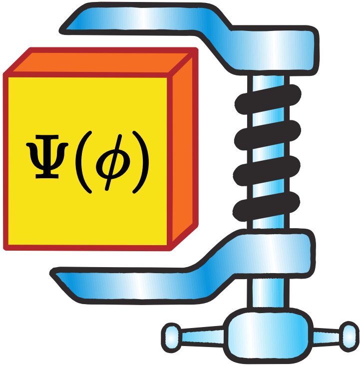
The Quantum Many Body Problem

and its recent solutions



Antoine Tilloy
November 18th, 2021
Séminaire du CAS, Mines ParisTech

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Quantum Mechanics in a nutshell

Principles

1. **System** – vector $|\psi\rangle$ in a Hilbert space $\mathscr{H}$
2. **Evolution** – generated by H self-adjoint on $\mathscr{H}$

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi_t\rangle = -\frac{i}{\hbar}H|\psi_t\rangle$$

3. **Measurement** – Ideal measurement $\equiv$ self-adjoint $\mathcal{O} = \sum_k \lambda_k P_k$

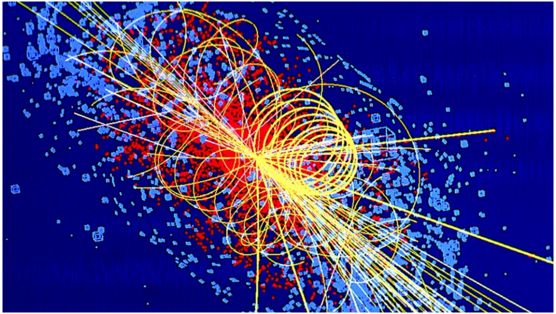
   Result k with probability $p_k = \langle\psi|P_k|\psi\rangle$ followed by collapse

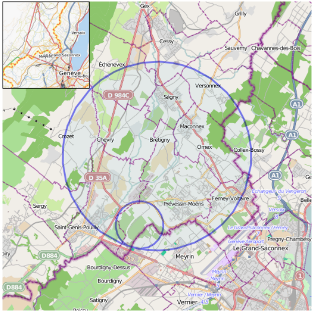
$$|\psi\rangle \longrightarrow \frac{P_k|\psi\rangle}{\|P_k|\psi\rangle\|}$$

Remark:

- Conceptual subtleties in 2 $\implies$ 3, "measurement problem"

The standard model of particle physics





The **standard model** is an instantiation of quantum mechanics that is potentially fundamental

1. Hilbert space $\mathscr{H}$ (the fundamental particles and their statistics)
2. Hamiltonian H (all the forces/interactions between the particles)

Completed by the independent detection of the Higgs boson by the Atlas and CMS collaborations at the LHC

The standard model: theory and practice

Theory: The standard model cannot be exact even in principle

1. no gravity
2. mathematically breaks down at (insanely) short distances
   (H does not exist as a self-adjoint operator on the $\mathscr{H}$ we would like, *even non-rigorously* with state of the art renormalization group theory)

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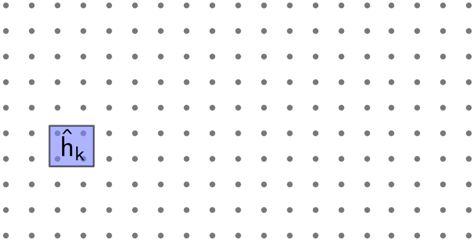
Practice: The standard model is exact for all practical purposes

- Electron - photon physics tested to 12 digits

$$g = 2.10011596521808 5(76)$$

- Ultra high energy subtleties irrelevant for realizable phenomena

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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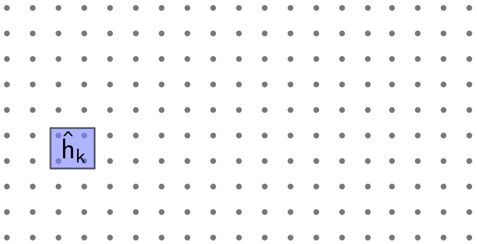

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Problem:

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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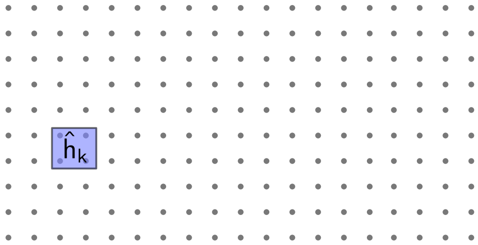

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Fugaku – 2 EFLOPS – 150 PB
cannot do $4 \times 4 \times 4$ spins

Perturbation theory

Main idea: usuall $H = H_0 + \lambda V$ where H_0 is diagnalizable exactly
$\rightarrow$ Taylor expand in λ

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Field theoretic perturbation theory

1. Interaction representation: $|\psi_t\rangle_I = e^{-iH_0 t}|\psi_t\rangle$ and $V_t = e^{-iH_0 t} V e^{iH_0 t}$

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$$|\psi_t\rangle_I = T \exp\left[-\frac{i\lambda}{\hbar}\int_0^t \mathrm{d}u \, V_u\right]|\psi_0\rangle_I$$

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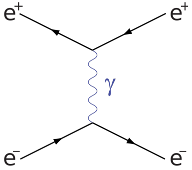
4. Dyson expansion
$$|\psi_t\rangle_I = \sum_{n=0}^{+\infty} \left(-\frac{i\lambda}{\hbar}\right)^n \int_{u_1 > u_2 > u_n} V_{u_1} V_{u_2} \cdots V_{u_n} \, |\psi_0\rangle_t$$

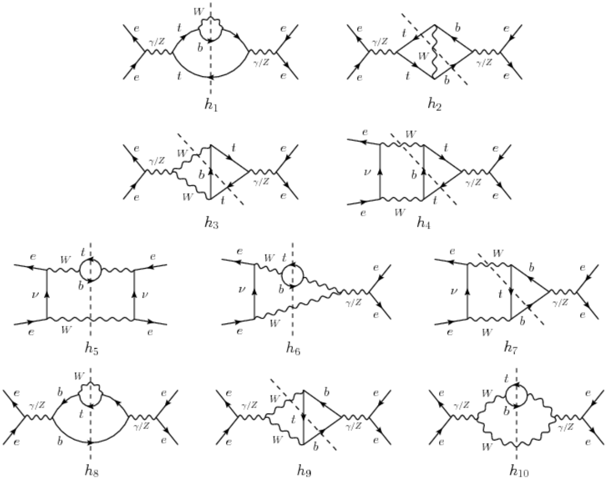
Diagrammatic reorganization of the expansion

Perturbation theory = Feynman diagrams

Order 2 in λ



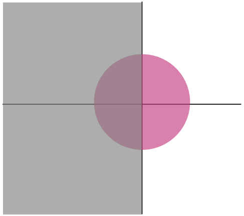
Order 6 in λ



Divergence of the expansion

First noted by Dyson in a 2 page letter

any physical quantity $= f(\lambda) \underset{\text{illicit}}{=} \sum_n a_n \lambda^n$ diverges $\forall\ \lambda$



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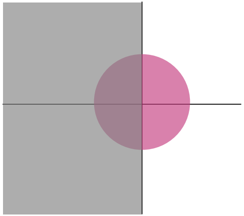


For ϕ_0^4

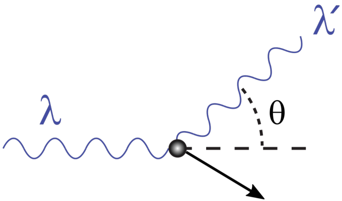
$$\int_{\mathbb{R}} d\phi\ \exp(-m^2\phi^2 - \lambda\phi^4) \underset{\text{illicit}}{=} \sum_{n=0}^{+\infty} \frac{(-\lambda)^n}{n!} \int_{\mathbb{R}} d\phi\, \phi^{4n} \exp(-m^2\phi^2)$$

$$= \sum_{n=0}^{+\infty} \frac{(-\lambda)^n}{n!\, m^{2n+1/2}} \int_0^{+\infty} du\, u^{2n+1/2} \exp(-u)$$

$$= \sum_{n=0}^{+\infty} \frac{(-\lambda)^n}{m^{2n+1/2}} \frac{\Gamma(2n+3/2)}{\Gamma(n+1)}$$

Successes

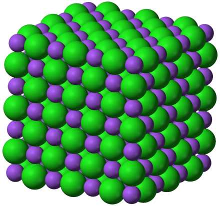
Fundamental Physics



Quantum electrodynamics

Nature is kind: $\lambda \simeq 1/137 \ll 1$
[electron-photon interaction is weak]

Condensed matter

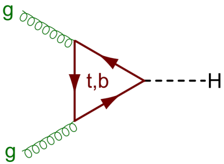


Metals/insulators/superconductors

Nature is kind: taking $\lambda = 0$ is fine
[electron-electron interaction weak]

Open problems

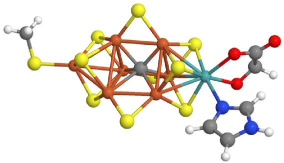
Fundamental Physics



Strong force between quarks and gluons

Nature semi-kind
$\lambda = \log[E_{\text{kin}}/E_0]$
$E_0 \simeq 200$ MeV
E_{kin} kinetic energy

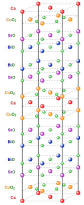
Chemistry



Atoms interacting to form molecules

Nature not kind $\lambda \sim 1$
but mean-field like approximations fairly efficient

Condensed matter

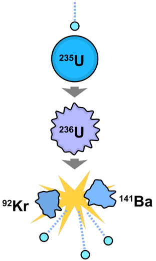


Cuprate perovskites superconductors

Nature not kind $\lambda \sim 1$
electrons interact strongly and get entangled

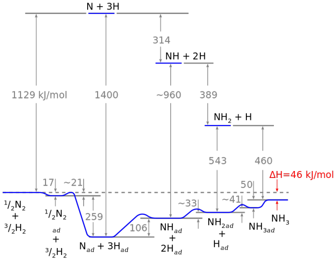
Consequences

Nuclear Physics



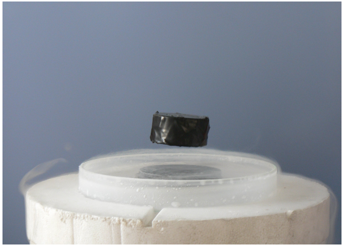
nuclei properties only measured in test reactors

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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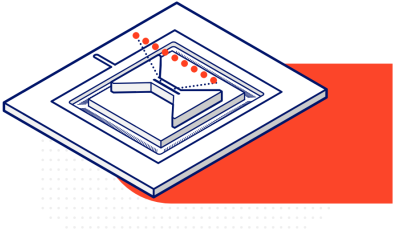
2 bleeding edge promising approaches

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

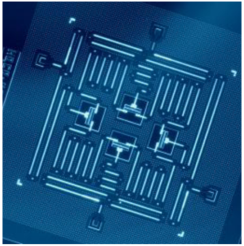
Quantum Computing

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

Aparté on quantum computing

DOES

1. Solve the quantum many-body problem directly
2. Factor prime numbers fast and break RSA
   - Turing Machines with best algorithm $t = C \exp\left(n^{1/3}\right)$
   - Shor's algorithm on quantum bits $t \propto n^3$

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DOES NOT

1. Solve by trying all solutions
   $\Longrightarrow$ only quadratic gain $n \rightarrow \sqrt{n}$ for search
2. Solve hard optimization problem in general
   $\Longrightarrow$ no exponential gain for NP-hard problems (conjecture)

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 $\nu = \text{argmin}_{\nu \in \mathcal{M}} \frac{\langle \nu | H | \nu \rangle}{\langle \nu | \nu \rangle}$ and get $|\text{ground state}\rangle \simeq |\nu\rangle$

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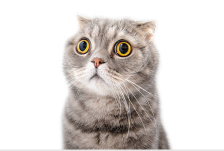
Reason for compression (classical)



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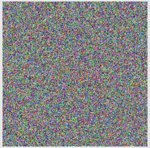

“typical” image

atypical $\implies$ compressible

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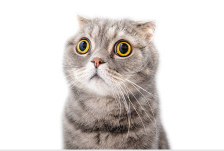

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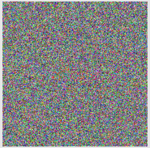

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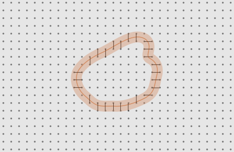
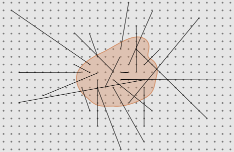
Reason for compression (quantum)



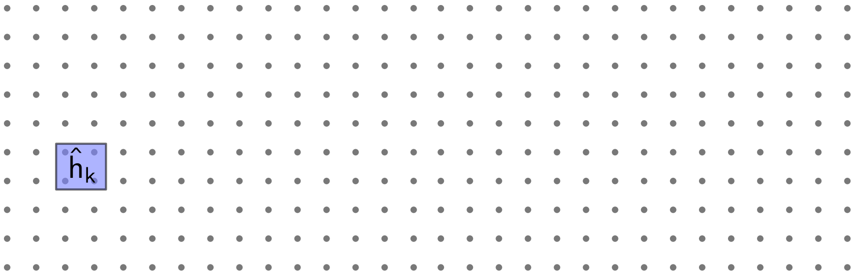
low energy state



random state

area law $=$ atypical $\Longrightarrow$ compressible

Many-body problem



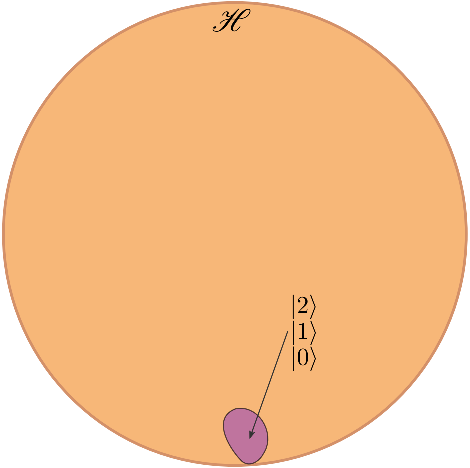
Problem

Finding low energy states of

$$\hat{H} = \sum_{k=1}^{N} \hat{h}_k$$

is **hard** because $\dim \mathscr{H} \propto 2^N$

Variational optimization



Generic (spin $1/2$) state $\in \mathscr{H}$:

$$|\psi\rangle = \sum_{i_1,\cdots,i_n=\pm 1} c_{i_1,i_2,\cdots,i_N} |i_1,\cdots,i_N\rangle$$

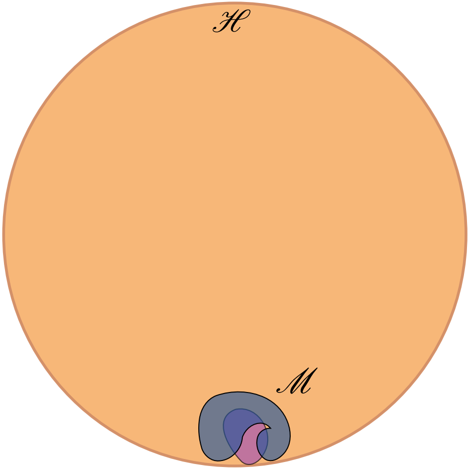
Exact variational optimization

To find the ground state:

$$|0\rangle = \min_{|\psi\rangle \in \mathscr{H}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

- $\dim \mathscr{H} = 2^N$

Variational optimization



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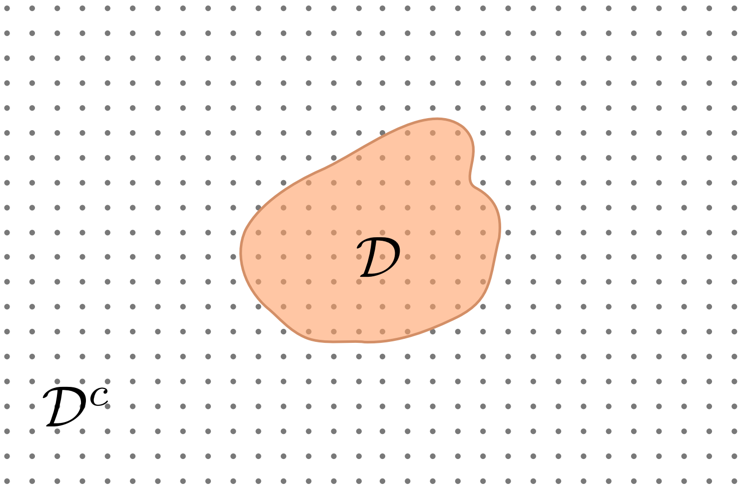
Approx. variational optimization

To find the ground state:

$$|0\rangle = \min_{|\psi\rangle\in\mathscr{M}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

- $\dim \mathscr{M} \propto \mathrm{Poly}(N)$ or fixed

Interesting states are weakly entangled



Low energy state

$|\psi\rangle = |0\rangle$ or $|1\rangle$ ...

Reduced density matrix
$\rho = \mathrm{tr}_{\mathcal{D}^c}\left[|\psi\rangle\langle\psi|\right]$

Entanglement entropy
$S = -\mathrm{tr}\left[\rho \log \rho\right]$

Area law

$$S \propto |\partial \mathcal{D}|$$

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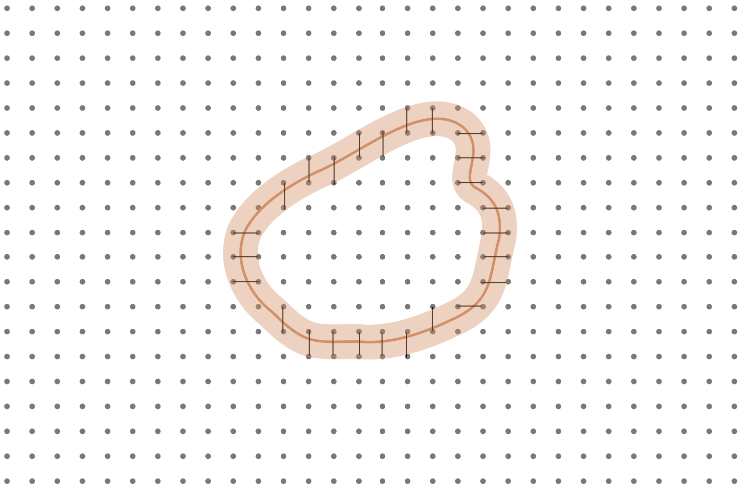

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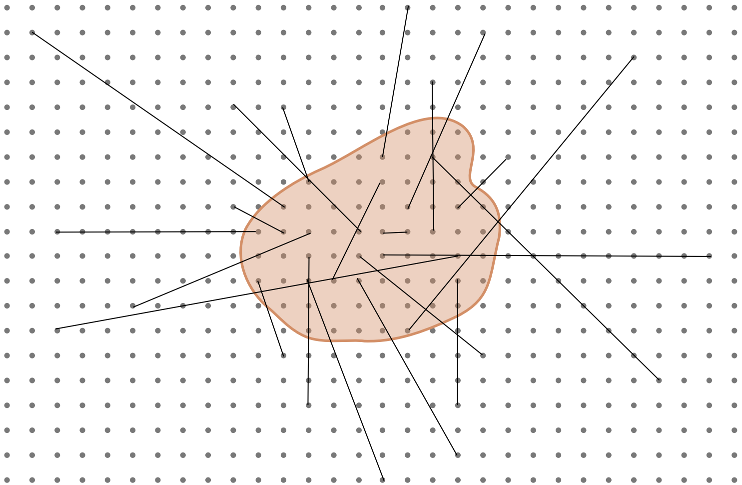
Typical states are strongly entangled



Random state

$|\psi\rangle = U_{\text{Haar}}|\text{trivial}\rangle$

Reduced density matrix

$\rho = \text{tr}_{\mathcal{D}^c}\left[|\psi\rangle\langle\psi|\right]$

Entanglement entropy

$S = -\text{tr}\left[\rho \log \rho\right]$

Volume law

$$S \propto |\mathcal{D}|$$

Matrix Product States (MPS) aka tensor trains

Definition

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

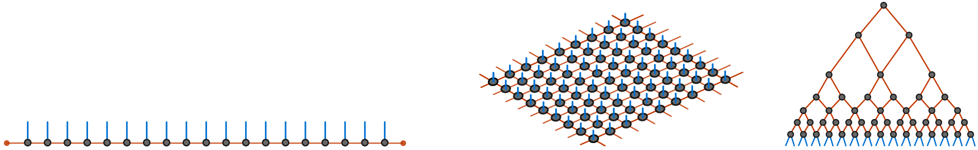
$$|\psi(A)\rangle := \sum_{i_1, i_2, \ldots, i_N} \mathrm{tr}\left[A_{i_1} A_{i_2} \cdots A_{i_N}\right] |i_1, i_2, \ldots, i_N\rangle$$

where A_i 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



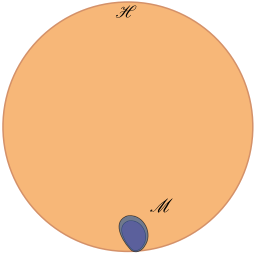
1. **Exponential reduction:** $2^N \longrightarrow N \times D^{2d}$ parameters
   [N number of spins, D amount of entanglement, d space dimension $(1, 2, 3)$]

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 $T = 0$]

Some facts

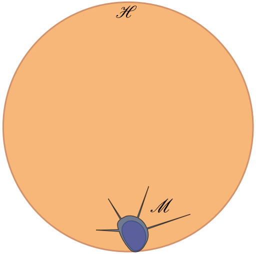
$d = 1$ spatial dimension



Theorems (colloquially)

1. For gapped H, TNS $|A\rangle$ approximate well $|0\rangle$ with D fixed
2. **All** $|A\rangle$ are ground states of gapped H

$d \geqslant 2$ spatial dimension



Folklore

1. For gapped H, TNS $|A\rangle$ approximate well $|0\rangle$ with D fixed
2. **Most** $|A\rangle$ are ground states of gapped H

State of the art

Dense: all states approximable (trivial)
Efficient: cost $Poly(D)$ error $1/superPoly(D)$

It's all a matter of prefactors and exponents

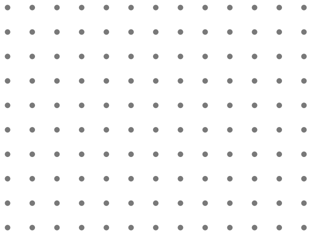
- 1 space dimension $\rightarrow D \geqslant 1000 \rightarrow$ machine precision (MPS results "numerically exact")
- 2 space dimensions $\rightarrow D \sim 10 \rightarrow$ efficient (PEPS efficient to $10^{-2} - 10^{-6}$ depending on problems)
- 3 space dimensions $\rightarrow D \sim 3 \rightarrow$ theoretically efficient but too expensive

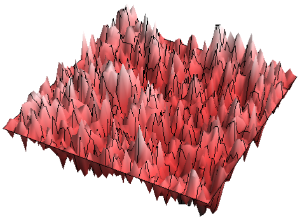
Summary

- We know the laws of Nature for all practical purposes
- But solving them is hard because of the tensor product structure in QM
- Perturbation theory saved the day for many problems
- Many crucial problems are blocked by our inability to simulate large N QM
- Quantum computing is a solution
- Classical compression based on tensor networks is another

The quantum many-body problem in the continuum

From the lattice to the continuum and Quantum Field Theory (QFT)





$$|\Psi\rangle = \sum_{i_1,i_2,\cdots,i_N} c_{i_1 i_2 \cdots i_N} |i_1 i_2 \cdots i_N\rangle \quad \longrightarrow \quad |\Psi\rangle = \int \mathcal{D}\phi \; \psi(\phi) \, |\phi\rangle$$

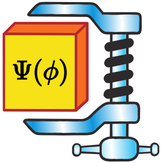
New problem: 2^N $\mathbb{C}$-parameters $\rightarrow$ $\dim \mathscr{H} = \infty^\infty$ even at finite size!

Question Can one compress ∞^∞ down to a manageable number of parameters?

Grand challenge

Grand challenge

Compress field wavefunctions $\psi(\phi)$ and use them to solve the continuous-many-body problem directly leveraging a continuous generalization of tensor networks

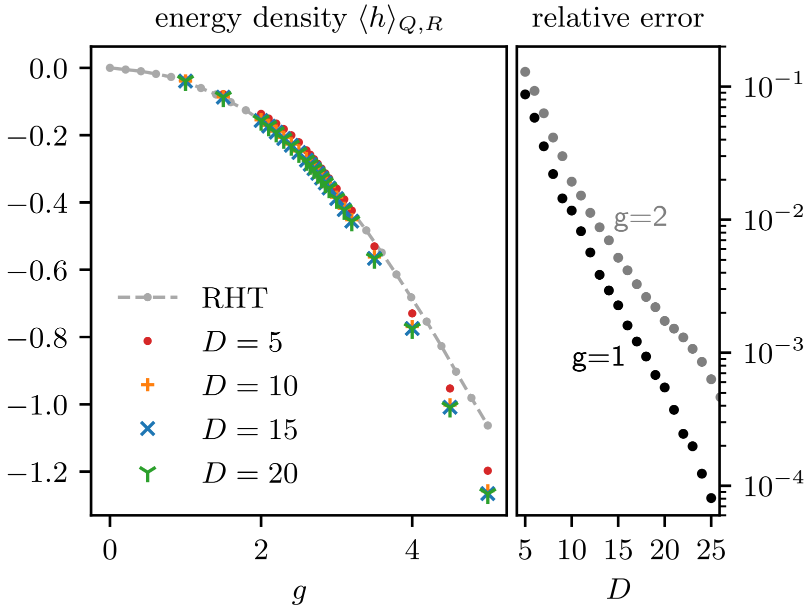


Ambitious but sound– first insights in 2010 and recent progress

	non-relativistic	relativistic	critical
$d = 1$ space	Verstraete-Cirac 2010	Tilloy 2021	
$d \geqslant 2$ space	Tilloy-Cirac 2019		

no idea	heuristics	clear definition	fast algorithm

Numerics



energy density $\langle h \rangle_{Q,R}$
relative error
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
−1.2
RHT
$D = 5$
$D = 10$
$D = 15$
$D = 20$
0
2
4
g
g=2
g=1
10^{-1}
10^{-2}
10^{-3}
10^{-4}
5
10
15
20
25
D