding:
dimensionality

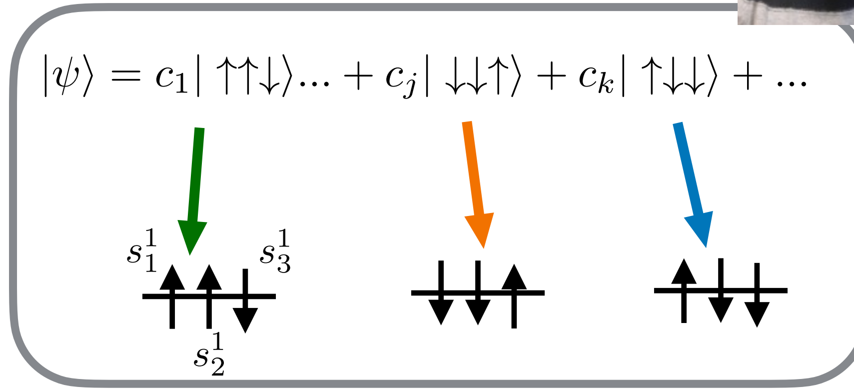
??????

See also works on persistent homology: SciPost Phys. 11, 060 (2021); 17, 100 (2024)

New tool: wave function networks

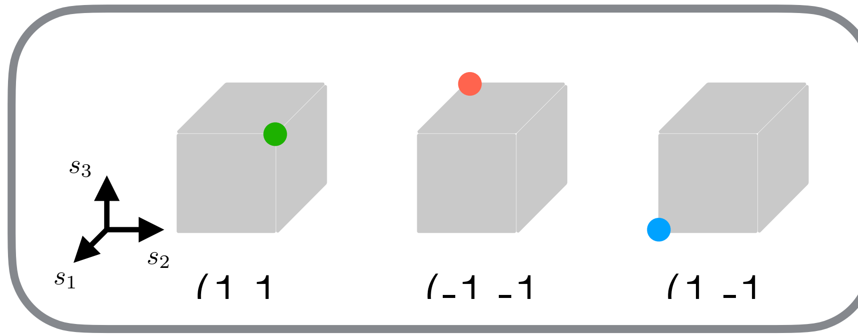
Collection of **wave function snapshots**

(Stochastic sampling of a wave function)



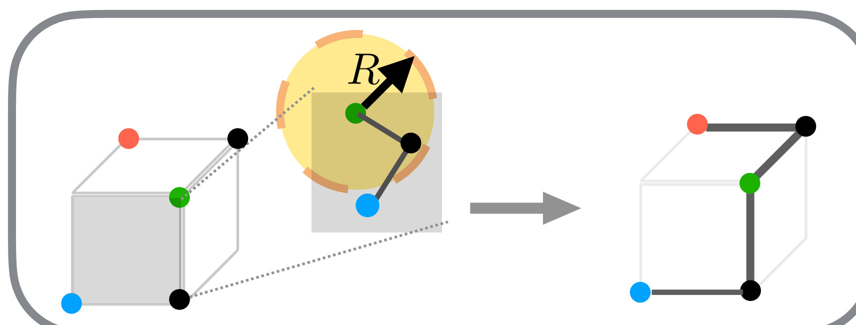
Interpretation of those in data space

(e.g.: Fock space)



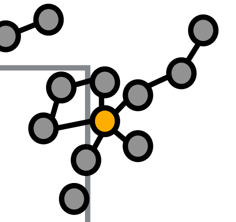
Mapping to **networks**

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



Scale-free network conjecture

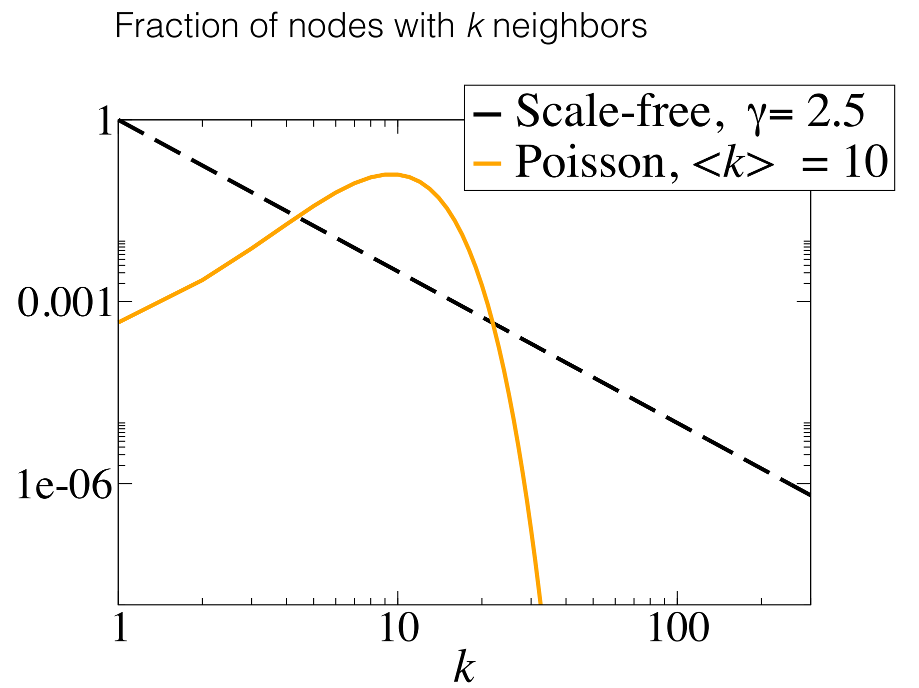
The wave function snapshots of strongly correlated quantum matter are described by **scale-free networks**



Quantum Computers/ simulators:

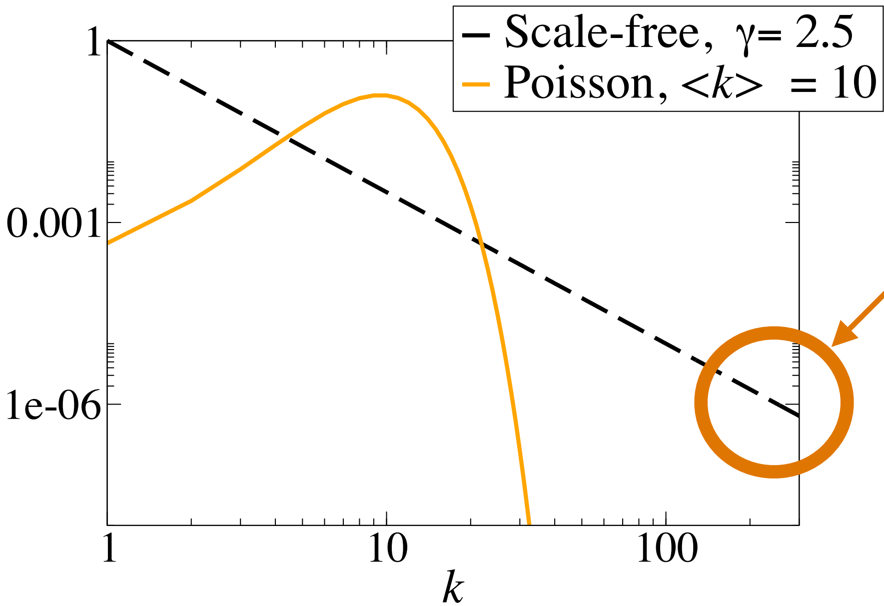
- Spin systems
- Hubbard models
- Lattice gauge theories
- All architectures alike (cQED, atoms, ions, etc.)

Barabasi, *Network Science*



What is a scale free network?

Fraction of nodes with k neighbors

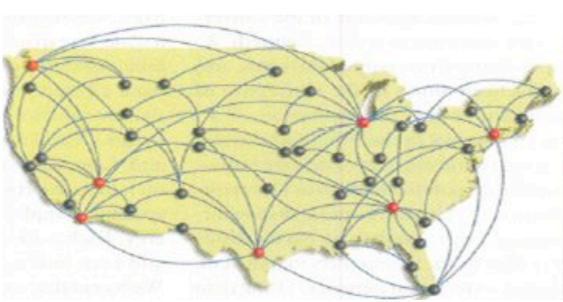


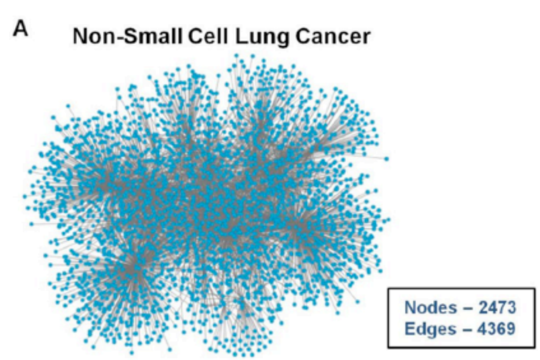
(1) Large number of hubs!

(2) Strong fluctuations

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

(Example: friends on Facebook)

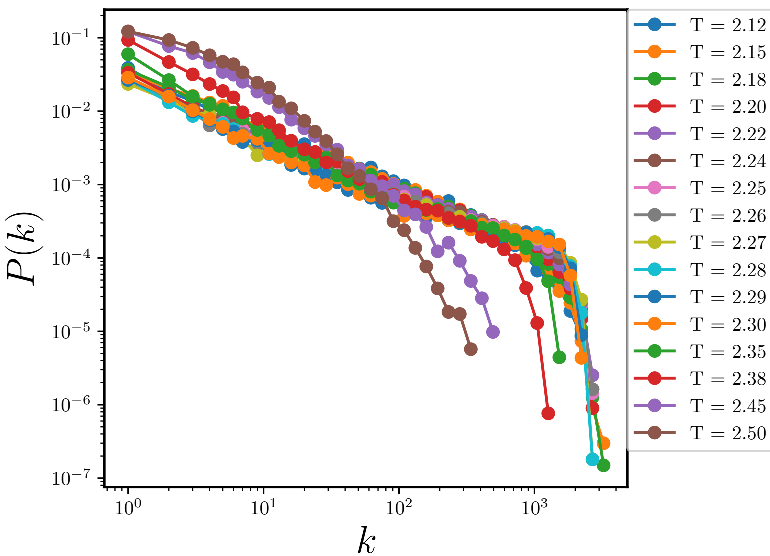




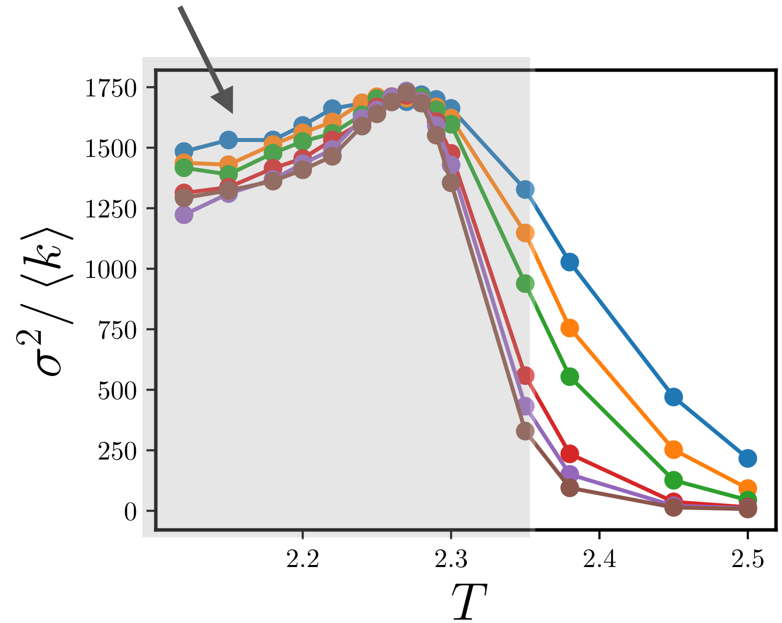
Known examples:
- Social networks
- Power grids
- Airports
- Ecological systems
- Cell dynamics…
- **Quantum computers and simulators!**

Emergence of scale-free networks: classical sanity checks

Classical statmech / 2D Ising



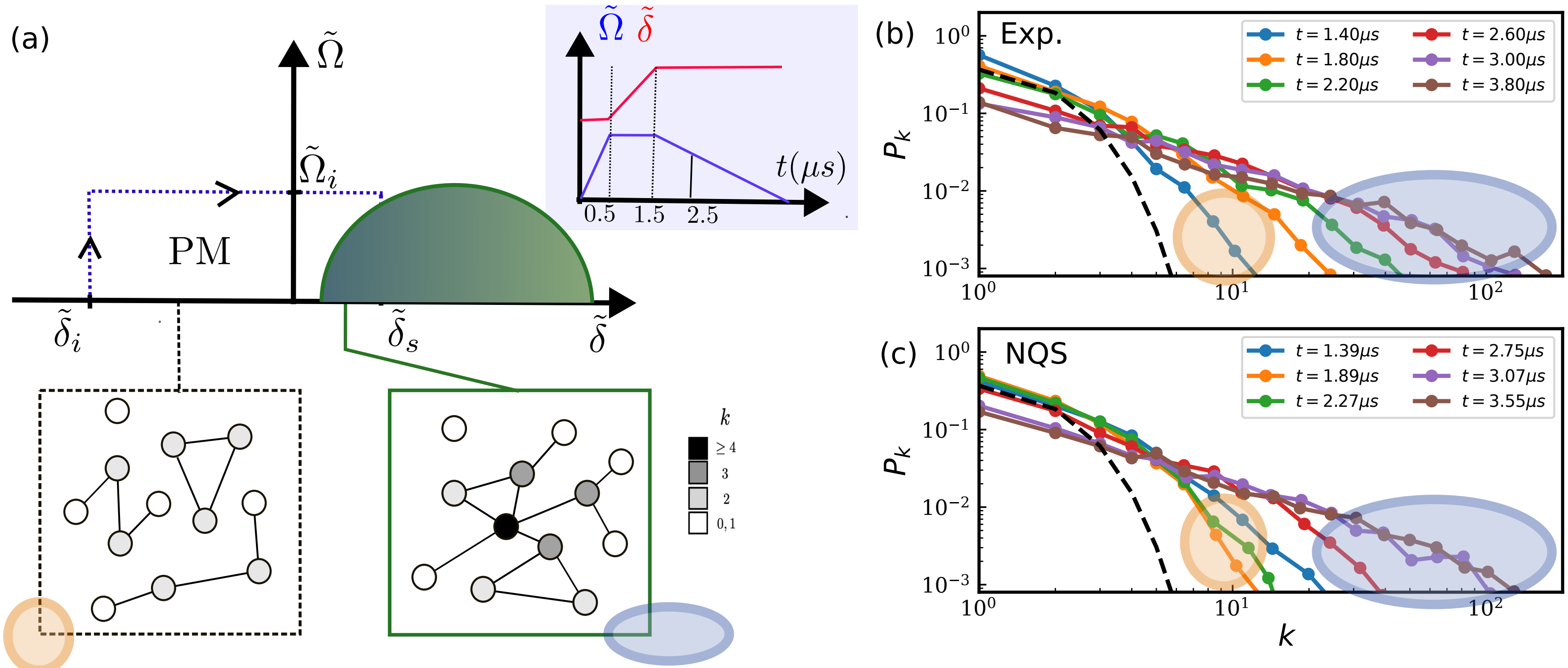
Both critical and ordered regimes are scale free!



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

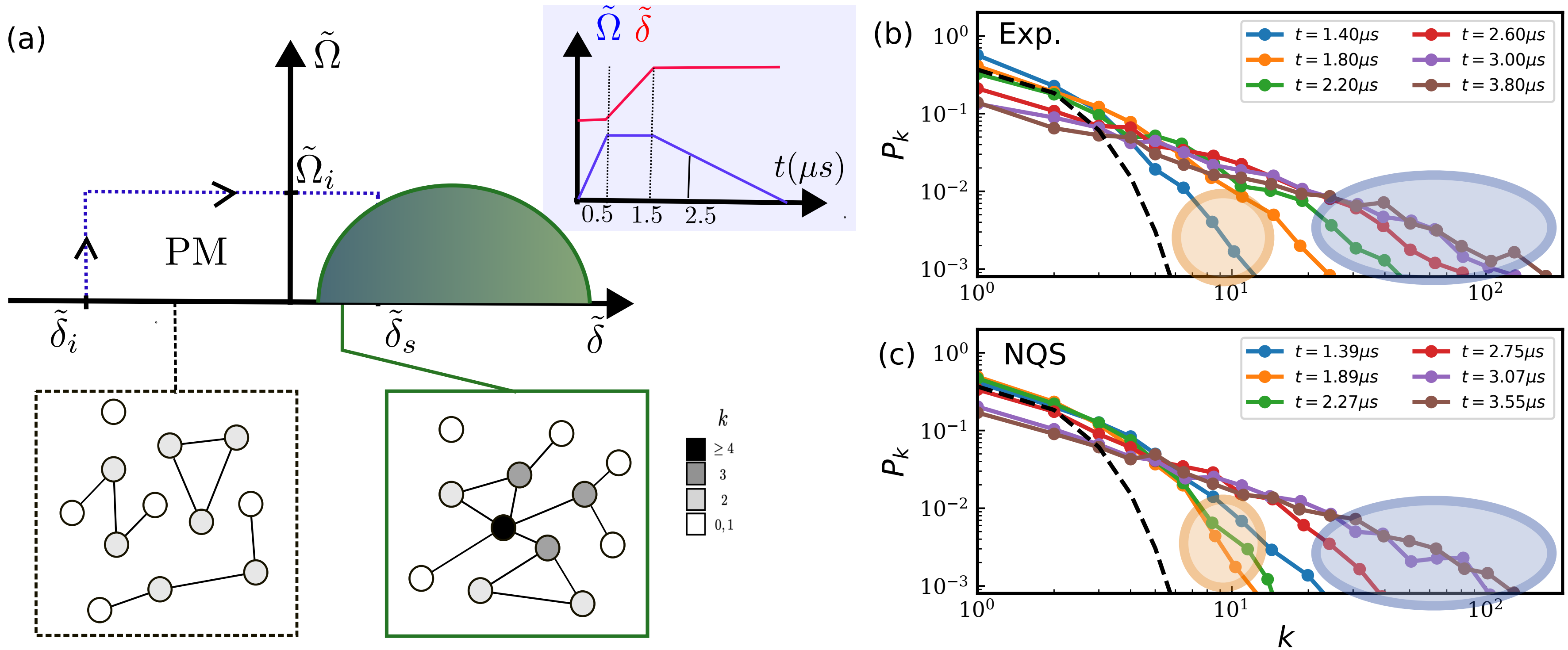
Emergence of scale-free networks: experiments



Short times: random network

After that: emergent scale-free network

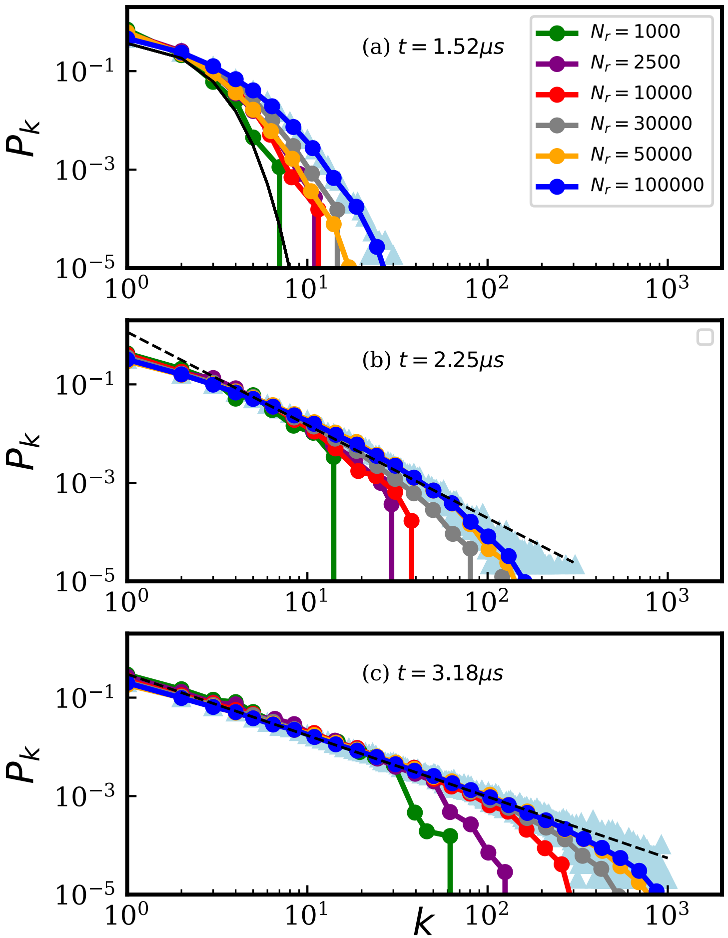
Emergence of scale-free networks: experiments



Short times: random network

After that: emergent scale-free network

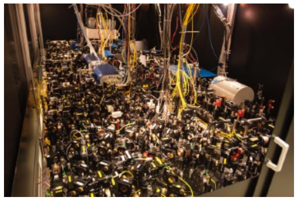
Is this an effect of finite sampling?

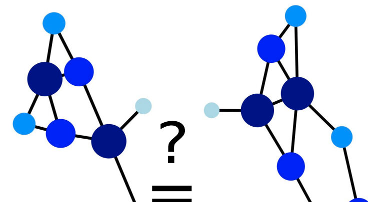


Scale-free is a robust feature, at least according to our simulations based on Neural network states

Markus Schmitt

Quantum information tools: cross-platform verification



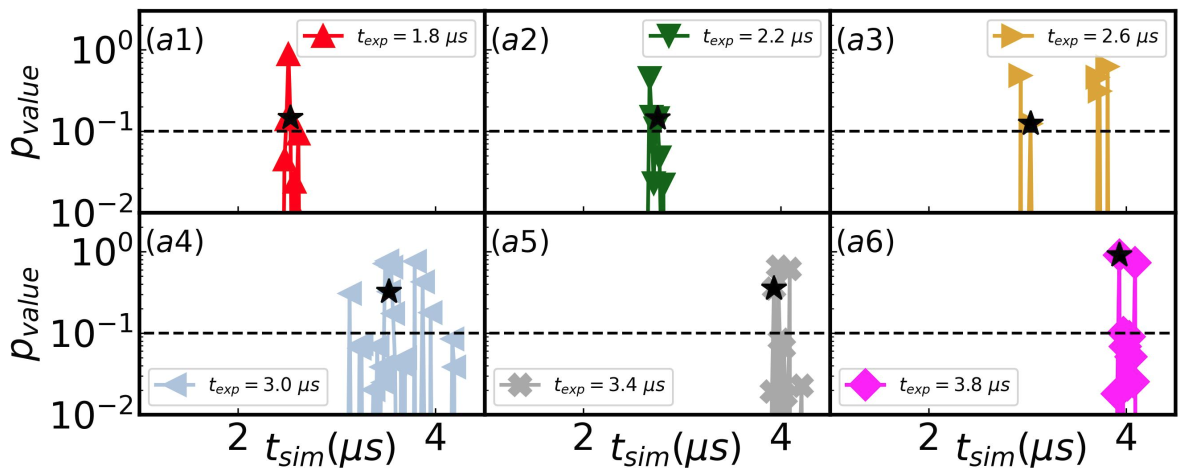


Cross-platform verification up to timescales where simulations become not fully reliable

Epps-Singleton test of compatibility between probability distributions

$p_v > 0.1$

Compatible



Statements

For classical stat mech sampling,

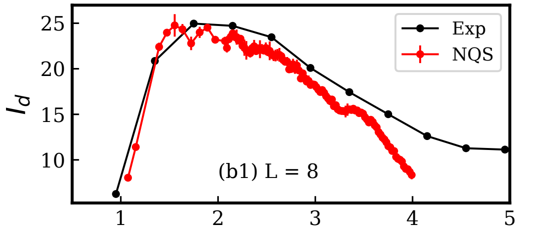
Kolmogorov complexity <—> intrinsic dimension

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

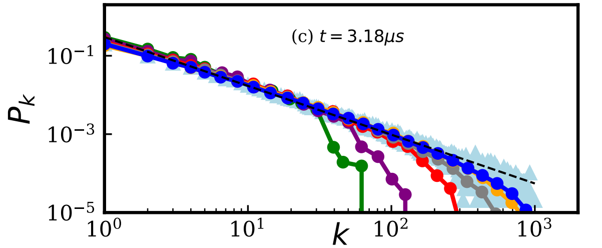
Complexity is minimal for field theories / critical points

—> **Emergent simplicity**

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



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



Is there a classification of matter based on photos?

Traditional classification schemes

Ginzburg-Landau criterion: symmetry breaking

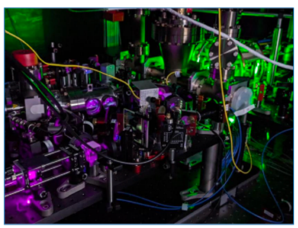
Gapless matter: critical behavior, field theory

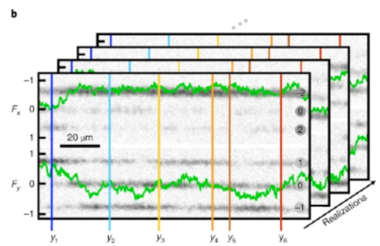
80's: topological matter
- free theories: Altland-Zirnbauer and topological insulators
- Interacting theories: symmetry-protected-topological phases
- Interacting theories: topological order - projective symmetry group

All of these relate certain wave function properties (sometimes coarse-grained) to response, under specific posits (symmetry, constraints on emergent gauge structure, dimensionality)

Excellent review: Wen's book

Can we do the same with partial information?

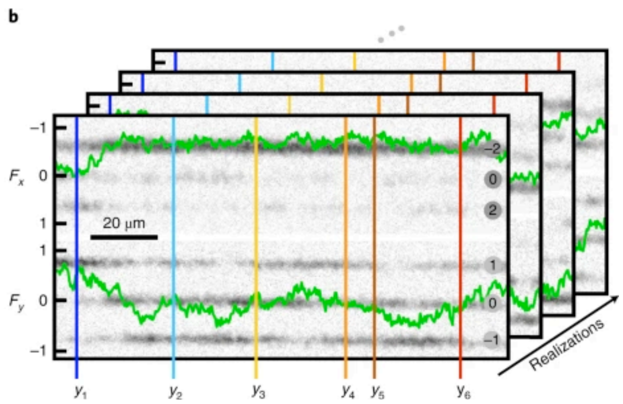




?

$$N_{\text{snapshot}} << 2^{N}$$

Our working principle: Occam's razor

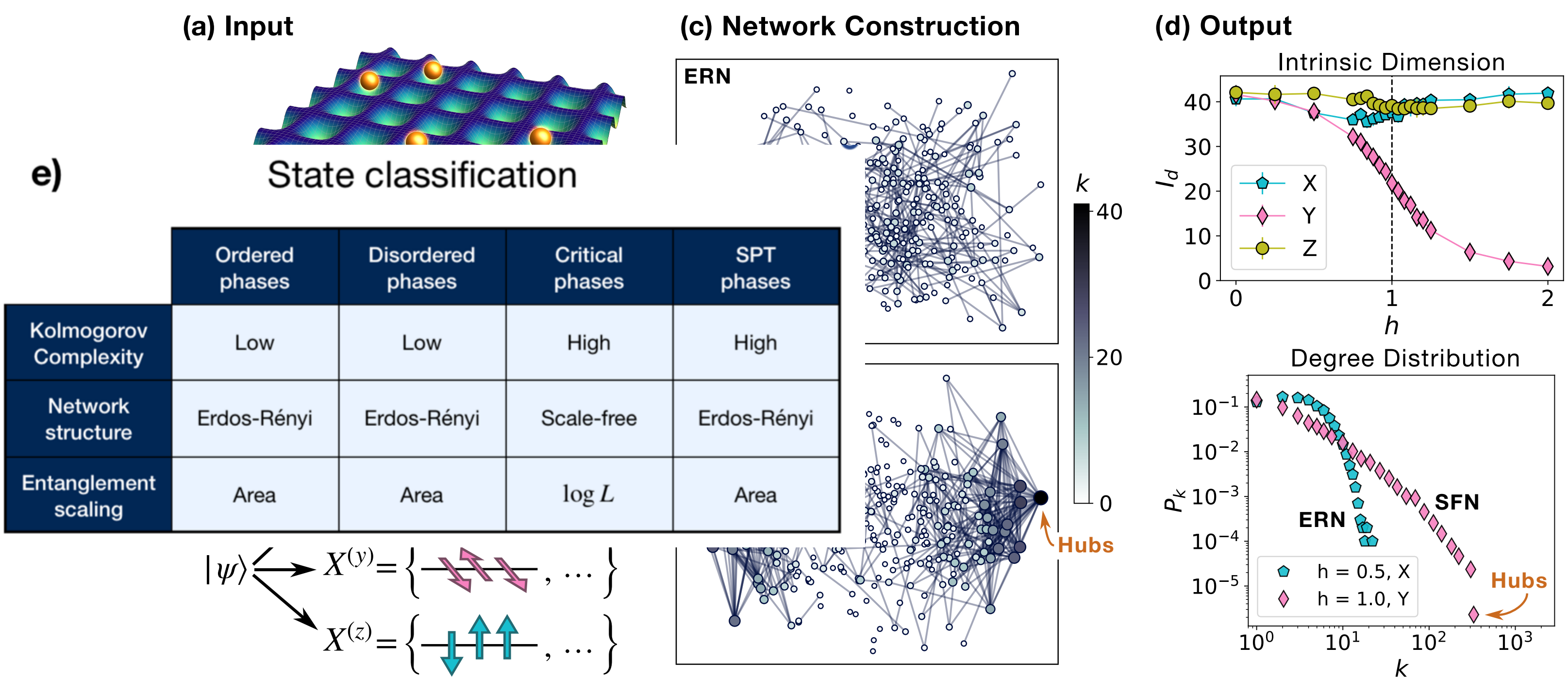


Entia non sunt multiplicanda praeter necessitatem

Classify a many-body wave function according to the basis which requires the minimal number of variables

Stochastic classification of quantum matter in one dimension

Step 1: determine minimal complexity basis



	Ordered phases	Disordered phases	Critical phases	SPT phases
Kolmogorov Complexity	Low	Low	High	High
Network structure	Erdos-Rényi	Erdos-Rényi	Scale-free	Erdos-Rényi
Entanglement scaling	Area	Area	$\log L$	Area

Step 2: analize minimal complexity basis network

Summary and outlook

Plenty of potential for fruitful interactions between (unsupervised) machine learning and physics!

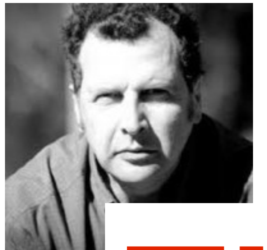
New conceptual "angle": data complexity and relation to many body

Future:

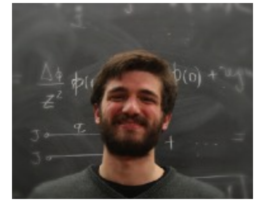
- Role of complexity in variational states
- Relation between complexity and out of equilibrium
- Use in experiments
- And more!

ICTP and SISSA

Adriano Angelone
(-> Sorbonne)



Sar

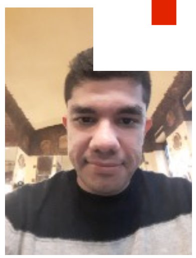


Schmitt
ısburg)

Markus Heyl
(Augsburg)

Thank you!

Vittorio Vitale
(-> Grenoble)



Tiago Mendes-Santos (-> Augsburg)

Rajat Panda
(-> UniTs)

Roberto Verdel Aranda

Devendra Singh Bhakuni

Ronald Cortez

Asja Jelic

Andrea Gambassi

Riccardo Andreoni

Cristiano Muzzi

Classical stat mech: Phys. Rev. X 11, 011040 (2021), 2308.13604, SciPost Phys. Core 6, 086 (2023).
Quantum stat mech: Phys. Rev. X Quantum 2, 030332 (2021);
Topology and data spaces: Phys Rev. E 109, 034102 (2024).
Rydberg experiments: Phys. Rev. X 14, 021029 (2024);
Cold atom experiments: Phys. Rev. B 109, 075152 (2024)

Key collaborations with Browayes's, Aidelsburger's and Oberthaler's groups