Applications of machine learning in condensed matter

Fabien Alet

Laboratoire de Physique Théorique, Toulouse

pdf of the talk & list of references

SCAN ME

Mostly a review + works with
Hugo Théveniaut & Sylvain Capponi (LPT)

GDR MEETICC Conférence plénière 2022
Jun. 2022, Ax-les-thermes

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Some Applications of machine learning in condensed matter

Disclaimer: *as seen by an amateur*

- Too many methods / ideas / techniques / attempts ….
- An (already old, not specific) review

REVIEWS OF MODERN PHYSICS

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Acc

Machine learning and the physical sciences*

Giuseppe Carleo, Ignacio Cirac, Kyle Cranmer, Laurent Daudet, Maria Schuld, Naftali Tishby, Leslie Vogt-Maranto, and Lenka Zdeborová

Rev. Mod. Phys. **91**, 045002 – Published 6 December 2019

- More recent (but not entirely specific)

arXiv > quant-ph > arXiv:2204.04198

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Quantum Physics

[Submitted on 8 Apr 2022]

Modern applications of machine learning in quantum sciences

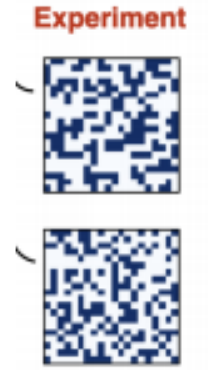
Anna Dawid, Julian Arnold, Borja Requena, Alexander Gresch, Marcin Płodzień, Kaelan Donatella, Kim Nicoli, Paolo Stornati, Rouven Koch, Miriam Büttner, Robert Okuła, Gorka Muñoz-Gil, Rodrigo A. Vargas-Hernández, Alba Cervera-Lierta, Juan Carrasquilla, Vedran Dunjko, Marylou Gabrié, Patrick Huembeli, Evert van Nieuwenburg, Filippo Vicentini, Lei Wang, Sebastian J. Wetzel, Giuseppe Carleo, Eliška Greplová, Roman Krems, Florian Marquardt, Michał Tomza, Maciej Lewenstein, Alexandre Dauphin

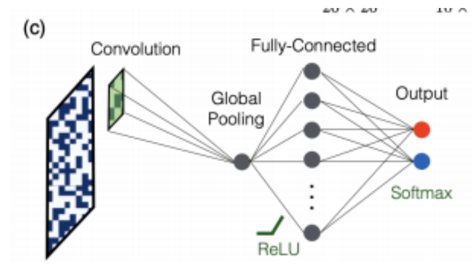
In these Lecture Notes, we provide a comprehensive introduction to the most recent advances in the application of machine learning methods in quantum sciences. We cover the use of deep learning and kernel methods in supervised, unsupervised, and reinforcement learning algorithms for phase classification, representation of many-body quantum states, quantum feedback control, and quantum circuits optimization. Moreover, we introduce and discuss more specialized topics such as differentiable programming, generative models, statistical approach to machine learning, and quantum machine learning.

Some Applications of Machine learning in quantum physics

Analysis of data generated in condensed matter / AMO

Experimental images (STM, quantum gas microscope)

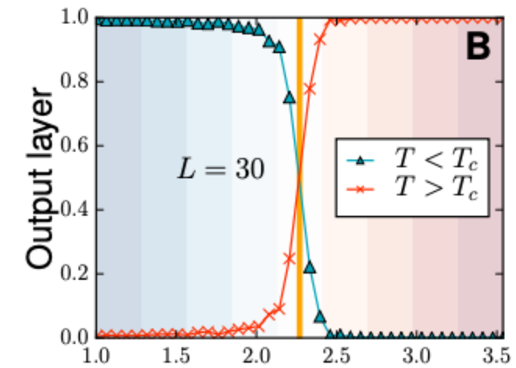




Zhang *et al.*, Nature (2019)

Khatami *et al.*, PRA (2020)

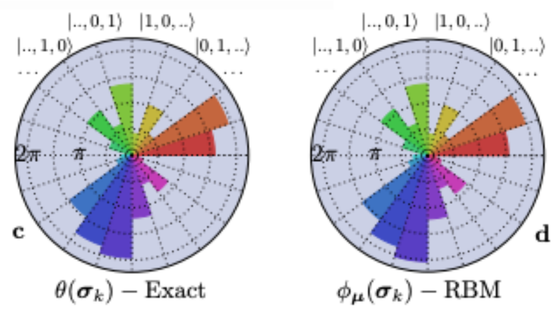
Synthetic data (e.g. Monte Carlo snapshots)



Carrasquilla, Melko., Nat. Phys. (2017)

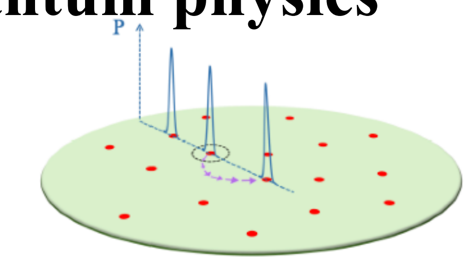
Quantum state tomography

Torlai *et al.*, Nat. Physics (2018)



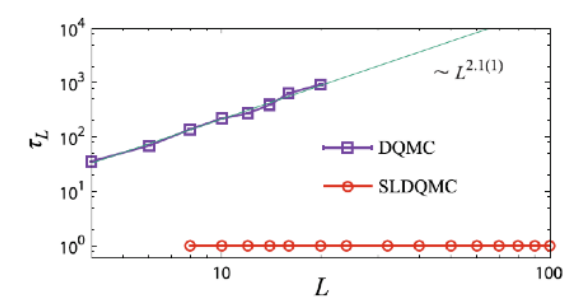
Computational quantum physics

Supervized/Reinforcement learning to find efficient Monte Carlo moves



Xu et *al.*, PRB (2017)

Zhao et *al.*, PRE (2019)

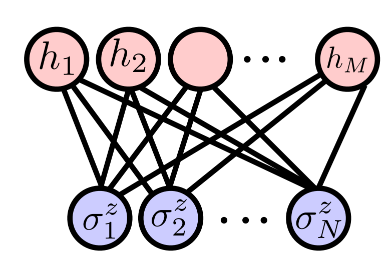


Neural Autoregressive Density estimators for perfect sampling

$$P(s_1, s_2, ..., s_N) = \prod_i p_i(s_i|s_{i-1}, ..., s_1)$$

Sharir e*t al.*, PRL (2020)

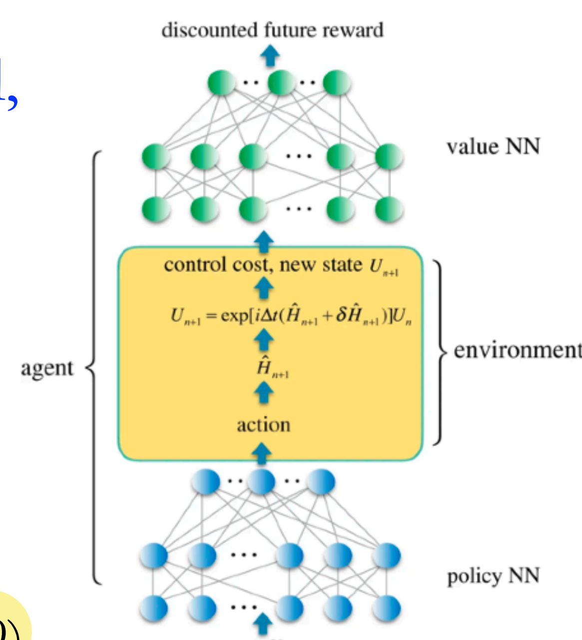
Neural quantum states as a variational ansatz



ML-based control/help of quantum experiments/ computations

Open or closed-loop control, in q. experiments

Quantum computing (optimisation of quantum gates, neural-network parameterized quantum circuit, quantum error correction)



Niu et al., NPJ Qu. Inf. (2019)

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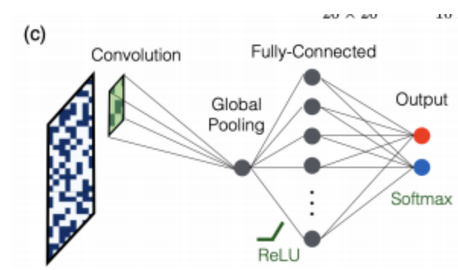

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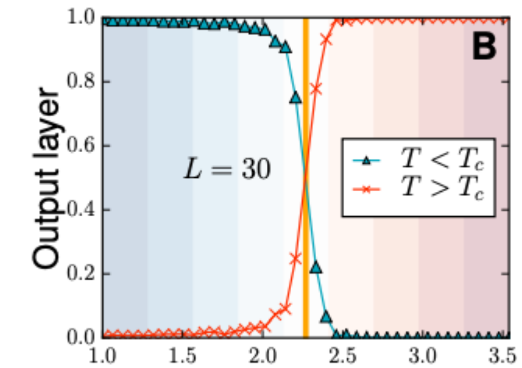
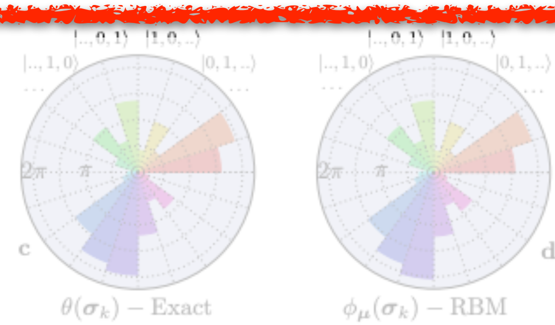


Part 1. Analysis of experimental / synthetic data

Quantum state tomography



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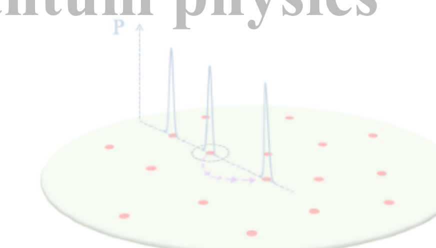

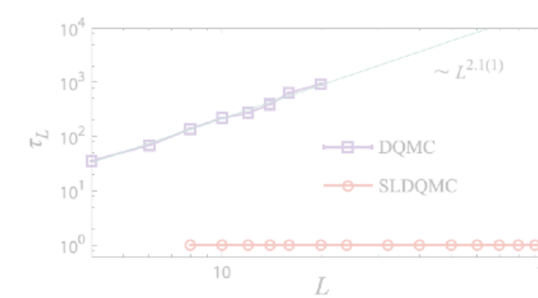

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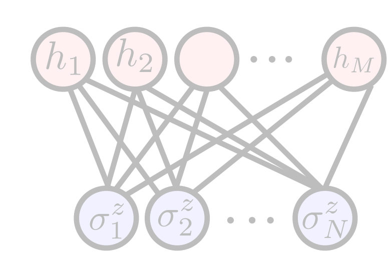

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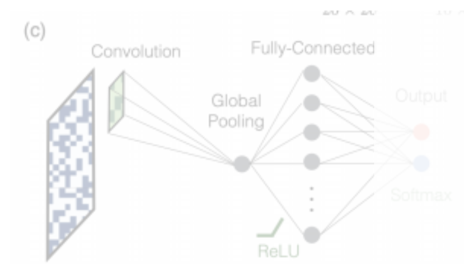

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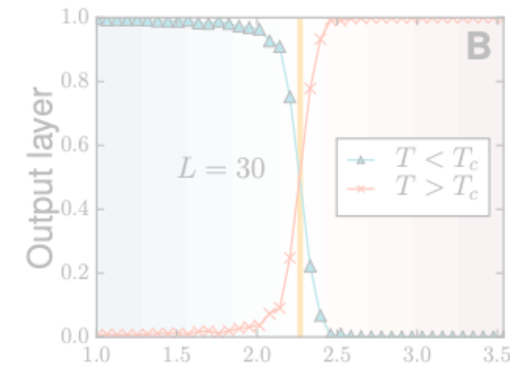

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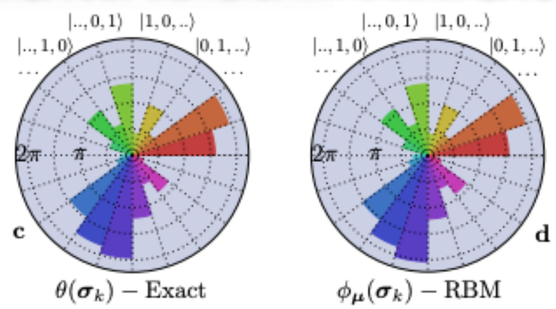
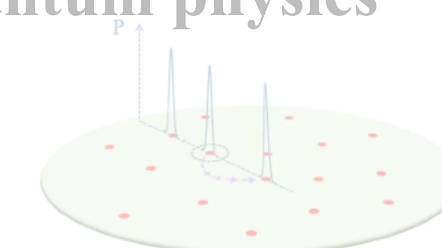
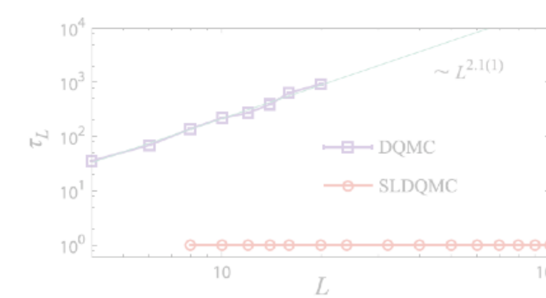


Part 2. Neural quantum states

Computational quantum physics

Supervized/Reinforcement learning to find efficient Monte Carlo moves





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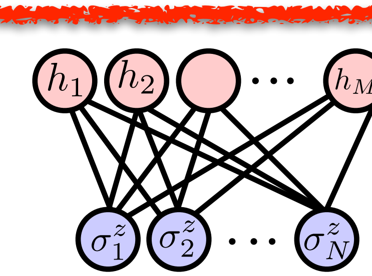

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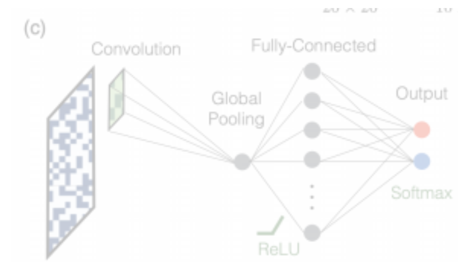

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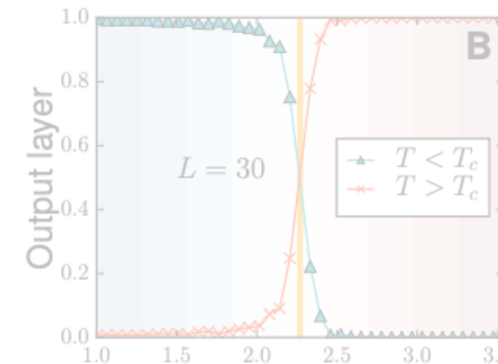
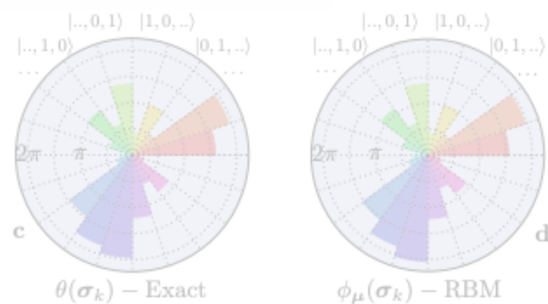


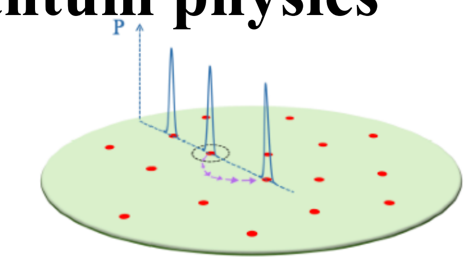
Quantum state tomography

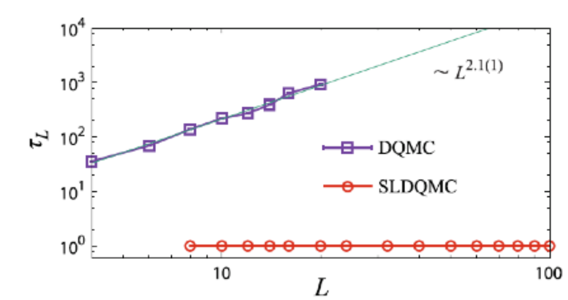


Part 3. Creation of improved algorithms

Computational quantum physics

Supervized/Reinforcement learning to find efficient Monte Carlo moves





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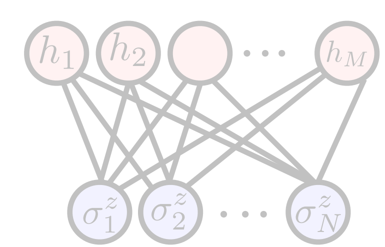


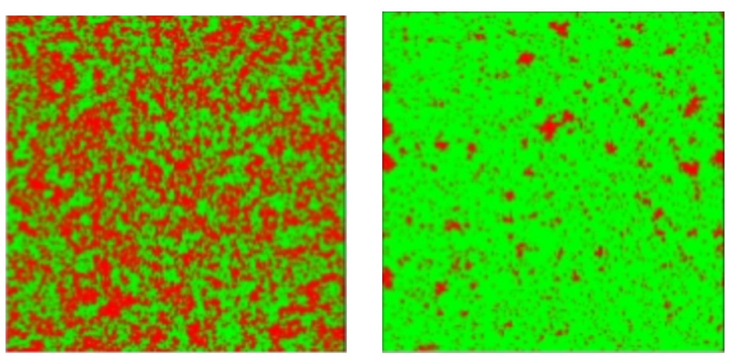
1. Analysis of experimental / synthetic data

Automatic detection of phases and phase transitions

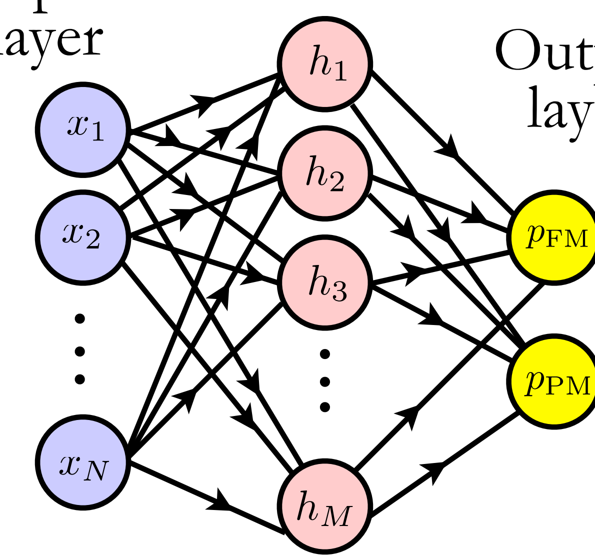
- **Idea :** Machine learning is good at classifying images. Let's try to classify **different phases of matter**, given some input (ideally « pictures »)

Example 1 (synthetic data) : Snapshots of Monte Carlo samples of 2d Ising model

Training at extremal regions of phase space

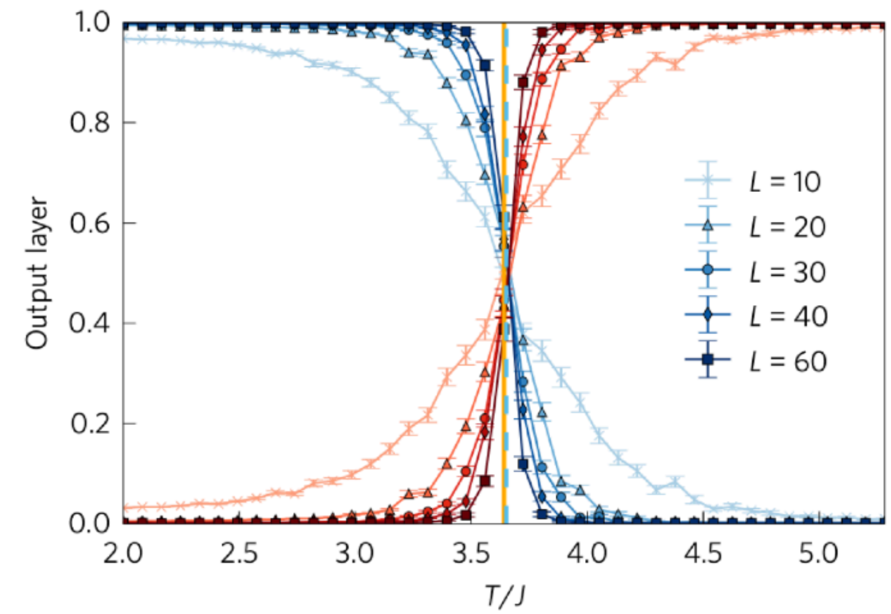


High temperature   Low temperature



Carrasquilla, Melko, Nature Physics (2017)

Prediction over the whole phase space



- Conclusion : Very simple networks pick the critical temperature (& critical exponents) with good accuracy (even if trained only at low / high T)
- More sophisticated networks & architectures can be used
- More complex phases have been detected (topological phases, disordered localized phases) albeit often with feature-engineered data (physics based)

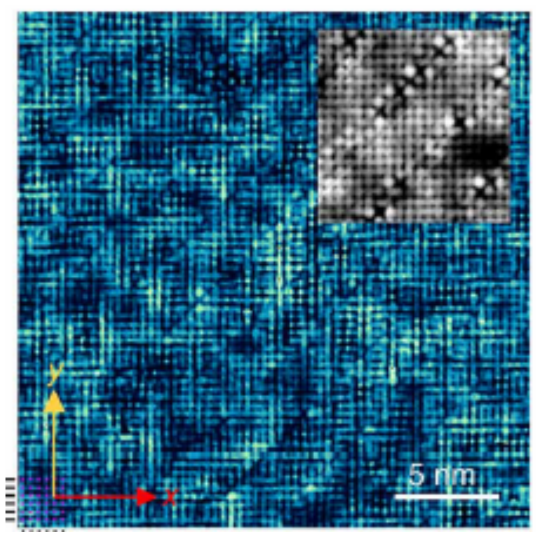
Automatic detection of phases and phase transitions

- **Idea :** Local probes in physics generate a large amount of data/images that ML can exploit

Example 2 (experimental data) : STM images on high-temperature superconductors

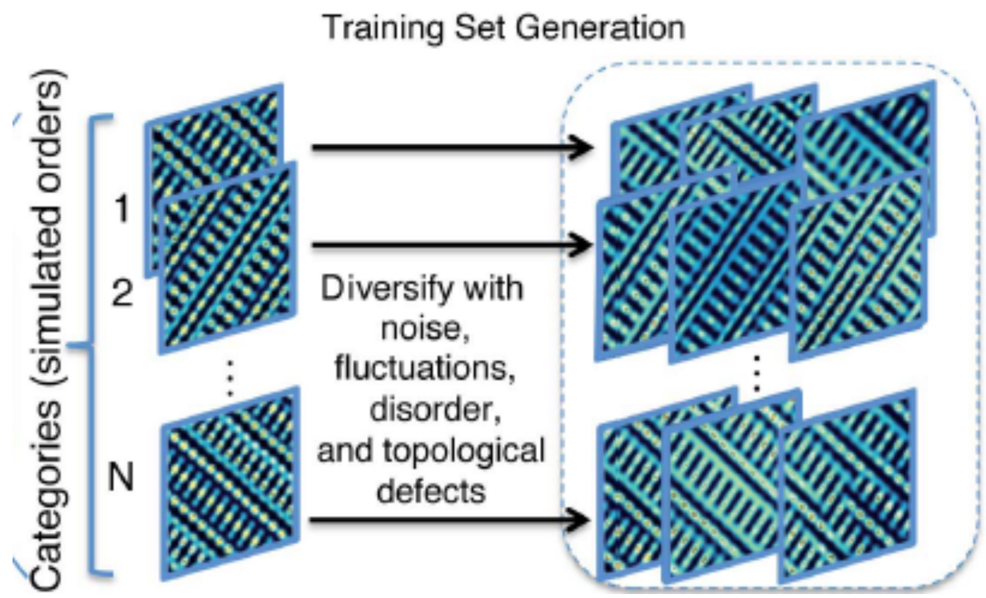
- **Physics question:** is electronic density showing a modulation? Important to discriminate theories
- Fourier analysis is not precise enough

Zhang *et al.*, Nature (2019)

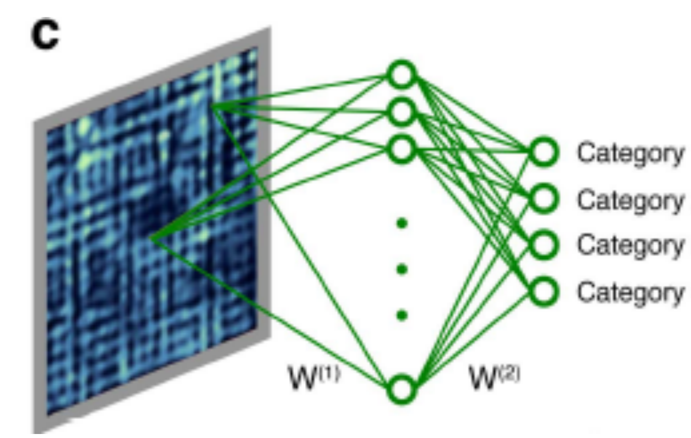


Typical STM image

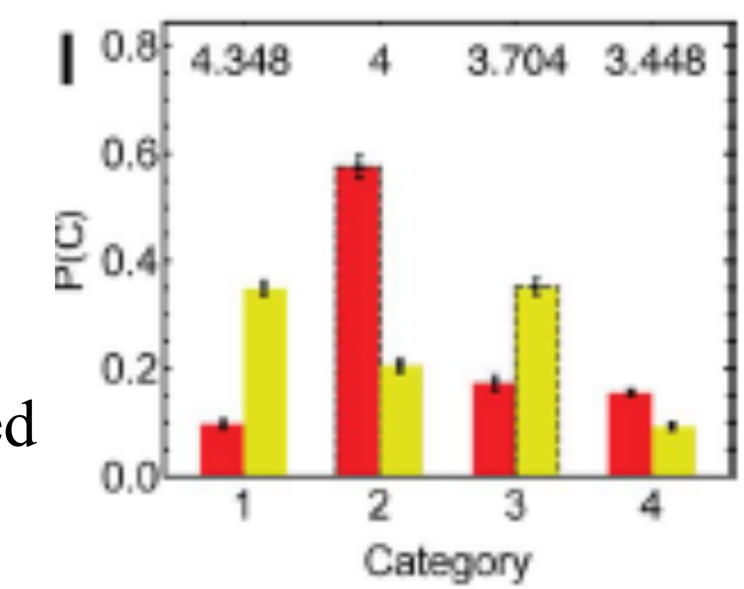
$Bi_2Sr_2CaCu_2O_8$



Train with different test modulations (« categories »)



Prediction: Category output



- **Physics conclusion 1: Fixed commensurate modulation at 4a** in the pseudo-gap phase for a large parameter regime.

- Moreover, different output probabilities depending on images presented in x or y direction. **Physics conclusion 2 : electronic nematic state**

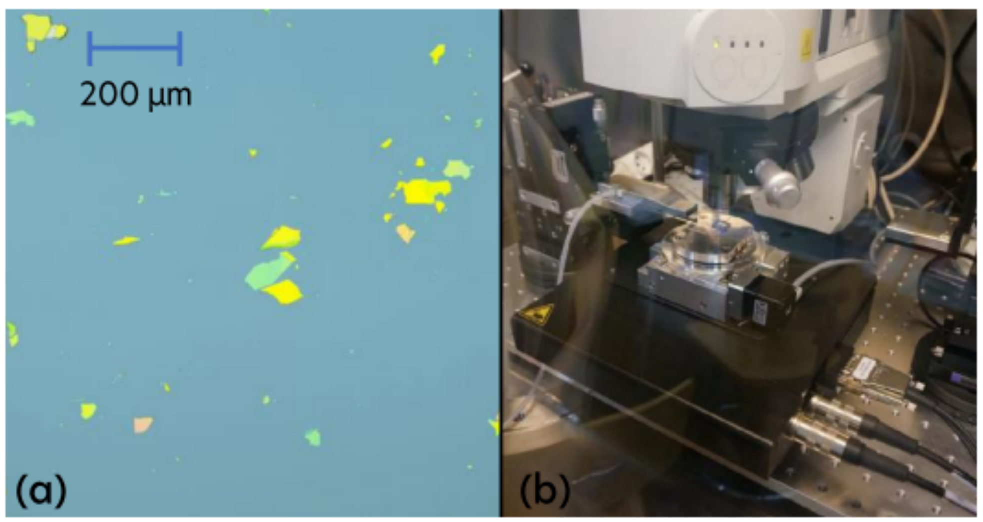
Automatic detection of « good samples »

- **Idea :** Some laborious part of experiments can be easily automated

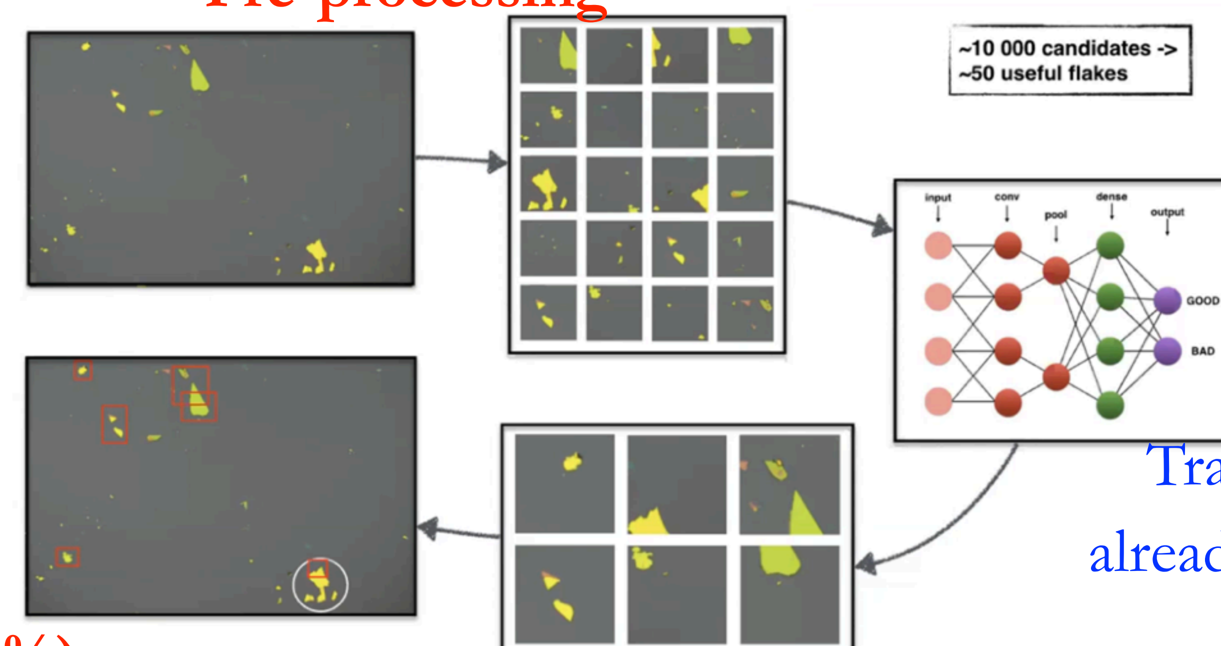
Example 3 (experimental data) : Detection of flakes in 2d material physics

Greplova *et al.*, PR Applied (2020)

- **Problem:** Prepare 2d materials by selecting flakes in exfoliated hbN on a silicon waffer
- Difficult and lengthy task because of the diversity of the data and the sparsity of « good » flakes



Pre-processing



Training already made

Validation by user (acceptance rate = 50%)

Prediction of candidate flakes

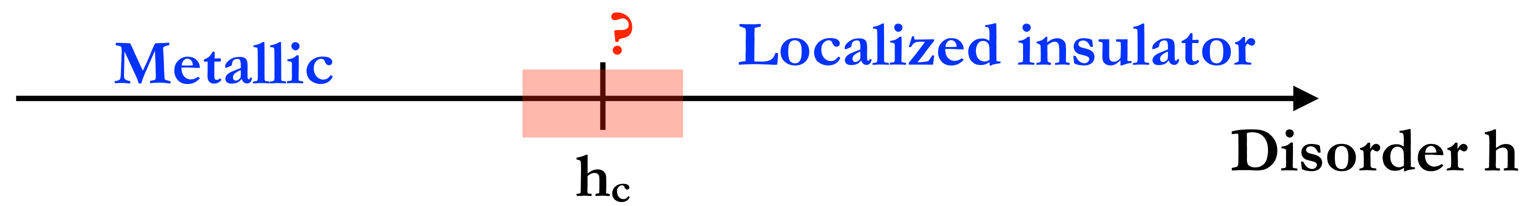
- Rk: The sparsity (< 1%) of good flakes requires a careful training
- Robustness: against changes in the microscopy conditions (illumination, color balance etc)
- Transfer learning: good transferability to other systems to speed up training

Related work in other experimental setups: Han *et al.*, NPJ Adv. Mater. (2020) Masubuchi *et al.*, NPJ 2d Mater. (2020)

Our work: Characterize the many-body localization transition

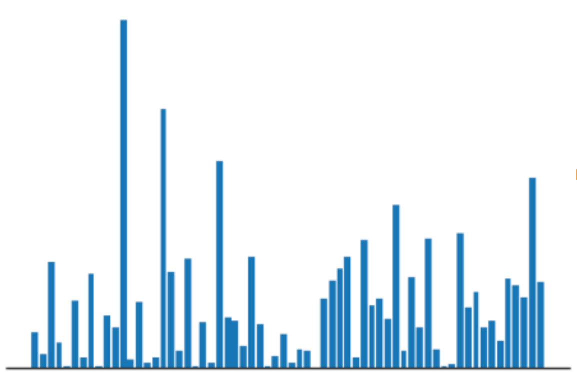
- **Many-body localization:** due to strong disorder, a metallic system can become insulating (even at very high energies!)

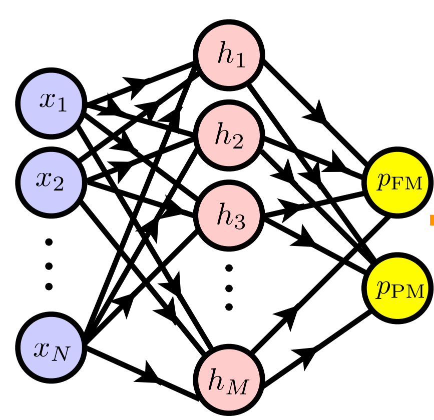
Model = Quantum spin chain + random magnetic field of strength h

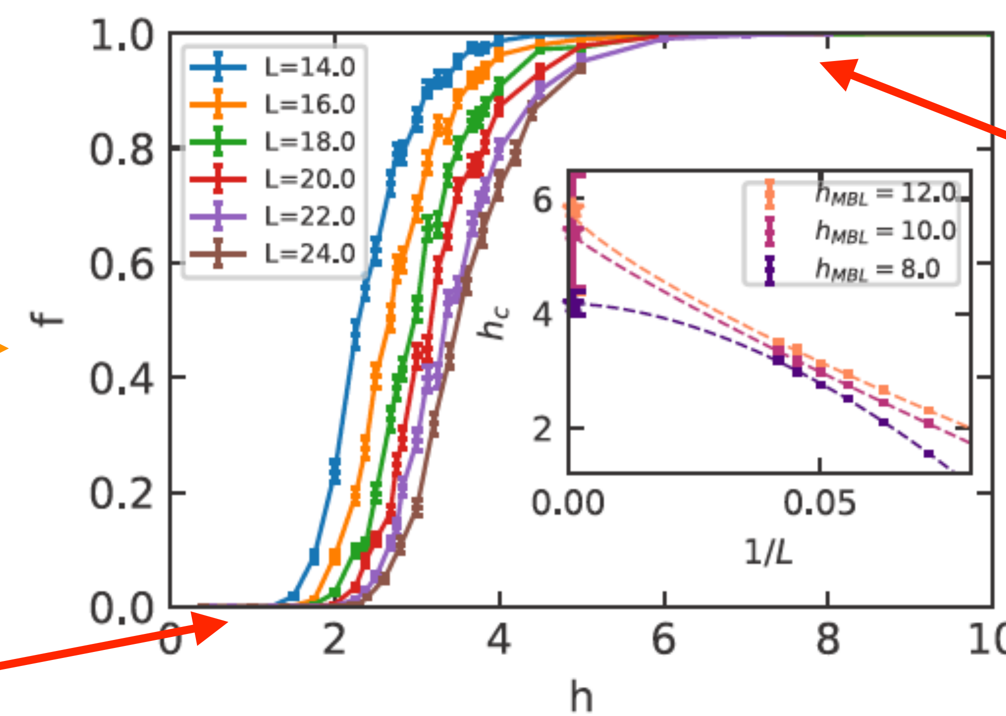


- **Motivation:** Reasonable estimate (but not precise) of the transition point from physics analysis. Universality class unknown (reasons: Simulations only on small samples + No known order parameter)
- **Guidelines for ML analysis:** Least possible human bias (we include no physics). Scalability with system size, interpretability if possible

Input:
Eigenstate amplitudes







Insulating prediction

Théveniaut, FA, PRB (2019)

Metal prediction

Overall phase diagram relatively well recognized (with strongly metallic and insulating phases)

Our work: Characterize the many-body localization transition

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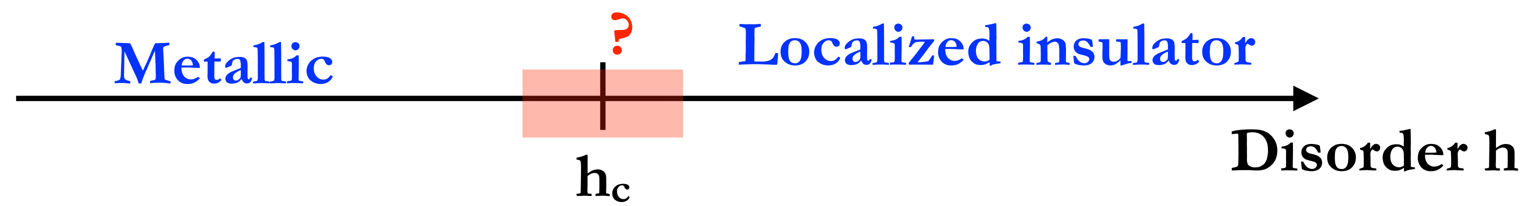

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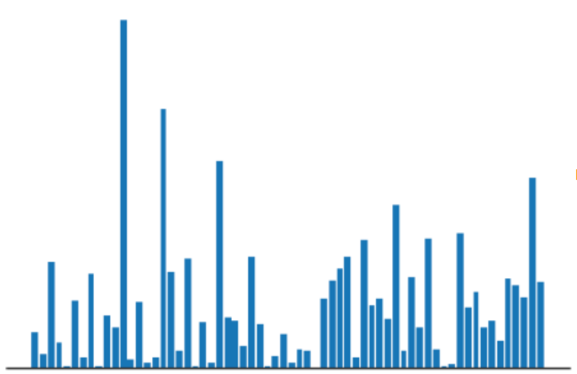
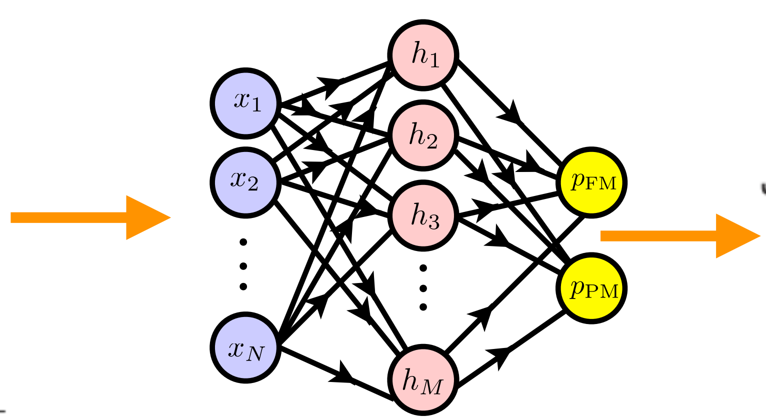
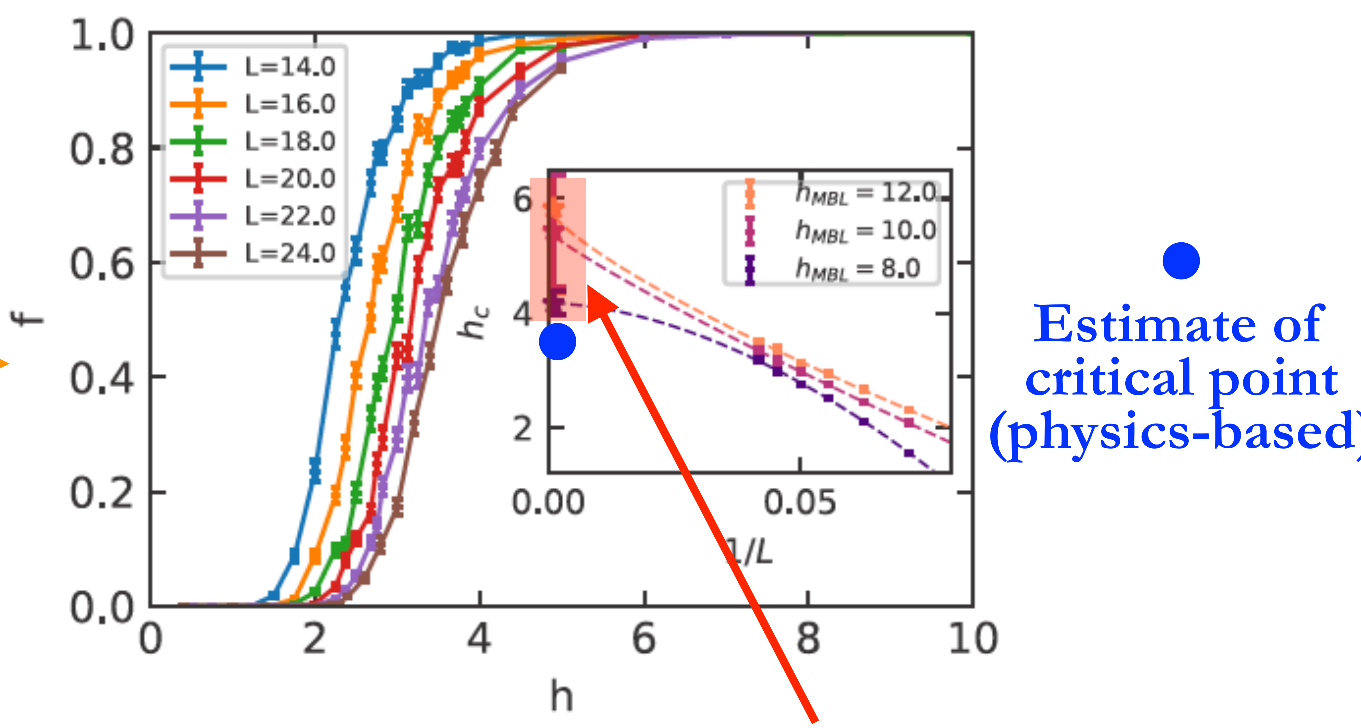






Théveniaut, FA, PRB (2019)

Large error bars on critical point

- **Conclusions *(for this problem)*:** 1. Difficult to obtain precise results without bias (e.g. input data)
  2. ML does not free from finite-size effects

2. Neural quantum states

Learning $|\Psi\rangle$

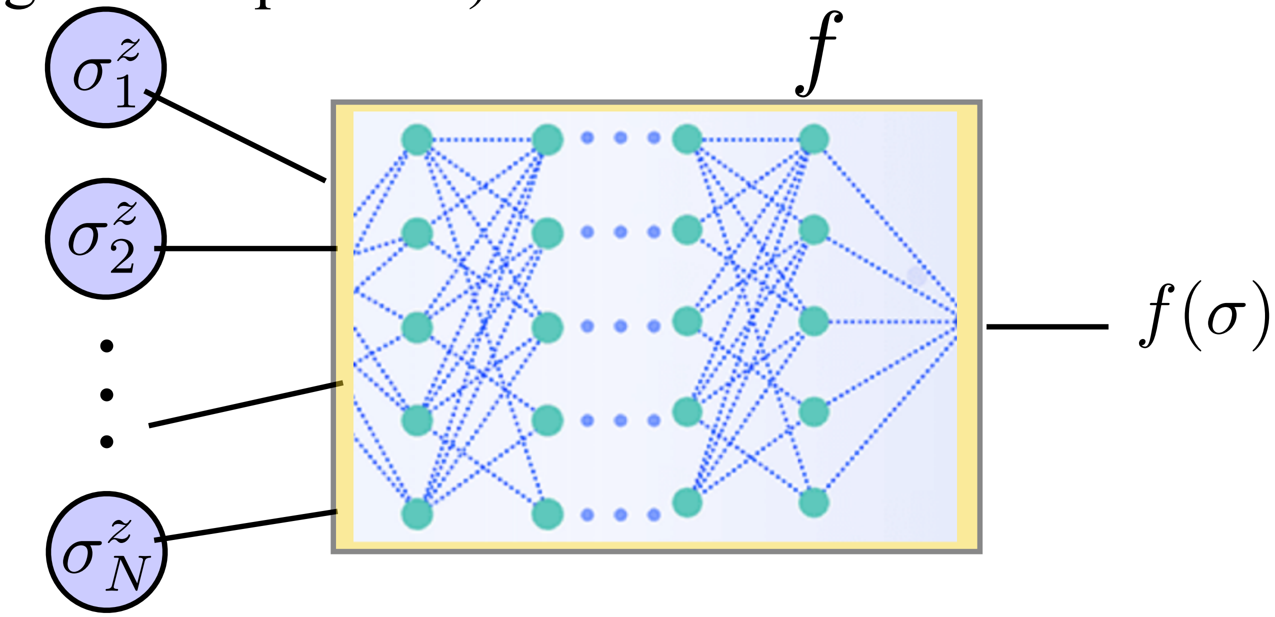
Neural quantum states

Carleo & Troyer, Science (2017)

- Parametrization of a quantum wave-function (e.g. for N spins 1/2) with a neural network

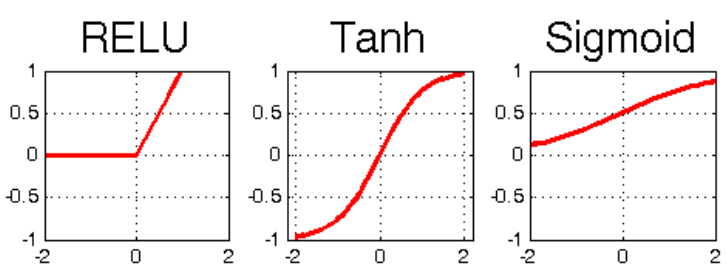
$$|\Psi\rangle = \sum_{\sigma} f(\sigma)|\sigma\rangle$$

$$\sigma = \{\sigma_1^z, ..., \sigma_N^z\}$$



$$f_{\mathrm{NN}}(|\sigma\rangle) = g_L \circ \mathbf{W}_L\, g_{L-1} \circ \ldots \mathbf{W}_2\, g_1 \circ \mathbf{W}_1 |\sigma\rangle$$

- **g non-linear function**



Element-wise

$$g|\sigma\rangle = \begin{bmatrix} g(\sigma_1^z) + b_1 \\ g(\sigma_2^z) + b_2 \\ \vdots \\ g(\sigma_N^z) + b_N \end{bmatrix}$$

- **W = Matrices of "weights"**

In general complex

$$W|\sigma\rangle = \begin{bmatrix} W_{11} & W_{12} & \ldots & W_{1N} \\ W_{21} & W_{22} & \ldots & W_{2N} \\ \ldots & \ldots & \ldots & \ldots \\ W_{r1} & W_{r2} & \ldots & W_{rN} \end{bmatrix} \begin{bmatrix} \sigma_1^z \\ \sigma_2^z \\ \vdots \\ \sigma_N^z \end{bmatrix}$$

- The architecture of the network (number & size of layers, choice of non-linear function) is free

In general fixed

- The weights **W** and bias **b** are variational parameters to optimise upon

Some examples

Simplest example: Restricted Boltzmann Machine (RBM)

Carleo & Troyer, Science (2017)

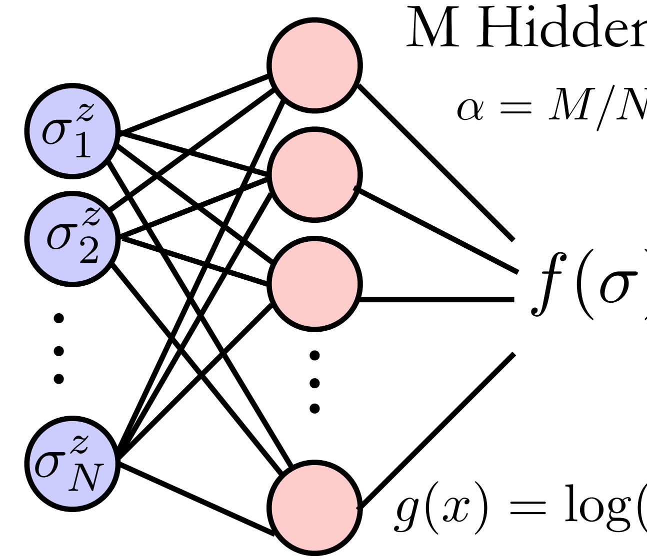
$$\Psi(\sigma) = \sum_{h_i} \exp[\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{i,j} W_{ij} h_i \sigma_j^z]$$

$$= \prod_i \left[\cosh(\sum_j W_{ij}\sigma_j^z + b_i)\right] \exp(\sum_j a_j \sigma_j)$$

$\sigma_i^z = \pm 1$

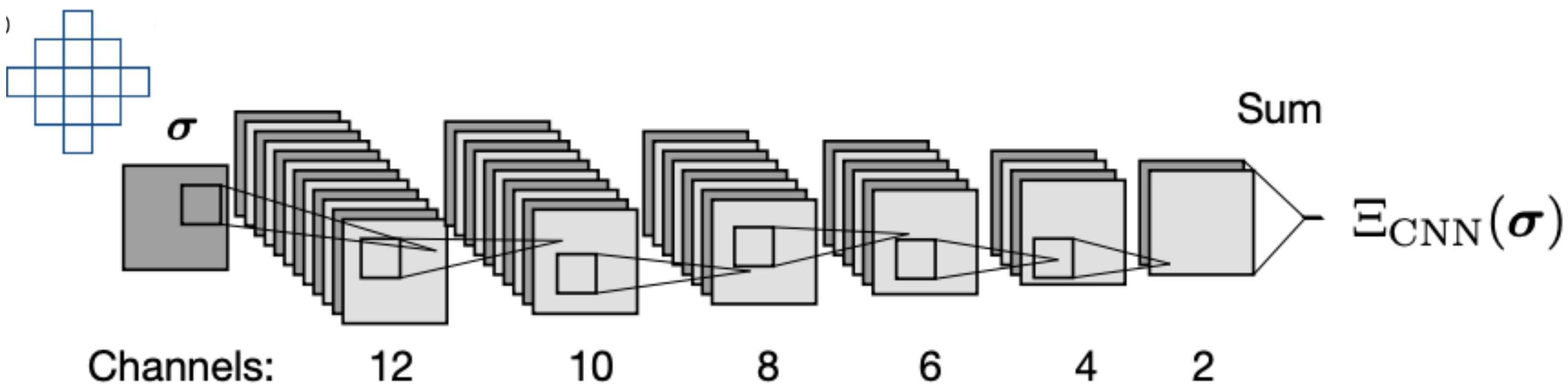
M Hidden neurons

$\alpha = M/N \sim 1, ..., 10$



$g(x) = \log(\cosh(x))$

Convolutional neural network (CNN)



$$\mathsf{h}^{(q)}_{i,j,k} = F\left(\sum_{l,m_y,m_x} \mathsf{h}^{(q-1)}_{l,j+m_y,k+m_x} \mathsf{K}^{(q)}_{i,l,m_y,m_x}\right)$$

$$:= F\left(\mathsf{K}^{(q)} * \mathsf{h}^{(q-1)}\right)$$

Choo *et al.*, 2019

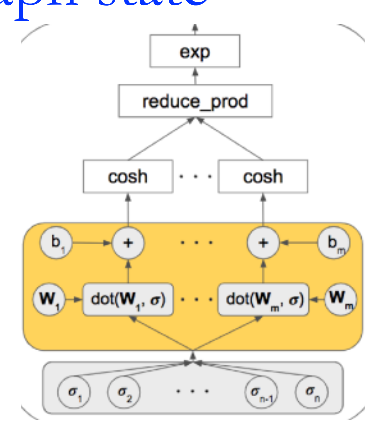
Takes explicit advantage of locality through **filters**
Calculations are lighter-weight

Computational graph states

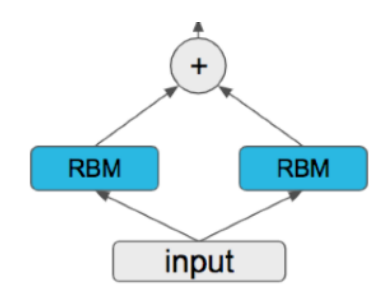
Useful to define neural network as computational graphs states : allows to combined and modify architectures efficiently

Kochkov & Clark, arXiv:1811.12423

RBM as a computational graph state



Combining 2 RBM



Why quantum neural states?

- Universal representation theorems for multi-layer networks

…

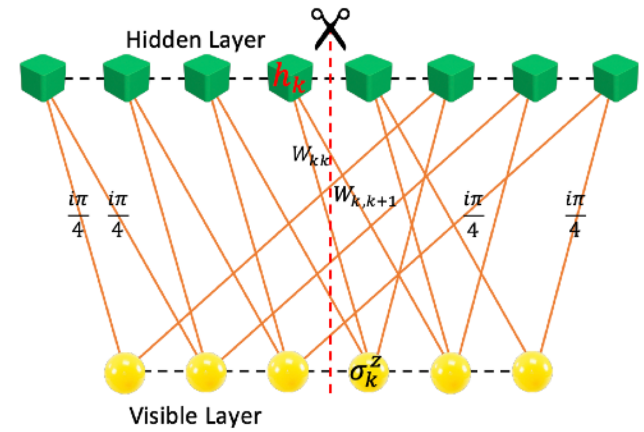
Does not necessarily help in building this network in practice

Cautions about too shallow networks

- Physical arguments: (Deep) neural networks can have volume-law entanglement

Levine et al., PRL (2019)

Deng, Li, Das Sarma., PRX (2017)



With order N parameters

- Relation to other approaches:

  Many of your favorite variational wave-functions can be combined with/translate into NQS

  Relation between NQS and tensor-network states

  Efficient contractible TNS can be constructed as NN (with polynomial size) — Sharir et al., arXiv:2103.10293

  RBM (and deep BM) can be represented as 2d TNS — Li *et al.*., arXiv:2105.04130

- Computational advantage: Harness all advances by ML community
  - Algorithms (automatic differentiation, backpropagation, optimisers…)
  - Software (TensorFlow, Pytorch, Keras, Jax etc)
  - Hardware (TPUs, GPUs)

- Starting in practice:

  How To Use Neural Networks To Investigate Quantum Many-Body Physics

  Juan Carrasquilla and Giacomo Torlai

  PRX Quantum **2**, 040201 – Published 12 November 2021

  Tutorial

  Carleo *et al.*, Software X (2019)

  Efficient Python library (spins models)

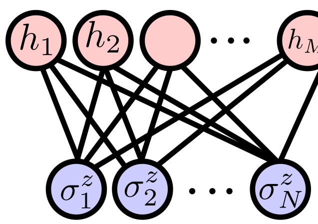
2. Neural quantum states

Application 1 : Variational ansatz for ground-states of strongly correlated systems

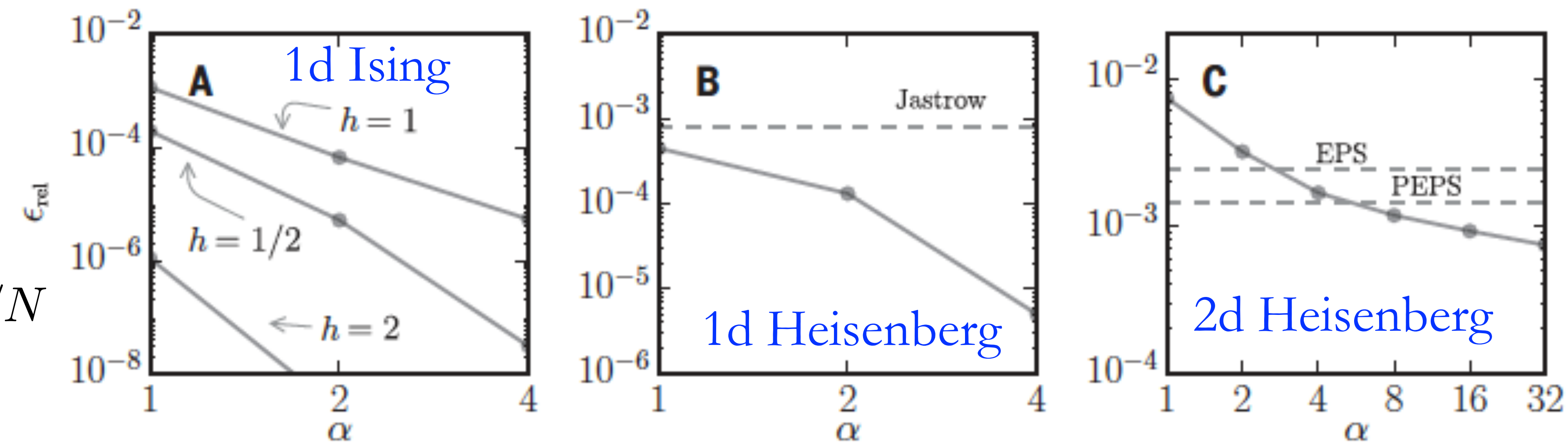
Variational efficiency of neural quantum states in practice

First simulations on quantum magnets (RBM)

Carleo & Troyer, Science (2017)



$\alpha = M/N$



RBM + Pair Projected

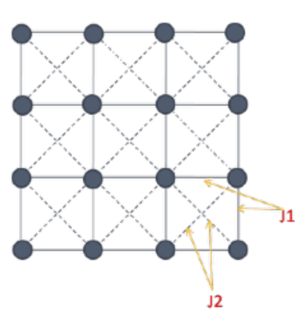
$$\Psi(\sigma) = \phi_{\rm RBM}(\sigma)\psi_{\rm PP}(\sigma)$$

$$|\psi_{\rm PP}\rangle = P_{\rm G}\left(\sum_{i,j} f_{ij}^{\uparrow\downarrow} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger\right)^{N_{\rm site}/2}|0\rangle$$

Frustrated magnets: Convolutional neural networks

Choo *et al.*, 2019

2d J1-J2 model



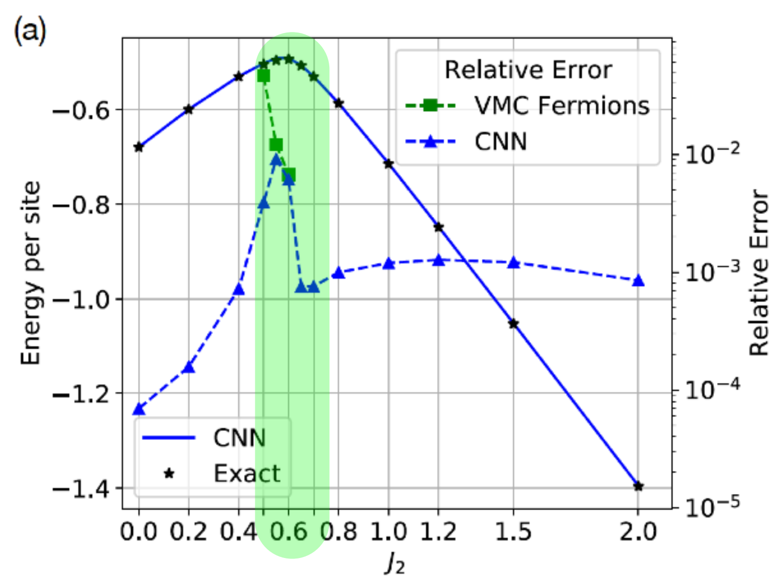


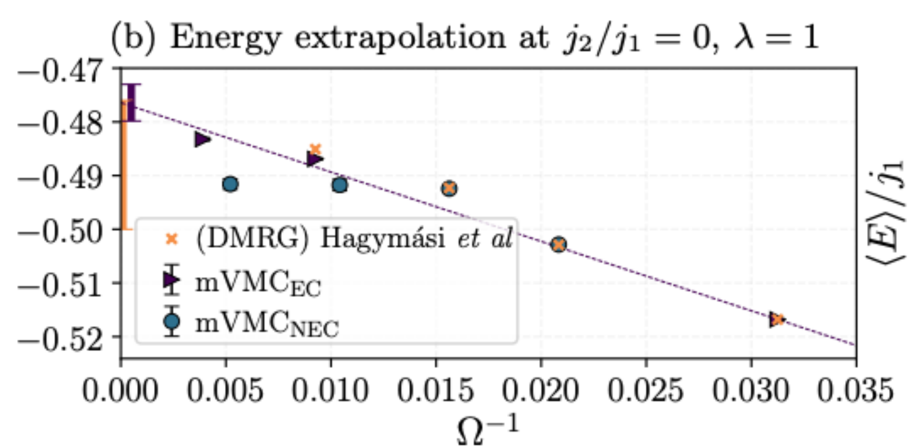
TABLE II. Comparison of ground-state energy for the 10×10 lattice at $J_2 = 0.5$ among different wave functions. The wave functions in bold font use neural networks. In Ref. [18], p-th order Lanczos steps are applied to the VMC wave function.

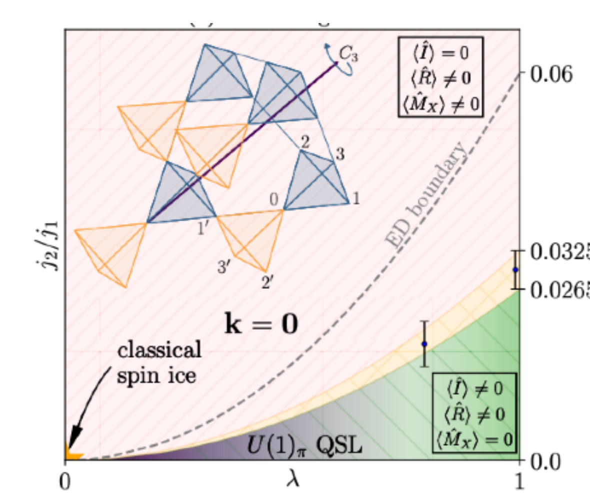
Energy per site	Wave function	Referen
−0.494757(12)	**Neural quantum state**	65
−0.49516(1)	**CNN**	60
−0.49521(1)	VMC(p=0)	18
−0.495530	DMRG	22
−0.49575(3)	**RBM-fermionic w.f.**	63
−0.497549(2)	VMC(p=2)	18
−0.497629(1)	**RBM+PP**	presen

Nomura, Imada (2021)

3d Pyrochlore

Astrakhantsev *et al.* PRX (2021)



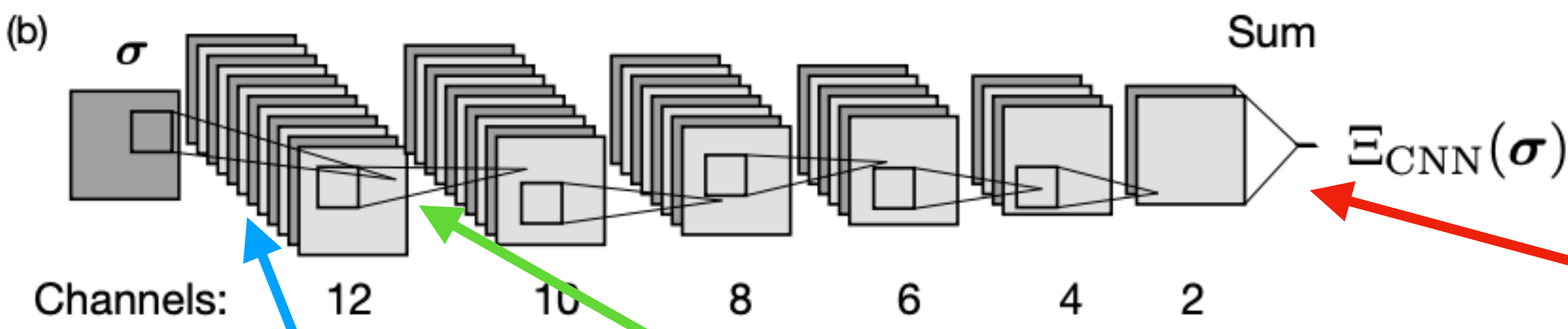


2. Neural quantum states

Intermezzo 1 : Symmetries

Implementing symmetries

Convolutional Neural networks (CNN) for translation invariance



Last pulling layer averages over all channels

Ensure translation invariance

Different channels = Various positions of the filters

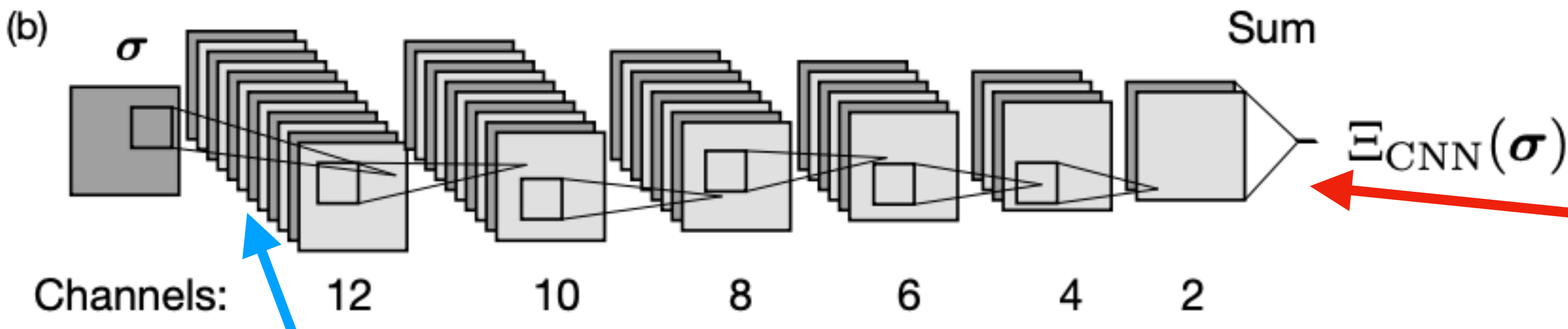
Less weights = less parameters = computations faster

$$\mathsf{h}^{(q)}_{i,j,k} = F\left(\sum_{l,m_y,m_x} \mathsf{h}^{(q-1)}_{l,j+m_y,k+m_x} \mathsf{K}^{(q)}_{i,l,m_y,m_x}\right)$$

$$:= F\left(\mathsf{K}^{(q)} * \mathsf{h}^{(q-1)}\right)$$

Implementing symmetries

Group Convolutional Neural networks (GCNN) for all symmetry operations



Add characters of the irrep at the final computation

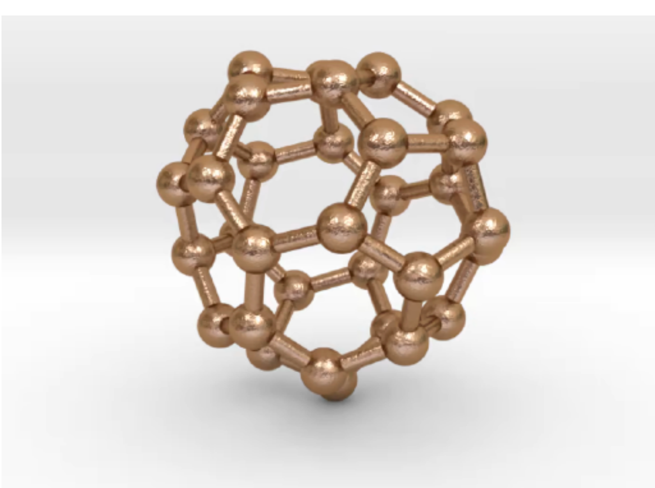
Roth, McDonald

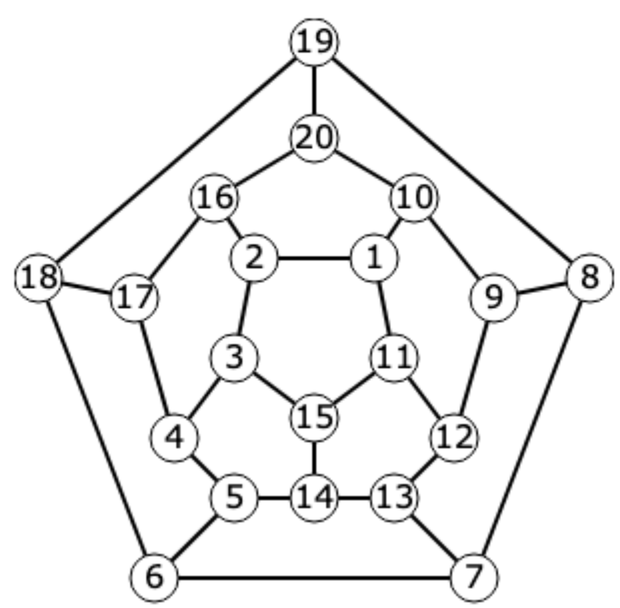
Variational computations for ground-states in all irreps

https://netket.org

Ex. Heisenberg spin 1/2 model on fullerene molecules

C_{32}





	E	mult.	irrep.	S
-15.93(1)	−15.93723	1	$A''_{1,s}$	0
-15.78(2)	−15.81192	2	E'_{s}	0
-15.74(2)	−15.77366	1	$A'_{2,a}$	1
-15.71(2)	−15.73368	1	$A'_{1,s}$	0
-15.58(2)	−15.63730	2	E'_{a}	1
	−15.60167	2	E'_{a}	1
-15.51(2)	−15.57485	2	E''_{s}	0
-15.51(3)	−15.56589	2	E''_{a}	1
	−15.54070	2	E''_{a}	1
-15.48(1)	−15.50045	1	$A''_{2,a}$	1
	−15.49288	1	$A''_{1,s}$	0
	−15.46219	1	$A''_{1,s}$	0
	−15.45437	1	$A'_{2,a}$	1
-15.44(1)	−15.45317	1	$A'_{1,a}$	1
	−15.42185	2	E''_{s}	0
	−15.39363	1	$A''_{2,a}$	1
	−15.38231	1	$A''_{2,a}$	1
	−15.38020	2	E''_{a}	1

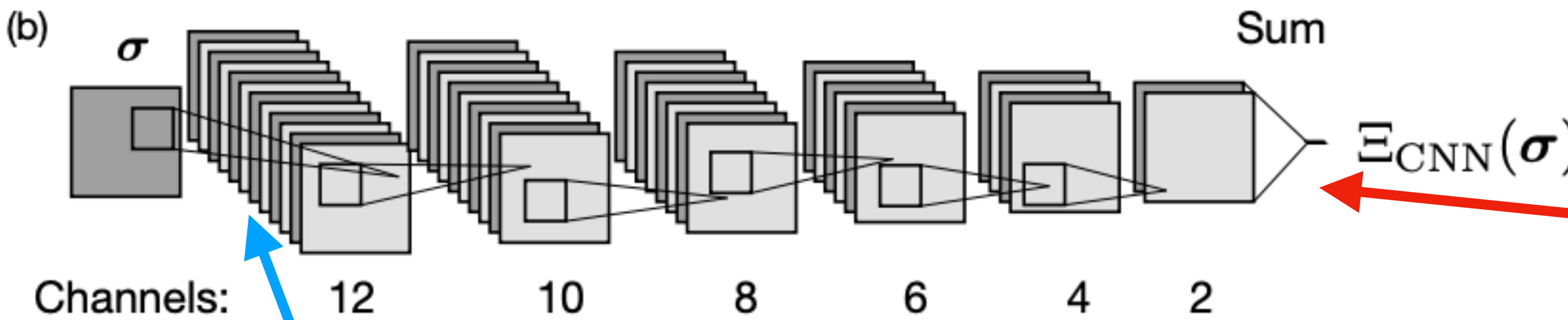
Relative error ~ 2.10^{-3}

Work in progress

D3h symmetry

Implementing symmetries

Group Convolutional Neural networks (GCNN) for all symmetry operations



All symmetry operations

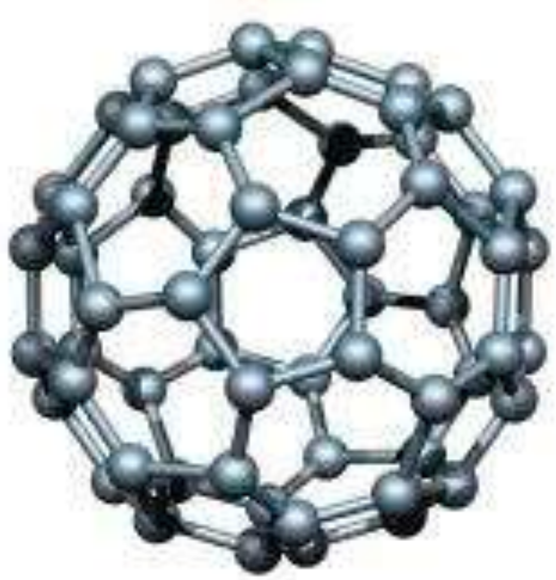
Add characters of the irrep at the final computation

Roth, McDonald

Variational computations for ground-states in all irreps

https://netket.org

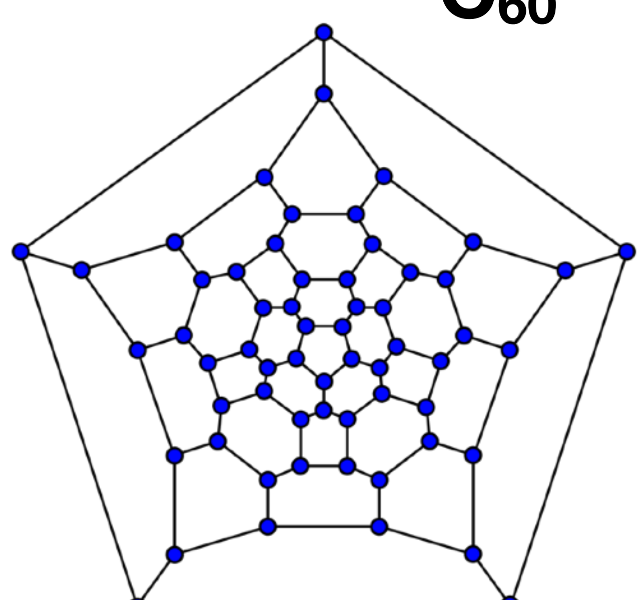
Ex. Heisenberg spin 1/2 model on fullerene molecules



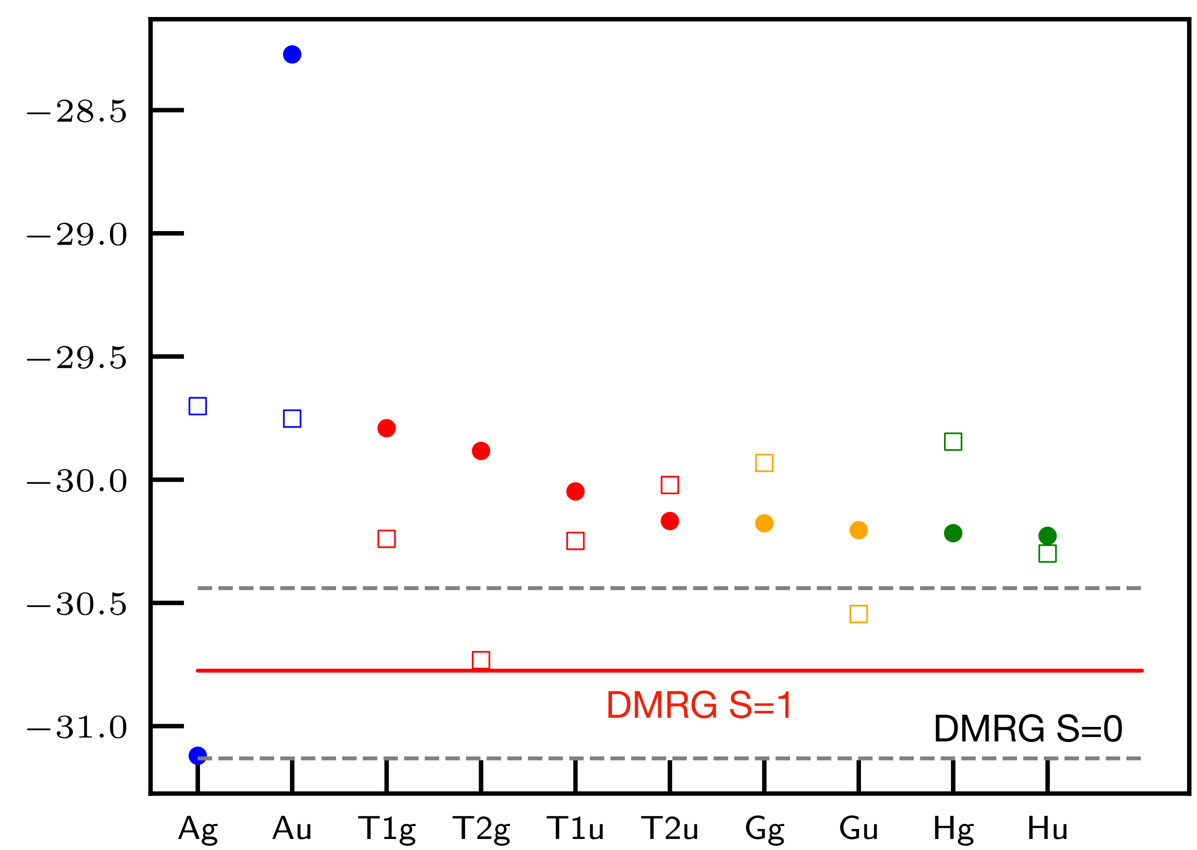
S. Capponi, FA

Work in progress

C_{60}



I_h symmetry



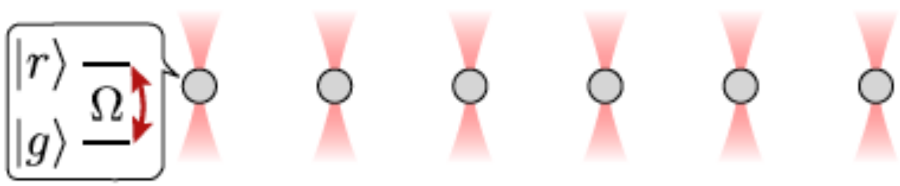
2. Neural quantum states

Application 2 : Tomography / Reconstruction of quantum states

Applications of neural quantum states

Application 2 : Tomography / Reconstruction of quantum states

- **Physical context:** Model a programmable quantum simulator (array of ~ 10 Rydberg atoms) including known experimental errors.



$$\hat{H}(\Omega,\Delta) = -\Delta \sum_{i=1}^{N} \hat{n}_i - \frac{\Omega}{2}\sum_{i=1}^{N}\hat{\sigma}_i^x + \sum_{i<j}\frac{V_{nn}}{|i-j|^6}\hat{n}_i\hat{n}_j,$$

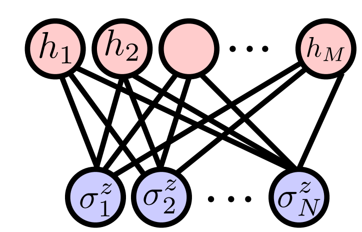
Detuning Rabi freq. vdW interactions

+ Decoherence (single-atom decay, dephasing)

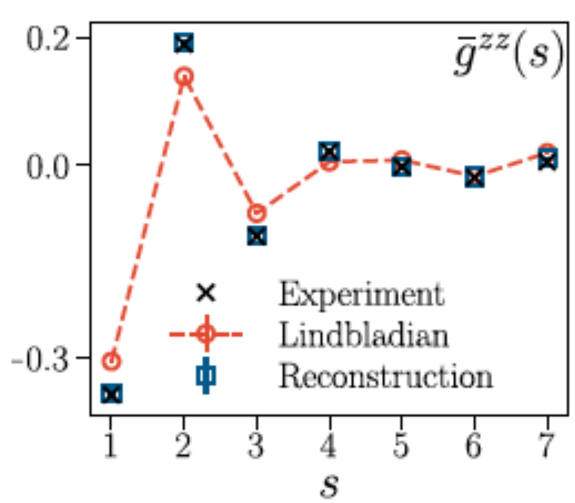
Torlai *et al.*, (2019)

- **Steps:** **1. Experimental Measurement** of n_i = projector in Rydberg state for atom i

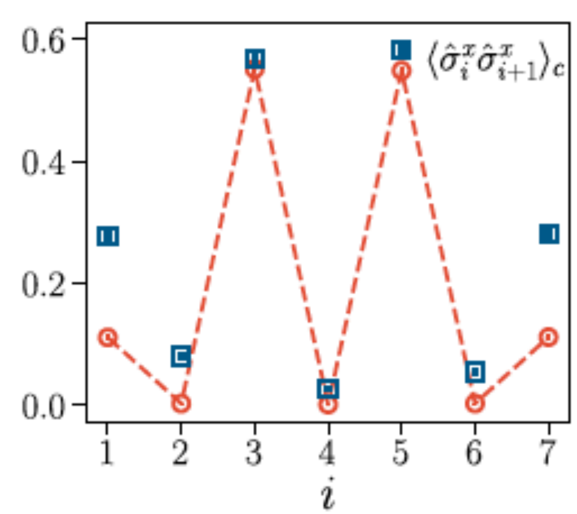
  2. Optimize RBM to reproduce the measurement

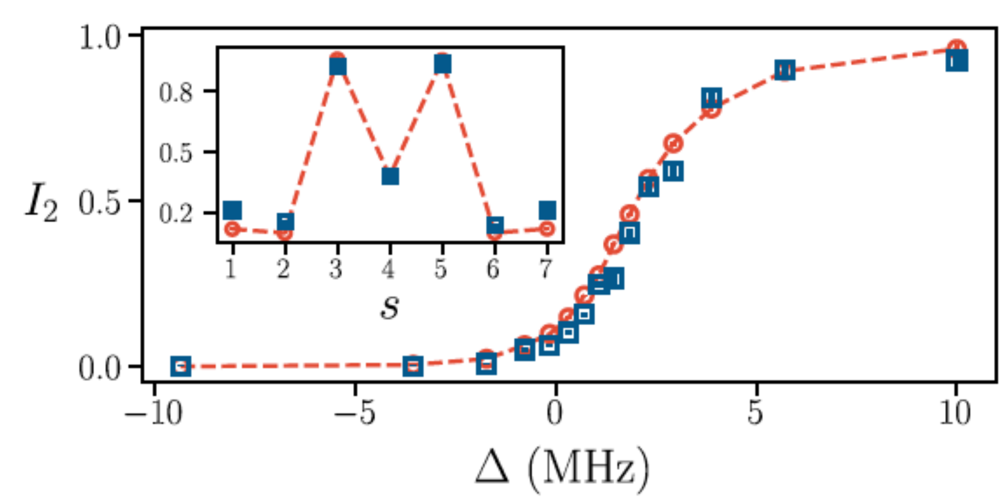


  3. Sample the RBM to **compute observables that can't be measured** experimentally



Diagonal correlations
(can be measured)





Off-Diagonal correlations and Entanglement entropy
(can't be measured)

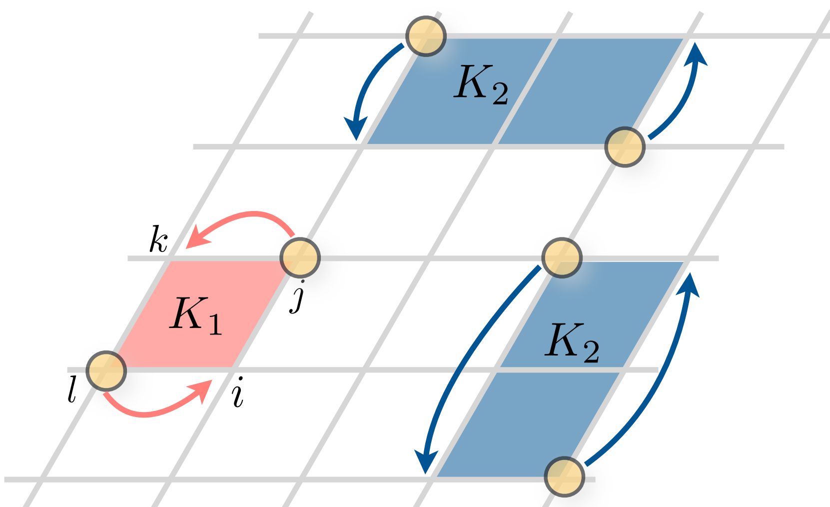
2. Neural quantum states

Intermezzo 2 : Combining with other methods

Our work: Exotic liquid state and Diffusion Monte Carlo

- **Goal:** Study a 2d bosonic model which hosts an exotic liquid phase. Can RBM capture this ?

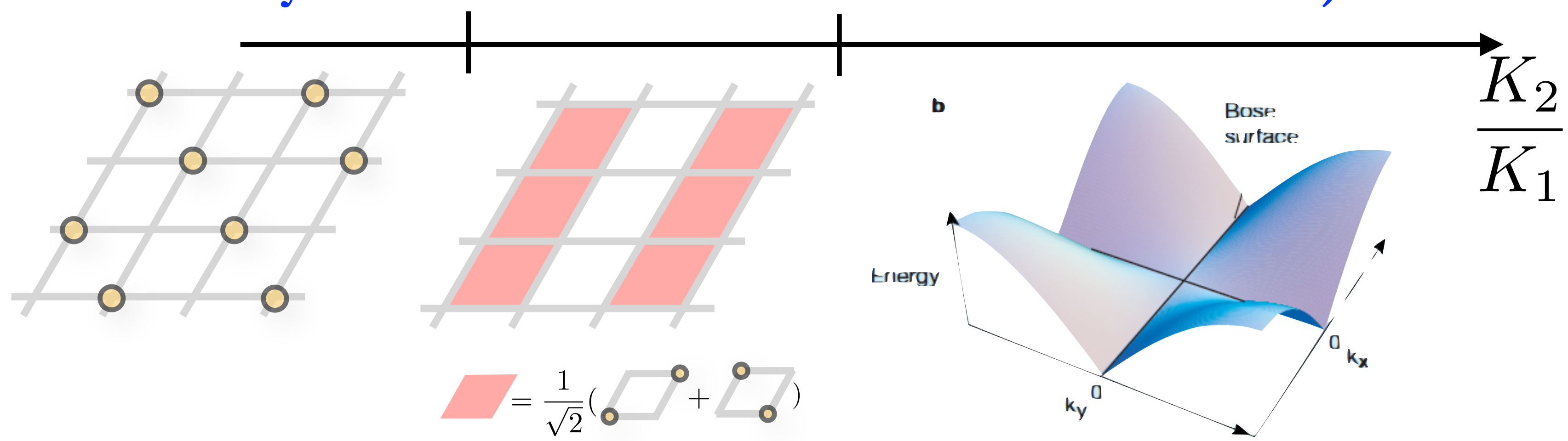
Bosons with competing ring exchanges



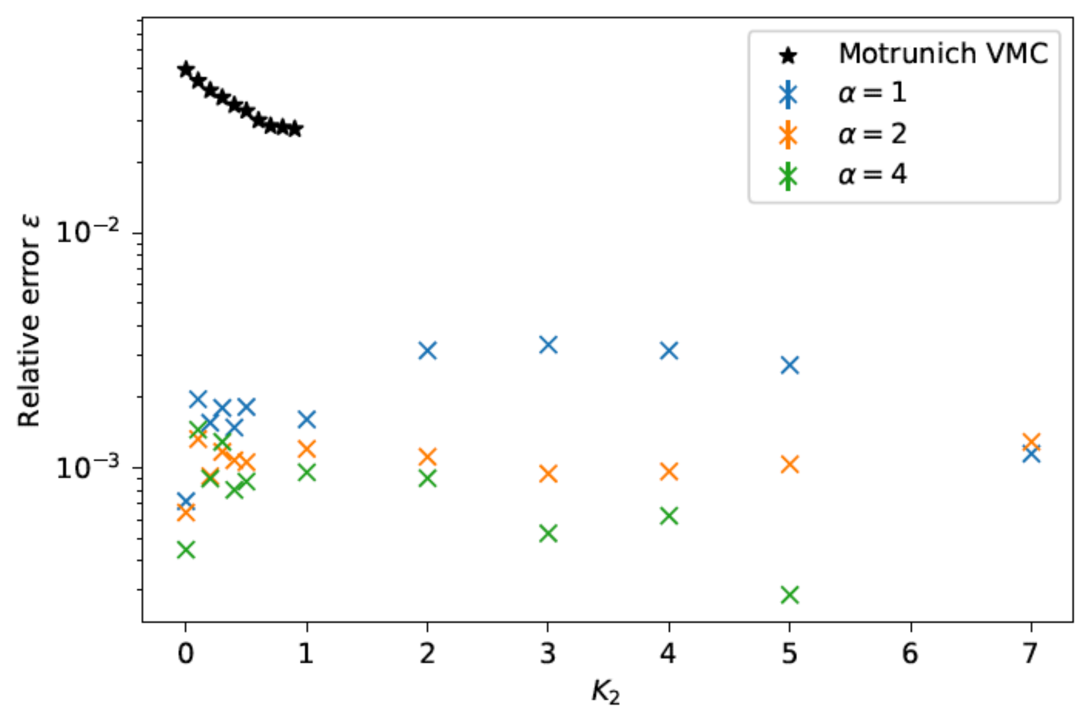
$$\mathcal{H}_{K_1,K_2} = -K_1 \sum_{\square} P^{1\times 1} - K_2 \sum_{\square,\square} (P^{1\times 2} + P^{2\times 1})$$

Suggested Ground-state

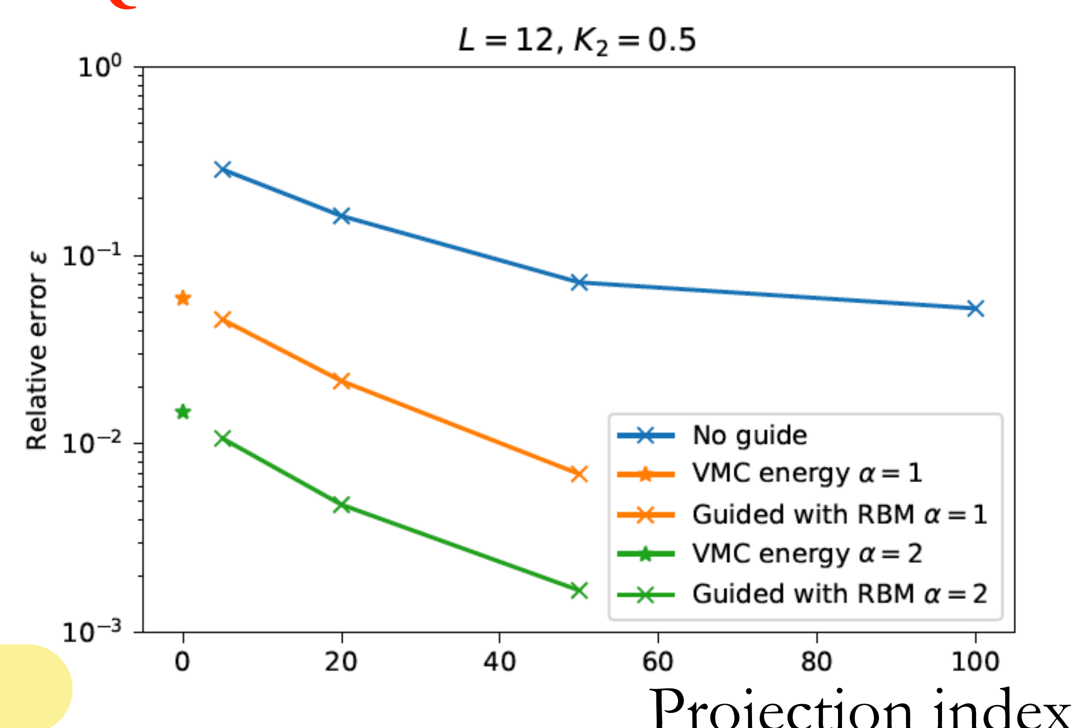
Charge density wave | **Plaquette state** | **Bose liquid (with « Bose surface »)**



- **Result 1:** RBM outperforms other variational methods



- **New Idea :** Can use **RBM as guiding wave-function for Quantum Monte Carlo**



Théveniaut, FA, WIP

3. Creation of improved algorithms

Improving Monte Carlo simulations

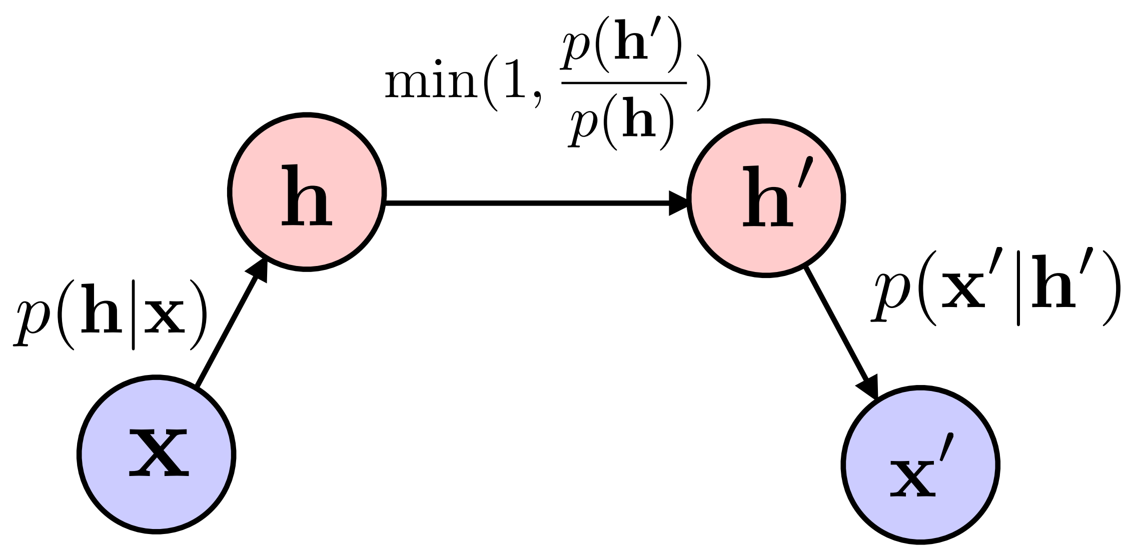
- **Monte Carlo simulations** ubiquitous in physical sciences. However, sometimes ...
  - A single Monte Carlo step is **costly** (and may not be accepted)

e.g. Fermionic determinant quantum MC : one step N^3

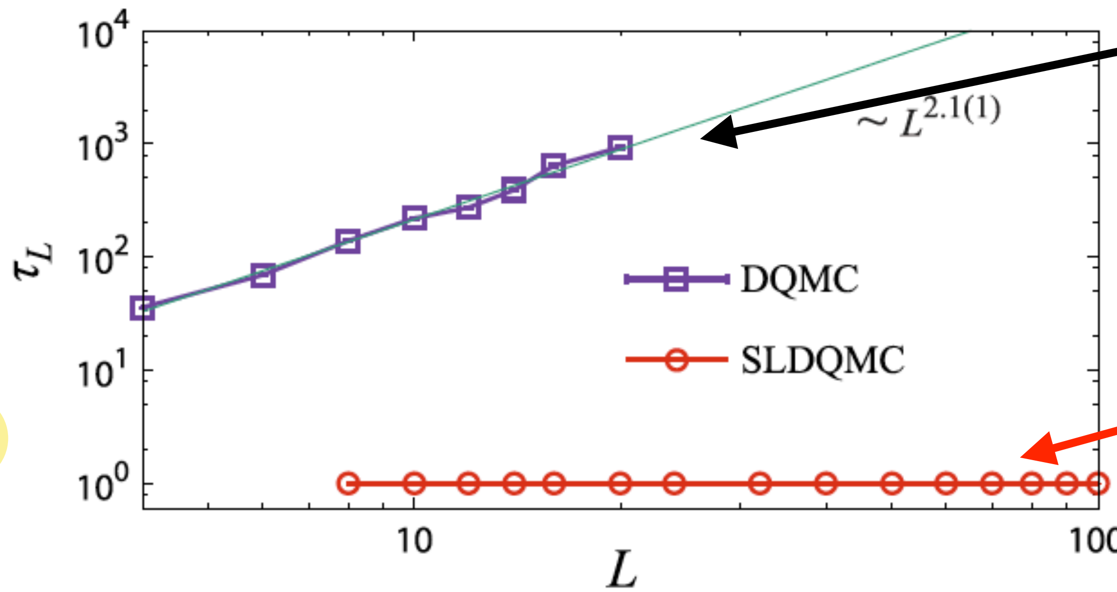
leads to **strong autocorrelations**

e.g. near phase transition

- **Idea:** Couple the physical system to an hidden one (e.g. through a RBM) easier to sample and which can propose large moves in phase space. Coupling parameters are machine learned.



Fermions coupled to transverse field Ising model in 2d



Standard QMC: Large autocorrelations, max. size 20^2

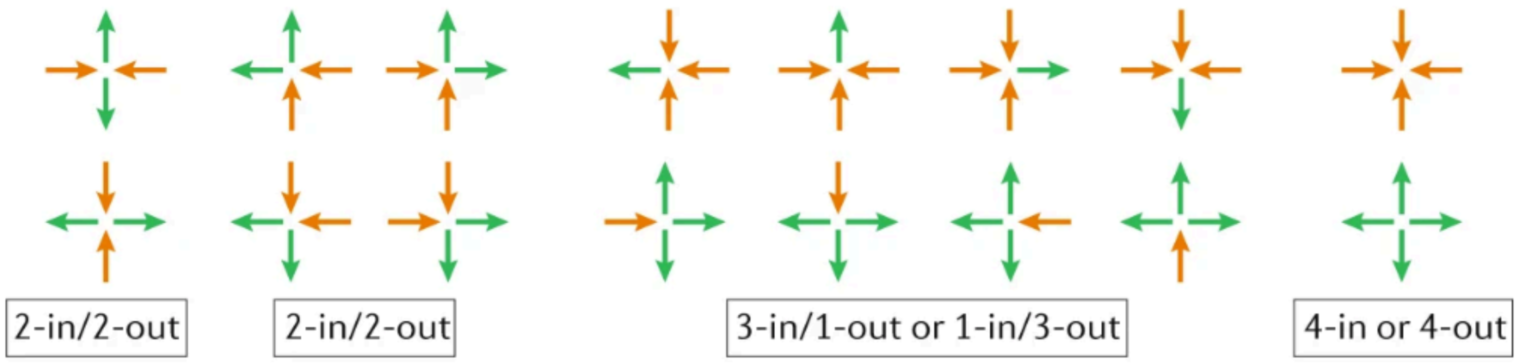
Machine-learning guided QMC: No autocorrelations, max. size 100^2

Xu *et al.*, PRB (2017)

Improving Monte Carlo simulations : Challenges

Reinforcement learning to help finding complex MC moves

- **Physical context:** Some magnets obey the (spin) ice rules at low temperature

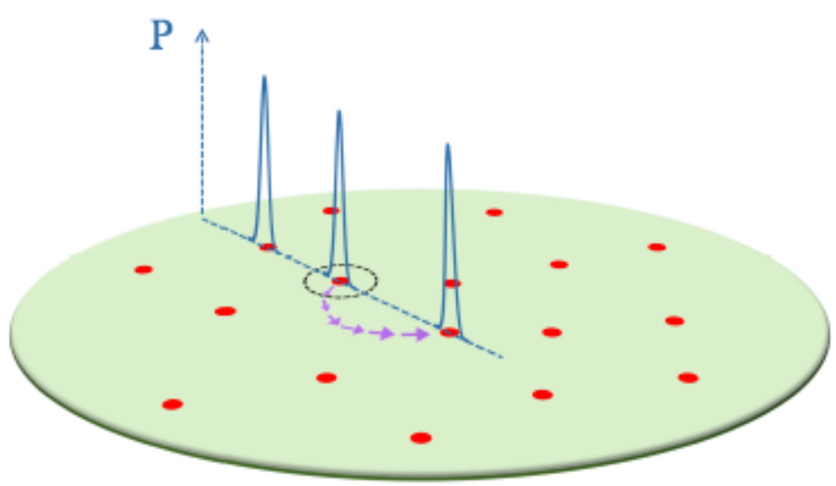


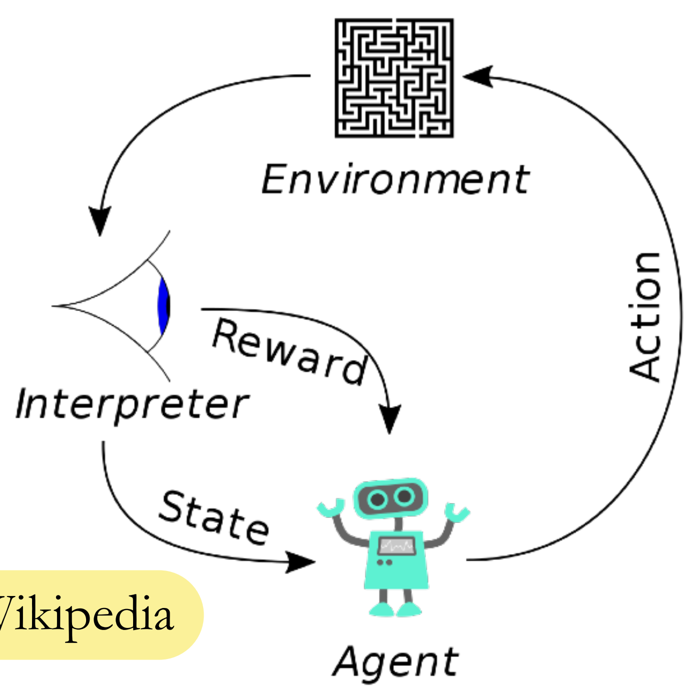
Only configurations with 2in-2out everywhere are allowed

- **Computational problem:** How to sample this 2-in 2-out manifold efficiently ?

- **Reinforcement learning**

Balance between exploration (of phase space) and exploitation (of knowledge of valid configurations through penalty/reward).





Wikipedia

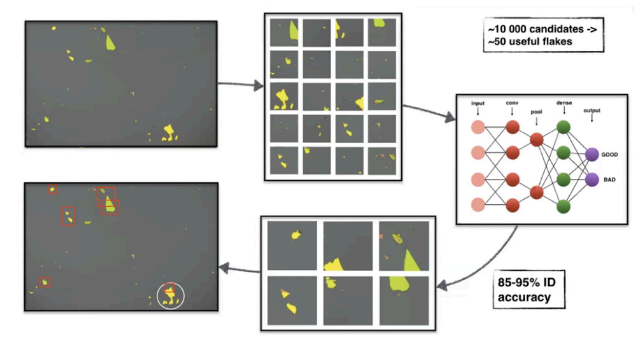
The agent learns by itself the rules of this manifold and finds complex MC moves to navigate through it

Zhao *et al.*, 2019

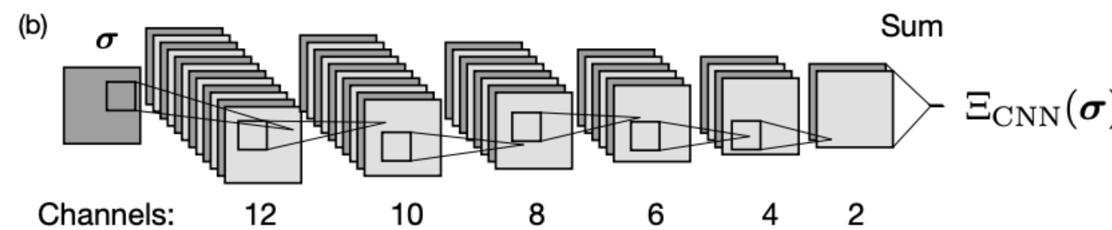
Summary

A new tool in the box of experimental and computational physicists

- Many recent applications of ML in quantum physics / condensed matter
- Some works go beyond the hype and obtain first non-trivial results
- Some straight-forward applications in data mining / image processing, some less straight-forward



- Neural quantum states : efficient (benefit from ML advances), albeit not fully understood



- My take: **Once you know what you want to do (method)**, entering the field is easy : many tutorials, examples, lectures, open source codes online

pdf of the talk &
list of references

SCAN ME

Perspectives

- **Outlook 1 :** Most of the ML techniques used so far are quite basic (from the AI point of view). Room for using state-of-the-art ML (GAN, VAE, Deep RL …) and improve performances

E.g. Autoregressive density samplers could strongly reduce the computational cost of sampling neural quantum states

Sharir *et al.*, PRL (2020)

Hibat Allah *et al.*, PRR (2020)

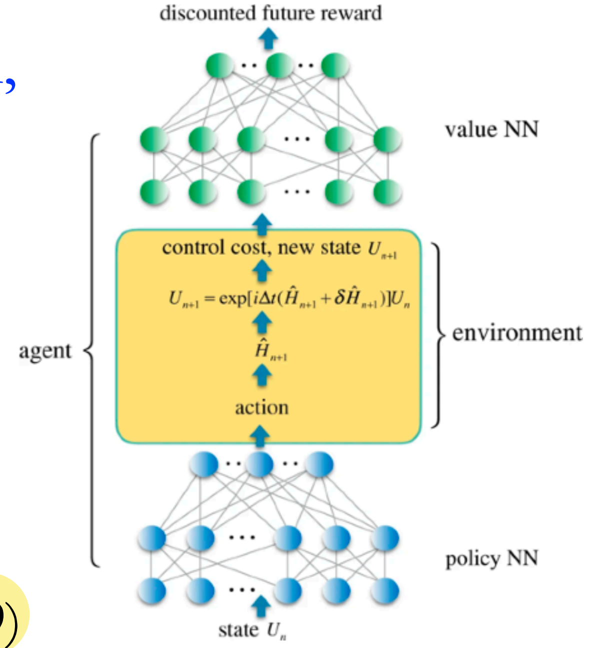
- **Outlook 2 :** ML inside truly quantum mechanical setups: Quantum computing + ML marriage

ML-based control/help of quantum experiments/ computations

Open or closed-loop control, in q. experiments

Quantum computing (optimisation of quantum gates, neural-network parameterized quantum circuit, quantum error correction)

Niu et al., NPJ Qu. Inf. (2019)



Perspectives

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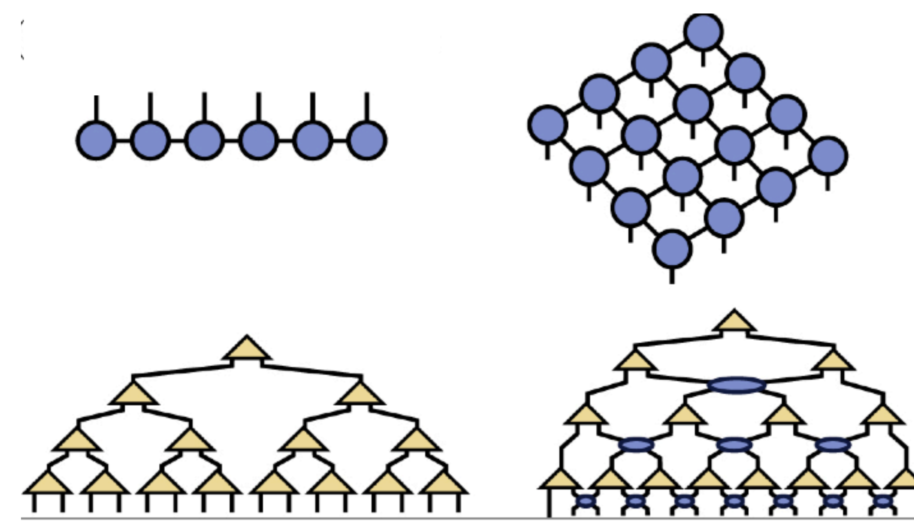
Sharir *et al.*, PRL (2020)

Hibat Allah *et al.*, PRR (2020)

- **Outlook 2 :** ML inside truly quantum mechanical setups: Quantum computing + ML marriage
- **Outlook 3: Can quantum physics help (classical) ML ?**

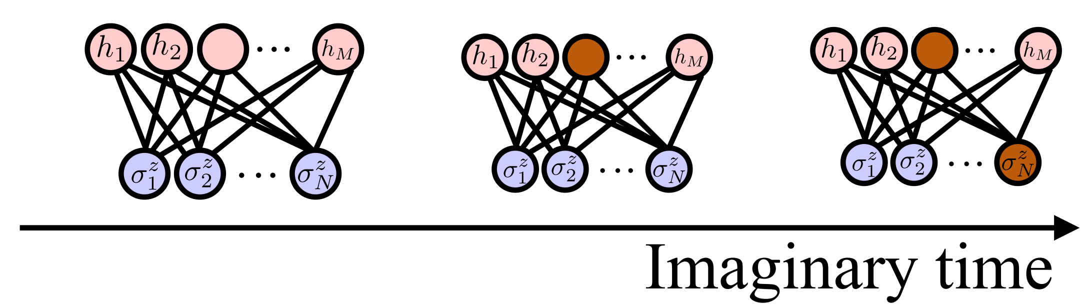
  - 1. Typical quantum methods (Matrix-Product States, DMRG) have been repurposed to perform ML tasks (classification, time-series modeling)

  Stoudenmire *et al.*, …



  - We know how to improve these quantum methods (e.g. tensor networks) and when they work / fail ? (few / a lot of quantum entanglement). Can this help characterize or design new ML methods and architectures ?

  - 2. Construct quantum version of networks (e.g. quantum Boltzmann machine).



$$H = \sum_j a_j \sigma_j^z + \sum_i b_h h_i^z + \sum_{ij} W_{ij} h_i^z \sigma_i^z + \Gamma_h \sum_i h_i^x + \Gamma_s \sum_i \sigma_i^x$$