LEARNING QUANTUM STATES WITH GENERATIVE MODELS

Juan Carrasquilla

@carrasqu

Physics Next: Machine Learning October 8-10, 2018

Hyatt Place Long Island hotel, Riverhead, NY

VECTOR INSTITUTE | INSTITUT VECTEUR

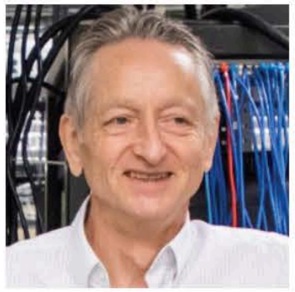
UNIVERSITY OF WATERLOO

VECTOR INSTITUTE | INSTITUT VECTEUR

About

- The Vector Institute is an independent, not-for-profit entity dedicated to research in artificial intelligence with a focus on excellence in machine learning and deep learning including applications in natural sciences.
- Vector launched in 2017 with support from the Government of Ontario, Government of Canada, and the private sector.

Researchers

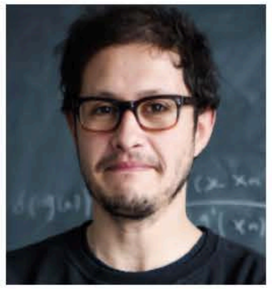


Geoffrey Hinton
Chief Scientific Advisor

Richard Zemel
Research Director

Alán Aspuru-Guzik

Jimmy Ba

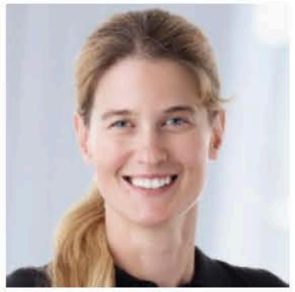


Juan Carrasquilla

David Duvenaud

Murat Erdogdu

Amir-massoud Farahmand



Sanja Fidler

David Fleet

Brendan Frey

Marzyeh Ghassemi

Anna Goldenberg

Roger Grosse

Alireza Makhzani

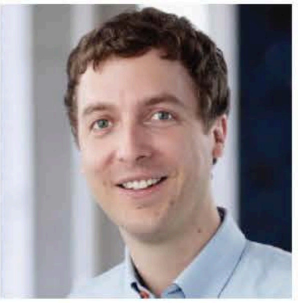
Quaid Morris

Sageev Oore

Pascal Poupart

Daniel Roy

Frank Rudzicz



Graham Taylor

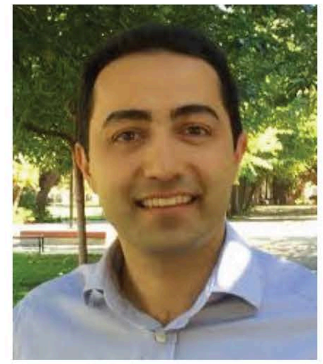
Raquel Urtasun

Over the next few years it is expected that Vector will grow to include several hundred researchers, students, engineers and others.

MACHINE LEARNING/MANY-BODY PHYSICS FRIENDS

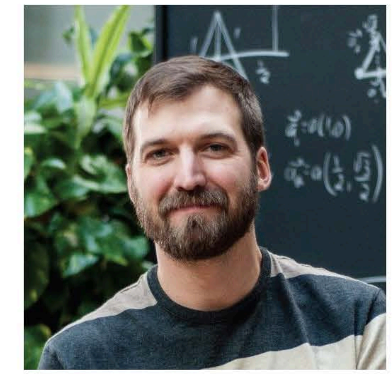
Guglielmo mazzola (ETH)

Giuseppe Carleo (Flatiron Institute)

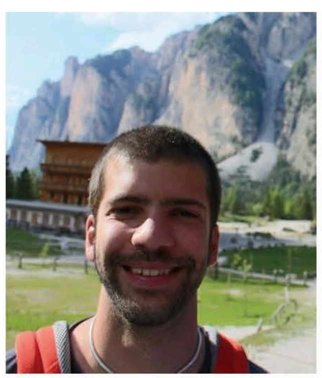


Ehsan Khatami (San Jose State U)

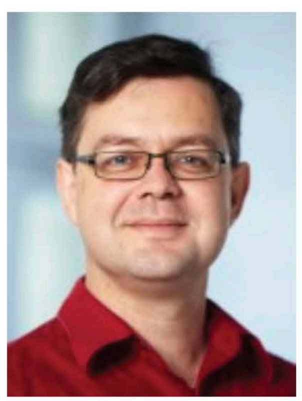
Leandro Aolita Universidade Federal do Rio de Janeiro



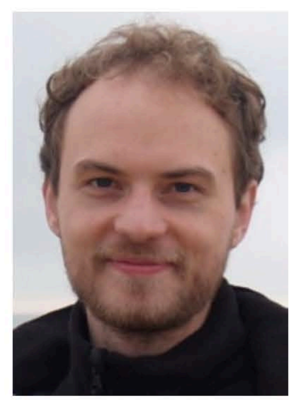
Roger Melko (U. Waterloo and Perimeter)



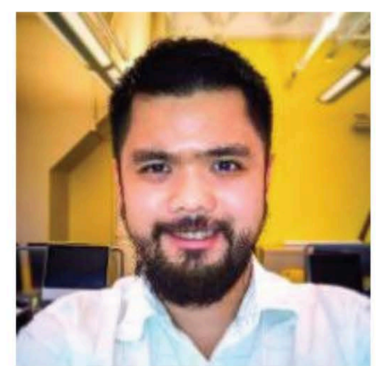
Giacomo Torlai (U. Waterloo and Perimeter)



Matthias Troyer (Microsoft, ETH)



Peter Broecker (U. Cologne)



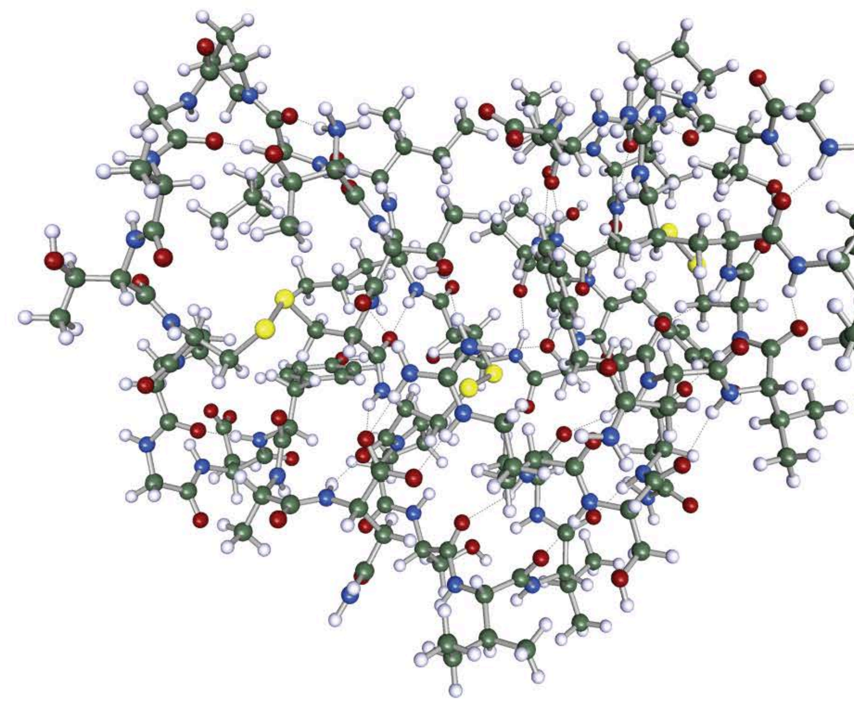
Kelvin Chng (San Jose State U)

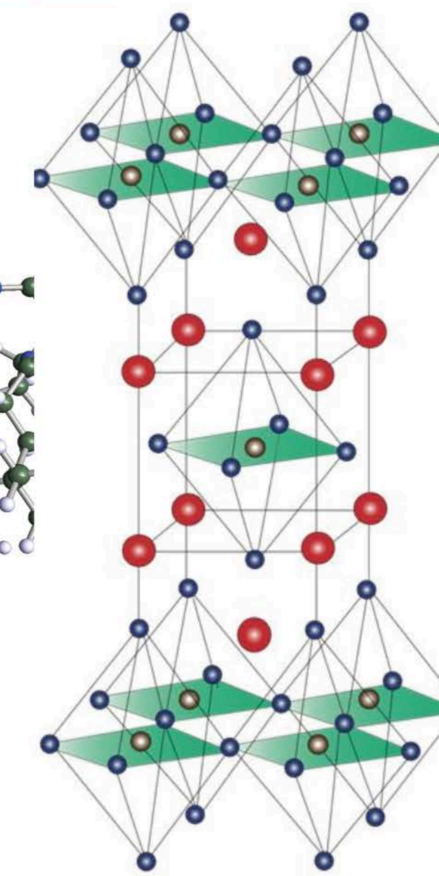
Simon Trebst (U. Cologne)

THE MANY-BODY PROBLEM IN QUANTUM MECHANICS

- Generic specification of a quantum state requires resources exponentially large in the number of degrees of freedom N
- Today's best supercomputers can solve the wave equation **exactly** for systems with a maximum of ~45 particles.
- Storing the state of a 273 spin system requires a computer with more bits than there are atoms in the universe
- Yet, technologically relevant problems in chemistry, condensed matter physics, and quantum computing are much larger than 273.
- Quantum computing

$|\Psi\rangle$ *vector with* 2^N

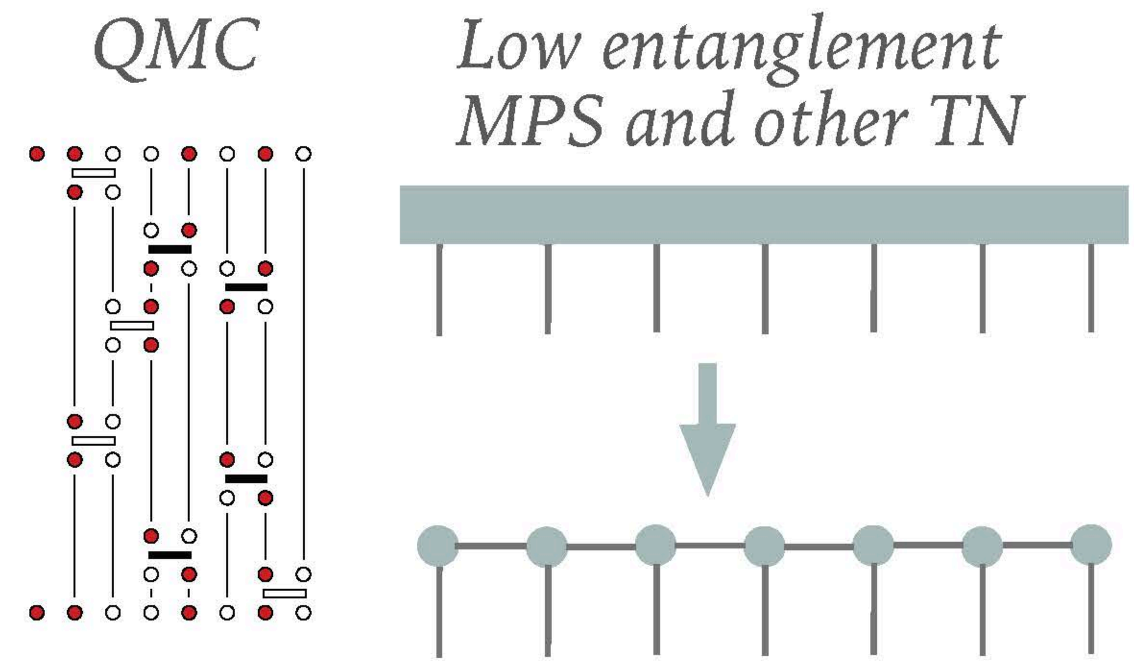


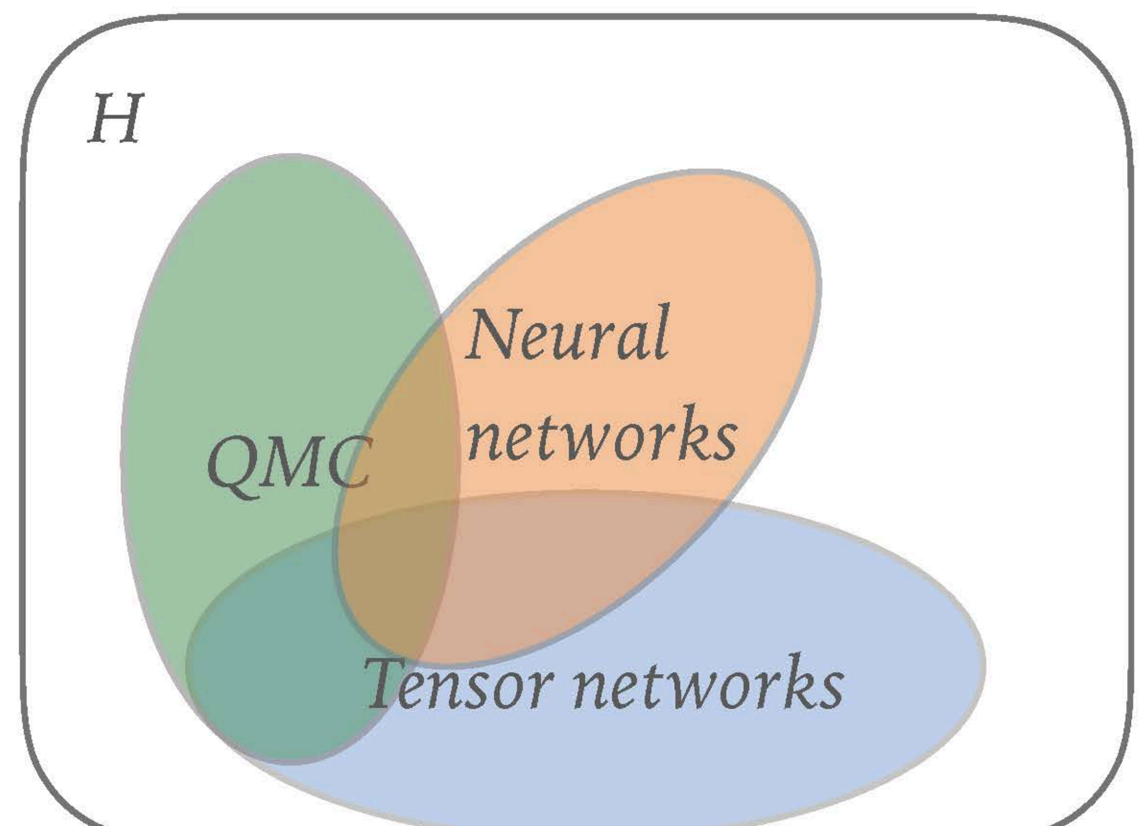


THERE IS STILL HOPE FOR CLASSICAL ALGORITHMS

- Nature is sometimes compassionate: many-body systems can be typically characterized by an amount of information smaller than the maximum capacity of the corresponding state space.
- Quantum Monte Carlo and other numerical methods based on Tensor Networks exploit this fact and are able to accurately study large quantum system in practice with limited amount of resources.
- Machine learning community deals with equally high dimensional problems ($N \sim 2^{256}$) and battle the curse of dimensionality successfully with impressive results in a wide spectrum of scientific and technologically relevant areas of research.

$|\Psi\rangle$ *vector with* 2^N



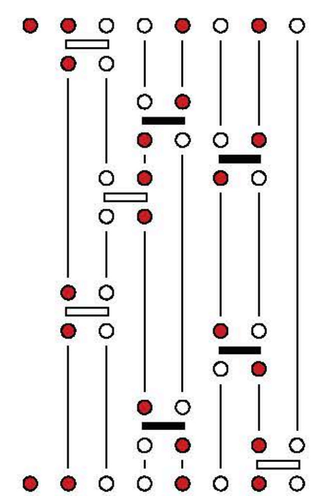


THERE IS STILL HOPE FOR CLASSICAL ALGORITHMS

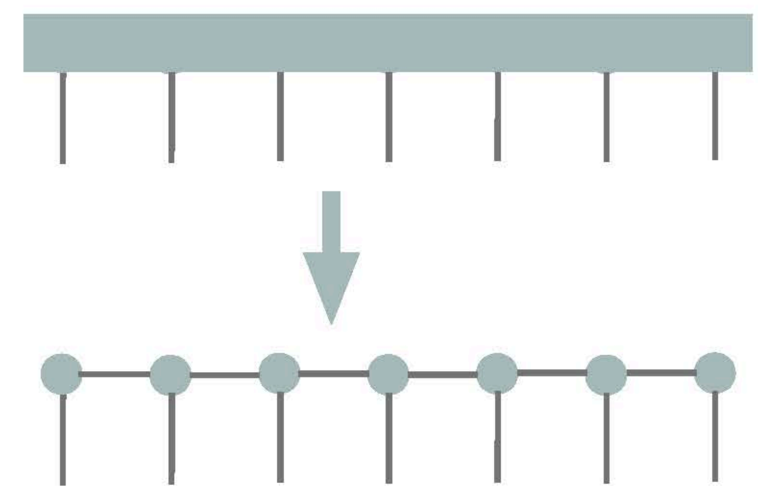
- Nature is sometimes compassionate: many-body systems can be typically characterized by an amount of information smaller than the maximum capacity of the corresponding state space.
- Quantum Monte Carlo and other numerical methods based on Tensor Networks exploit this fact and are able to accurately study large quantum system in practice with limited amount of resources.
- Machine learning community deals with equally high dimensional problems and battle the curse of dimensionality successfully with impressive results in a wide spectrum of scientific and technologically relevant areas of research.

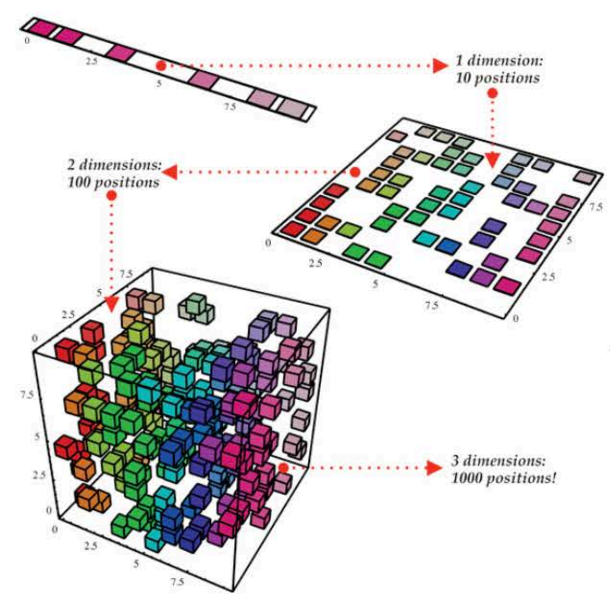
$|\Psi\rangle$ *vector with* 2^N

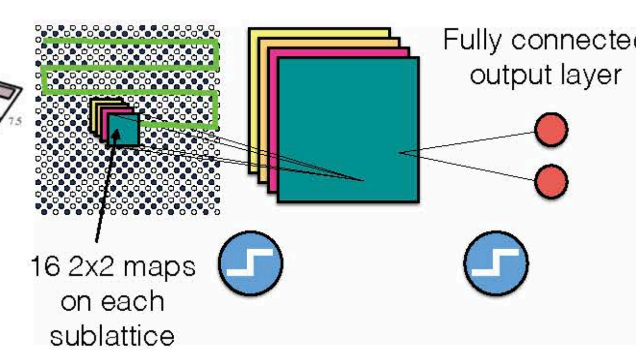
QMC



Low entanglement MPS and other TN







QUANTUM AND CLASSICAL MANY-BODY PHYSICS HAS NOT BEEN THE EXCEPTION

- ML phases of matter/phase transitions (Carrasquilla, Melko 1605.01735, Wang 1606.00318, Zhang, Kim, 1611.01518)
- New ML inspired ansatz for quantum many-body systems (Carleo, Troyer 1606.02318, Deng, Li, Das Sarma, 1701.04844, Deng, Li, Das Sarma 1609.09060, Carrasquilla, Melko 1605.01735)
- Accelerated Monte Carlo simulations (Huang, Wang 1610.02746)
- Quantum state preparation guided by ML (Bukov, Day, Sels, Weinberg, Polkovnikov and Mehta 1705.00565)
- Renormalization group analyses, RBMs, PCA (Bradde, Bialek 1610.09733, Koch-Janusz, Ringel 1704.06279,Mehta, Schwab,1410.3831)
- Quantum state tomography based on RBMs (Torlai, Mazzola, Carrasquilla, Troyer, Melko, Carleo, 1703.05334)
- ML based decoders for topological codes (Torlai, Melko 1610.04238, Varsamopoulos, Criger, Bertels, 1705.00857)
- Supervised Learning with Quantum-Inspired Tensor Networks (Stoudenmire, Schwab 1605.05775, Novikov, Trofimov, Oseledets, 1605.03795)
- Quantum Boltzmann machines (Amin, Andriyash, Rolfe, Kulchytskyy, Melko, 1601.02036, Kieferova, Wiebe, 1612.05204,)
- Quantum machine learning algorithms to accelerate learning (Biamonte, Wittek, Pancotti, Rebentrost, Wiebe, Lloyd, 1611.09347)

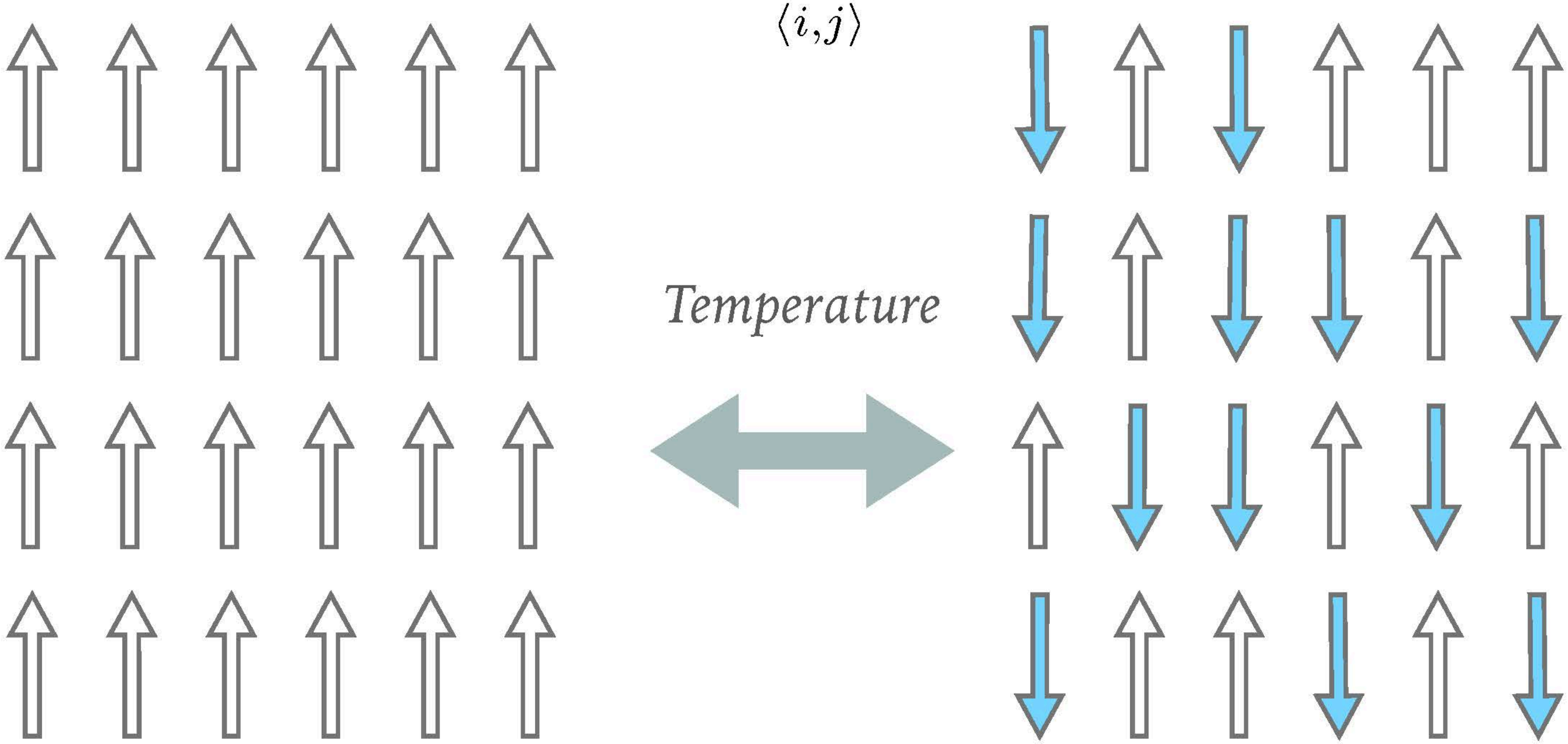
And many more

FROM SUPERVISED LEARNING TO QUANTUM STATES

PHASES, PHASE TRANSITIONS, AND THE ORDER PARAMETER

Ising ferromagnet in two dimensions

$$E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \qquad \sigma_i = \pm 1$$

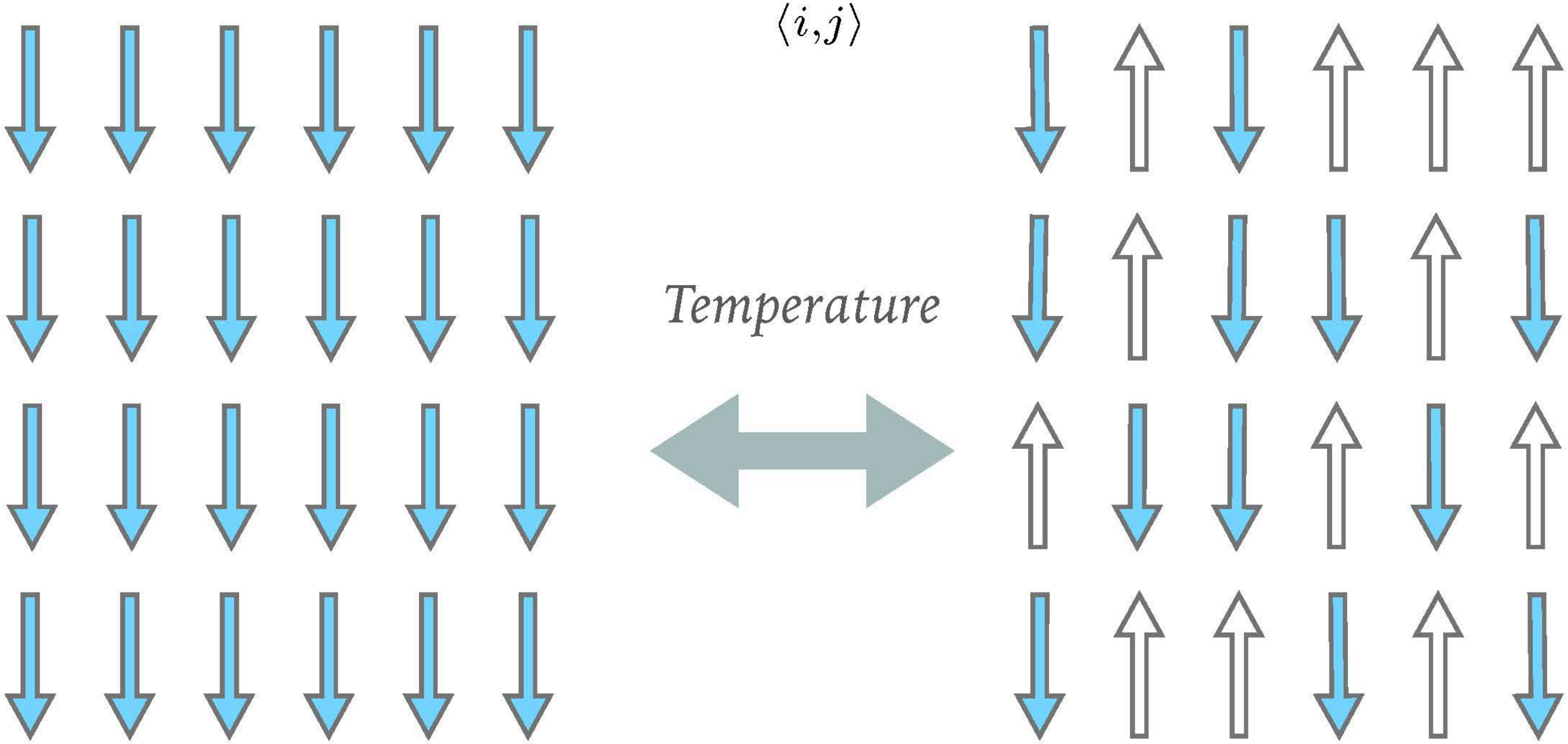


Ferromagnet *Lars Onsager Phys. Rev. 65, 117* **Paramagnet**

PHASES, PHASE TRANSITIONS, AND THE ORDER PARAMETER

Ising ferromagnet in two dimensions

$$E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

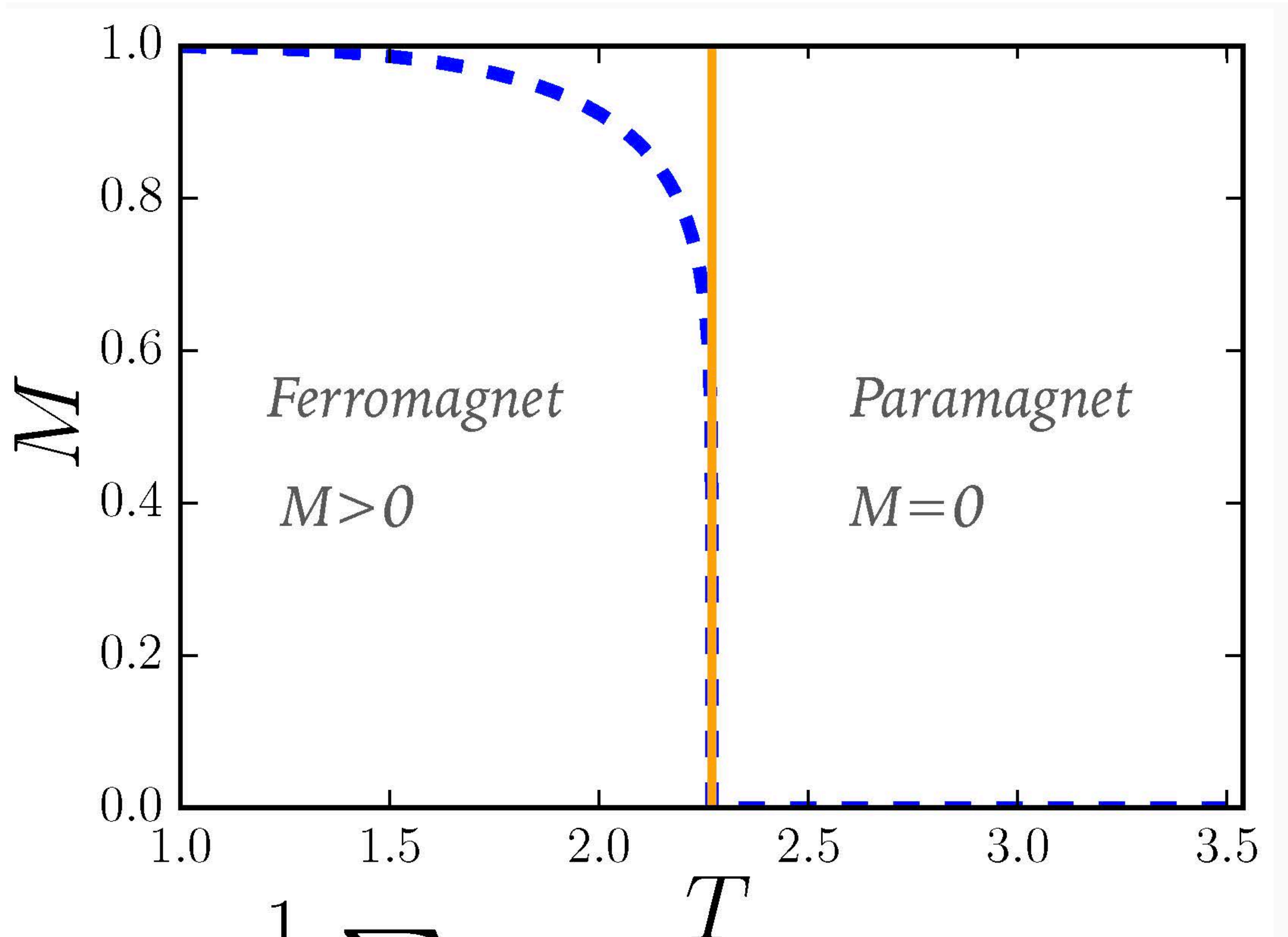


Ferromagnet

Paramagnet

PHASES, PHASE TRANSITIONS, AND THE ORDER PARAMETER

Ferromagnetic transition: order parameter

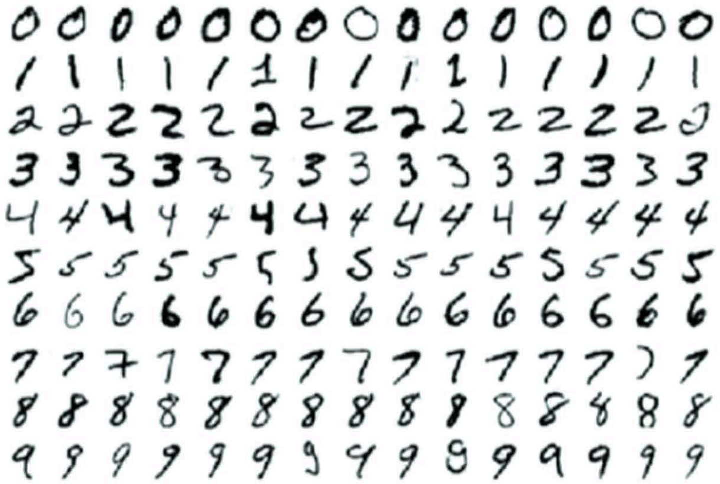


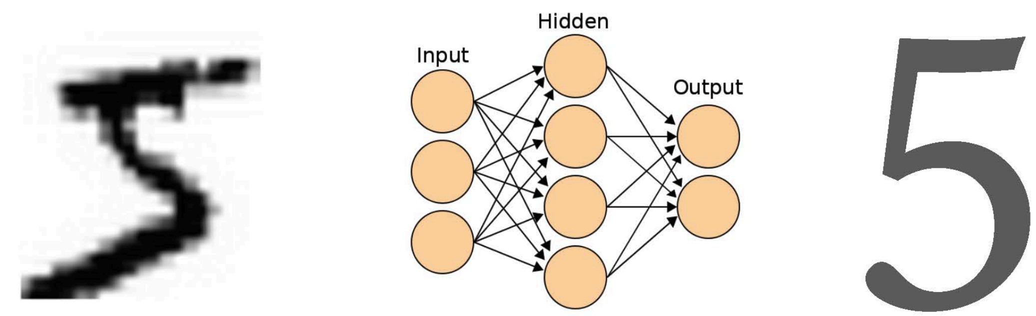
It is a measure of the degree of order in the system

$$M = \frac{1}{N}\sum_i \langle \sigma_i \rangle, \qquad \sigma_i = \pm 1$$

Lars Onsager Phys. Rev. 65, 117 (1944)

FLUCTUATIONS HANDWRITTEN DIGITS (MNIST)

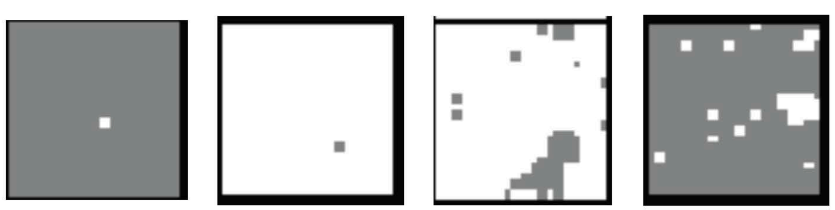




ML community has developed powerful supervised learning algorithms

 $= 5 + \textit{fluctuations}$

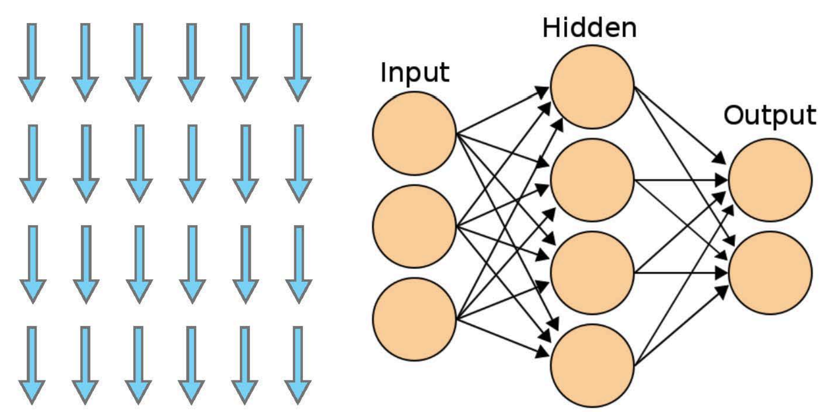
FM phase



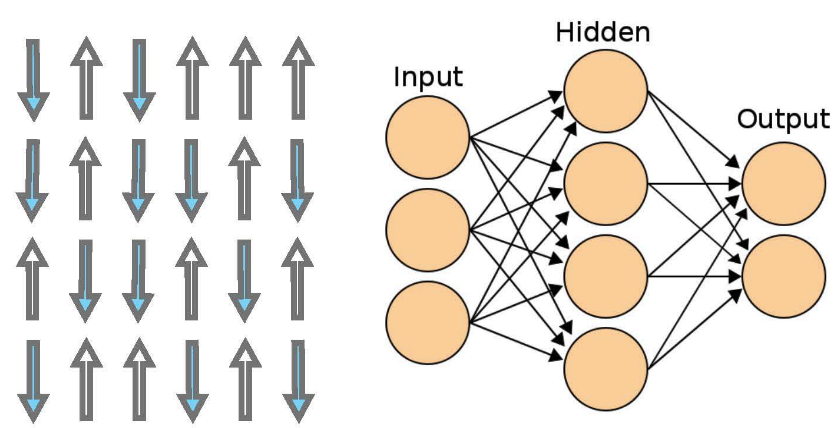
High T phase

gray=spin up

white=spin down



FM (0)

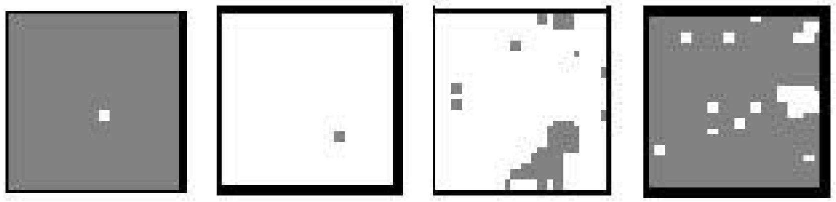


PM (1)

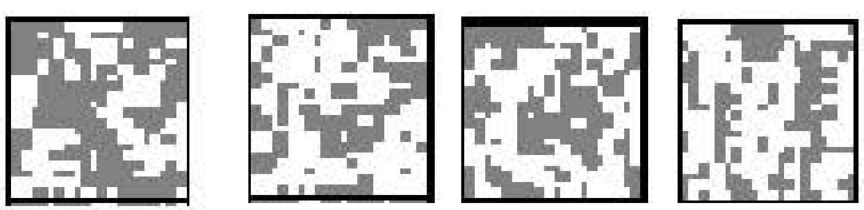
J. Carrasquilla and R. G. Melko. Nature Physics 13, 431–434 (2017)

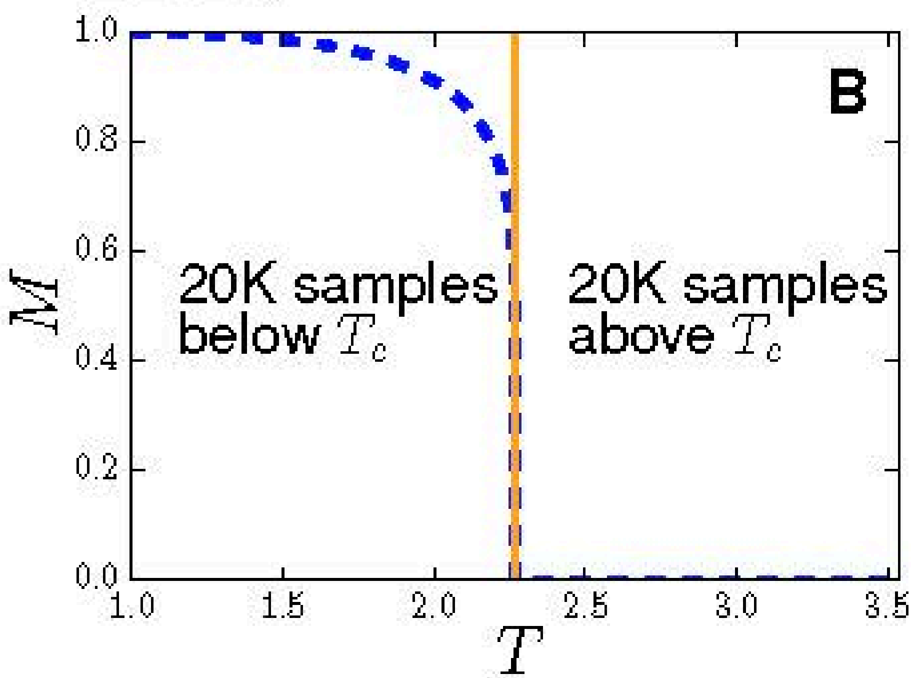
RESULTS: SQUARE LATTICE ISING MODEL (TEST SETS)

2D Ising model in the ordered phase



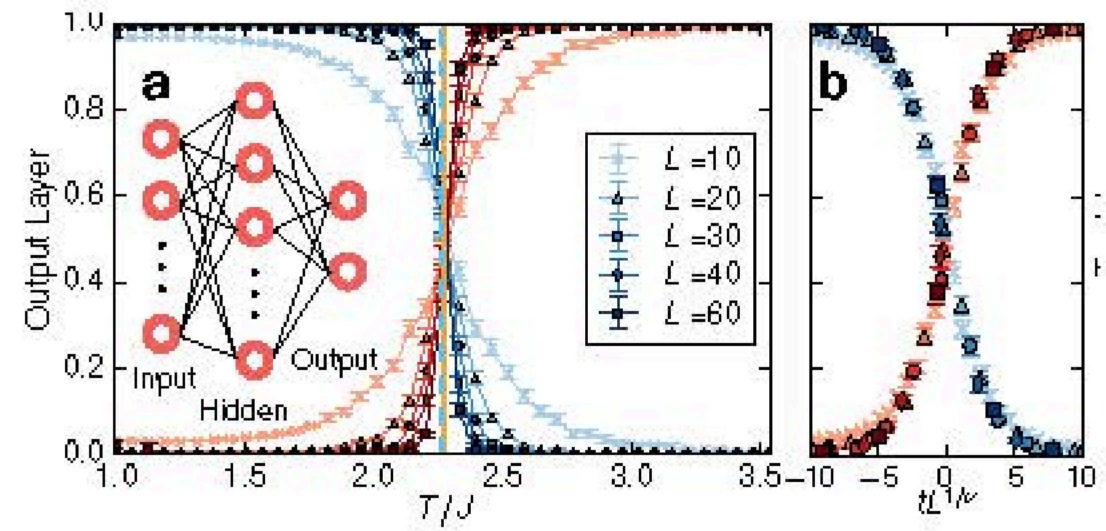
2D Ising model in the disordered phase

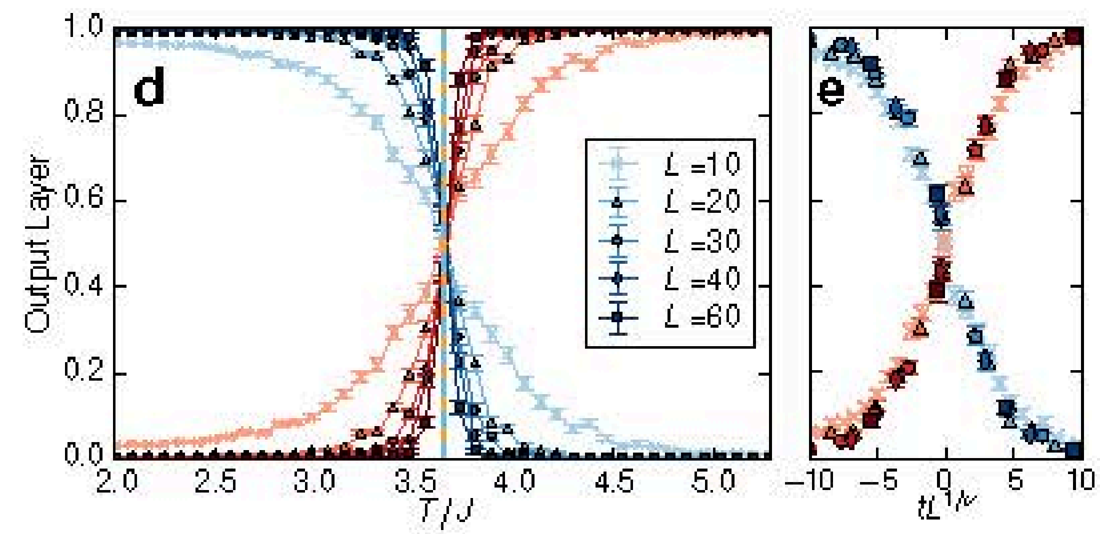




Analytical understanding: toy model with 3 analytically trained neutrons. NN relies on the **magnetization** of the system

$$T_c/J = 2/\ln\left(1+\sqrt{2}\right)$$





Tc of Triangular within <1%

NN knows about criticality

$\nu \approx 1$

J. Carrasquilla and R. G. Melko. Nature Physics 13, 431–434 (2017)

PHASES OF MATTER WITHOUT AN ORDER PARAMETER AT T=0

- Topological phases of matter. Examples: Fractional quantum hall effect, quantum spin liquids, Ising gauge theory. Potential applications in topological quantum computing. Interestingly, these phases defy the Landau symmetry breaking classification.

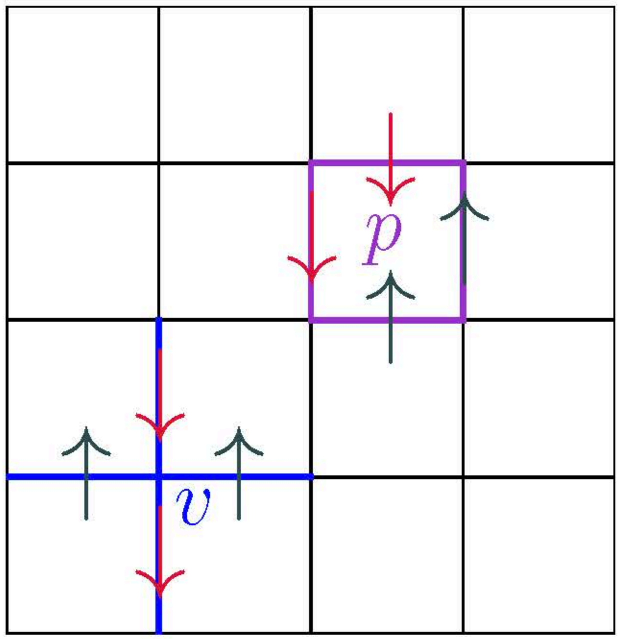
PHASES OF MATTER WITHOUT AN ORDER PARAMETER AT T=0,∞

Wegner's Ising gauge theory:

$$H = -J \sum_p \prod_{i \in p} \sigma_i^z$$

F.J. Wegner, J. Math. Phys. 12 (1971) 2259

(Kogut Rev. Mod. Phys. 51, 659 (1979))



The ground state is a highly degenerate manifold with exponentially decaying spin–spin correlations.

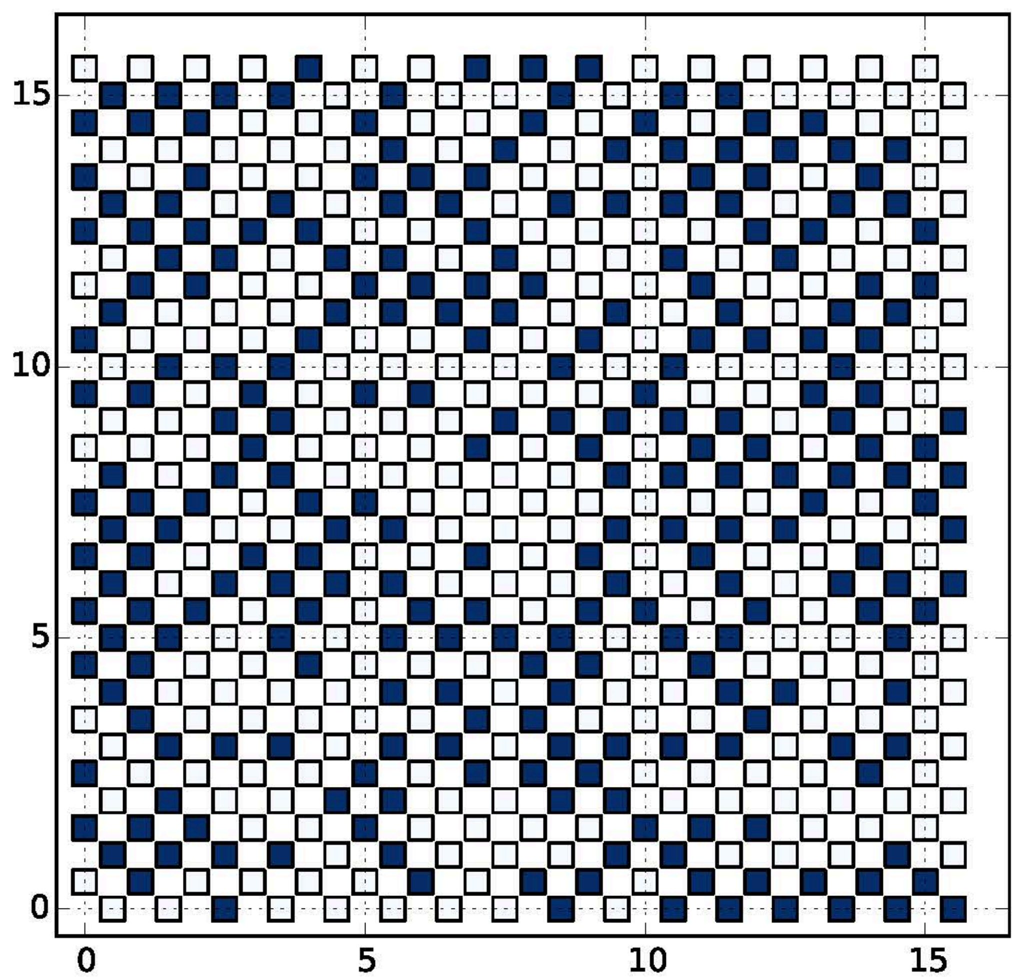
The grandmother of all lattice models for topological quantum computation

Ground state is a classical disordered topologically ordered phase

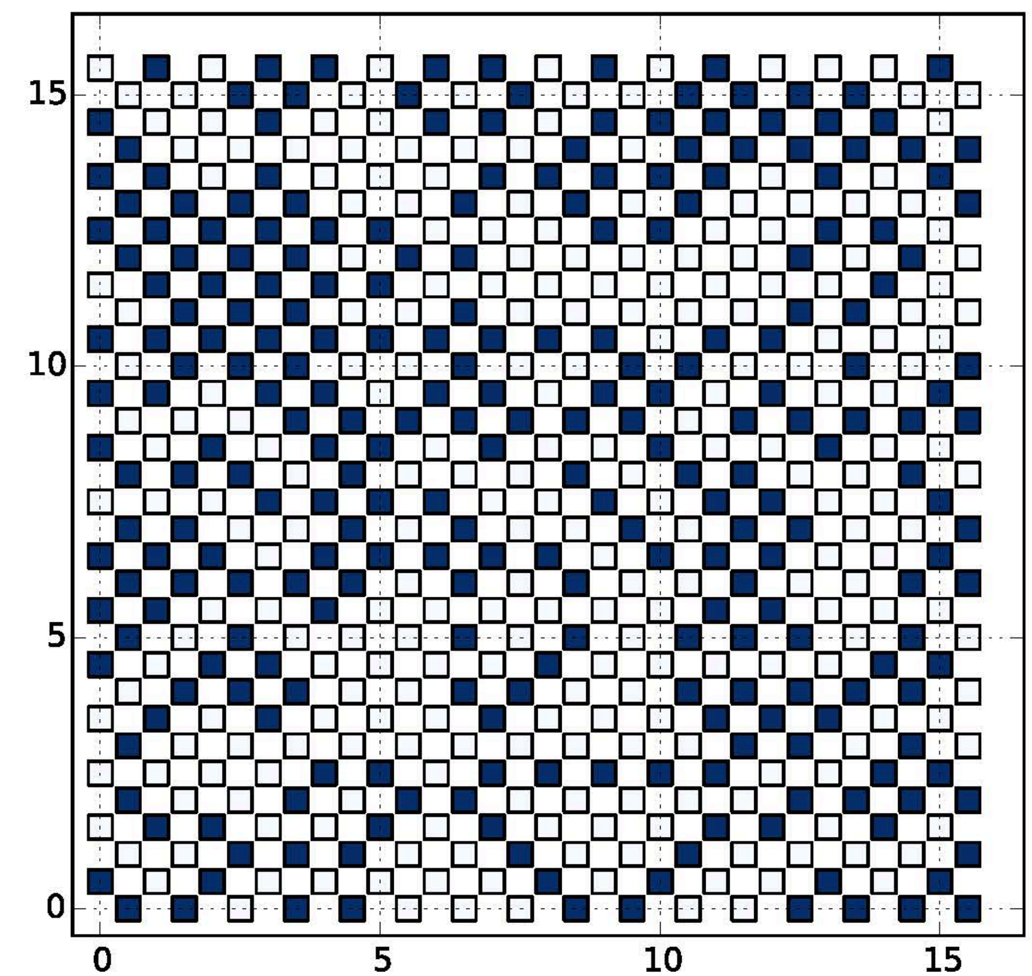
Castelnovo and Chamon Phys. Rev. B 76, 174416 (2007)

T=0 **high temperature phase** *T=infinity*

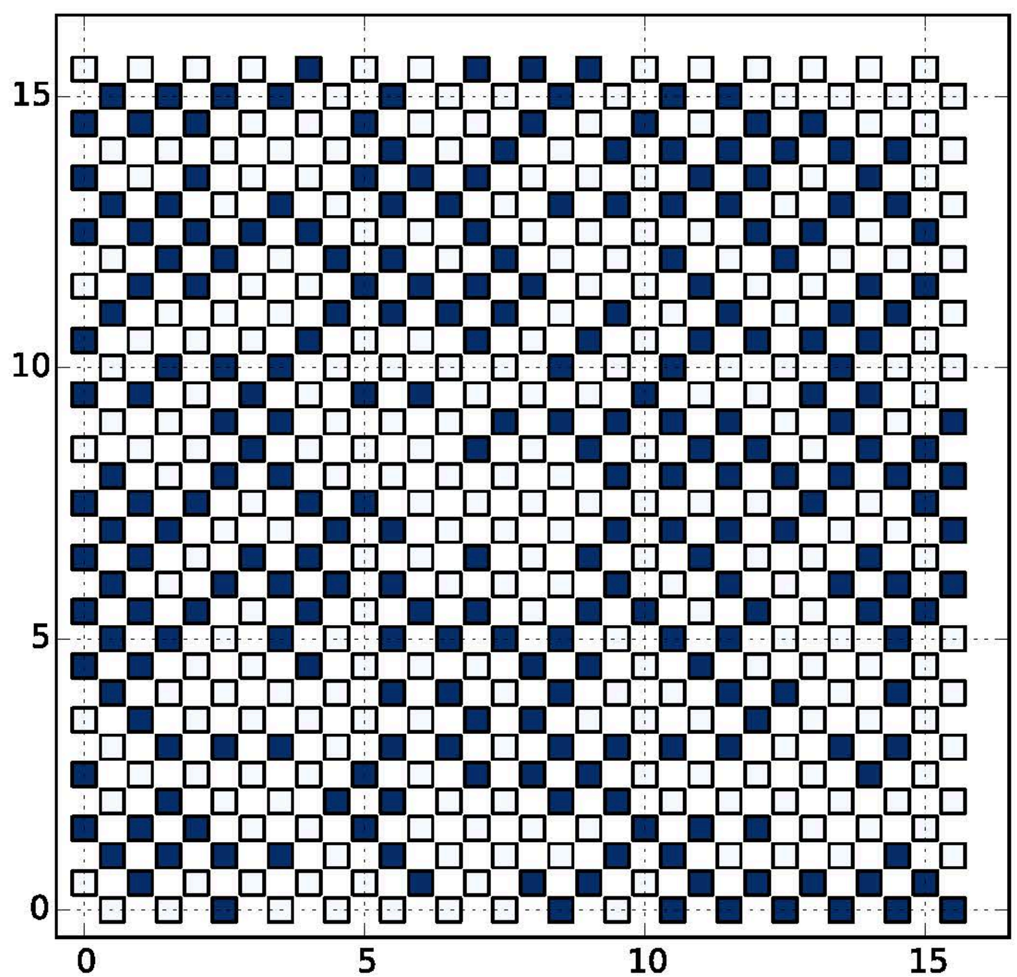
For two configurations



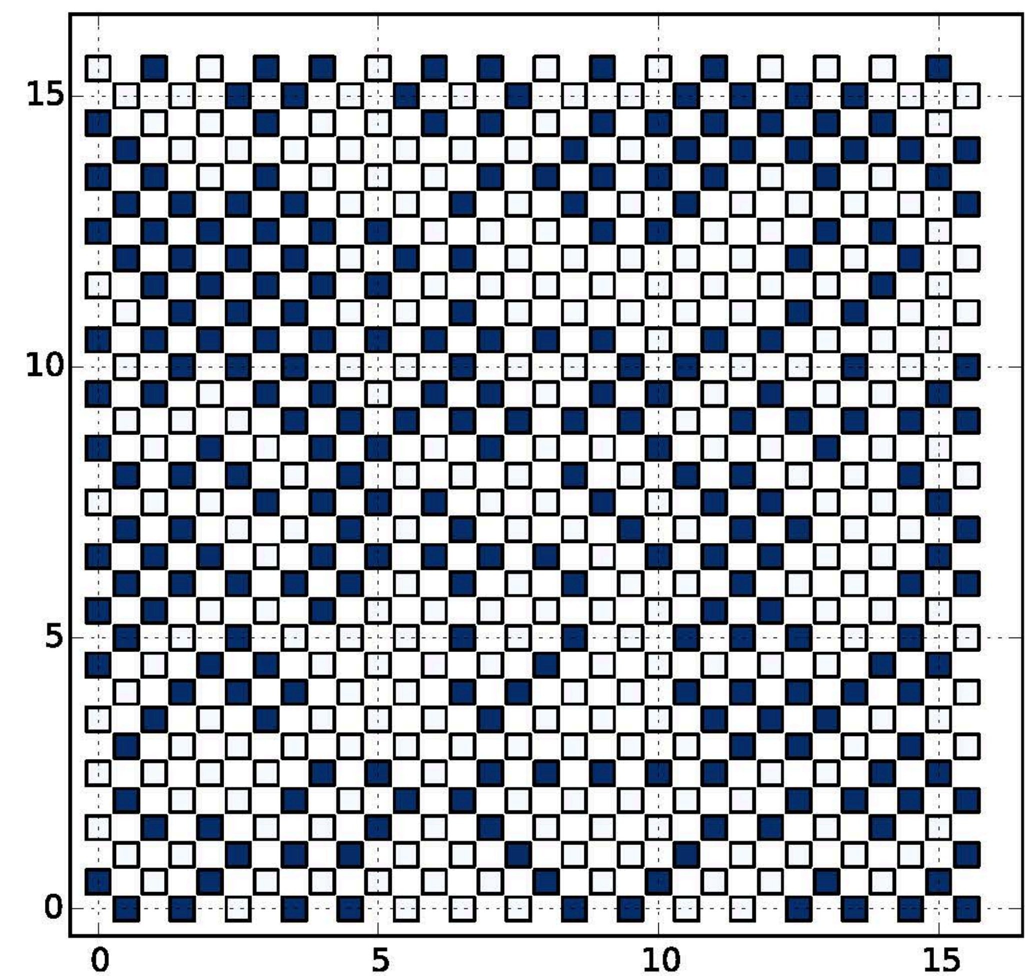
?



For two configurations



?



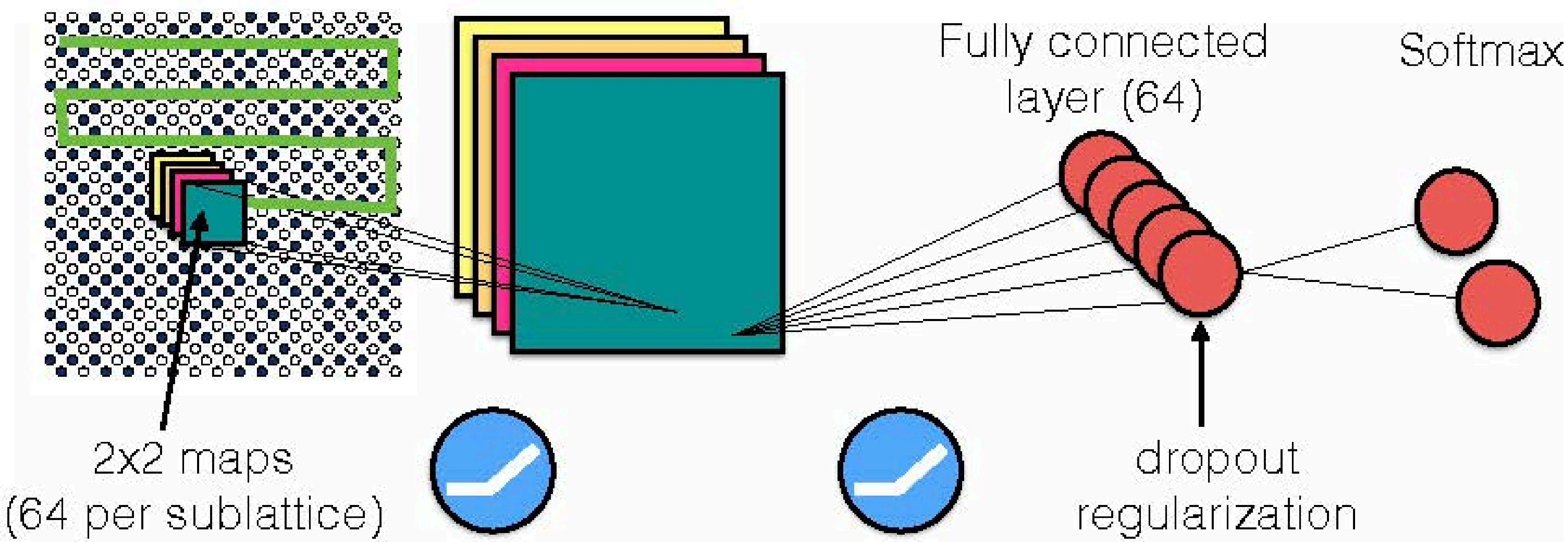
high-temperature state

Ground state

Feedforward NN are difficult to apply to this problem and lead to 50% accuracy

ISING GAUGE THEORY *F.J. Wegner, J. Math. Phys. 12 (1971) 2259*

$$H = -J \sum_p \prod_{i \in p} \sigma_i^z$$



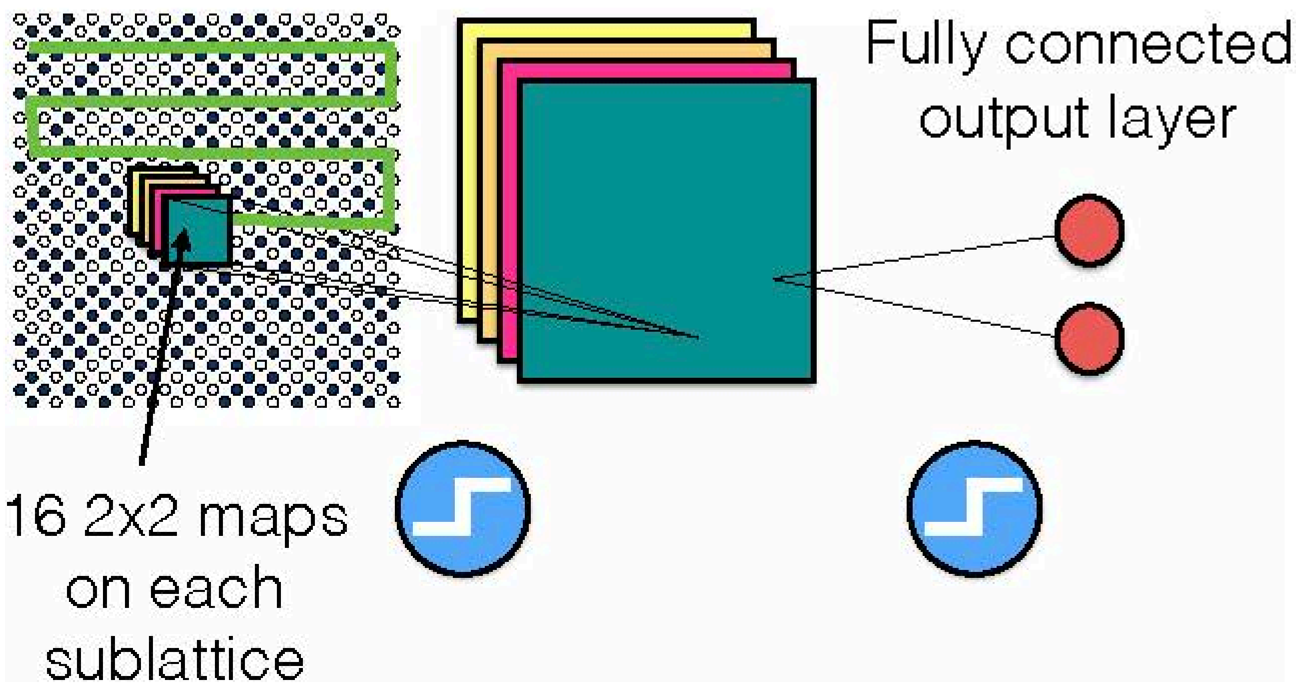
99% accuracy
easy to train

The picture we draw for what the CNN is using to distinguish the phases is that of the detection of satisfied local constraints. In few words, the neural network figures out the energy and uses it to classify states

ANALYTICAL UNDERSTANDING: WHAT DOES THE CNN USE TO MAKE PREDICTIONS?

- Based on this observation we derived the weights of a streamlined convolutional network *analytically* designed to work well for this problem:

$$O_{\text{cold}}(\sigma_1, \ldots, \sigma_N) \propto \lim_{\beta \to \infty} \exp \beta J \sum_p \prod_{i \in p} \sigma_i^z$$

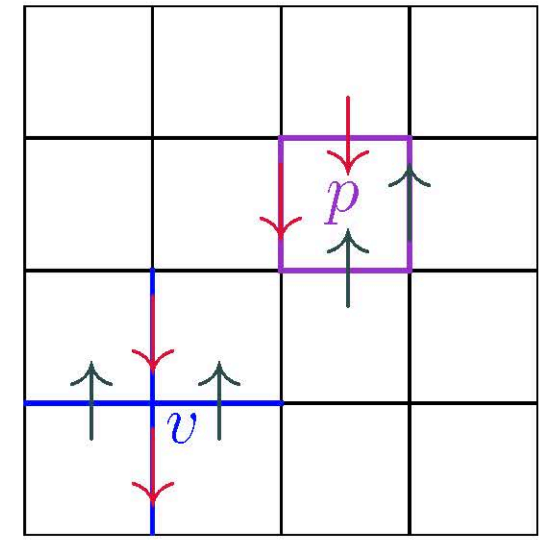


100% accuracy on test sets

J. Carrasquilla and R. G. Melko. Nature Physics 13, 431–434 (2017)

KITAEV'S QUANTUM ERROR CORRECTING CODE WITH CONVOLUTIONAL NEURAL NETWORKS

KITAEV'S TORIC CODE GROUND STATE

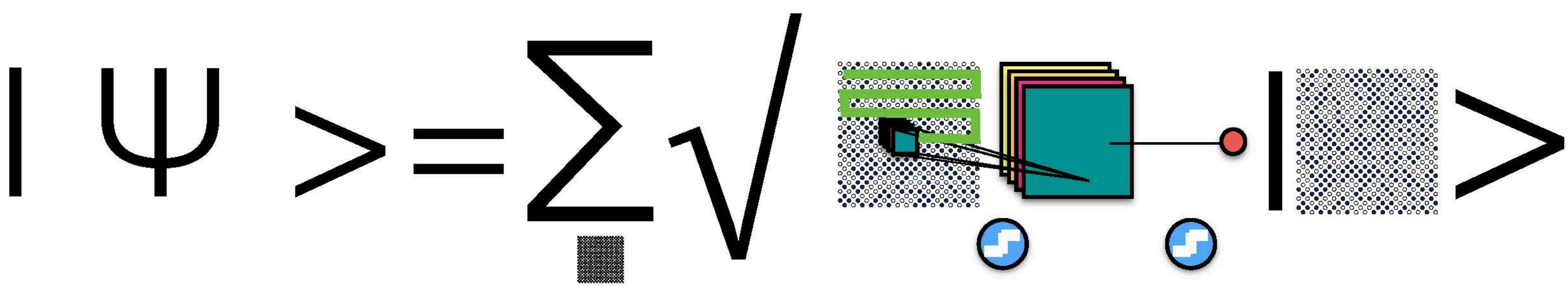


$$H = -J_p \sum_p \prod_{i \in p} \sigma_i^z - J_v \sum_v \prod_{i \in v} \sigma_i^x$$

$$|\Psi_{\mathrm{TC}}\rangle \propto \lim_{\beta \to \infty} \sum_{\sigma_1, \ldots, \sigma_N} e^{\frac{\beta}{2} J \sum_p \prod_{i \in p} \sigma_i^z} |\sigma_1, \ldots, \sigma_N\rangle$$

PEPS : *F. Verstraete, M. M. Wolf, D. Perez-Garcia, J. I. Cirac Phys. Rev. Lett. 96, 220601 (2006).*

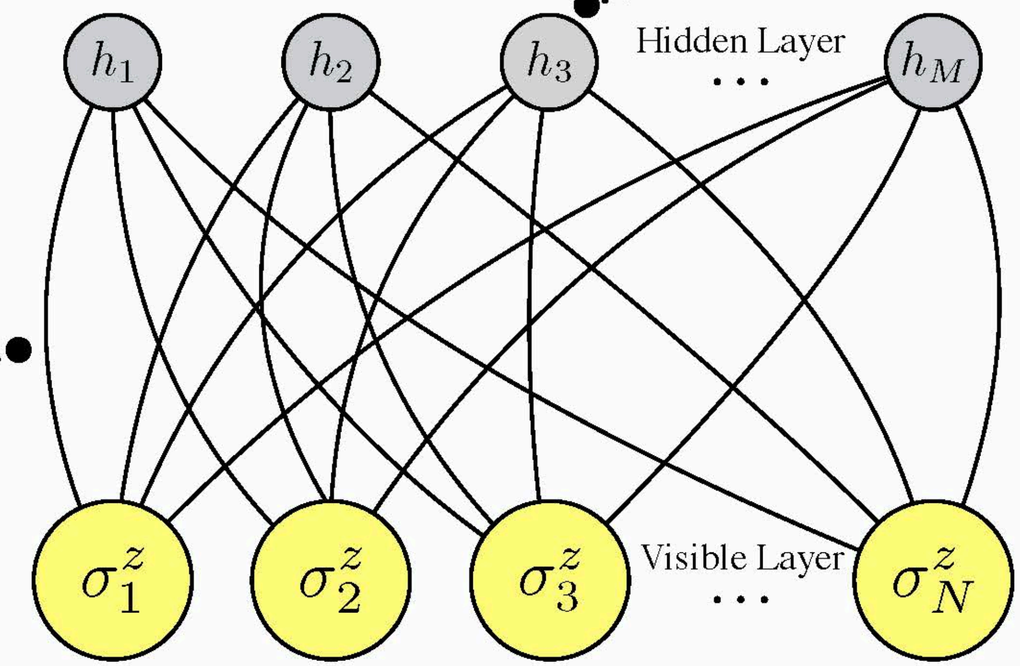
$$O_{\mathrm{cold}}(\sigma_1, \ldots, \sigma_N) \propto \lim_{\beta \to \infty} \exp \beta J \sum_p \prod_{i \in p} \sigma_i^z$$



J. Carrasquilla and R. G. Melko. Nature Physics 13, 431–434 (2017)
Dong-Ling Deng et al Phys. Rev. X 7, 021021 (2017)
Jing Chen, Song Cheng, Haidong Xie, Lei Wang, Tao Xiang arXiv:1701.04831 RBMs

EXTENDING RESTRICTED BOLTZMANN MACHINES TO THE QUANTUM DOMAIN

Carleo, and Troyer
Science 355, 602 (2017)



M Hidden Neurons (Auxiliary Spin Variables)

More Hidden Neurons Make it Smarter (and more accurate)

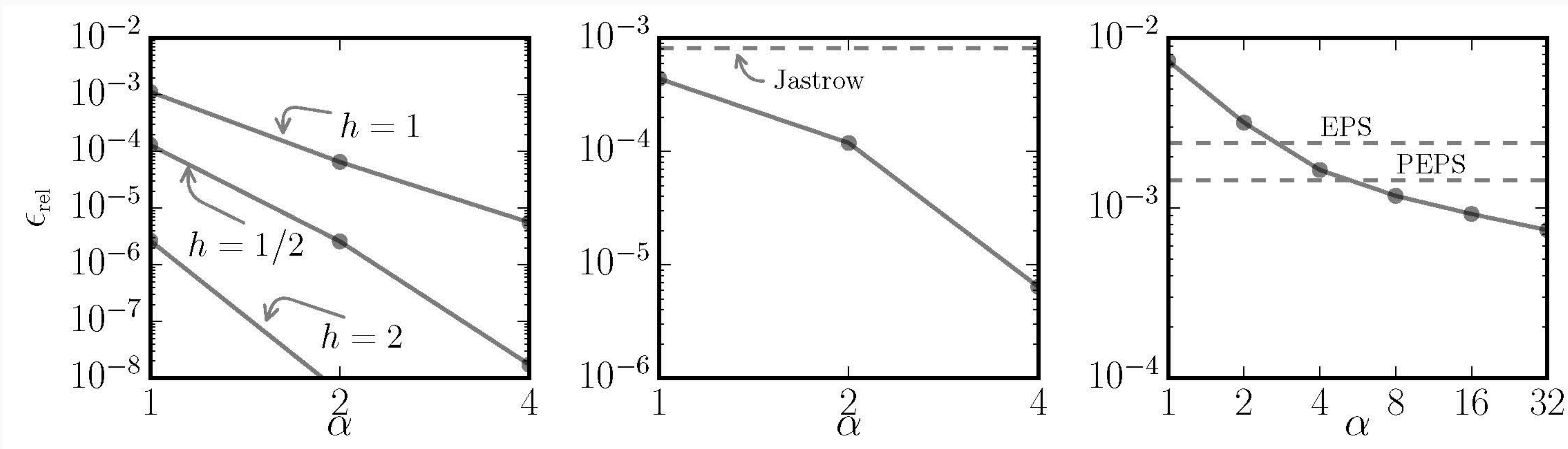
Restricted Boltzmann Machine

[Hinton et al.]

$$\Psi(\sigma_1^z, \sigma_2^z, \ldots \sigma_N^z; \mathbf{W}) = \sum_{\{h_i\}} e^{\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z}$$

Variational Parameters

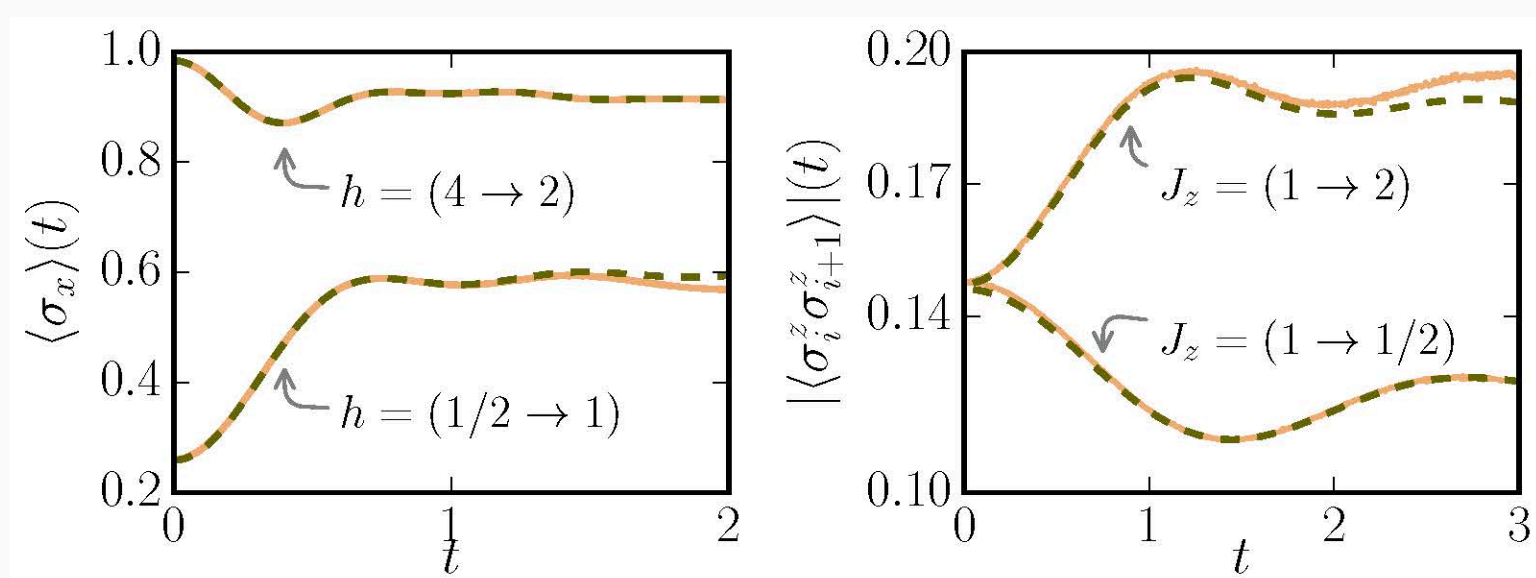
VARIATIONAL MONTE CARLO



1D Transverse-Field Ising

1D Heisenberg Model

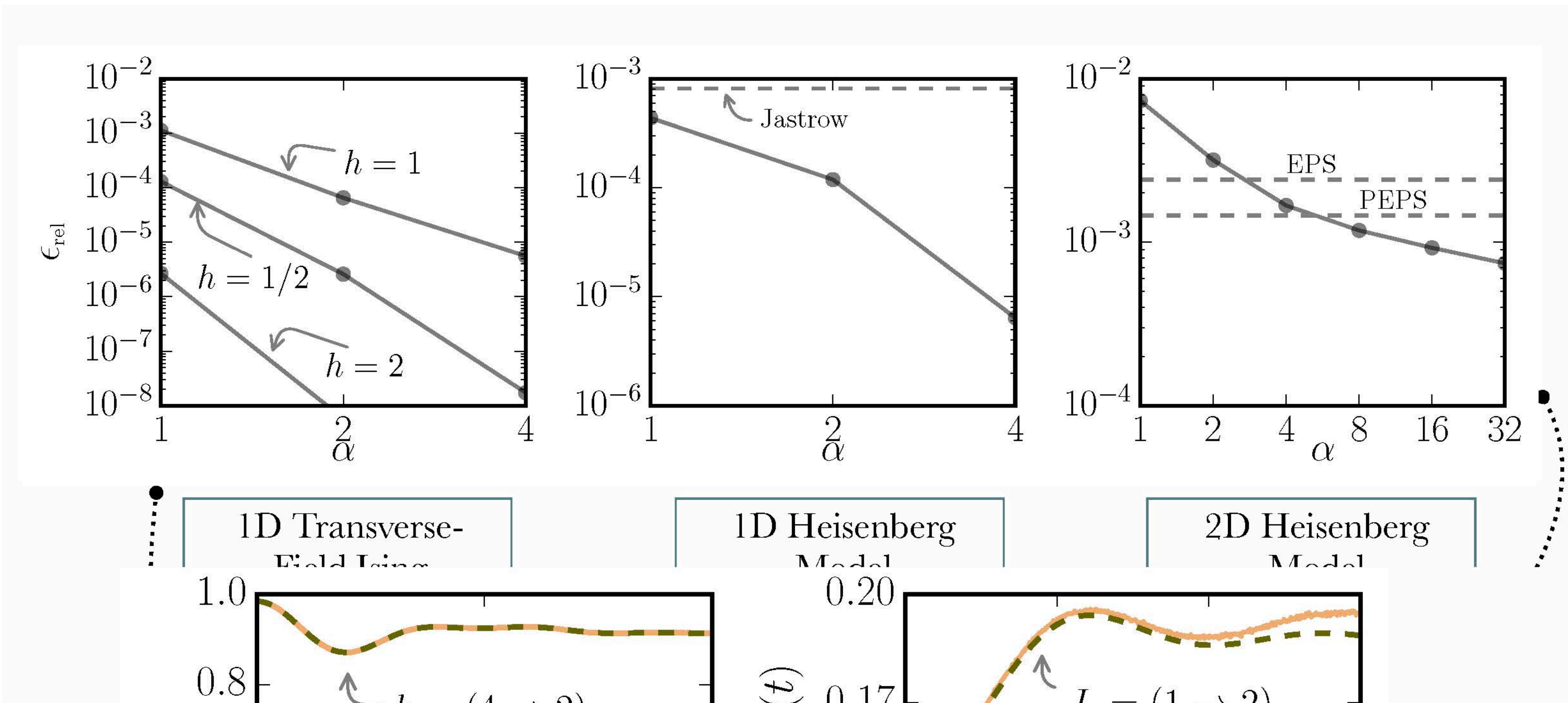
2D Heisenberg Model



1D Transverse-Field Ising

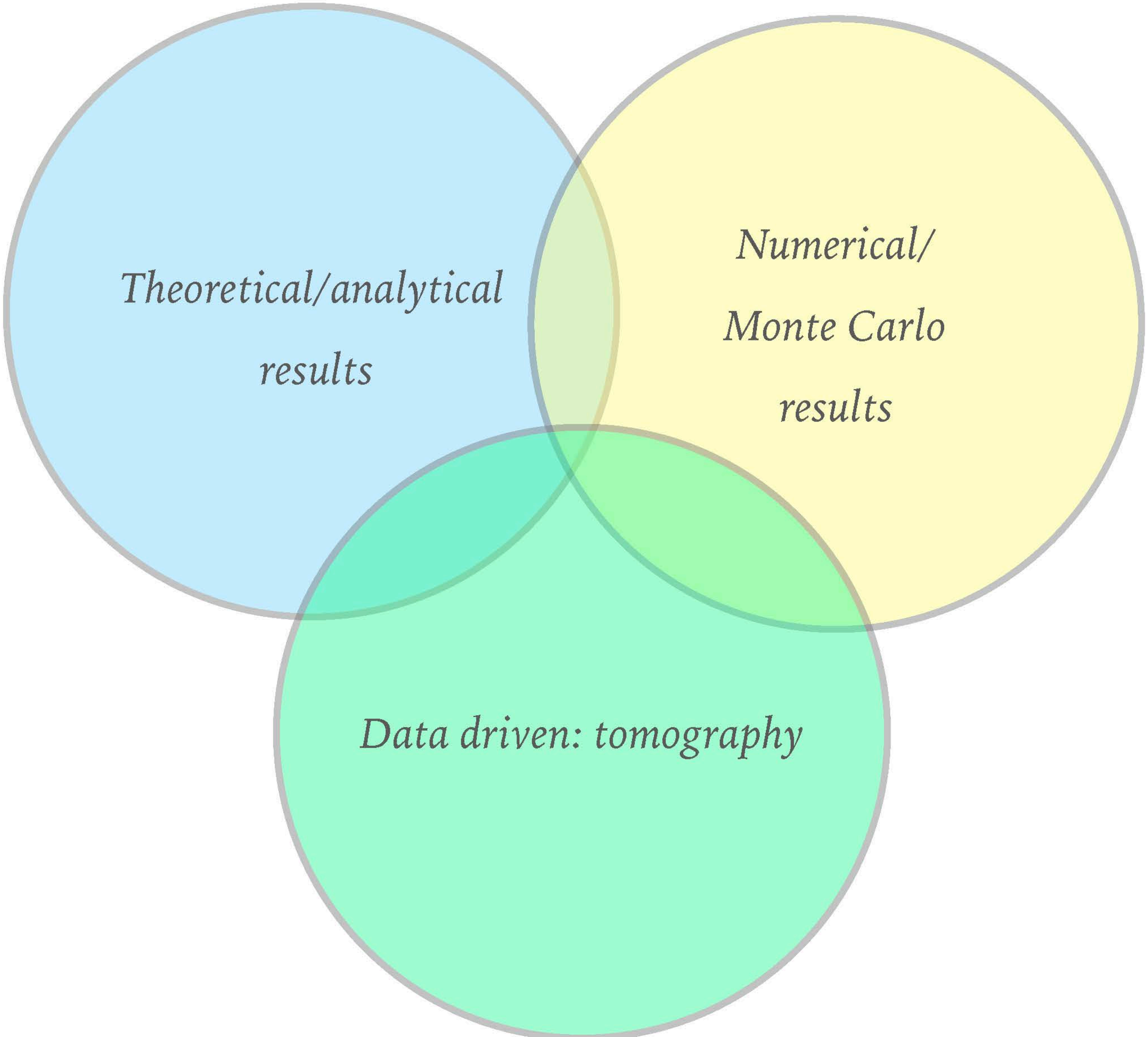
1D Heisenberg Model

COMBINE NEURAL NETWORKS WITH STANDARD VARIATIONAL MONTE CARLO



Promising research area

NEURAL NETWORK QUANTUM STATES



NEURAL NETWORK QUANTUMS TATES

Theoretical/analytical results

Equivalence of restricted Boltzmann machines and tensor network states
J Chen, S Cheng, H Xie, L Wang, T Xiang - Physical Review B, 2018 - APS
The restricted Boltzmann machine (RBM) is one of the fundamental building blocks of deep learning. RBM finds wide applications in dimensional reduction, feature extraction, and recommender systems via modeling the probability distributions of a variety of input data …
Cited by 50 Related articles All 8 versions

Machine learning topological states
DL Deng, X Li, SD Sarma - Physical Review B, 2017 - APS
Artificial neural networks and machine learning have now reached a new era after several decades of improvement where applications are to explode in many fields of science, industry, and technology. Here, we use artificial neural networks to study an intriguing …
Cited by 47 Related articles All 8 versions

[HTML] Efficient representation of quantum many-body states with deep neural networks
X Gao, LM Duan - Nature communications, 2017 - nature.com
Part of the challenge for quantum many-body problems comes from the difficulty of representing large-scale quantum states, which in general requires an exponentially large number of parameters. Neural networks provide a powerful tool to represent quantum many …
Cited by 48 Related articles All 7 versions

Quantum entanglement in neural network states
DL Deng, X Li, SD Sarma - Physical Review X, 2017 - APS
Abstract Machine learning, one of today's most rapidly growing interdisciplinary fields, promises an unprecedented perspective for solving intricate quantum many-body problems. Understanding the physical aspects of the representative artificial neural-network states has …
Cited by 55 Related articles All 5 versions

Neural network representation of tensor network and chiral states
Y Huang, JE Moore - arXiv preprint arXiv:1701.06246, 2017 - arxiv.org
We study the representational power of a Boltzmann machine (a type of neural network) in quantum many-body systems. We prove that any (local) tensor network state has a (local) neural network representation. The construction is almost optimal in the sense that the …
Cited by 38 Related articles All 6 versions

Neural-network quantum states, string-bond states, and chiral topological states
I Glasser, N Pancotti, M August, ID Rodriguez, JI Cirac - Physical Review X, 2018 - APS
Neural-network quantum states have recently been introduced as an Ansatz for describing the wave function of quantum many-body systems. We show that there are strong connections between neural-network quantum states in the form of restricted Boltzmann …
Cited by 22 Related articles All 5 versions

[PDF] Deep Learning and Quantum Physics: A Fundamental Bridge
Y Levine, D Yakira, N Cohen… - arXiv preprint arXiv …, 2017 - pdfs.semanticscholar.org
Deep convolutional networks have witnessed unprecedented success in various machine learning applications. Formal understanding on what makes these networks so successful is gradually unfolding, but for the most part there are still significant mysteries to unravel. The …
Cited by 4 Related articles

NEURAL NETWORK QUANTUM STATES

Numerical/
Monte Carlo
results

Self-learning monte carlo method
J Liu, Y Qi, ZY Meng, L Fu - Physical Review B, 2017 - APS
Monte Carlo simulation is an unbiased numerical tool for studying classical and quantum many-body systems. One of its bottlenecks is the lack of a general and efficient update algorithm for large size systems close to the phase transition, for which local updates …

Approximating quantum many-body wave functions using artificial neural networks
Z Cai, J Liu - Physical Review B, 2018 - APS
In this paper, we demonstrate the expressibility of artificial neural networks (ANNs) in quantum many-body physics by showing that a feed-forward neural network with a small number of hidden layers can be trained to approximate with high precision the ground states …

Solving the Bose–Hubbard model with machine learning
H Saito - Journal of the Physical Society of Japan, 2017 - journals.jps.jp
Motivated by the recent successful application of artificial neural networks to quantum many-body problems [G. Carleo and M. Troyer, Science 355, 602 (2017)], a method to calculate the ground state of the Bose–Hubbard model using a feedforward neural network is …

Neural-network quantum states, string-bond states, and chiral topological states
I Glasser, N Pancotti, M August, ID Rodriguez, JI Cirac - Physical Review X, 2018 - APS
Neural-network quantum states have recently been introduced as an Ansatz for describing the wave function of quantum many-body systems. We show that there are strong connections between neural-network quantum states in the form of restricted Boltzmann …

Restricted Boltzmann machine learning for solving strongly correlated quantum systems
Y Nomura, AS Darmawan, Y Yamaji, M Imada - Physical Review B, 2017 - APS
We develop a machine learning method to construct accurate ground-state wave functions of strongly interacting and entangled quantum spin as well as fermionic models on lattices. A restricted Boltzmann machine algorithm in the form of an artificial neural network is …

Constructing exact representations of quantum many-body systems with deep neural networks
G Carleo, Y Nomura, M Imada - arXiv preprint arXiv:1802.09558, 2018 - arxiv.org
We develop a constructive approach to generate artificial neural networks representing the exact ground states of a large class of many-body lattice Hamiltonians. It is based on the deep Boltzmann machine architecture, in which two layers of hidden neurons mediate …

NEURAL NETWORK QUANTUM STATES

Data driven: tomography

[HTML] Learning hard quantum distributions with variational autoencoders
A Rocchetto, E Grant, S Strelchuk, G Carleo… - npj Quantum …, 2018 - nature.com
The exact description of many-body quantum systems represents one of the major challenges in modern physics, because it requires an amount of computational resources that scales exponentially with the size of the system. Simulating the evolution of a state, or …
Cited by 5 Related articles All 3 versions

Neural-network quantum state tomography
G Torlai, G Mazzola, J Carrasquilla, M Troyer, R Melko… - Nature Physics, 2018 - nature.com
The experimental realization of increasingly complex synthetic quantum systems calls for the development of general theoretical methods to validate and fully exploit quantum resources. Quantum state tomography (QST) aims to reconstruct the full quantum state from simple …
Cited by 18 Related articles All 5 versions

Latent Space Purification via Neural Density Operators
G Torlai, RG Melko - Physical Review Letters, 2018 - APS
Abstract Machine learning is actively being explored for its potential to design, validate, and even hybridize with near-term quantum devices. A central question is whether neural networks can provide a tractable representation of a given quantum state of interest. When …
Cited by 4 Related articles All 4 versions

QUANTUM STATE TOMOGRAPHY

QUANTUM STATE TOMOGRAPHY

Quantum state tomography is the process of reconstructing the quantum state by **measurements** on the system. It "is the gold standard for verification and benchmarking of quantum devices"*

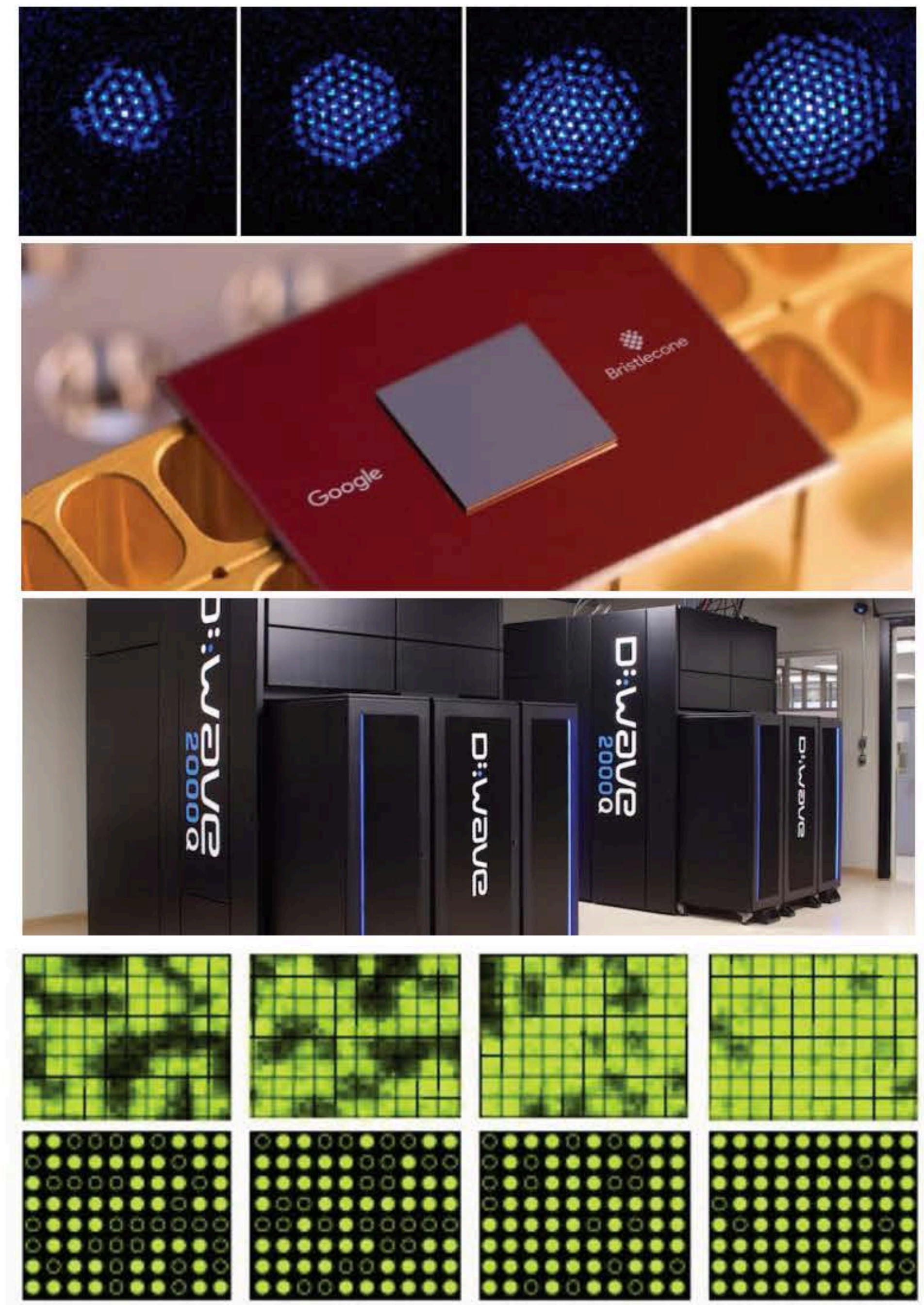
Useful for:

- Characterizing optical signals
- Diagnosing and detecting errors in state preparation, e.g. states produced by quantum computers reliably.
- Entanglement verification

* Efficient quantum state tomography. Marcus Cramer, Martin B. Plenio, Steven T. Flammia, Rolando Somma, David Gross, Stephen D. Bartlett, Olivier Landon-Cardinal, David Poulin & Yi-Kai Liu. Nature Communications volume 1, Article number: 149

NEED TO GO BEYOND STANDARD QUANTUM STATE TOMOGRAPHY

- Progress in controlling large quantum systems.
- Availability of arbitrary measurements performed with great accuracy.
- The bottleneck limiting progress in the estimation of states: curse of dimensionality.



SYNTHETIC QUANTUM DEVICES ARE GROWING FAST

nature.com > nature > articles > article

nature
International journal of science

Article | Published: 29 November 2017

Probing many-body dynamics on a 51-atom quantum simulator

Hannes Bernien, Sylvain Schwartz, Alexander Keesling, Harry Levine, Ahmed Omran, Hannes Pichler, Soonwon Choi, Alexander S. Zibrov, Manuel Endres, Markus Greiner, Vladan Vuletić & Mikhail D. Lukin

Nature **551**, 579–584 (30 November 2017) | Download Citation

nature.com > nature > letters > article

nature
International journal of science

Letter | Published: 29 November 2017

Observation of a many-body dynamical phase transition with a 53-qubit quantum simulator

J. Zhang, G. Pagano, P. W. Hess, A. Kyprianidis, P. Becker, H. Kaplan, A. V. Gorshkov, Z.-X. Gong & C. Monroe

Nature **551**, 601–604 (30 November 2017) | Download Citation

nature.com > nature > letters > article

nature
International journal of science

Letter | Published: 22 August 2018

Observation of topological phenomena in a programmable lattice of 1,800 qubits

Andrew D. King, Juan Carrasquilla, [...] Mohammad H. Amin

Nature **560**, 456–460 (2018) | Download Citation

PHYSICAL REVIEW X

Highlights Recent Subjects Accepted Collections Authors Referees Search Press About Staff

Open Access

Quantum Chemistry Calculations on a Trapped-Ion Quantum Simulator

Cornelius Hempel, Christine Maier, Jonathan Romero, Jarrod McClean, Thomas Monz, Heng Shen, Petar Jurcevic, Ben P. Lanyon, Peter Love, Ryan Babbush, Alán Aspuru-Guzik, Rainer Blatt, and Christian F. Roos

Phys. Rev. X **8**, 031022 – Published 24 July 2018

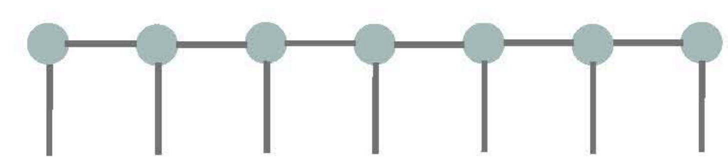
162

More

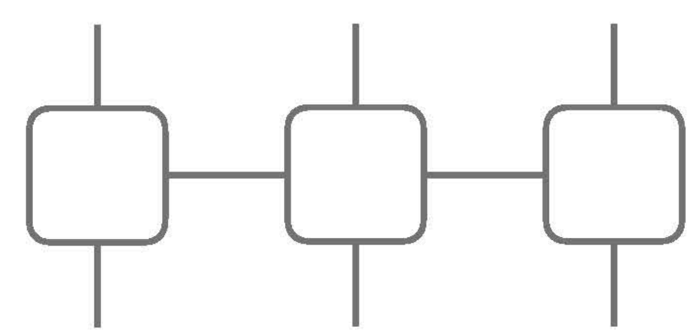
APPROACHES TO MAKE QST EFFICIENT: TENSOR NETWORKS

- Introduce a parametrization of the quantum state with good scaling if non-trivial structural information on the quantum systems under consideration is utilized: MPS[1] and MPO[2] tomography

[1] Efficient quantum state tomography. Marcus Cramer, Martin B. Plenio, Steven T. Flammia, Rolando Somma, David Gross, Stephen D. Bartlett, Olivier Landon-Cardinal, David Poulin & Yi-Kai Liu. Nature Communications volume 1, Article number: 149



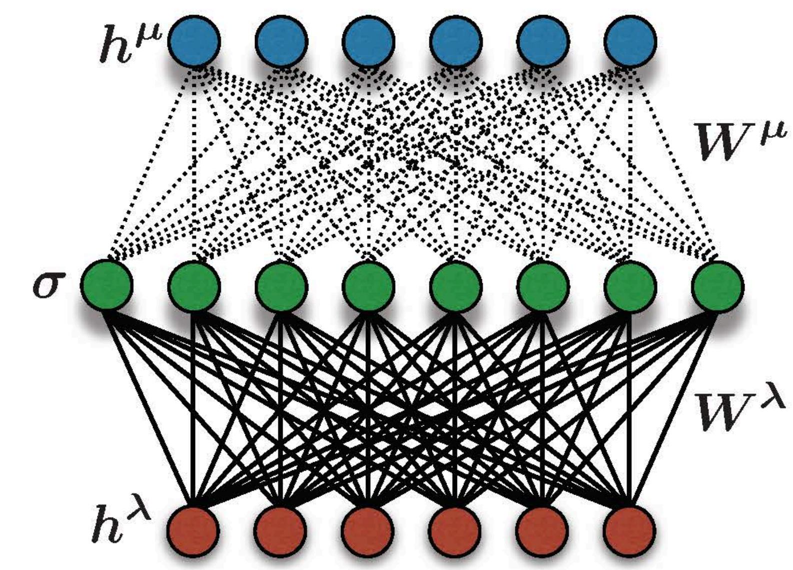
[2] A scalable maximum likelihood method for quantum state tomography T Baumgratz1, A Nüßeler, M Cramer and M B Plenio. New Journal of Physics, Volume 15, December 2013



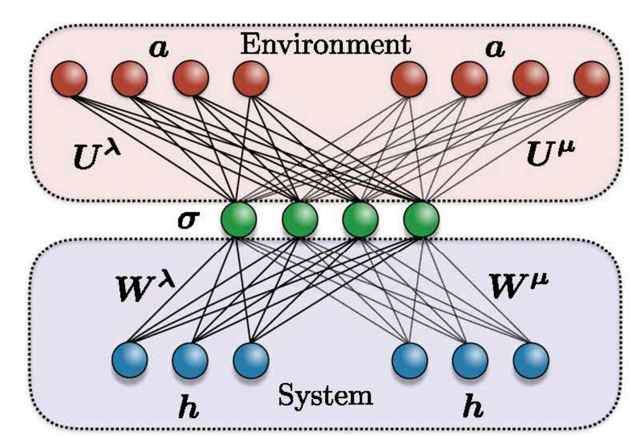
APPROACHES TO MAKE QST EFFICIENT: NEURAL NETWORKS

- Introduce a parametrization of the quantum state with good scaling if non-trivial structural information on the quantum systems under consideration is utilized: Restricted Boltzmann machines both for pure[3] states and mixed states[4]

[3] Neural-network quantum state tomography. G. Torlai, G. Mazzola, J. Carrasquilla, M. Troyer, R. Melko, and G. Carleo, Nat. Phys. 14, 447 (2018).



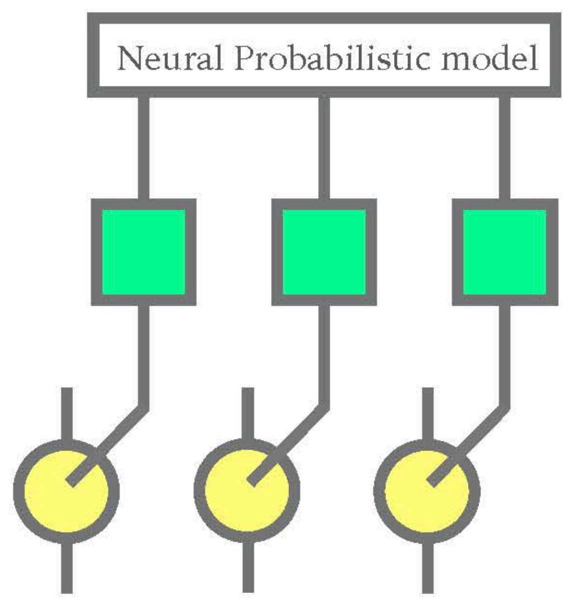
[4] Latent Space Purification via Neural Density Operators. Giacomo Torlai and Roger G. Melko. Phys. Rev. Lett. 120, 240503 (2018)



A NEW APPROACH: COMBINE NEURAL AND (EASY) TENSOR NETWORKS

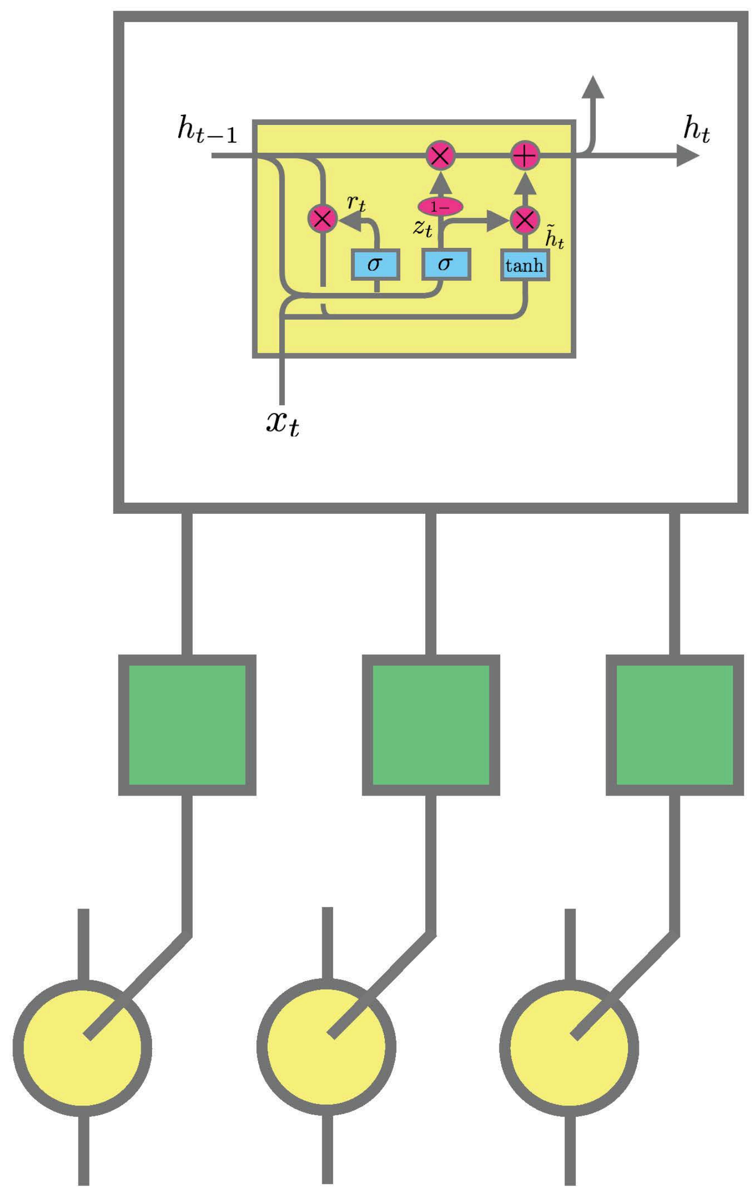
- ~~Parametrize the quantum state~~ We parametrize the Born's rule in terms of generative models. Measurements: informationally complete positive operator valued measures (POVM)

$$\rho_{\mathrm{model}} = (\mathbf{T}^{-1} P_{\mathrm{model}})^T \mathbf{M}$$



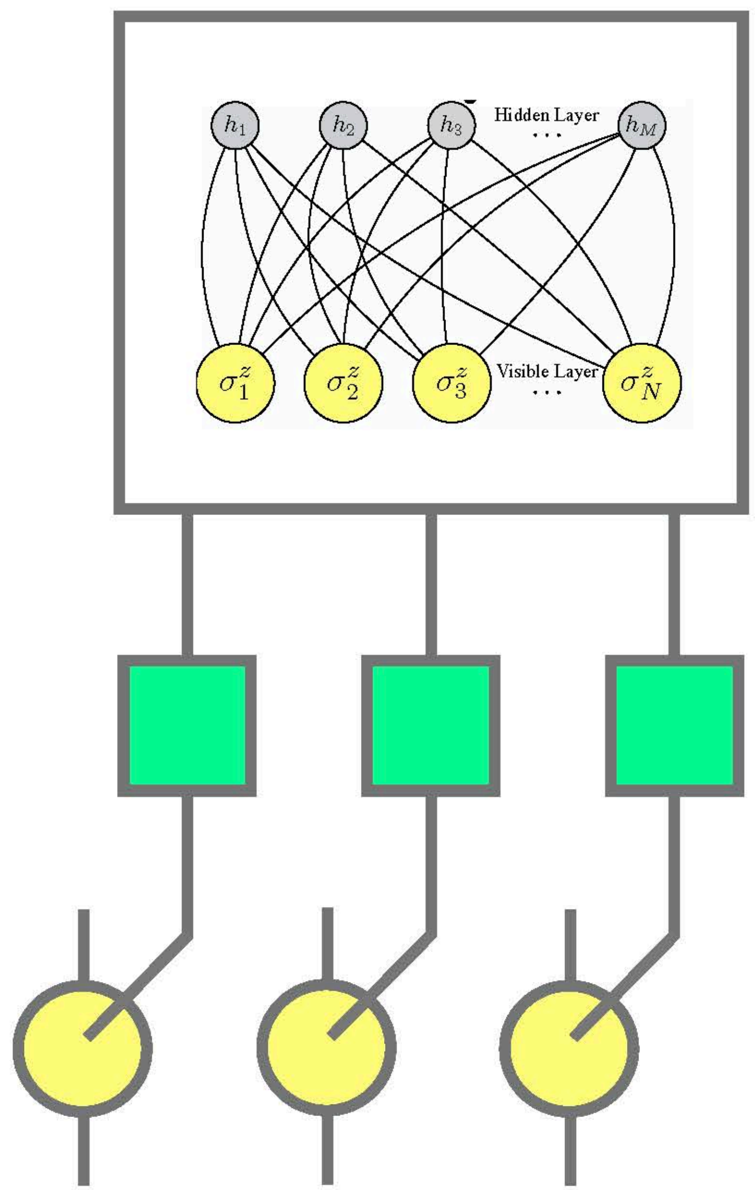
A NEW APPROACH: COMBINE NEURAL AND (EASY) TENSOR NETWORKS

- ~~Parametrize the quantum state~~ We parametrize the Born's rule in terms of generative models. Measurements: informationally complete positive operator valued measures (POVM)



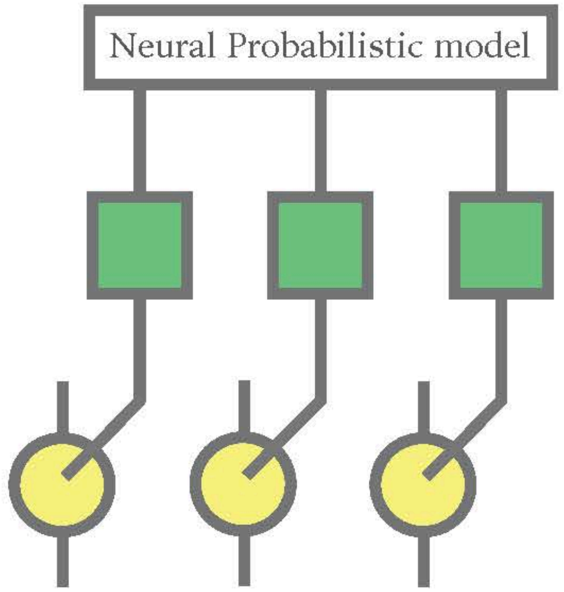
A NEW APPROACH: COMBINE NEURAL AND (EASY) TENSOR NETWORKS

- ~~Parametrize the quantum state~~ We parametrize the Born's rule in terms of generative models. Measurements: informationally complete positive operator valued measures (POVM)



LEARNING MIXED STATES USING POSITIVE OPERATOR VALUED MEASURE

$\rho_{\text{model}} = (\mathbf{T}^{-1} P_{\text{model}})^T \mathbf{M}$

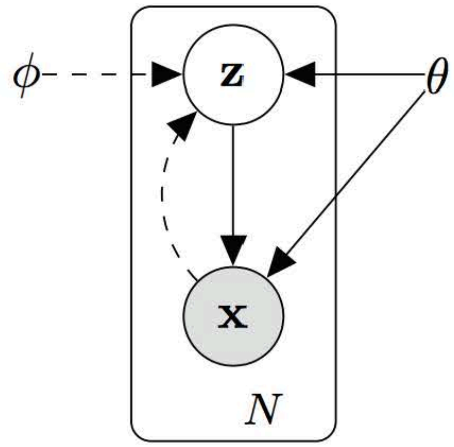


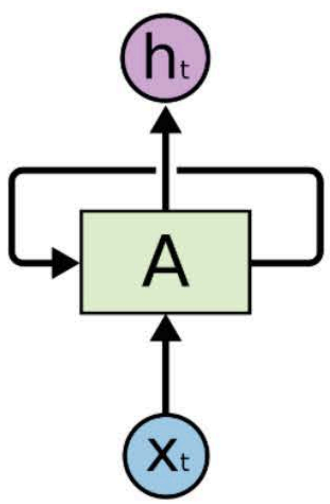
The statistics of the measurements is given by **Born rule**

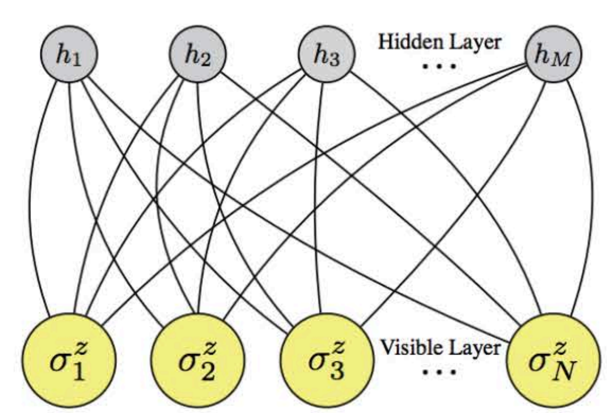
$$P(\mathbf{a}) = \mathrm{Tr}\, \rho M^{\mathbf{a}}$$

=> Unsupervised learning of P(a)

$P_{\text{model}}(\mathbf{a})$ ⟶ **VAE, RBM, GAN, autoregressive models, any model**







Goodfellow et al. Deep Learning (2016)

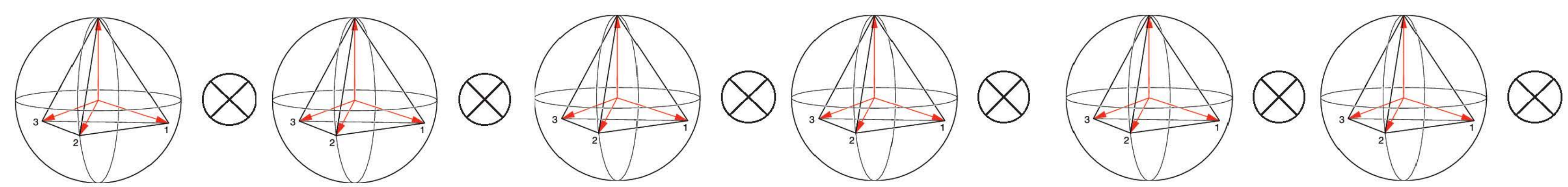
MEASUREMENTS: POSITIVE OPERATOR VALUED MEASURES (POVM)

Measurements: $\mathbf{M} = \{M^{(a)} \mid a \in \{1, ..., m\}\}$

Informationally complete POVMs $\sum_i M^{(a)} = \mathbb{1}$ m is at least $D^2 = 2^{2N}$ and M should span the entire Hilbert space

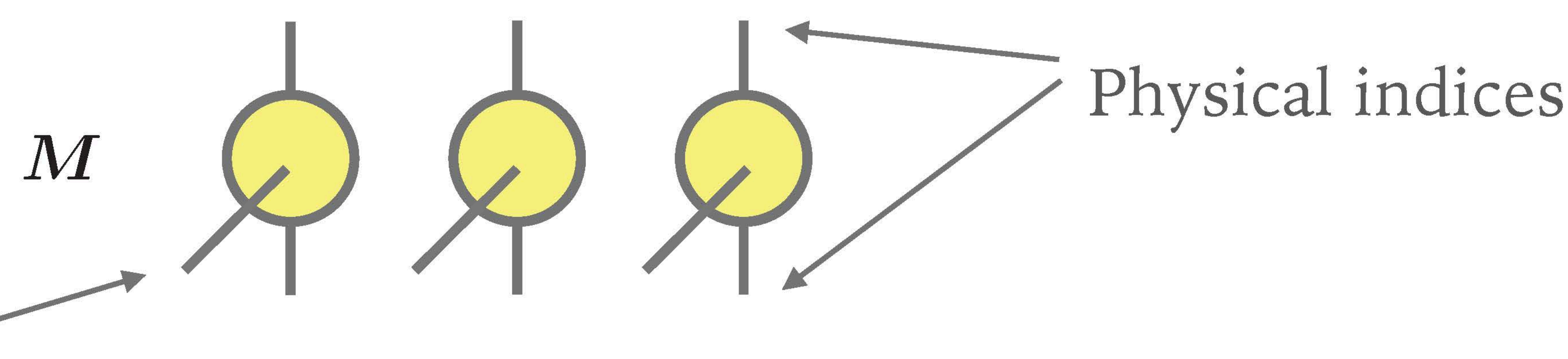
$P(\mathbf{a}) = \mathrm{Tr}\, \rho M^{\mathbf{a}}$ Born rule. Defines a distribution over the generalized measurements

For multiqubit systems



$$\boldsymbol{M} = \left\{M^{(a_1)} \otimes M^{(a_2)} \otimes \ldots M^{(a_N)}\right\}_{a_1,\ldots a_N}$$

Tensor network representation of the POVM



Experimental schemes see: Phys. Rev. A 86, 062107 (2012), Phys. Rev. A 83, 051801(R) (2011), Phys. Rev. A 91, 042101 (2015)

INFORMATIONAL COMPLETENESS AND HOW TO INVERT BORN RULE

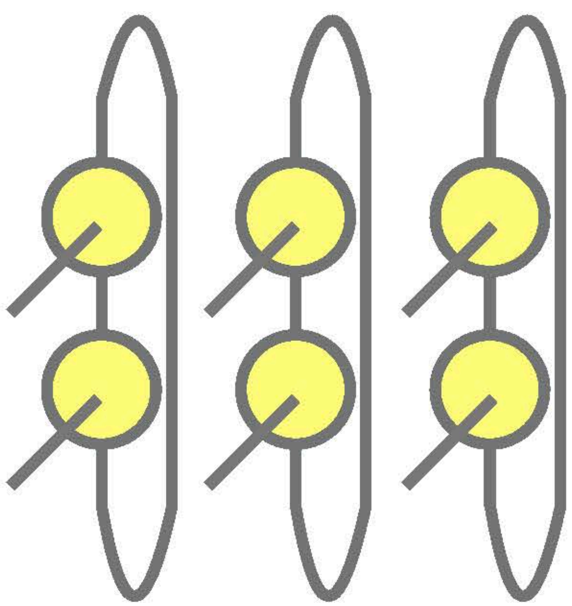
If the POVM is informationally complete then

$$\rho = \sum_a O_\rho(a) M^{(a)}$$

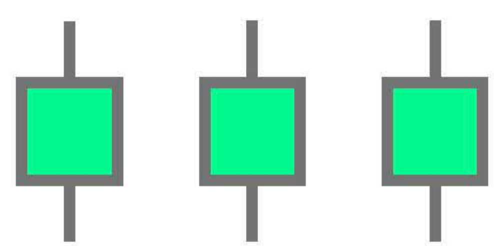
Insert this relation into Born's rule $\quad P(a) = \sum_{a'} O_\rho(a') Tr[M^{(a)} M^{(a')}] = \sum_{a'} O_\rho(a') T_{a'a}$

$$\rho = \sum_{a,a'} T^{-1}_{a,a'} P(a') M^{(a)},$$

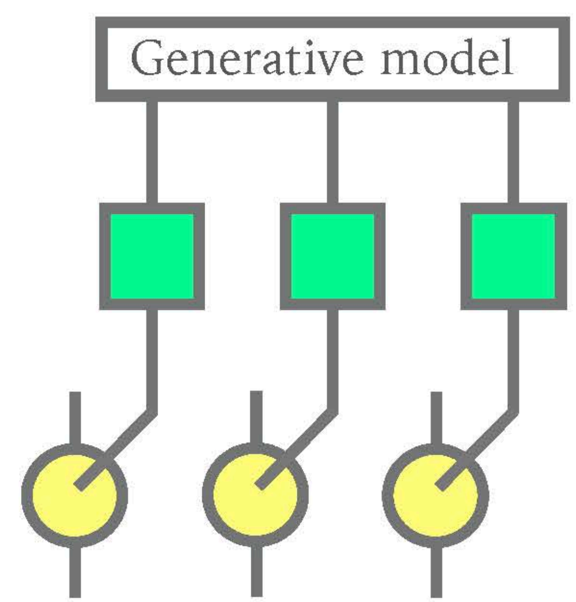
$T_{\alpha,\beta} = \mathrm{Tr}\ M^\alpha M^\beta$



$\mathbf{T}^{-1}$

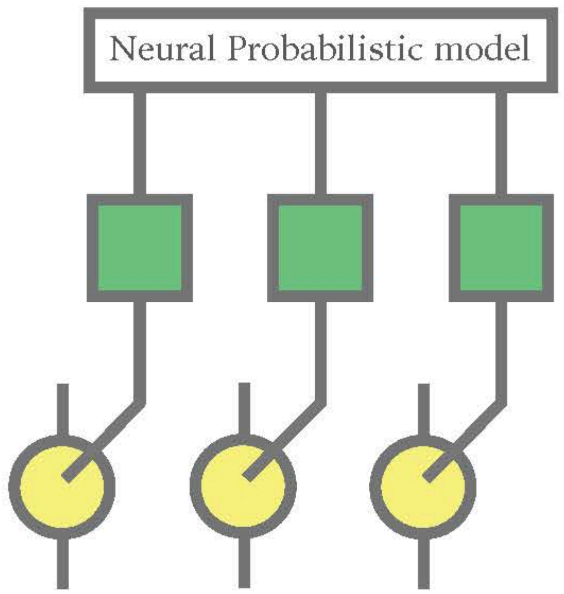


$\rho_{\mathrm{model}} = (\mathbf{T}^{-1} P_{\mathrm{model}})^T \mathbf{M}$



LEARNING MIXED STATES USING POSITIVE OPERATOR VALUED MEASURE

$\rho_{\text{model}} = (\mathbf{T}^{-1} P_{\text{model}})^T \mathbf{M}$



The statistics of the measurements is given by **Born rule**

$$P(\mathbf{a}) = \text{Tr}\, \rho M^{\mathbf{a}}$$

=> Unsupervised learning of P(a)

Any probabilistic model works in this framework

Goodfellow et al. Deep Learning (2016)

RESULTS ON SYNTHETIC DATASETS FOR GHZ STATES

Pure GHZ

$$|\Psi_0\rangle \equiv \alpha\,|0\rangle^{\otimes N} + \beta\,|1\rangle^{\otimes N}$$

$$\begin{aligned}\varrho_0 &:= |\Psi_0\rangle\,\langle\Psi_0| \\ &= |\alpha|^2\,|0\rangle\,\langle 0|^{\otimes N} + |\beta|^2\,|1\rangle\,\langle 1|^{\otimes N} + \left(\alpha\beta^*\,|0\rangle\,\langle 1|^{\otimes N} + \text{ h.c.}\right)\end{aligned}$$

GHZ with

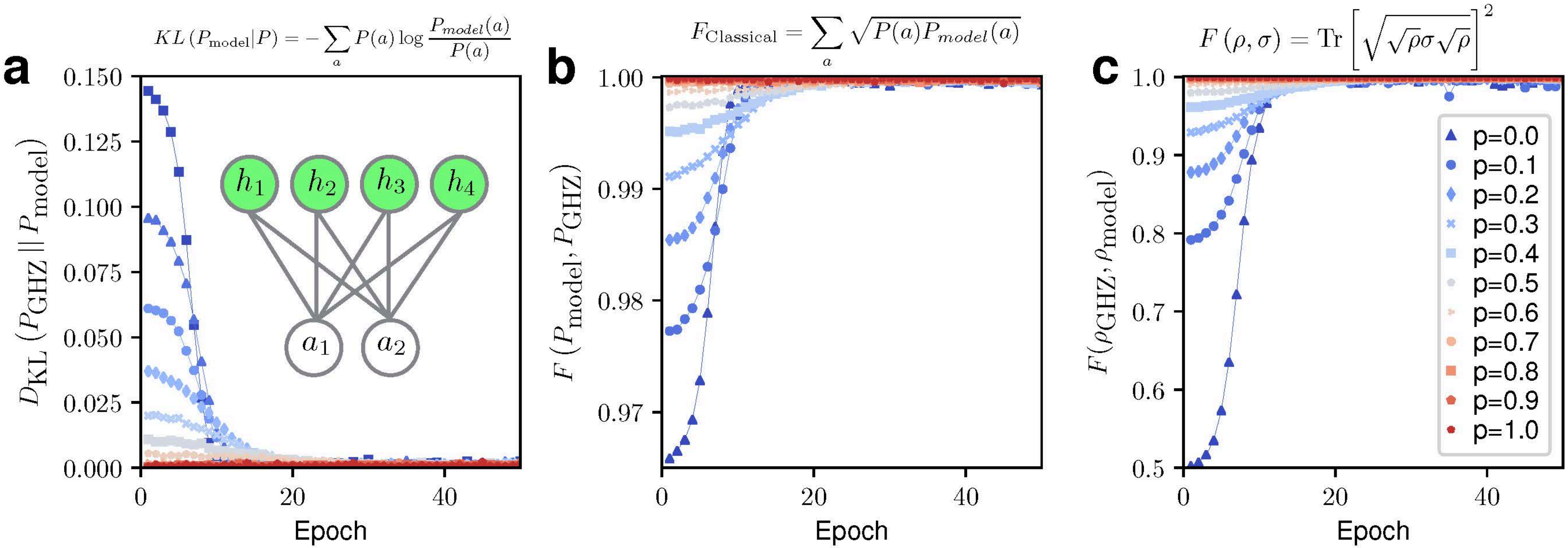
Locally depolarized

generalized GHZ

$$\mathcal{E}_i\varrho_0 = (1-p)\,\varrho_0 + \frac{p}{3}\left(\sigma_i^{(1)}\,\varrho_0\,\sigma_i^{(1)} + \sigma_i^{(2)}\,\varrho_0\,\sigma_i^{(2)} + \sigma_i^{(3)}\,\varrho_0\,\sigma_i^{(3)}\right)$$

states : a model of a decohering qubit where with probability 1 − p the qubit remains intact, while with probability p an “error” occurs.

LEARNING 2 QUBIT LOCALLY DEPOLARIZED GHZ



This result is obtained by parametrizing the P(a) with an RBM with multinomial visible units (4 states per qubit for the corresponding to the outcomes of the POVMs)

$$v_i = 0, 1, 2, 3, 4$$

$$h_j = 0, 1$$

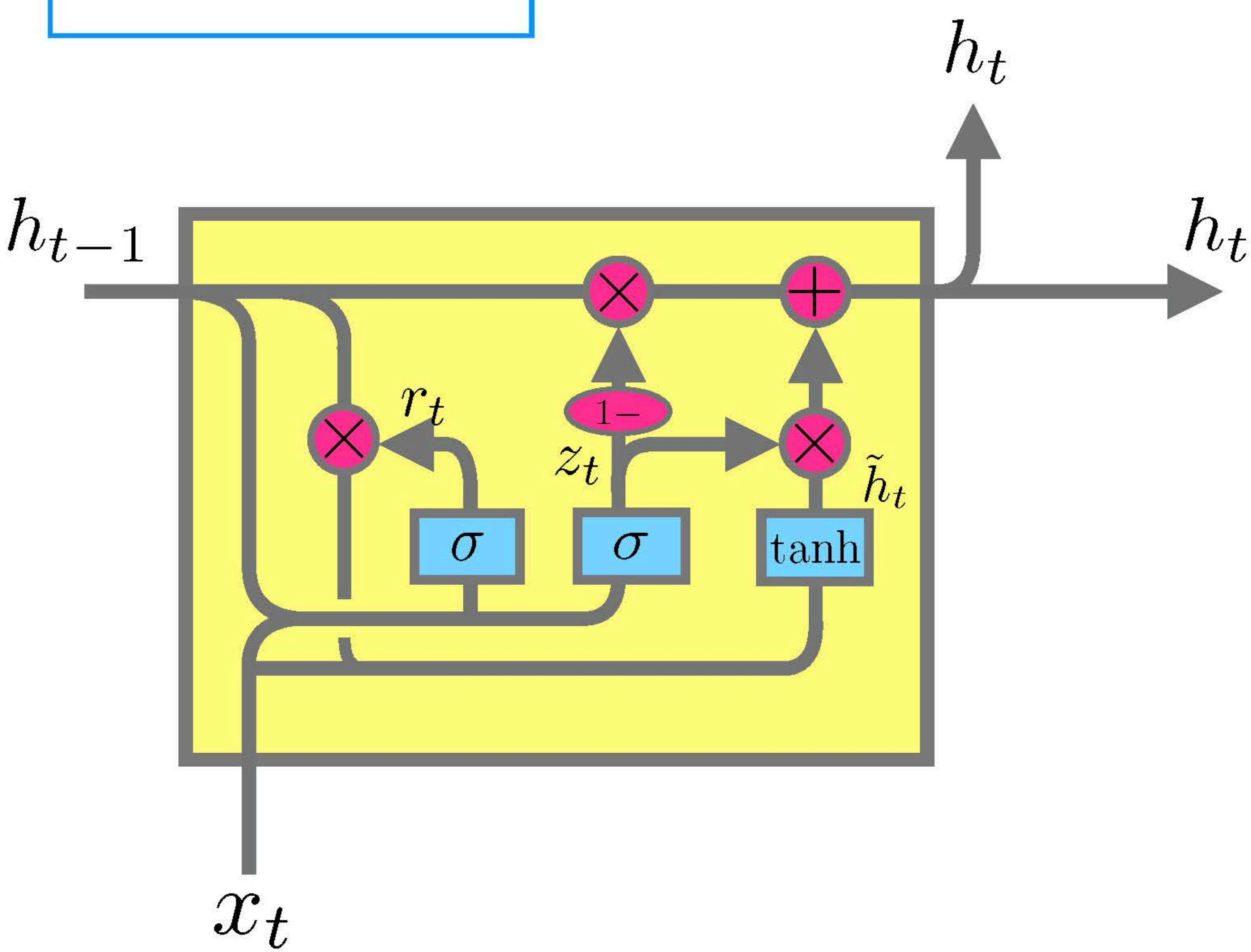
Restricted Boltzmann Machines for Collaborative Filtering. Salakhutdinov, Mnih, Hinton. 2007

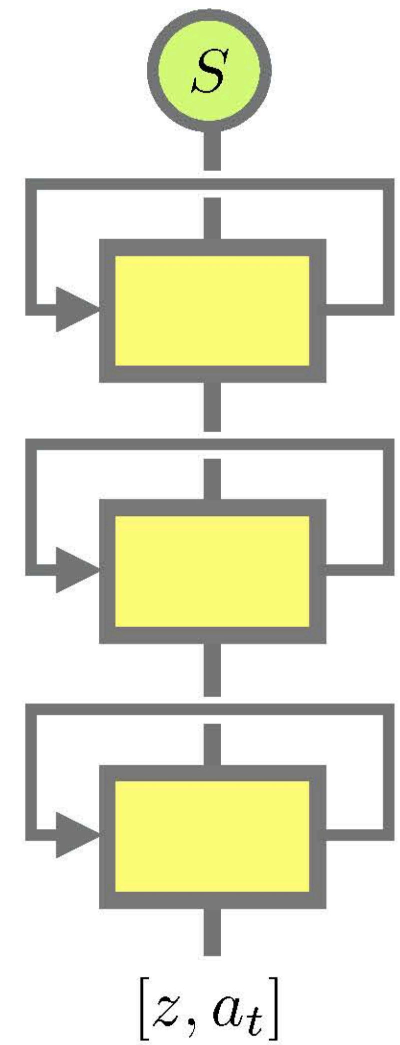
RECURRENT NEURAL NETWORK MODEL AND RESULTS

GHZ results

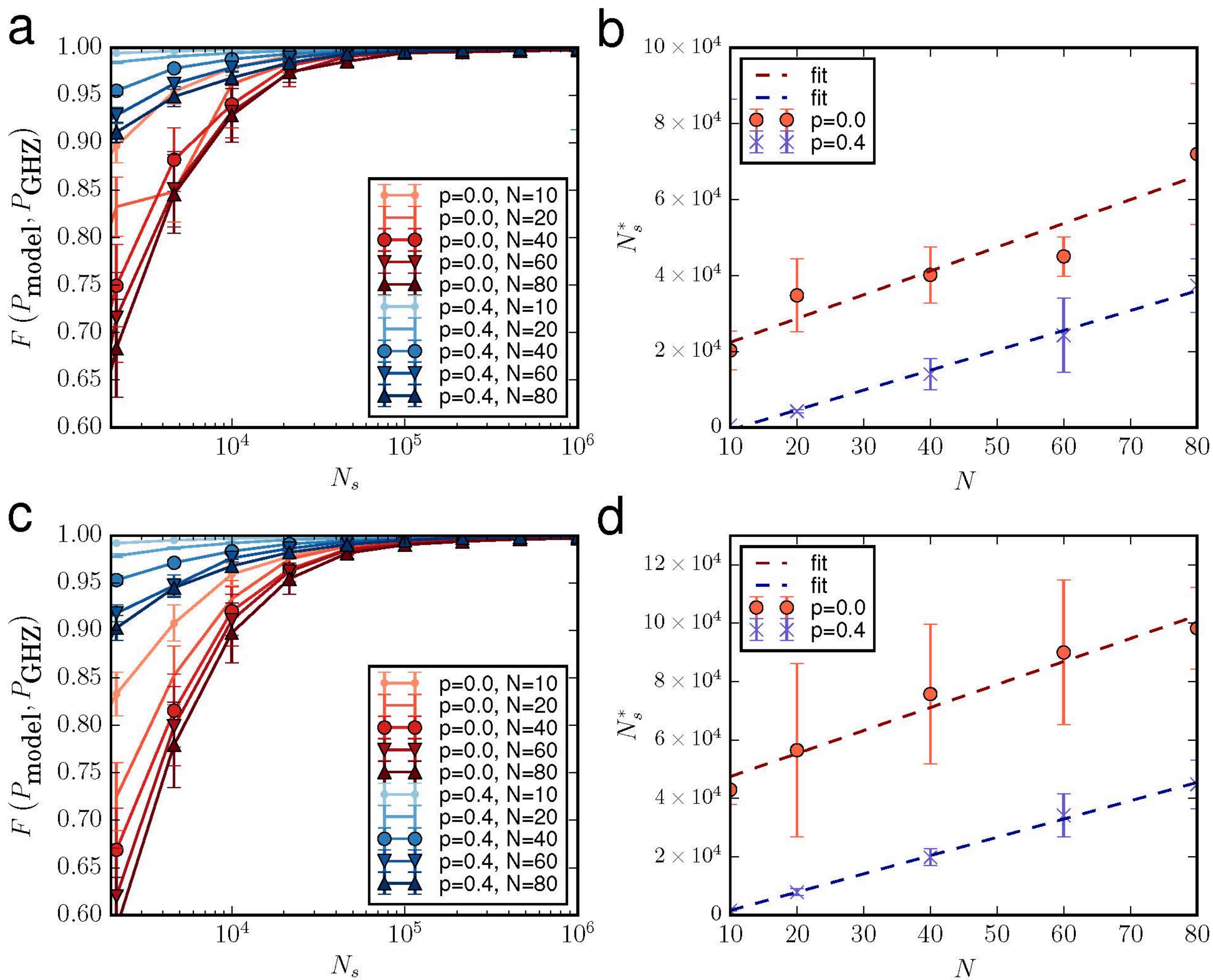
40 qubit p=0
Fc = 0.9992(4)
80 qubits p =0.01
Fc = 0.9988(1)
KL = 0.0050(2)

Full model stacks three of these units and adds a softmax dense layer at each time step



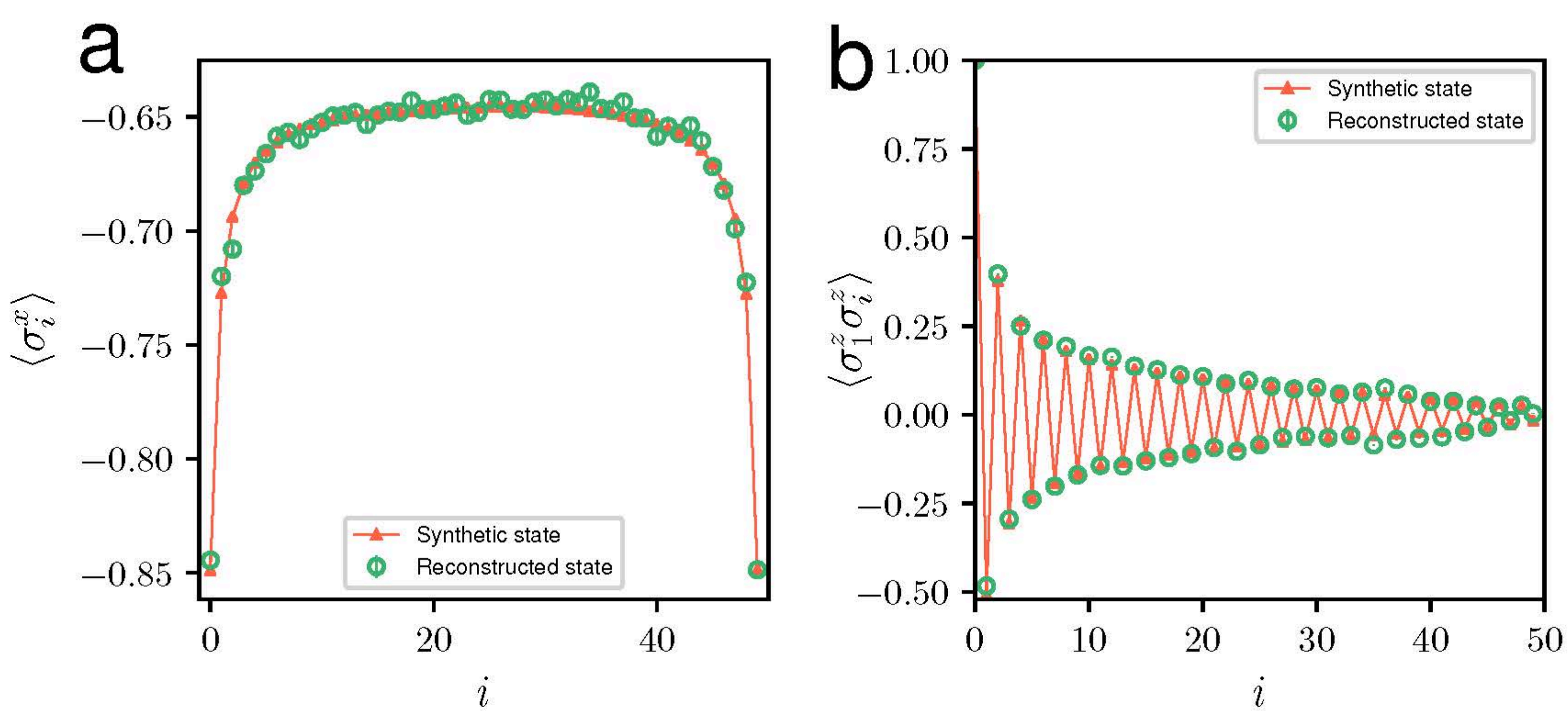


NUMERICAL INVESTIGATION OF THE SAMPLE COMPLEXITY OF LEARNING



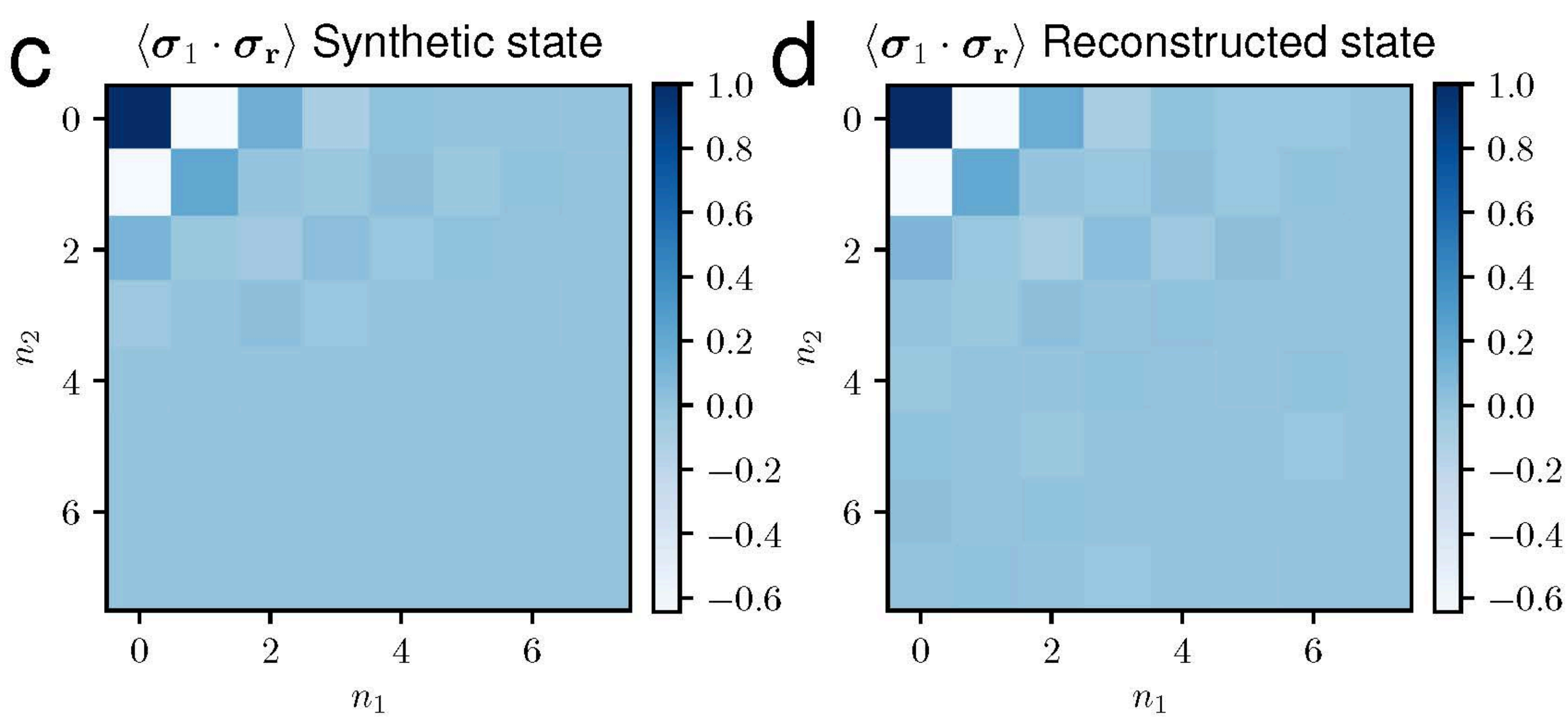
Favorable scaling!

GROUND STATES OF LOCAL HAMILTONIANS

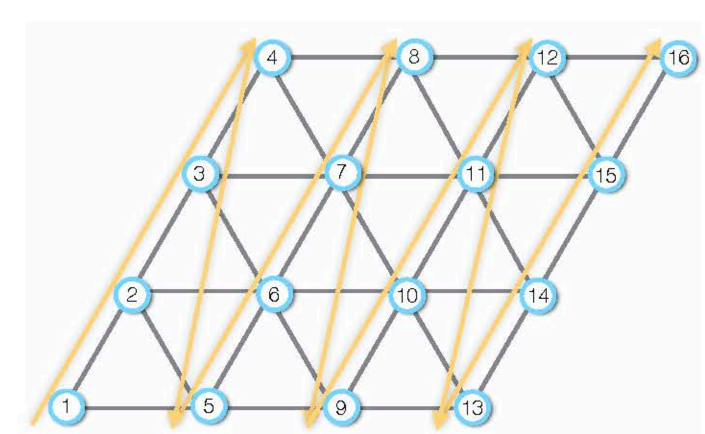


$$\mathcal{H} = J \sum_{ij} \sigma_i^z \sigma_j^z + h \sum_i \sigma_i^x$$

N=50 spins. P(a) is a deep (3 layer GRU) recurrent neural network language model.



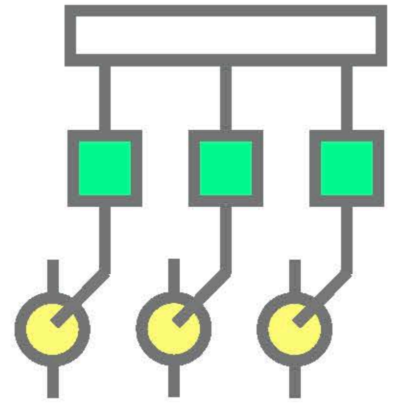
$$H = J \sum_{i,j} \boldsymbol{\sigma}_i . \boldsymbol{\sigma}_j$$



CONCLUSION

- We are starting to explore a machine learning perspective on many-body problems in classical and quantum physics.
- We can discriminate phases and phase transitions, both conventional and topological, using neural network technology.
- We have performed QST based on neural networks with results that are better than the state-of-the-art methods and which enable us to study of 2- and potentially 3-dimensional quantum systems and quantum devices
- I believe there are a lot of opportunities for us physicists. **⟨ PHYSICS | MACHINE LEARNING ⟩**

$$\rho_{\mathrm{model}} = (\mathbf{T}^{-1} P_{\mathrm{model}})^{T} \mathbf{M}$$



2 PhD positions and short-term visits

- If you know students interested in working at the intersection between machine learning, condensed matter theory, numerical simulations of quantum many-body systems, and quantum computers
- Possibility to interact and collaborate with ML and quantum computing experts
- Possibility to interact with industry if you want
- Get in touch with me carrasqu@vectorinstitute.ai
- https://vectorinstitute.ai/team/juan-felipe-carrasquilla/

REGULARIZATION ISSUES

Requisite to specifying a quantum state through P(a), one must have an understanding of the allowed probabilities since not every choice of P(a) will give rise to positive semi-definite density matrix.

Requires regularization that is tricky to perform for large systems

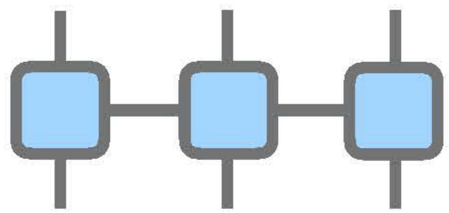
For this tomography problem in particular we just use a lot of data

$$\rho = \sum_{a,a'} T^{-1}_{a,a'} P(a') M^{(a)}$$

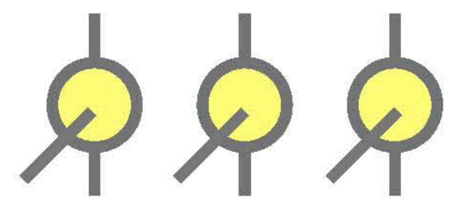
FOR LARGER GHZ STATES USE MPS/MPO

GENERATING **SYNTHETIC** DATA FOR BIG SYSTEMS EFFICIENTLY USING TENSOR NETWORKS

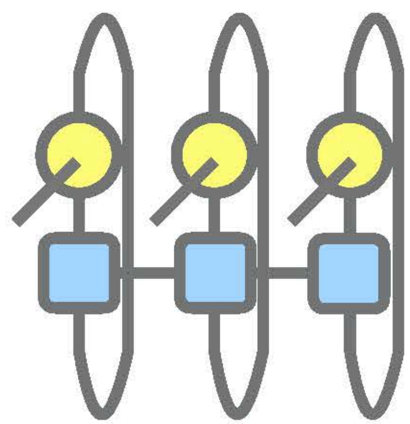
ρ



$\mathbf{M}$

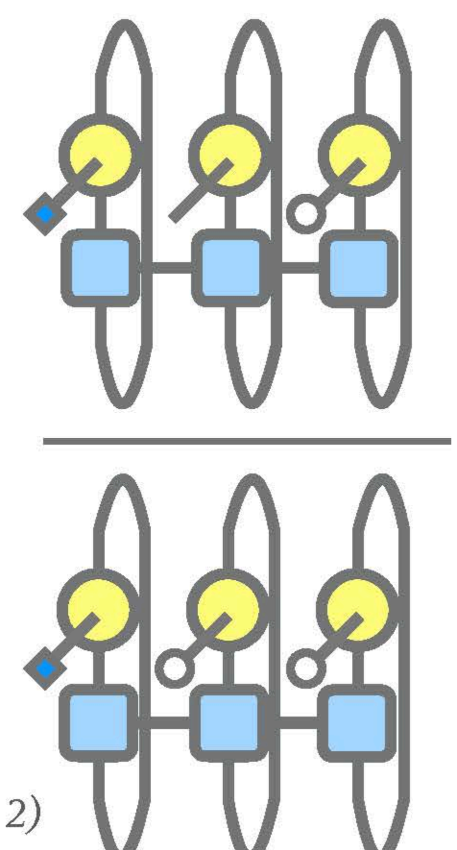


$$P\left(\mathbf{a}\right) = \mathrm{Tr}\,\rho M^{\mathbf{a}}$$



Can be sampled in polynomial time exactly (zipper algorithm)

$$P(a_i|a_{<i}) = \frac{\sum_{a_{j>i}} P(\mathbf{a})}{\sum_{a_{j\geq i}} P(\mathbf{a})}$$

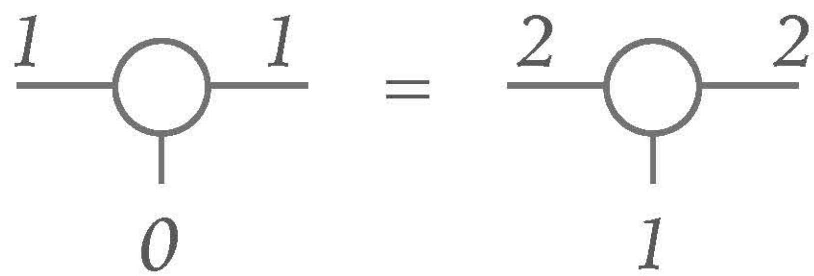


$P(a_2|a_1)$

AJ Ferris and G. Vidal. PRB 85, 165146 (2012)

FOR LARGER GHZ STATES USE MPS/MPO

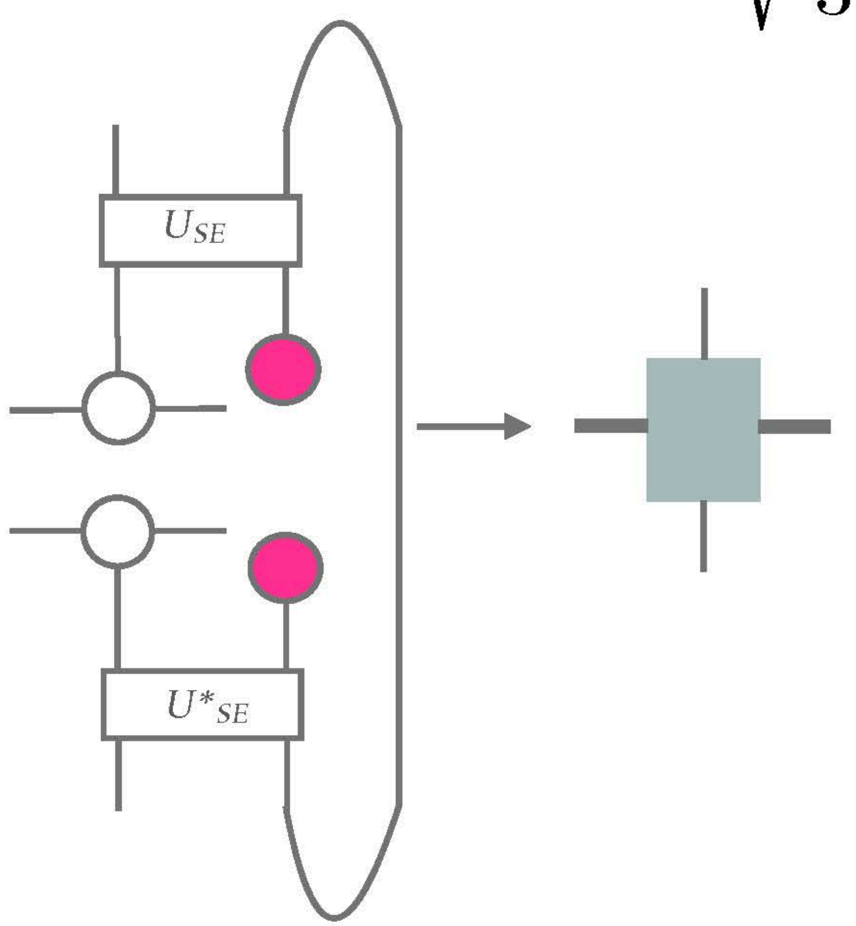
Pure GHZ = MPS

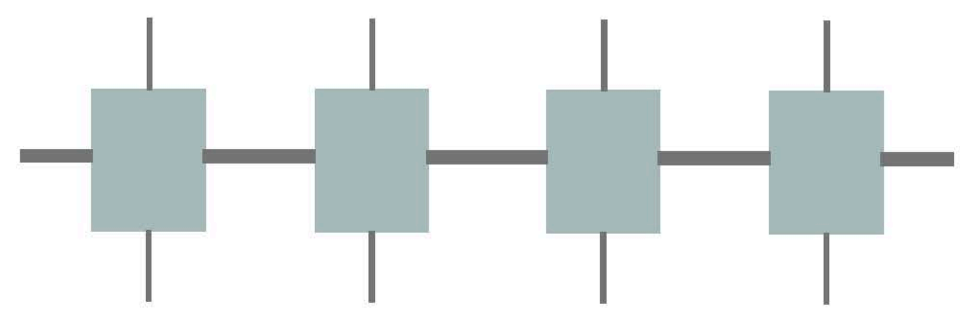


$= 2^{-1/(2N)}$

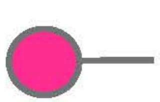
Locally depolarized GHZ

$$U_{SE} = \mathbb{1}_S \otimes |0\rangle\langle 0|_E + \sqrt{\frac{p}{3}}\,(\sigma_S^x \otimes |1\rangle\langle 0|_E + \sigma_S^y \otimes |2\rangle\langle 0|_E + \sigma_S^z \otimes |3\rangle\langle 0|_E)$$





Locally depolarized GHZ = MPO

 = *(1 0 0 0)*

Preskill's notes http://www.theory.caltech.edu/people/preskill/ph219/

DEPOLARIZING CHANNEL

3.4.1 Depolarizing channel

The *depolarizing channel* is a model of a decohering qubit that has particularly nice symmetry properties. We can describe it by saying that, with probability $1-p$ the qubit remains intact, while with probability p an "error" occurs. The error can be of any one of three types, where each type of error is equally likely. If $\{|0\rangle, |1\rangle\}$ is an orthonormal basis for the qubit, the three types of errors can be characterized as:

1. Bit flip error: $\begin{smallmatrix} |0\rangle \mapsto |1\rangle \\ |1\rangle \mapsto |0\rangle \end{smallmatrix}$ or $|\psi\rangle \mapsto \boldsymbol{\sigma}_1 |\psi\rangle, \boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$,

2. Phase flip error: $\begin{smallmatrix} |0\rangle \mapsto |0\rangle \\ |1\rangle \mapsto -|1\rangle \end{smallmatrix}$ or $|\psi\rangle \mapsto \boldsymbol{\sigma}_3 |\psi\rangle, \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$,

3. Both: $\begin{smallmatrix} |0\rangle \mapsto +i|1\rangle \\ |1\rangle \mapsto -i|0\rangle \end{smallmatrix}$ or $|\psi\rangle \mapsto \boldsymbol{\sigma}_2 |\psi\rangle, \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$.

If an error occurs, then $|\psi\rangle$ evolves to an ensemble of the three states $\boldsymbol{\sigma}_1|\psi\rangle, \boldsymbol{\sigma}_2|\psi\rangle, \boldsymbol{\sigma}_3|\psi\rangle$, all occurring with equal likelihood.

Unitary representation. The depolarizing channel mapping qubit A to A can be realized by an isometry mapping A to AE, where E is a four-dimensional environment, acting as

$$\begin{aligned} \boldsymbol{U}_{A\to AE} : |\psi\rangle_A \mapsto & \sqrt{1-p}\; |\psi\rangle_A \otimes |0\rangle_E \\ & + \sqrt{\frac{p}{3}} \left(\boldsymbol{\sigma}_1 |\psi\rangle_A \otimes |1\rangle_E + \boldsymbol{\sigma}_2 |\psi\rangle_A \otimes |2\rangle_E + \boldsymbol{\sigma}_3 |\psi\rangle_A \otimes |3\rangle_E \right). \end{aligned} \tag{3.83}$$

Preskill's notes http://www.theory.caltech.edu/people/preskill/ph219/

NEUMARK'S DILATION THEOREM

How one can implement a general quantum measurement by performing a unitary on the system of interest and an ancilla, followed by a von Neumann measurement of the ancilla.

$$P(a) = \mathrm{Tr}\rho M^{(a)} = \mathrm{Tr}\left[\mathbf{I}_s \otimes |a\rangle\langle a|_p U_{sp}\rho \otimes |0\rangle\langle 0|_p U_{sp}^{\dagger}\right]$$

- Requires projective measurements in only one basis set

Experimental schemes see: Phys. Rev. A 86, 062107 (2012), Phys. Rev. A 83, 051801(R) (2011), Phys. Rev. A 91, 042101 (2015)