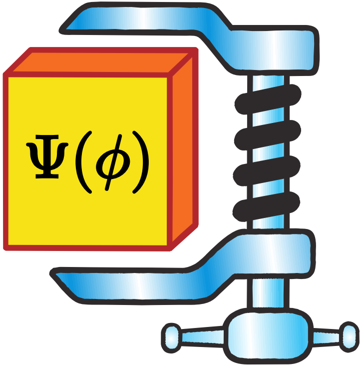
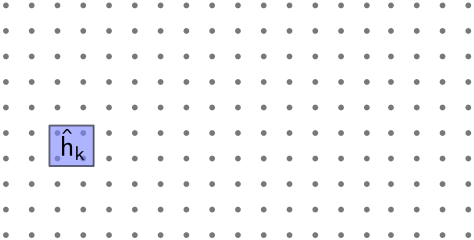
Tensor network states

to compress the many body problem



Antoine Tilloy
November 19th, 2021
Défi EQIP, Inria

Quantum many-body problem on the lattice



Typical many-body problem

N spins on a lattice

$\mathscr{H} = \bigotimes_{j=1}^{n} \mathscr{H}_j$ with $\mathscr{H}_j = \mathbb{C}^2$

$|\psi\rangle = \sum c_{i_1, i_2, \cdots, i_n} |i_1, i_2, \cdots i_N\rangle$

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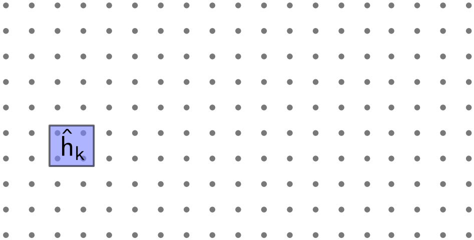

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Problem:

Finding the low energy states of

$$H = \sum_{k=1}^{N} h_k$$

is **hard** because $\dim \mathscr{H} = 2^N$ for spins

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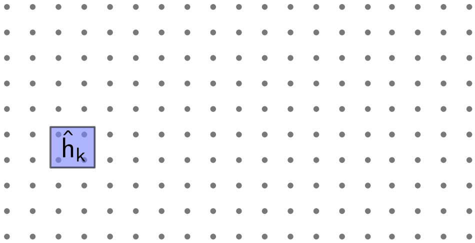

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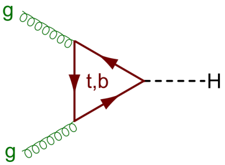
Fugaku – 2 EFLOPS – 150 PB
cannot do $4 \times 4 \times 4$ spins

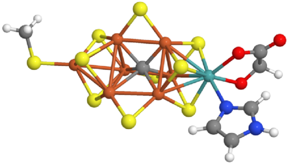
Open problems in theoretical physics

Fundamental Physics



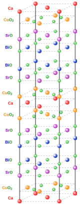
Strong force between quarks and gluons

Chemistry



Atoms interacting to form molecules

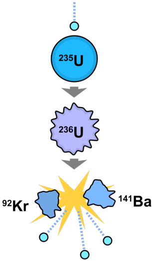
Condensed matter



Cuprate perovskites superconductors

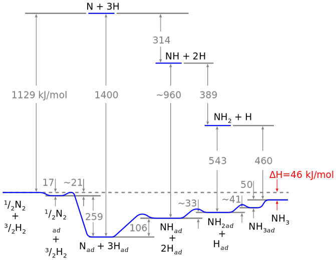
Consequences

Nuclear Physics



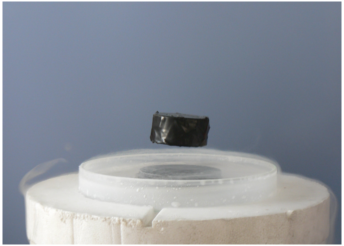
nuclei properties only measured in test reactors

Catalysis



Ammonia costly to produce
1% of CO2 prod.

High T_c superconductors



No room temp. supra
No flying cars
Costly electricity transport

Many options

Many popular approximations to go beyond standard perturbation theory

- Dynamical mean field theory (DMFT) for condensed matter
- Density functional theory (DFT) for chemistry
- Quantum Monte-Carlo
- Diagrammatic Monte-Carlo
- Resummation/resurgence

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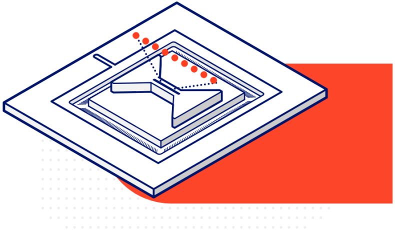
2 bleeding edge promising approaches

1. Quantum computing
2. Classical compression (variational method)

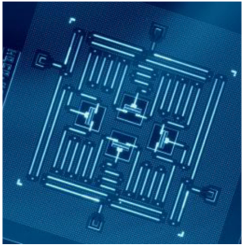
Quantum Computing

If quantum mechanics is difficult to simulate, make the simulator quantum mechanical

Trapped ions
(ionQ, Maryland,Honeywell)



Superconducting circuits
(IBM, Google, QUANTIC, Alice&Bob)



- **highly non trivial**: not just analog simulation, ultimately digital quantum computation with error correction

The direct compression approach

Variational method for ground state search

1. Guess a manifold $\mathcal{M} \subset \mathscr{H}$ with few parameters ν *i.e.* $\dim \mathcal{M} \ll \dim \mathscr{H}$
2. Tune ν to minimize energy $\nu = \operatorname{argmin}_{\nu \in \mathcal{M}} \frac{\langle \nu | H | \nu \rangle}{\langle \nu | \nu \rangle}$ and get $|\text{ground state}\rangle \simeq |\nu\rangle$

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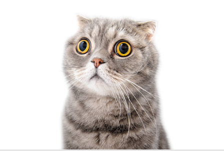
Reason for compression (classical)



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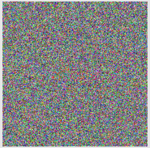

"typical" image

atypical $\Longrightarrow$ compressible

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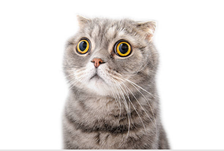

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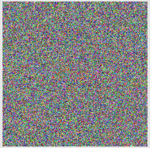

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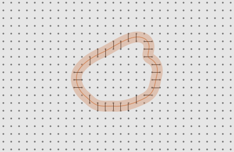
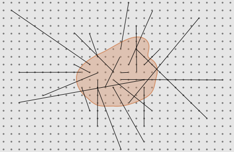
Reason for compression (quantum)



low energy state



random state

area law = atypical $\Longrightarrow$ compressible

Matrix Product States (MPS) aka tensor trains

Definition

A MPS for a translation invariant chain of N spins/qubits ($\mathscr{H}_k = \mathbb{C}^2$) with periodic boundary conditions is a state

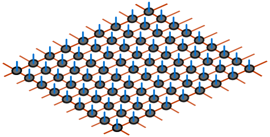
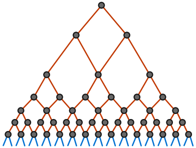
$$|\psi(A)\rangle := \sum_{i_1, i_2, \ldots, i_N = \{0,1\}} \mathrm{tr}\left[A_{i_1} A_{i_2} \cdots A_{i_N}\right] |i_1, i_2, \ldots, i_N\rangle$$

where A_0 and A_1 are 2 matrices $\in \mathcal{M}_D(\mathbb{C})$.

- The matrices A_i for $i = \pm 1$ are the free parameters
- The size D of the matrices is the **bond dimension** (quantifies freedom)
- Correlation functions (and $\langle H \rangle$) efficiently computable
- Optimizing over A provably gives good results for gapped H

Tensor network states in a nutshell

.zip or **.jpg** for complex quantum states that appear in Nature

1. **Exponential reduction:** $2^N \longrightarrow N \times D^{2d}$ parameters
   [N number of spins, D amount of entanglement, d space dimension $(1, 2, 3)$]

2. **Efficient compression:** compression error $\leqslant e^{-D}$ or $1/\text{superpoly(D)}$
   [For a large number of *a priori* non-trivial problems]

[History: 1992 for $d = 1$, 2004 for $d \geqslant 2$, 2016 for 2d-Hubbard at $T = 0$]

Tensor network states in QUANTIC

2 potential uses for the many-body problem

1. **direct** – Use tensor networks to solve many instances of the many body problem directly
2. **indirect** – Use tensor networks to simulate small clusters of physical qubits, to find the best error tolerant blocks, to then make a full fledged quantum computer, to then solve all instances of the many body problem