A sample of numerical methods for strongly correlated matter

Stakes, numerical challenges & few examples

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DISCLAIMER

This informal talk will mostly :

- present results of small-scale projets (1-5 persons)
- focus on ad-hoc techniques …
- … that burn a lot of CPU time
- only superficially touch machine learning

Actually quite representative of condensed-matter theory & numerics

albeit not always the case …

Introduction to condensed matter & strongly correlated quantum systems

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Motivations

Models

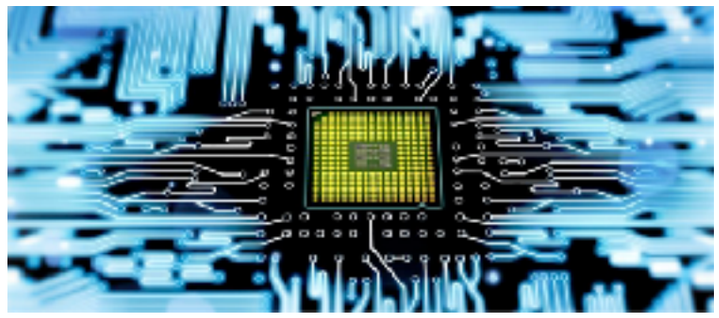
Numerical challenges

Condensed matter theory

- Condensed matter theory = Understand the material world around us, using a description at the atomic level

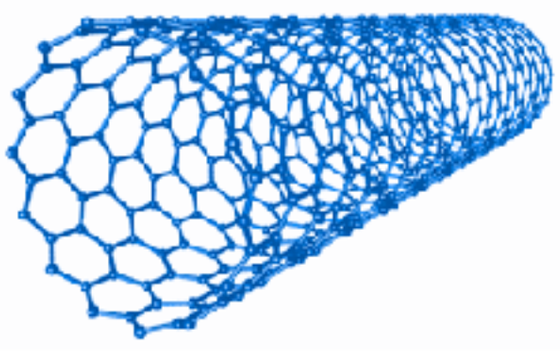
- Quantum mechanics MUST be taken into account and is the source of beautiful / useful phenomena at the electronic scale

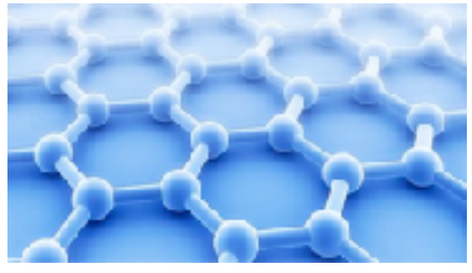
Superconductivity



Semiconductors

Quantum computer





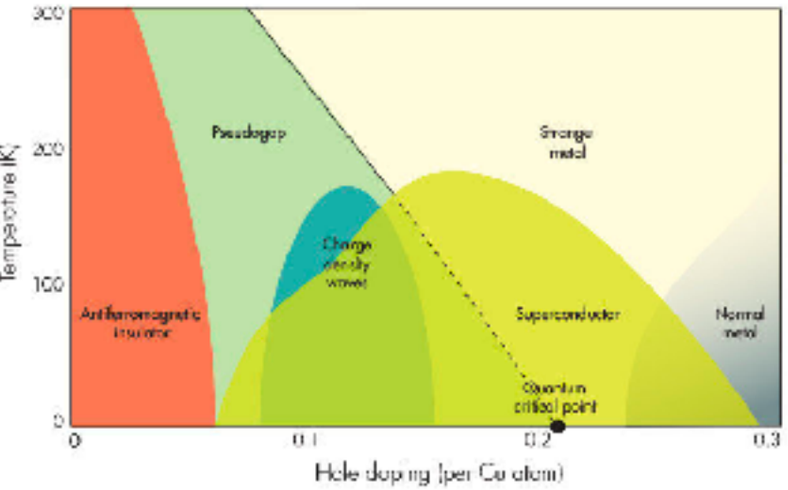
NanoEverything …

The many-electron problem

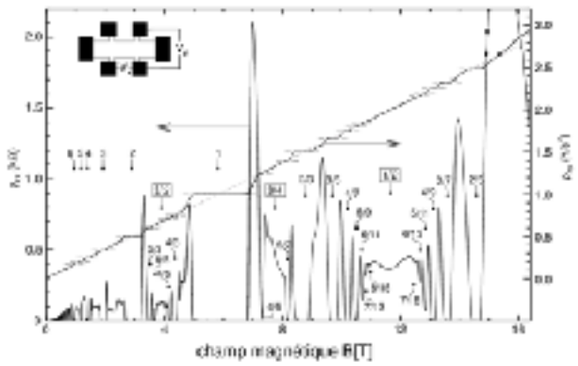
- Often, electrons moving in solids can be seen as independent
- However, in many cases, interactions between electrons are relevant

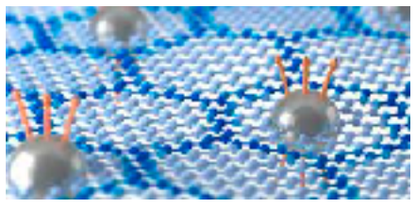
New phenomena and phases of matter emerge

High-Tc superconductors

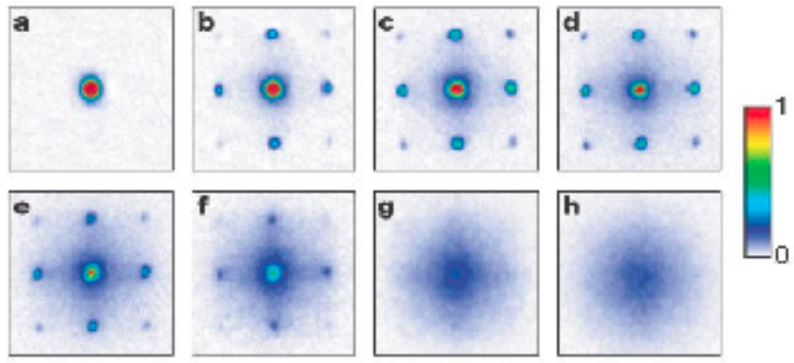


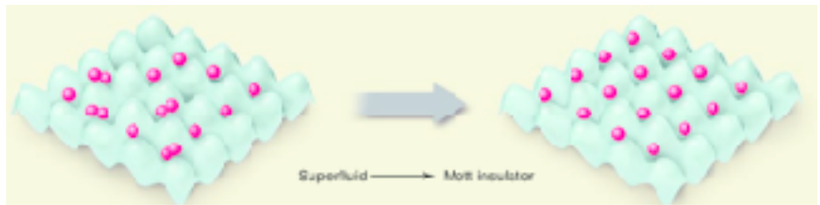
Fractional quantum Hall effect





Quantum phase transitions in ultracold atoms





- More is different

Defining the problem (« rules of the game ») is very easy, yet very hard to solve ! Emergence of complexity, collective solutions

More Is Different

P.W. Anderson (1972)

thinking is that the reductionist hypothesis does not by any means imply a "constructionist" one: The ability to reduce everything to simple fundamental laws does not imply the ability to start from those laws and reconstruct the universe. In fact, the more the ele-

The constructionist hypothesis breaks down when confronted with the twin difficulties of scale and complexity. The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear, and the understand-

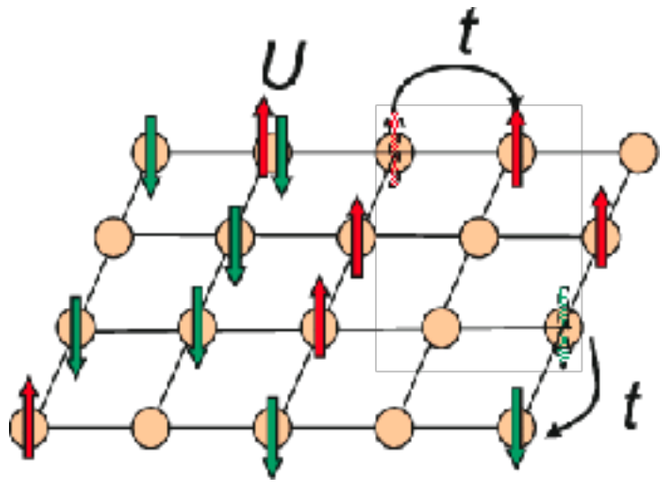
Solving the N electrons problem is NOT solving N times the one-electron problem

Models of strong correlations

- Simplified models for electrons and their spins defined on a lattice

- Hubbard model = Electrons moving on a lattice, with repulsion on the same site (simplification w.r.t Coulomb interactions)

$$H = -t \sum_{\langle i,j \rangle, \sigma=\uparrow,\downarrow} c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c. + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$



Competition between kinetic (electrons want to move) and potential energy (electrons localize)

- Prototypical model of material with strong correlations, high-Tc superconductors …

- Complexity = Size of Hilbert space = 4^N (N number of lattice sites)

- Simple questions … : what is the ground-state, low-lying excitations ? Do they break any symmetry ? If yes, which one(s) ?

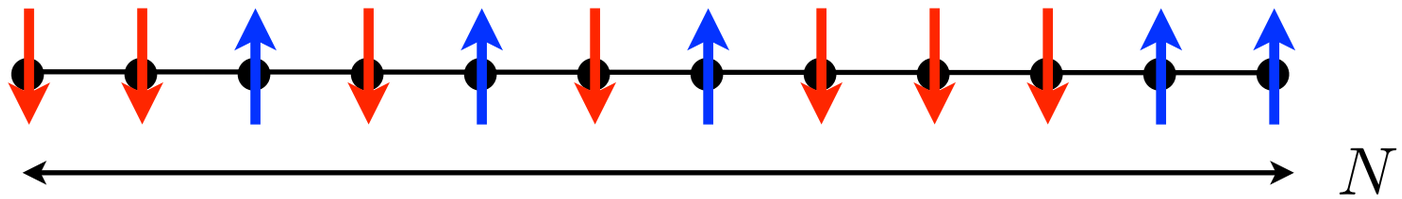
  - … but no simple answers: model can only be solved in 1d. We don't know the phase diagram in d>1 in general.

Models of strong correlations

- Heisenberg model = Electrons are localized, can exchange their spins

Describe magnetic properties of insulators : (anti-)ferromagnets

$$H = \sum_i \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z$$



- To each site, is associated a spin : Orientation = ↑ or ↓

3 Pauli matrices $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

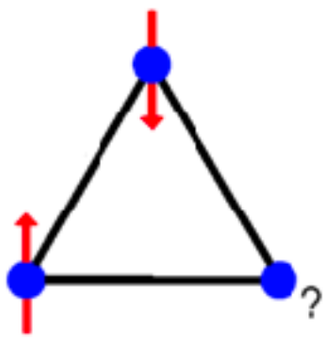
- For N spins : basis state $|\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\rangle = 001010100011$

- Complexity = 2^N
- Hamiltonian matrix does spin-flips on nearest-neighbours sites

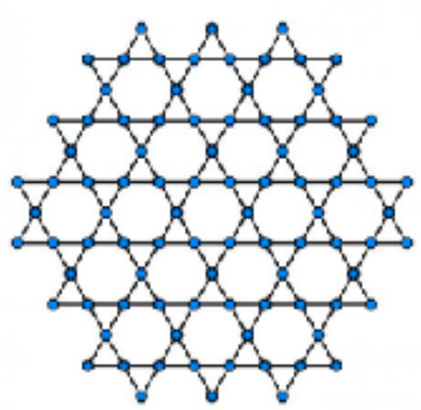
$|\cdots\downarrow\uparrow\cdots\rangle \leftrightarrow |\cdots\uparrow\downarrow\cdots\rangle$

- Exact solution only in 1d. We understand the physics / we can do good simulations when the lattice is bipartite.

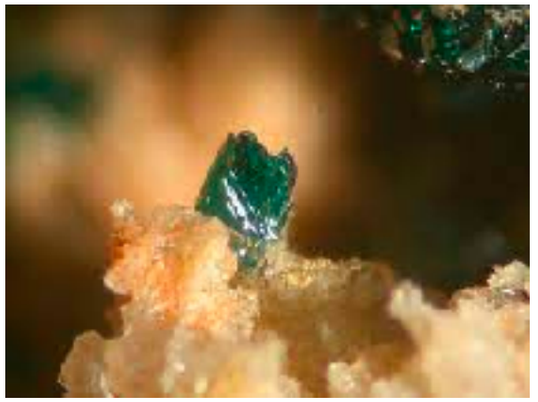
- Difficult situation : Frustrated antiferromagnets



Can already be seen at the « classical level »



Kagome lattice



Herbertsmithite

Some numerical methods to solve the (lattice) quantum many-body problem

« Exact » methods

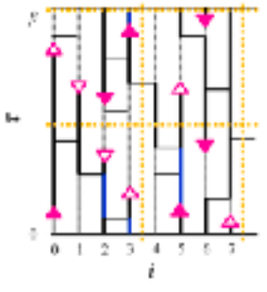
Variational methods

Numerical simulations of strongly correlated systems

- Large variety of methods to « solve » the quantum many-body problem

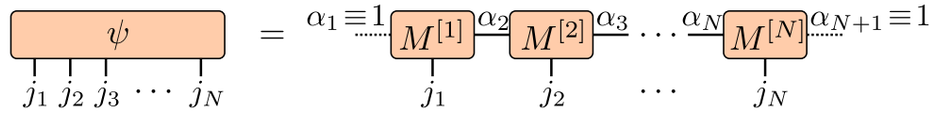
  - Exact Diagonalization : Solve exactly the eigenproblem. Small N only !

- Quantum Monte Carlo : avoids exponential complexity : up to N ~ 10^6, but often prohibited by a strong sign problem

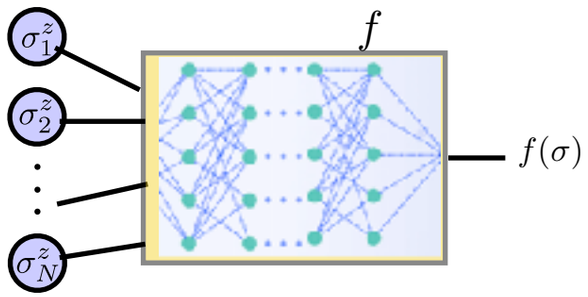


  - Variational methods : Based on good physical intuition or …

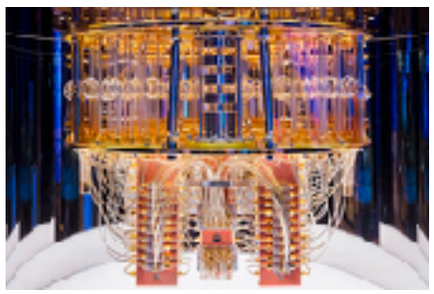
  - Matrix-Product States / Tensor-Network methods : compressing quantum information



  - Machine learning : Neural Quantum States



- Another way (not this talk) : analog simulations with quantum computers



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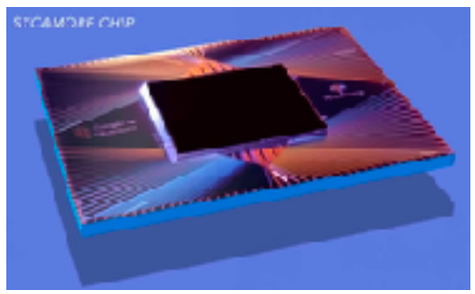

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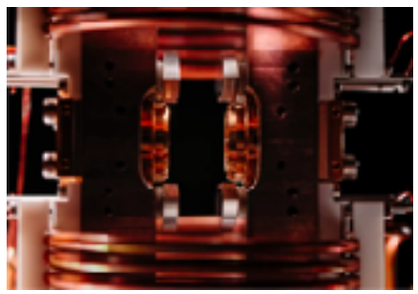


Pasqal

e.g. w. variational quantum eigensolver (VQE) algorithm

Exact diagonalization of strongly correlated systems (1/2)

- H is usually a big sparse matrix = Gold mine

  e.g. Heisenberg spin model : Each of 2^N lines has ~ N non-zero matrix elements

- Use all symmetries of the problem (H is block diagonal)

  Use standard sparse linear algebra techniques pushed to their limits

- Standard problems:
  - Full spectrum : #H max ~ 10^5 N = 24 (scalapack)
  - Low-energies: #H typique ~ 10^9, 10^{10} N = 36 Lanczos algorithm+openMP

    #H max ~ 5.10^{11} N = 50 Lanczos+MPI

    Sylvain Capponi

    1 vector ~ 1 TB of RAM

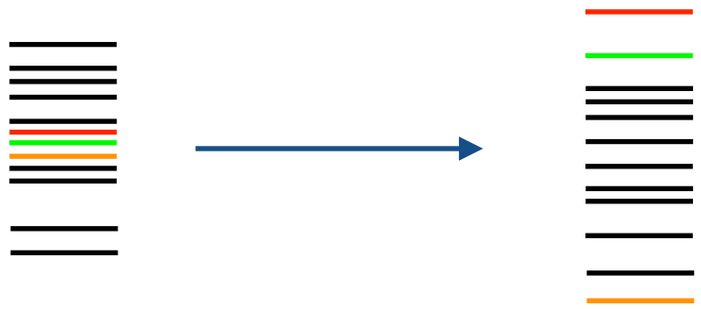
MESSAGE : Do NOT store Hamiltonian in memory (matrix-free methods)
Do NOT store eigenvectors on disk (analysis on the fly & cheapest to recompute)

Exact diagonalization of strongly correlated systems (2/2)

- H is usually a big sparse matrix

- Sometimes unusual problems …

  - Interior eigenvalues



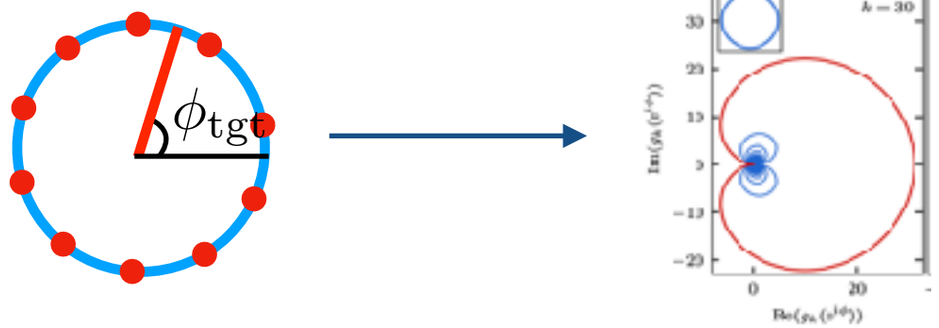
#H max ~ 10^7

N = 26

Spectral transforms

Nicolas Laflorencie, FA

  - Unitary problems



- Sometimes don't want eigenstates, but just to apply a fonction of H

e.g. time evolution, thermal typicality …

$$|\Psi(t)\rangle = \exp(-iHt)|\Psi(0)\rangle \qquad |\Psi(\beta)\rangle = \exp(-\beta H/2)|\mathrm{Random}\rangle$$

MESSAGE : Never diagonalise H, instead work in the Krylov basis

$$\mathrm{Span}\{|\Psi(0)\rangle, H|\Psi(0)\rangle, H^2|\Psi(0)\rangle, \ldots H^n|\Psi(0)\rangle\}$$

Sylvain Capponi, FA

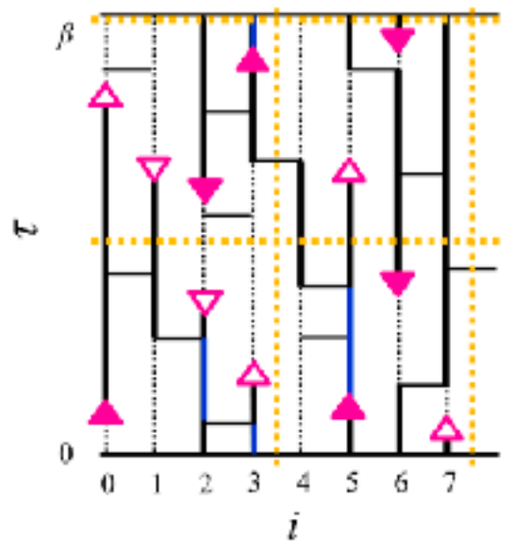
Quantum Monte Carlo methods (1/2)

- **Monte Carlo** ubiquitous in physical sciences, often to sample high-dimensional integrals
- « **Quantum Monte Carlo** » regroup a zoo of methods

  Determinant MC, Projection QMC, Green Function MC, Path integral MC …

$$Z = \mathrm{Tr}\exp(-\beta H) \equiv \sum_{\mathcal{C}} W(\mathcal{C})$$

Goal : Sample sum with Monte Carlo, according to the weight $W(\mathcal{C})$

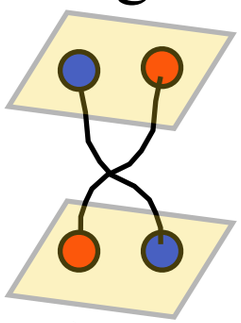


Quantum problem in dimension d → Classical stat-mech problem in dimension d+1

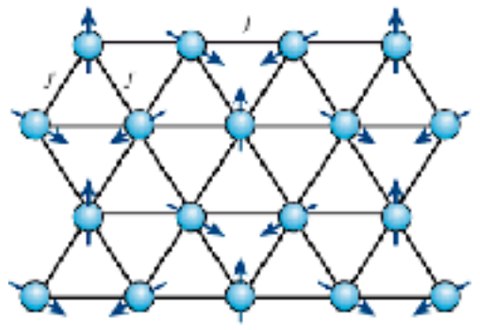
- Extremely efficient method when applicable …
- … but the weight $W(\mathcal{C})$ does not need to be positive !! → **Sign problem**

  Kills exponentially fast the MC sampling

Present in general for fermionic systems and frustrated magnets



$$\Psi_F(x_1, x_2) = -\Psi_F(x_2, x_1)$$



MESSAGE 1 : On a lattice, sign problem if one off-diagonal matrix element $H_{ij} > 0$

Quantum Monte Carlo methods (1/2)

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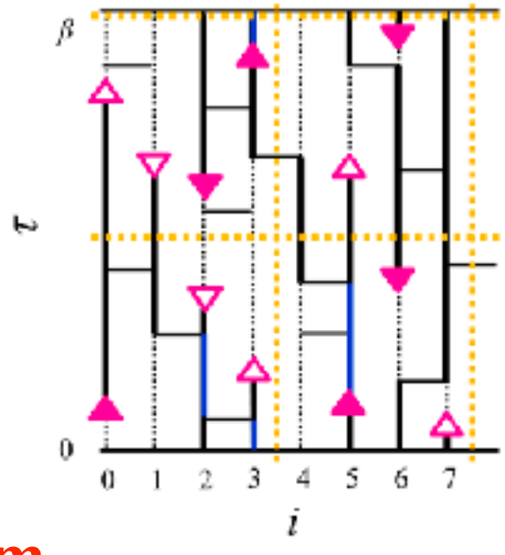


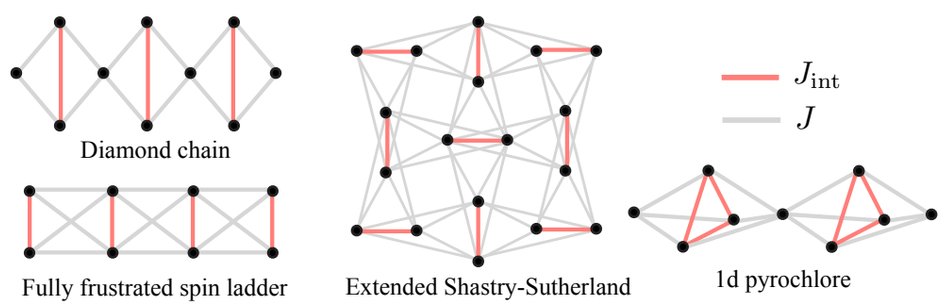
- … but the weight $W(\mathcal{C})$ does not need to be positive !! → **Sign problem**

  Present in general for fermionic systems and frustrated magnets

MESSAGE 1 : On a lattice, sign problem if one off-diagonal matrix element $H_{ij} > 0$

MESSAGE 2 : Sign problem is also a representation problem : depends on the basis!

Sometimes, symmetries or a clever reformulation can alleviate/ remove the sign problem



FA

MESSAGE 3 : Even without a sign problem, path integral can still be hard to sample !

e.g. systems with disorder (spin glasses), constrained systems…

Matrix Product methods (1/2)

- Matrix Product ansatz : **many-body states/operators** are products of local matrices
- Matrix Product states in one formula/picture

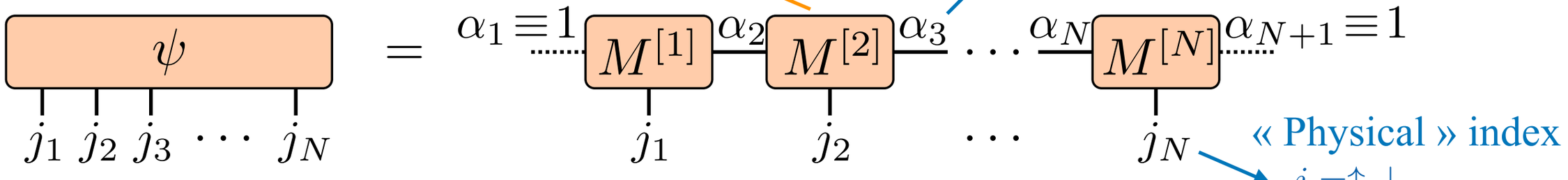
$$|\Psi\rangle = \sum_{j_1,j_2\ldots j_N} c_{j_1,j_2,\ldots,j_N} |j_1, j_2, \ldots, j_N\rangle = \sum_{j_1\ldots j_N} \sum_{\alpha_2\ldots\alpha_N} M^{[1]j_1}_{\alpha_1\alpha_2} M^{[2]j_2}_{\alpha_2\alpha_3} \ldots M^{[N]j_N}_{\alpha_N,\alpha_{N+1}} |j_1, j_2, \ldots, j_N\rangle$$

$$= \sum_{j_1\ldots j_N} M^{[1]j_1} M^{[2]j_2} \ldots M^{[N]j_N} |j_1, j_2, \ldots, j_N\rangle$$

e.g. $|\uparrow\uparrow\downarrow \ldots \downarrow\rangle$

$M^{[i]}$
$\chi \times \chi \times 2$ Tensor

« Virtual » index (summed over)
$\alpha = 1, \ldots, \chi$

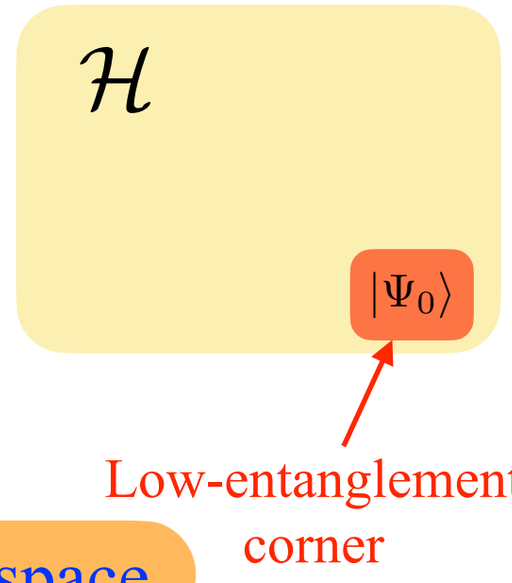


- Why should it work ? Low-energy states have small entanglement

$|\Psi(j_1, j_2)\rangle = M^{j_1} M^{j_2}$ Separable (unentangled) state

$|\Psi(j_1, j_2)\rangle = \sum_i M_i^{j_1} M_i^{j_2}$ Entangled state

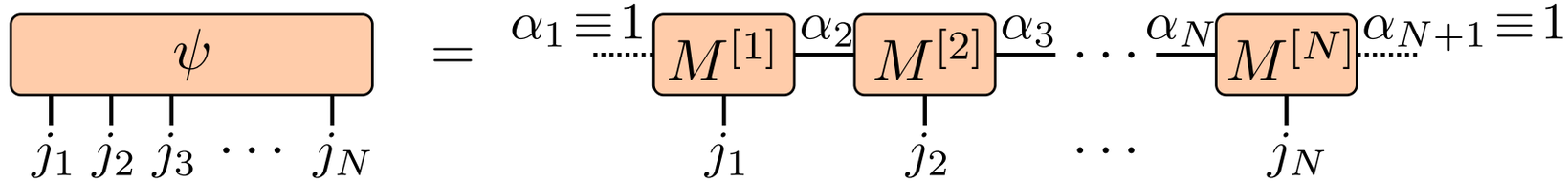
Small number of terms = Small entanglement



MESSAGE : Many-body ground states live in a corner of the Hilbert space

- Interest: Trade exponential # of coefficients with polynomial # of parameters to optimize upon (hopefully χ small)

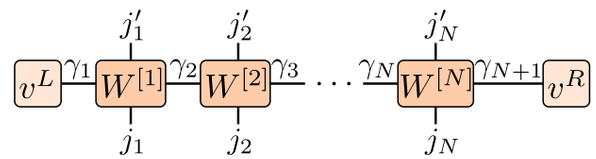
Matrix Product methods (2/2)



- MPS = Extremely efficient ansatz for one-dimensional systems
  - Optimization method: Density Matrix Renormalization Group

$$E_{\text{var}} = \min \frac{\langle \Psi_{\text{MPS}} | H | \Psi_{\text{MPS}} \rangle}{\langle \Psi_{\text{MPS}} | \Psi_{\text{MPS}} \rangle}$$

- Same idea can be applied to time-evolution, operator ansatz etc

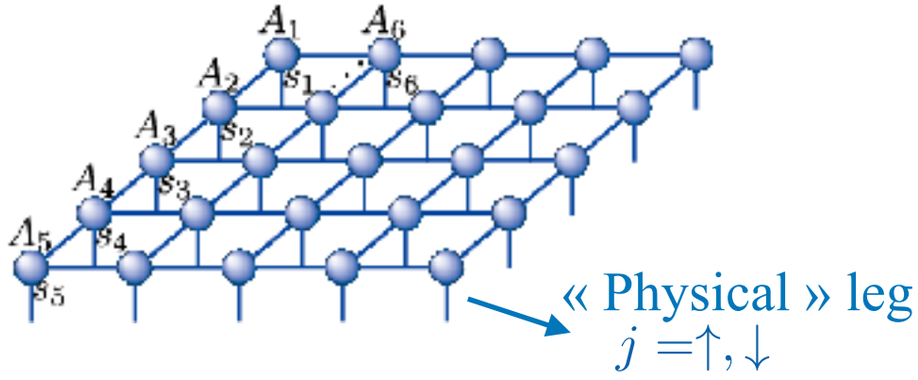


- More difficult in higher dimensions (tensor contraction is hard)

Projected Entangled Pair State (PEPS) ansatz

Didier Poilblanc, Matthieu Mambrini

Search for variational descriptions of exotic states of matter (e.g. chiral spin liquids) using these ansatz



MESSAGE : Such Tensor Networks representations of higher-dimensional tensors could be / have been adapted to other fields

Tensor trains in maths, supervised machine learning, continuum differential equations (Navier Stokes) …

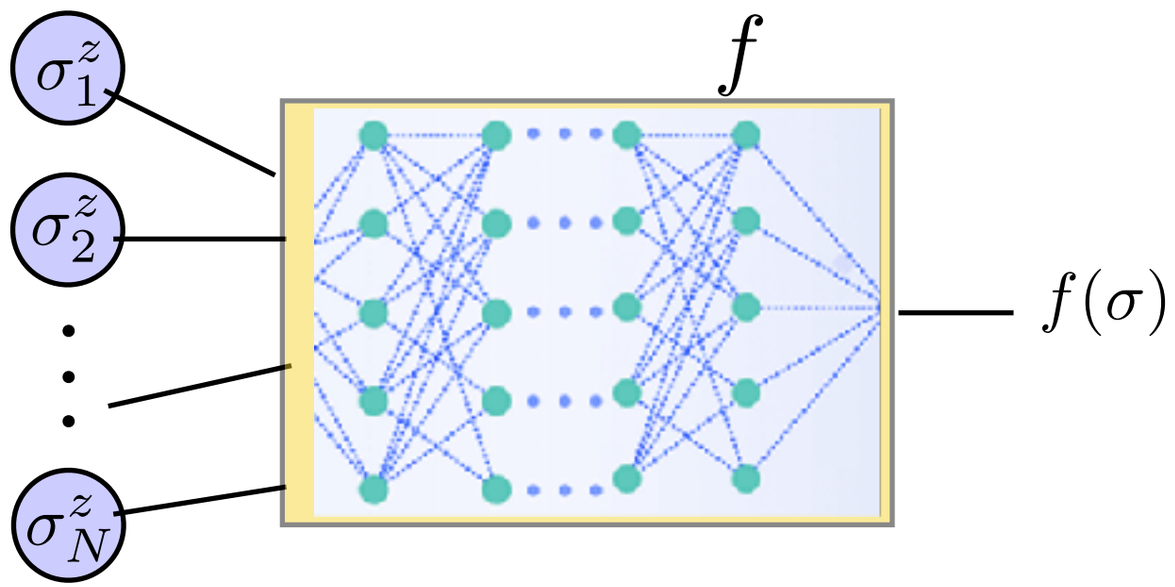
Machine learning $|\Psi\rangle$ = Neural quantum states

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

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

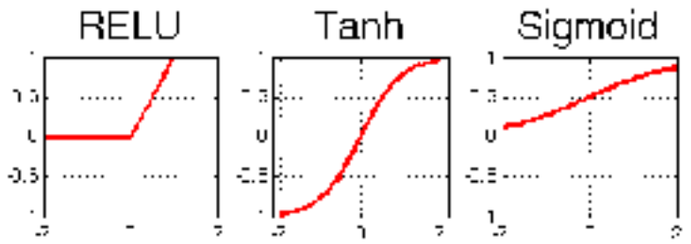
$$\sigma = \{\sigma_1^z, ..., \sigma_N^z\}$$

$\uparrow, \downarrow$



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

- **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

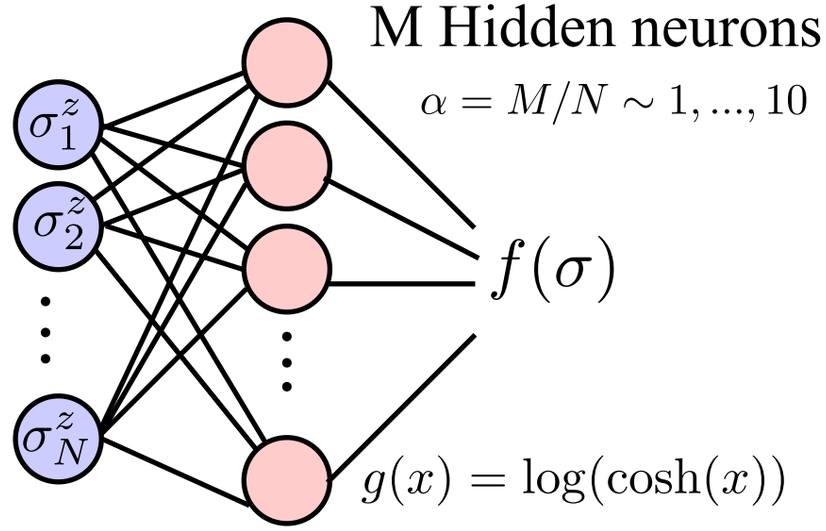
- Optimization through Variational Monte Carlo computation to e.g. minimise $E_{\mathrm{var}} = \dfrac{\langle \Psi_{\mathrm{NN}}|H|\Psi_{\mathrm{NN}}\rangle}{\langle \Psi_{\mathrm{NN}}|\Psi_{\mathrm{NN}}\rangle}$

Some examples

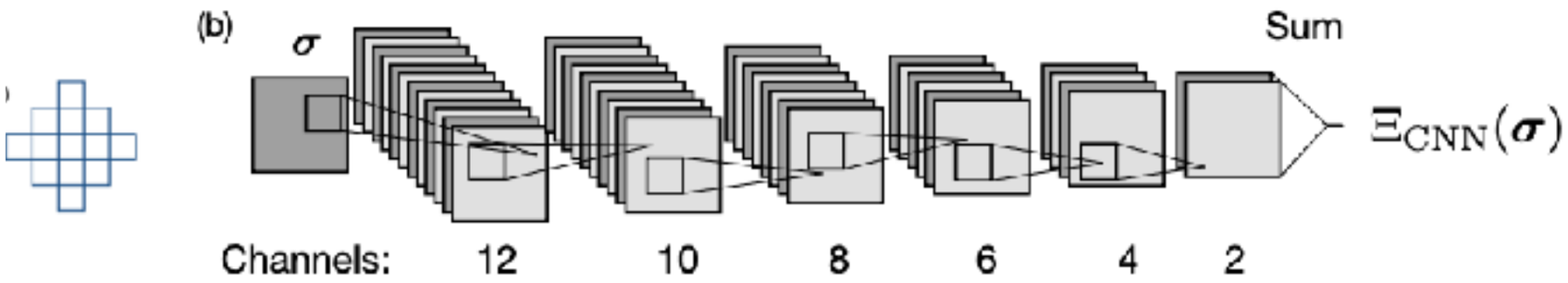
Simplest example: Restricted Boltzmann Machine (RBM)

$$\Psi(\sigma) = \sum_{h_i} \exp[\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{i,j} W_{ij} h_i \sigma_j^z] \qquad \sigma_i^z = \pm 1$$

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



Convolutional neural network (CNN)

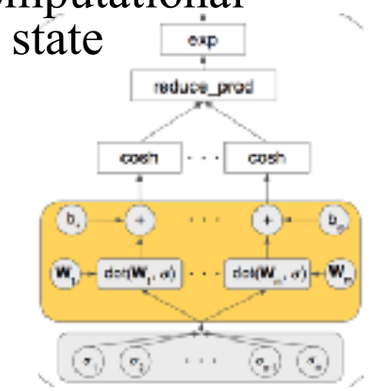


Takes explicit advantage of locality through **filters;** Calculations are lighter-weight

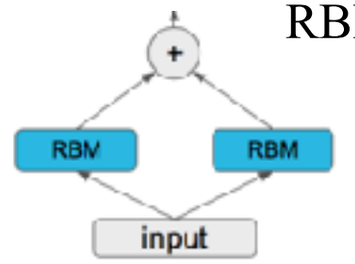
Computational graph states

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

RBM as a computational graph state



Combining 2 RBM



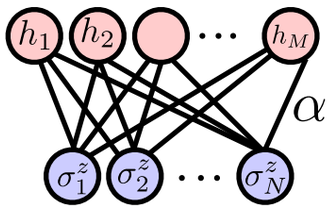
MESSAGE : We can harness all advances by ML community for variational computations

Algorithms (automatic differentiation, backpropagation, optimisers…)
Software (TensorFlow, Pytorch, Keras, Jax etc)
Hardware (GPUs)

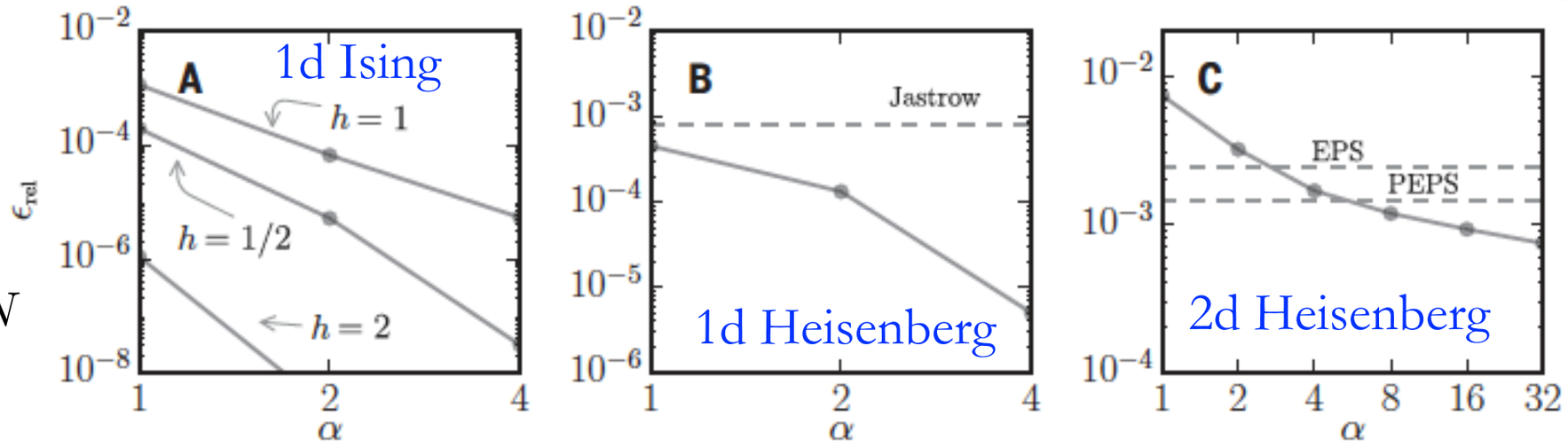
Variational efficiency of neural quantum states in practice

First simulations on quantum magnets (RBM)

Carleo & Troyer, Science (2017)



$\alpha = M/N$



RBM + Pair Projected

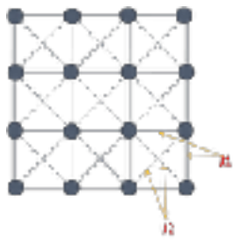
$$\Psi(\sigma) = \phi_{\rm RBM}(\sigma)\psi_{\rm PP}(\sigma)$$

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

Frustrated magnets: Convolutional neural networks

Choo *et al.*, 2019

2d J_1-J_2 model



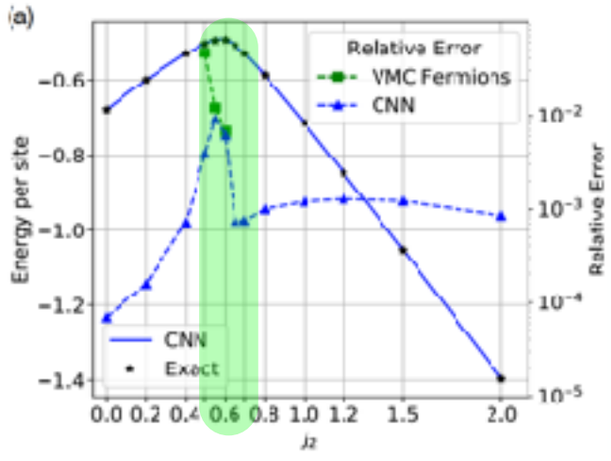
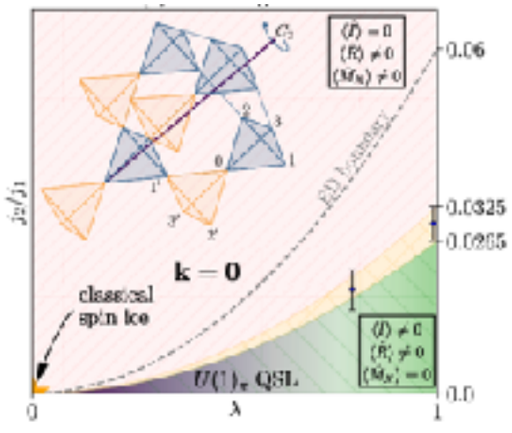


TABLE II. Comparison of ground-state energy for the 10×10 lattice at $J_2 = 0.5$ among different wave functions. The wave functions in bold font use neural networks. In Ref. [18], p-th order Lanczos steps are applied to the VMC wave function.

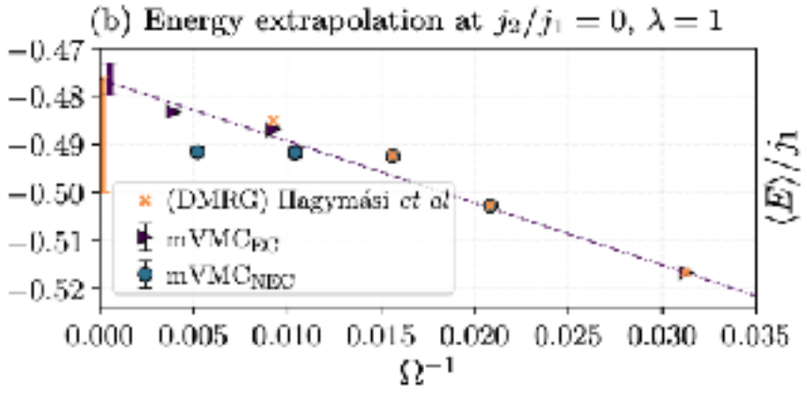
Energy per site	Wave function	Refere
−0.494757(12)	**Neural quantum state**	65
−0.498416(1)	**CNN**	60
−0.498921(1)	VMC(p=0)	18
−0.495530	DMRG	22
−0.49575(3)	**RBM-fermionic w.f.**	63
−0.497549(2)	VMC(p=2)	18
−0.497620(1)	**RBM+PP**	presen

Nomura, Imada (2021)



3d Pyrochlore

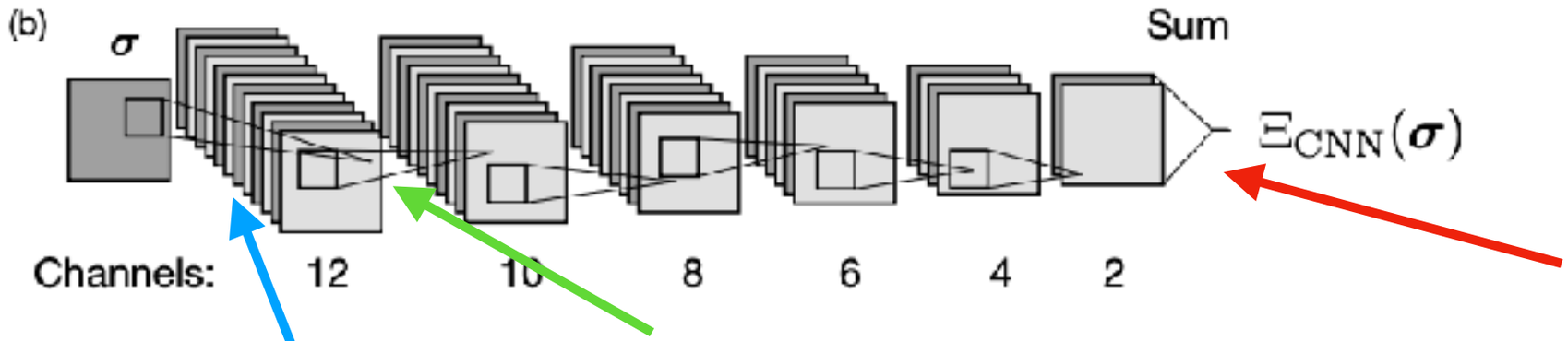
Astrakhantsev e*t al.* PRX (2021)



MESSAGE : Excellent wave-function ansatz from neural networks. No entanglement limitation

Implementing symmetries

Convolutional Neural networks (CNN) for translation invariance



Last pulling layer averages over all channels

Ensure translation invariance

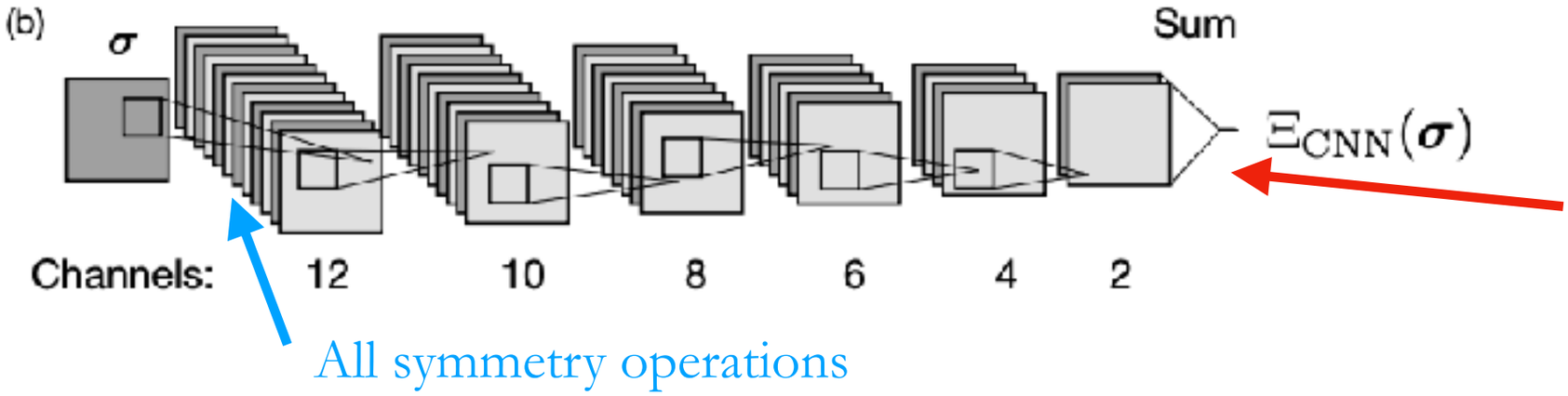
Different channels = Various positions of the filters

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

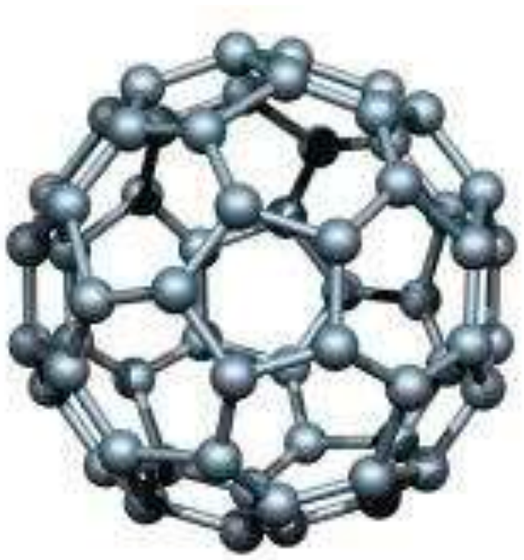


Add characters of the irrep at the final computation

Variational computations for ground-states in all irreps of arbitrary graphs

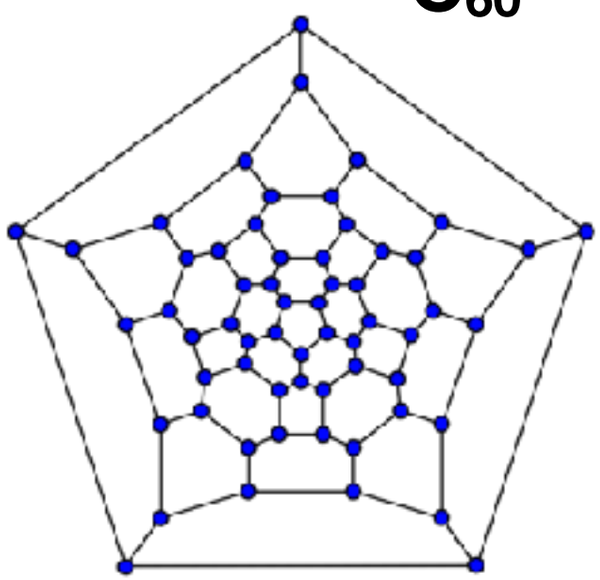
https://netket.org

Ex. Heisenberg spin 1/2 model on fullerene molecules

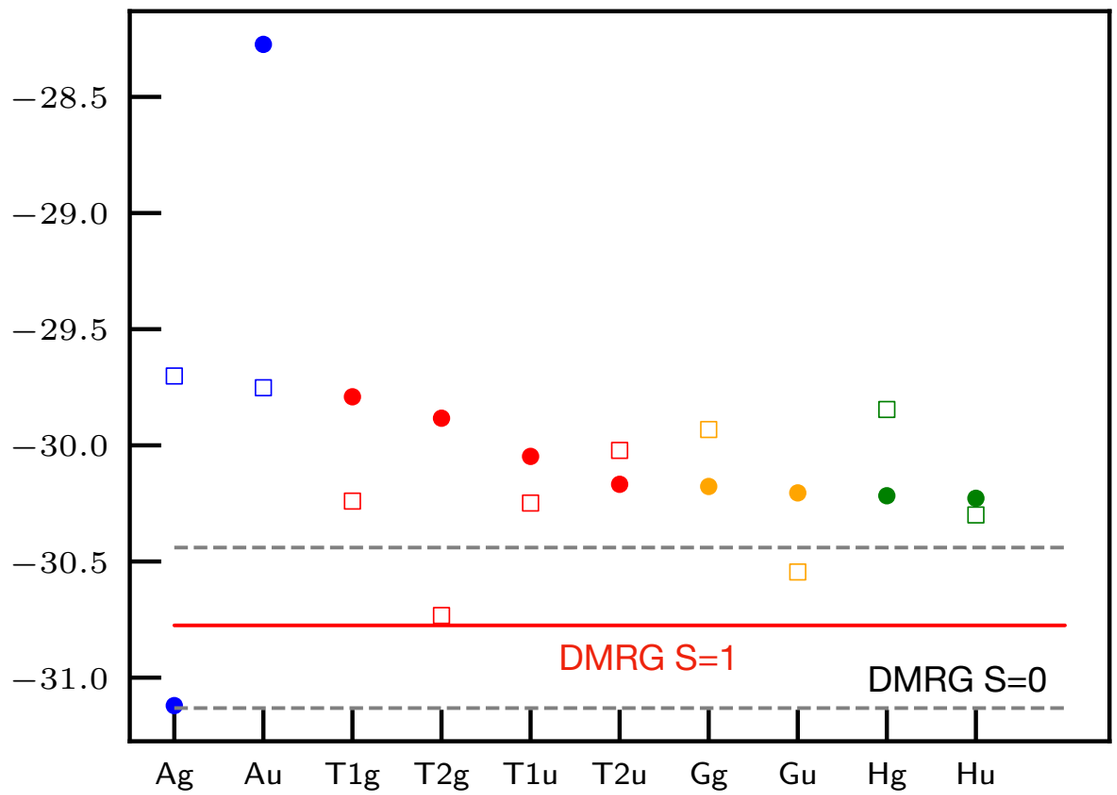


S. Capponi, FA

Work in progress



I_h symmetry



Conclusions

- Condensed matter theory & strongly correlated systems is a strong activity at LPT

- Condensed matter numerics: **a large variety of techniques**

  Many have close cousins (when not identical) in quantum chemistry, nuclear physics (nuclear many-body problem), astrophysics, statistical mechanics etc

Lots of inspiration / collaboration possible!