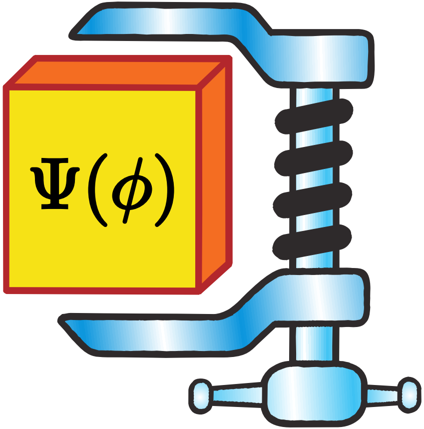
Tensor networks to compress the quantum many body problem



Antoine Tilloy

December 12th 2024

Subatech, Nantes

MINES PARIS | PSL
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erc

Content

Mostly from:

Very little of it is things I did!

The hardness and power of many-body quantum mechanics

Many-body quantum mechanics is hard

Quantum Mechanics of Many-Electron Systems.

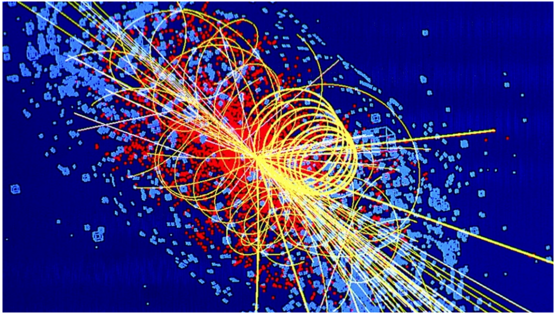
By P. A. M. Dirac, St. John's College, Cambridge.

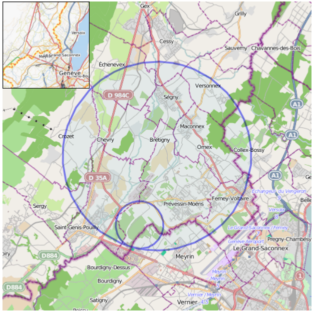
(Communicated by R. H. Fowler, F.R.S.—Received March 12, 1929.)

§ 1. *Introduction.*

The general theory of quantum mechanics is now almost complete, the imperfections that still remain being in connection with the exact fitting in of the theory with relativity ideas. These give rise to difficulties only when high-speed particles are involved, and are therefore of no importance in the consideration of atomic and molecular structure and ordinary chemical reactions, in which it is, indeed, usually sufficiently accurate if one neglects relativity variation of mass with velocity and assumes only Coulomb forces between the various electrons and atomic nuclei. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

Many-body Quantum mechanics is still hard today



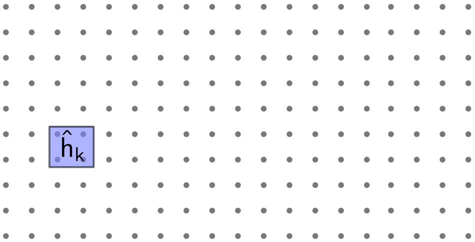


Since Paul Dirac in 1929, the **standard model of particle physics** has been completed with measurement at LHC

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

The problem is still the same

Quantum many-body problem: simplest setting



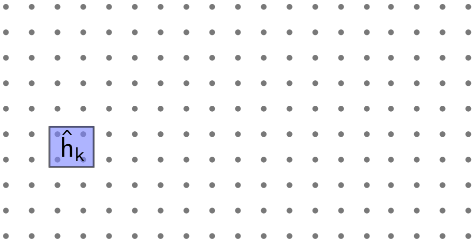
Quantum N-body problem

N spins on a lattice

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

2^N classical degrees of freedom

Quantum many-body problem: simplest setting



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N spins on a lattice

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

2^N classical degrees of freedom

Objective:

Finding the low energy states of

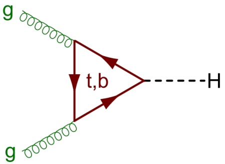
$$H = \sum_{k=1}^{N} h_k$$

difficult: H is a $2^N \times 2^N$ matrix

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

Open Problems in Theoretical Physics

Fundamental Physics

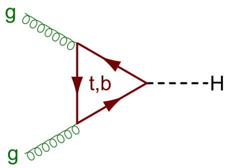


Strong interaction between quarks and gluons

Allows the formation of the nucleus

Open Problems in Theoretical Physics

Fundamental Physics



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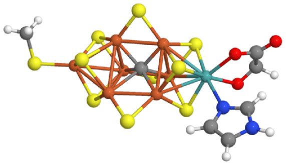
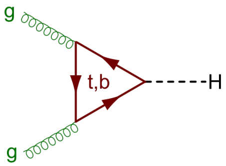


Interactions electrons - electrons and electrons - protons

Allows the formation of complex molecules

Open Problems in Theoretical Physics

Fundamental Physics



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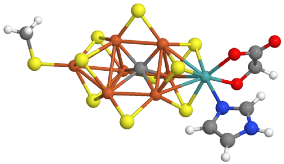

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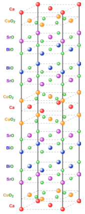
Condensed matter

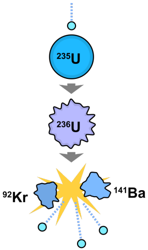


Strong interactions between electrons

Enables superconductivity in cuprate materials

Practical consequences

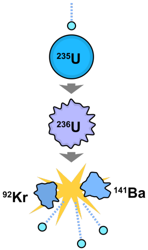
Nuclear Physics



Properties of nuclei
must be measured

Practical consequences

Nuclear Physics



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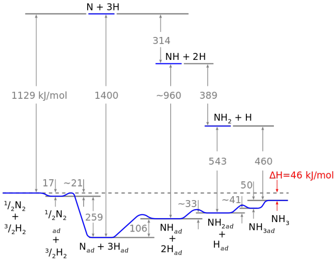
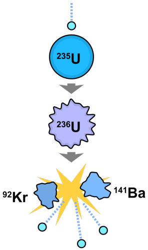
Catalysis



Ammonia is expensive
$\geqslant 1\%$ CO2 worldwide

Practical consequences

Nuclear Physics



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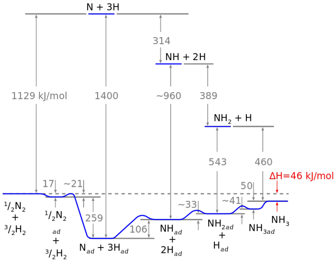

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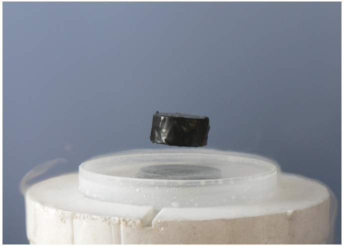
High T_c superconductors



No lossless electricity transfer

Quantum mechanics is only as hard as quantum mechanics

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

> *Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy*

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Feynman foresaw **Quantum Simulation**

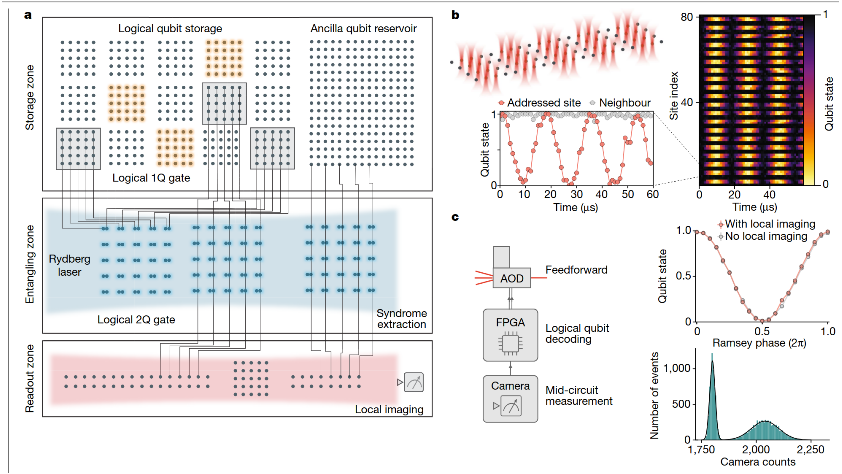
A wide range of options

Many ways to encode ψ

1. Electronic states of trapped ions
2. Electronic states of trapped cold neutral atoms
3. Mesoscopic currents in superconducting circuits
4. Spin states
5. Light states

Cold atoms

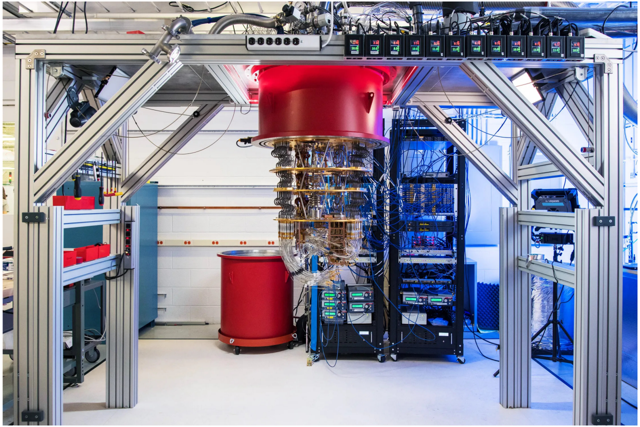
- Quera (Harvard spin-off)
- Pasqal (Institut d'optique spin-off)



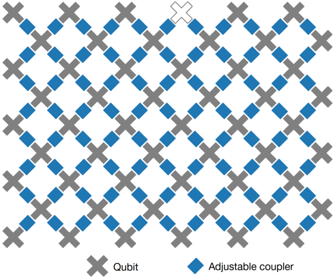
Blustein et al. Nature 2023

Superconducting circuits

- **Transmon qubits**: Google, IBM, Rigetti
- **Cat qubits** Amazon, Alice & Bob

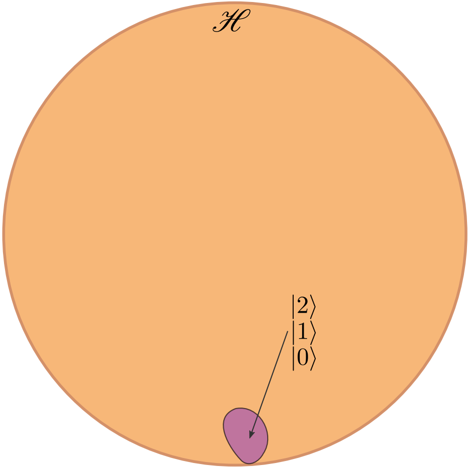


Google quantum computer



The variational method

Variational optimization



Generic state $\in \mathscr{H} = (\mathbb{C}^d)^{\otimes N}$:

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

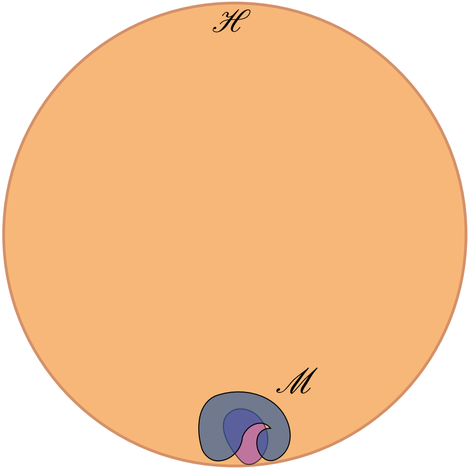
Exact variational optimization

To find the ground state:

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

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

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

An idea popular in many fields

- **Mean field** approximation (of which TNS are an extension)

$$\psi(x_1, x_2, \cdots, x_n) = \psi_1(x_1)\,\psi_2(x_2)\cdots\psi_n(x_n)$$

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$$\psi(x_1, x_2, \cdots, x_n) = \left\langle \hat{\phi}(x_1)\hat{\phi}(x_2)\cdots\hat{\phi}(x_n)\right\rangle_{\mathrm{CFT}}$$

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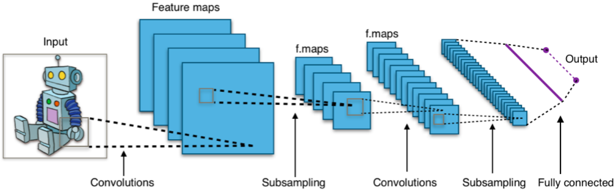
- Fully connected and convolutional **neural networks** used in machine learning



State compression and the area law

The room for compression

atypicality $\implies$ compressibility

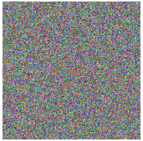
The room for compression

atypicality $\Longrightarrow$ compressibility

- For image classification, exponentially many classifiers $N_{\text{colors}}^{N_{\text{pixels}}}$ but

cat image

dog image



"typical" image

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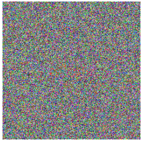
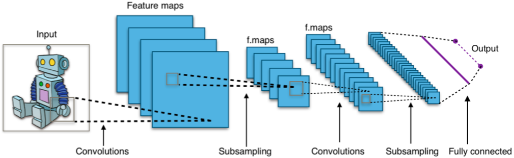


"typical" image

- efficient classifiers $f(x)$ with only $Poly(N_{\text{pixels}}) \ll N_{\text{colors}}^{N_{\text{pixels}}}$ parameters



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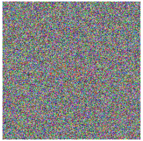

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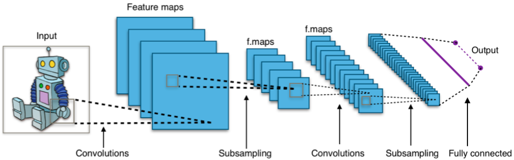
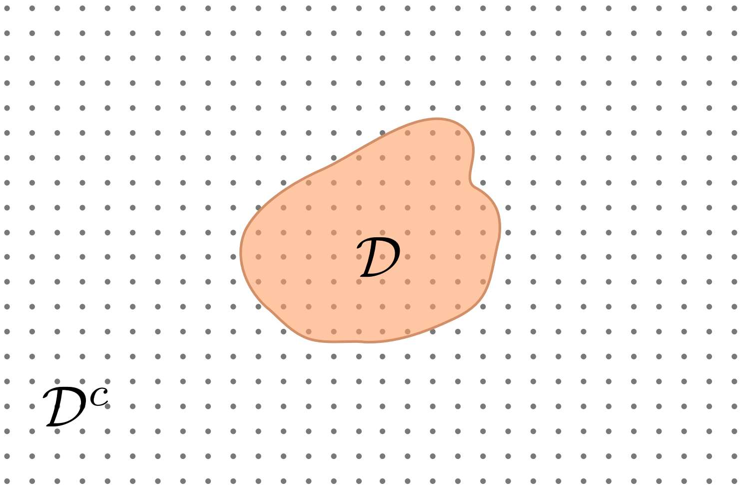


- What is the atypicality analog for quantum? $\rightarrow$ **Entanglement**

Interesting states are weakly entangled



Low energy state

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

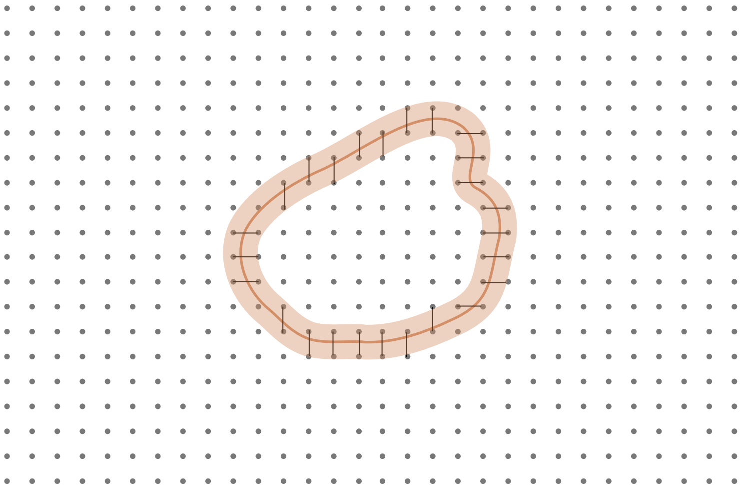
Reduced density matrix
$\rho = \mathrm{tr}_{\mathcal{D}^c}\left[|\psi\rangle\langle\psi|\right]$

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

Area law

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

Interesting states are weakly entangled



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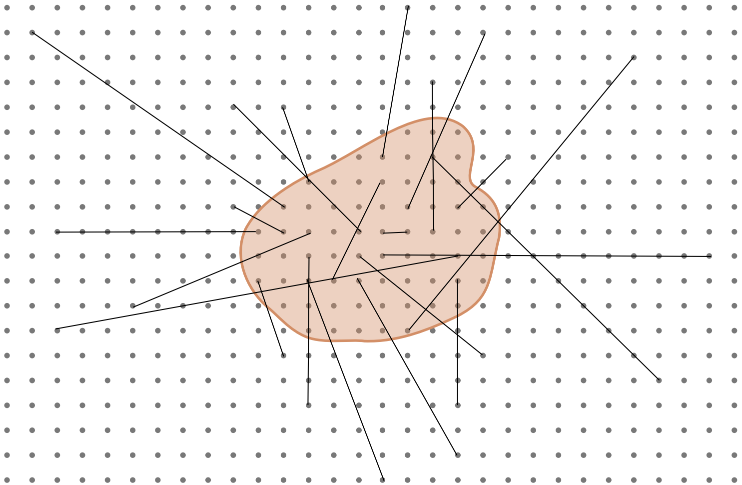
$$S \propto |\partial\mathcal{D}|$$

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

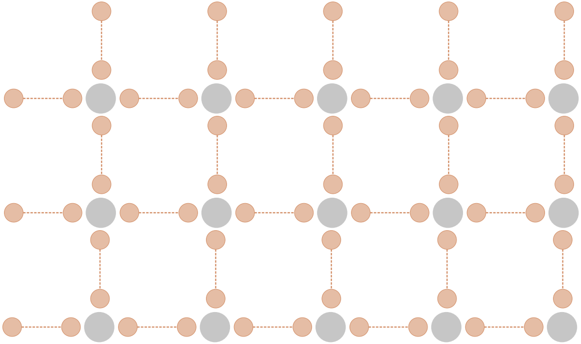
Volume law

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

Tensor network states

Constructing weakly entangled states

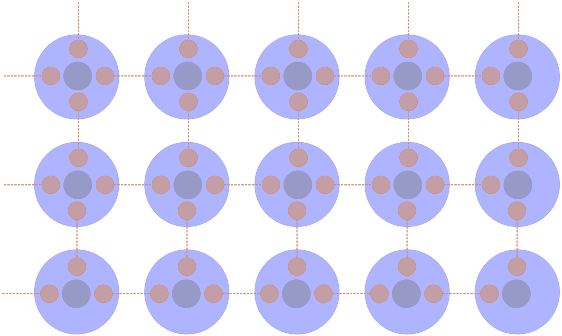
Constructing weakly entangled states



1. Put auxiliary **maximally entangled** states between sites

 $= \sum_{j=1}^{\chi} |j\rangle|j\rangle$

Constructing weakly entangled states



1. Put auxiliary **maximally entangled** states between sites

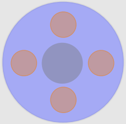
$$= \sum_{j=1}^{\chi} |j\rangle|j\rangle$$

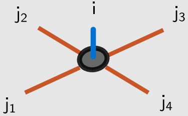
2. Map to initial Hilbert space on each site

$$= A : (\mathbb{C}^{\chi})^{\otimes 4} \to \mathbb{C}^{d}$$

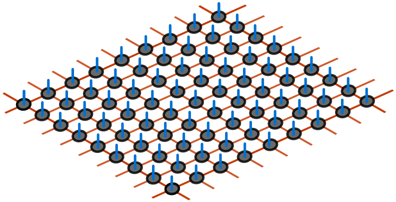
Tensor network states: definition

Why "tensor" network?





$$A : (\mathbb{C}^\chi)^{\otimes 4} \to \mathbb{C}^d \qquad \longrightarrow \qquad A^i_{j_1, j_2, j_3, j_4}$$

$|A\rangle =$ 

with tensor contractions on links

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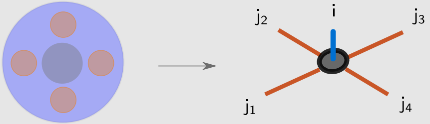

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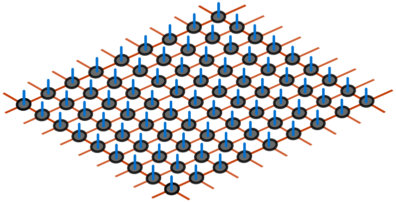


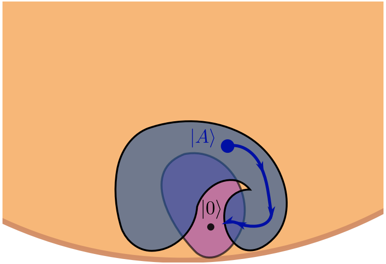
with tensor contractions on links

Optimization

Find best A for fixed χ $\quad$ ($d \times \chi^4$ coeff.)

$$E_0 \simeq \min_{A} \frac{\langle A|\widehat{H}|A\rangle}{\langle A|A\rangle}$$

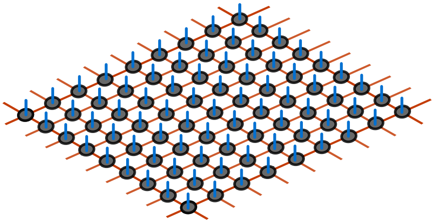
for example go down $\frac{\partial E}{\partial A^{i}_{j_1,j_2,j_3,j_4}}$



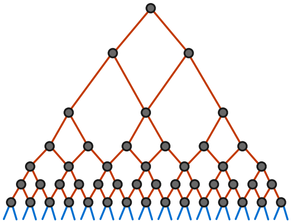
Generalizations: different tensor networks

Matrix Product States (MPS)

Projected Entangled Pair States (PEPS)

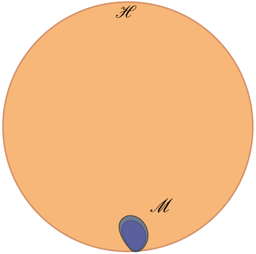


Multi-scale Entanglement Renormalization Ansatz (MERA)



Some facts

$d = 1$ spatial dimension



Theorems (colloquially)

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

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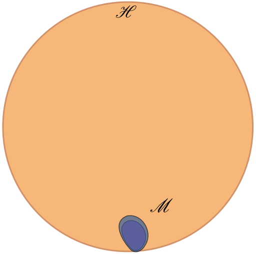
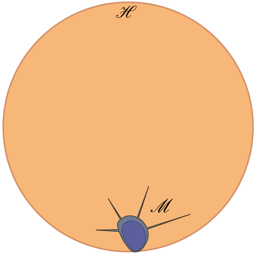
$d = 1$ spatial dimension



$d \geqslant 2$ spatial dimension



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Folklore

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

State of the art

Dense: all states approximable (trivial)
Efficient: cost *Poly*(χ) error *superPoly*(χ^{-1})

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It's all a matter of prefactors and exponents

- 1 space dimension $\rightarrow \chi \geqslant 1000 \rightarrow$ machine precision (MPS results "numerically exact")

State of the art

Dense: all states approximable (trivial)
Efficient: cost $\mathit{Poly}(\chi)$ error $\mathit{superPoly}(\chi^{-1})$

It's all a matter of prefactors and exponents

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

State of the art

Dense: all states approximable (trivial)
Efficient: cost $\mathit{Poly}(\chi)$ error $\mathit{superPoly}(\chi^{-1})$

It's all a matter of prefactors and exponents

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Beyond ground states

- Low-lying spectrum - excited states (on the G.S. tangent space)
- Thermal states (because area law)
- Real-time evolution (but no long time quench)

Beyond area law (no free lunch)

A sad fact

Scrambling of real-time evolution creates volume law entanglement even with local gapped H

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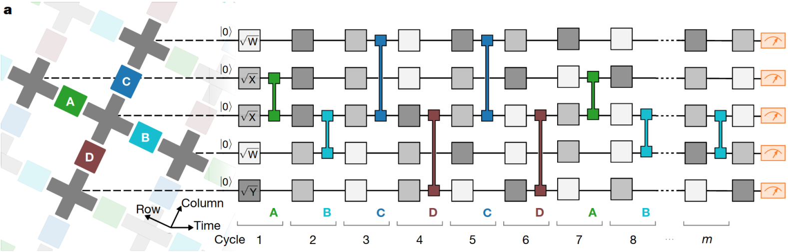
Motivates Google supremacy experiment [Nature, 2020]



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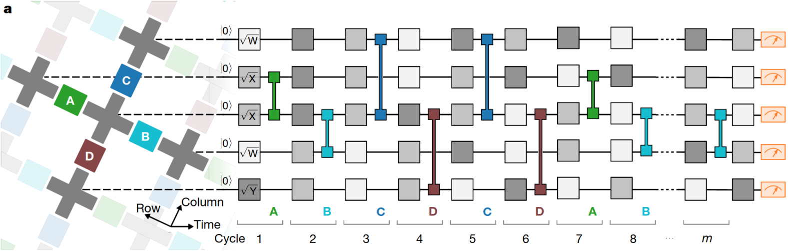


Still possible compression [Zhou, Stoudenmire, Waintal, PRX 2020]
but no exponential miracle **IF** errors low enough

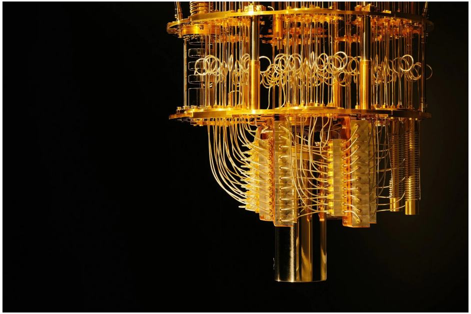
Right now? For useless tasks

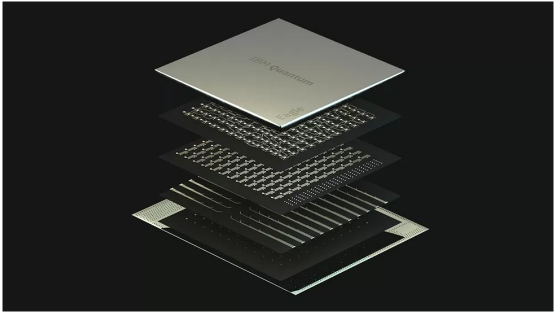
Best quantum computer is probably `Willow 105` by Google

- Previous `Sycamore 53` claimed supremacy but tensors fought back
- `Sycamore 72` wins for a carefully designed useless task
- `Willow 105` wins for a carefully designer useless task with a lot of margin

Right now

IBM – June 14th 2023 in *Nature*
Evidence for the utility of quantum computing before fault tolerance

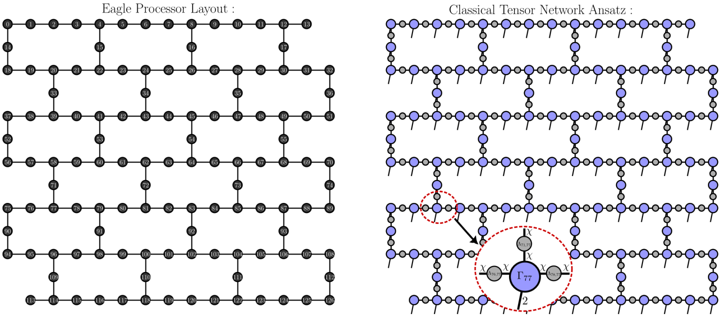




- 127 superconducting qubits
- First example of a useful case study

Right now?

Flatiron – June 26th 2023 on `ArXiv`
Efficient tensor network simulation of IBM's Eagle [...]

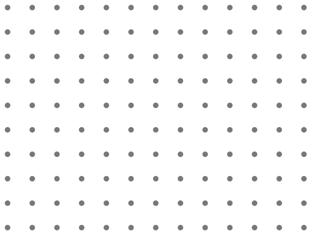


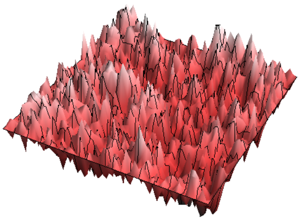
- Classical simulation via state compression
- Better precision than the quantum computer

Quantum Field Theory

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?

ϕ_2^4 testbed

Renormalized ϕ_2^4 theory

$$H = \int \mathrm{d}x \, \frac{:\pi^2:_a}{2} + \frac{:(\nabla\phi)^2:_a}{2} + \frac{m^2}{2} :\phi^2:_a + g :\phi^4:_a$$

ϕ_2^4 testbed

Renormalized ϕ_2^4 theory

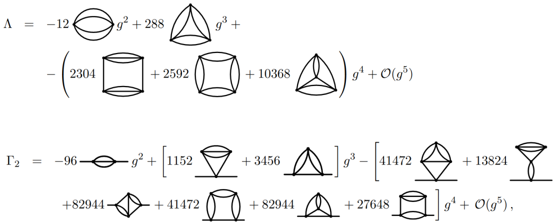
$$H = \int dx \, \frac{:\pi^2:_a}{2} + \frac{:(\nabla\phi)^2:_a}{2} + \frac{m^2}{2} :\phi^2:_a + g:\phi^4:_a$$

1. Rigorously defined relativistic QFT without cutoff (Wightman QFT)
2. Vacuum energy density finite
3. Very difficult to solve unless $g \ll m^2$ (perturbation theory)
4. Phase transition around $f_c = \frac{g}{4m^2} = 11$ i.e. $g \simeq 2.7$ in mass units

Two (main) games in town

Perturbation theory

+ resummation

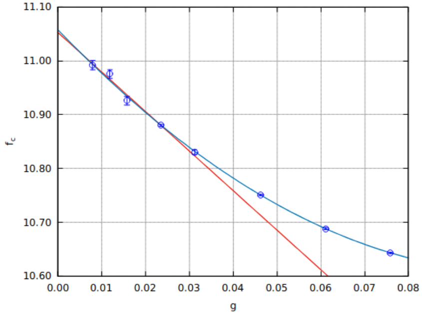


state of the art is $O(g^8)$

arXiv:1805.05882

Serone, Spada, Villadoro

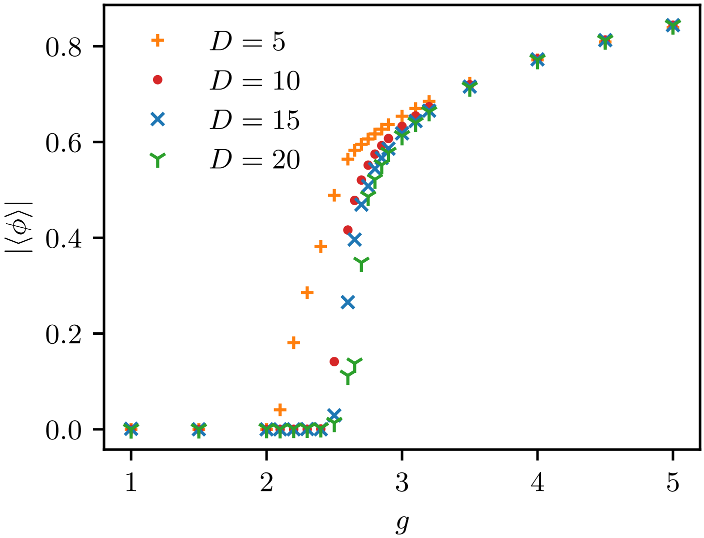
Lattice Monte-Carlo



arXiv:1807.03381

Bronzin, De Palma, Guagnelli

Results

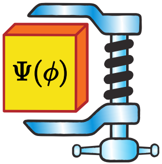


Number of parameters optimized: $2D^2$, cost $\propto D^3$

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



	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

Summary

To solve the quantum many-body problem:

- Quantum computer / simulators
- Classical compression

So far, best compression is tensor network states

- Works well in $d = 1$, ok in $d = 2$, not so well $d = 3$
- Works well for low energy, not so well for quenches

State of the art:

- For taylor made problems: current quantum computers win
- For physically relevant problems: current tensor network methods win