Solving topological quantum matter on a quantum computer

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Emergence in quantum materials

Topological materials







Quantum spin liquids



Fractional topological matter



Bi₂Se₃

Science, 325(5937), 178-181 (2009) UTe₂

Nature 579, 523–527 (2020) ZnCu₃(OH)₆Cl₂

Science 350(6261), 655-658 (2015) Twisted MoTe₂ Nature 622, 63–68 (2023)

Quantum excitations in quantum materials

Quantum materials made of electrons (spin = 1/2, charge = 1), protons, neutrons and photons

But in quantum materials, we can have emergent collective new excitations



Topological quantum matter

Ouantum Hall effect



Quantum Anomalous Hall effect

Cr-doped

(Bi,Sb)₂Te₃



Science 340.6129 (2013): 167-170

Weyl semimetal



Nature Physics 11, 724–727 (2015)

Quantum Spin Hall effect



Bi₂Se₃

Science 325.5937 (2009): 178-181

Topological superconductor



Science 346.6209 (2014): 602-607

Nodal line semimetals



Advanced Science 6.4 (2019): 1800897

All these states are described by effective isolated single-particle physics

Many-body topological quantum matter

Quantum spin liquids



Reports on Progress in Physics 80.1 (2016): 016502.

Fractional Chern insulators



Rev. Mod. Phys. 71, S298 (1999)

Parafermions



Annual Review of Condensed Matter Physics 7, 119-139 (2016)

Topological many-body quantum matter is an open challenge where quantum algorithms will potentially enable solving open challenges

Macroscopic topological effects

Chern topological insulators Superconductivity $\Phi = \frac{h}{2e} \quad \underline{\textbf{Quantization}} \text{ of flux}$ $\sigma_{xy} = \nu \frac{1}{h}$ **Quantization** of conductance

Macroscopic (topological) quantum phenomena determine fundamental physical constants with the highest precision

The computational challenge in topological matter

Single particle topological matter

$$H = \sum c_i^{\dagger} c_j$$

- N sites/atoms/orbitals
- $N\,$ computational resources

How can it be solved

Exact classical methods

Many-body topological matter

$$H = \sum c_i^{\dagger} c_j + V_{ijkl} c_i^{\dagger} c_j c_k^{\dagger} c_l$$

N sites/atoms/orbitals

 2^N computational resources

How can it be solved

Exact classical methods (tiny systems) Tensor network classical methods Quantum computers (?)

Introduction to topology in quantum materials

The Hall effect



Measure the current perpendicular to a voltage

The Hall conductivity

The Hall conductivity is obtained as

$$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_{\alpha} d^2 \mathbf{k}$$

The transverse conductivity is a topological invariant

This means, it must take integer values regardless of defects in an insulator

Hall conductivity in an insulator

$$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_{\alpha} d^2 \mathbf{k} = \sum_{\alpha} C_{\alpha} = C$$

The Chern number is quantized

$$C_{\alpha} = \int \Omega_{\alpha}(\mathbf{k}) d^2 \mathbf{k} = 0, \pm 1, \pm 2, \dots$$



An insulator can have a finite (and quantized) Hall conductivity

This is a simple example of a topological state of matter

The idea of topological invariants

Holes in a 3d surface

Knots in curves



Topology classifies object that cannot smoothly deformed into one another

Topology and holes



Topological invariant in a Hamiltonian

We can classify Hamiltonians according to topological invariants



The role of a topological invariant

Hamiltonians with different topological invariants can not be deformed one to another







The consequence of different topological invariants



Topological excitations appear between topologically different systems

The edge states of a Chern insualtor



The edge states of the quantum Hall effect are topological excitations

The edge states of a Chern insualtor



The edge states of the quantum Hall effect are topologically protected

Three important topological materials

Chern insulators



Electronics



Spintronics



Topological quantum computing

A minimal model for a topological insulator: the SSH model

The SSH model



Let us consider a finite dimerized chain

The two phases of the dimerized model

"Trivial" phase (gaped everywhere)



"Topological" phase (gapless zero modes)



The two phases of the dimerized model



Coupling the dimers



 $H = tc_0^{\dagger}c_1 + c_1^{\dagger}c_2 + tc_2^{\dagger}c_3 + c_3^{\dagger}c_4 + h.c.$

Does this Hamiltonian have a surface zero mode?

Coupling the dimers



For t<1, both Hamiltonians are topologically equivalent

They can be deformed into one another without closing the bulk gap

The bulk Hamiltonian in the dimerized model

For a finite system of this form



The unit cell is



The Hamiltonian is

$$H = \begin{pmatrix} 0 & t + e^{ik} \\ t + e^{-ik} & 0 \end{pmatrix}$$

The bulk invariant in the dimerized model

Hamiltonian Zak phase $H = \begin{pmatrix} 0 & t + e^{ik} \\ t + e^{-ik} & 0 \end{pmatrix} \qquad \phi = \int_{BZ} A dk$ $A = i \langle \Psi(k) | \partial_k | \Psi(k) \rangle$

Two different possible values for the Zak phase

 $\begin{array}{ll} \phi = 0 & t > 1 & \mbox{Trivial insulator} \\ \phi = \pm \pi & t < 1 & \mbox{Topological insulator} \end{array}$

The bulk-boundary correspondence in the dimerized model



Physical relevance of dimerized models

Some topological orders are equivalent to dimerized models upon a mathematical transformation

Topological superconductor

$$H = \sum_{n} c_{n}^{\dagger} c_{n+1} + c_{n} c_{n+1} + h.c. \qquad f$$
Conventional Majorana operator
$$c_{n} = \gamma_{2n-1} + i\gamma_{2n}$$

Topological quantum magnets

$$H = \sum_{n} \vec{S}_{n} \cdot \vec{S}_{n+1}$$
$$S \sim s_1 \otimes s_2$$
$$(S=1) \quad s_{1,2} = 1/2$$

$$f$$

$$s = 1/2$$

$$S = 1$$

The computational challenge of quantum many-body systems

The problem of dimensionality

In a many-body problem, the size of our vectors grows as

For a single-particle tight binding problem, we can reach up to $\,10^8$ sites in a laptop

For a many-problem, we cannot even store states for systems bigger than L=30 sites $2^{30}\sim 10^9$

The quantum many-body problem

Let us take a simple many-body problem

$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

And let us imagine that we have L different sites on our system and S=1/2

For example, for L=2 sites the elements of the basis are

 $|\uparrow\uparrow\rangle \quad |\uparrow\downarrow\rangle \quad |\downarrow\uparrow\rangle \quad |\downarrow\downarrow\rangle$

For L=3 sites the elements of the basis are

The quantum many-body problem

Let us take a simple many-body problem

$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

And let us imagine that we have L different sites on our system and S=1/2

For L=4 sites, the elements of the basis are

The quantum many-body problem

Let us take a simple many-body problem

$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

A typical wavefunction is written as

$$|\Psi\rangle = \sum c_{s_1,s_2,\ldots,s_L} |s_1,s_2,\ldots,s_L\rangle$$

We need to determine in total 2^L coefficients

Is there an efficient way of storing so many coefficients?

The fundamental idea of tensor-networks

A many-body wavefunction a is a very high dimensional object

$$|\Psi\rangle = \sum c_{s_1,s_2,\ldots,s_L} |s_1,s_2,\ldots,s_L\rangle$$

Tensor-networks allow "compressing" all that information in a very efficient way



"True wavefunction"



"Tensor-network wavefunction"

The matrix-product state ansatz

For this wavefunction
$$\ket{\Psi} = \sum c_{s_1,s_2,...,s_L} \ket{s_1,s_2,...s_L}$$

Let us imagine to propose a parametrization in this form

$$c_{s_1,s_2,...,s_L} = M_1^{s_1}M_2^{s_2}....M_L^{s_3}$$
 dimension 2^L dimension $\sim Lm^2$

(m dimension of the matrix)
State compression with tensor-networks

Given a many-body wavefunction, we can parametrice the components as

$$|\Psi\rangle = \sum_{\{s\}} \operatorname{Tr} \left[M_1^{(s_1)} M_2^{(s_2)} \cdots M_N^{(s_N)} \right] |s_1 s_2 \dots s_N\rangle$$



Matrix product state

The previous representation allows drastically reducing the memory required to store a state

Annals of Physics 326, 96 (2011)

Exponentially large algebra with tensor networks

Tensor network allow to (approximately) operate in exponentially large vector spaces



MPS as a parametrization of area law states

Full Hilbert space



$$c_{s_1,s_2,\dots,s_L} = M_1^{s_1} M_2^{s_2} \dots M_L^{s_3}$$

MPS have an entanglement entropy bounded by the bond dimension

 $S \sim \log(m)$

A controlled way of parametrizing the Hilbert space

Sketch of the space parametrized with bond dimension D



The matrix-product state ansatz

- This ansatz enforces a maximum amount of entanglement entropy in the state $S \sim \log m$
- One-dimensional problems have ground states that can be captured with this ansatz

$$c_{s_1,s_2,\ldots,s_L} = M_1^{s_1} M_2^{s_2} \ldots M_L^{s_3}$$

This ansatz can be generalized for time-evolution, excited states, or typical thermal states

The Heisenberg model with tensor-networks

 $\mathcal{H} = \sum_{n} J(n) \vec{S}_{n} \cdot \vec{S}_{n+1}$ $J(n) \stackrel{n}{=} J_{0} + \delta \cos \Omega n$ Non-uniform Heisenberg model $\frac{1}{2} \frac{1}{2} \frac{1}$ 50 100 150 200 \mathcal{N}

Tensor networks allow solving a 200 many-body spin model in a few seconds in a laptop

Many-body dynamical correlators

One dimensional Heisenberg Hamiltonian



Tensor networks allow computing dynamical correlators

 $\mathcal{S}(N,\omega) = \langle GS | S_N^z \delta(\omega - \mathcal{H} + E_0) S_N^z | GS \rangle$

Dynamical structure factor of a Heisenberg model

S=1/2 chain

S=1 chain



Open-source software for tensor-network many-body algorithms

dmrgpy

```
from dmrgpy import spinchain
spins = ["S=1" for i in range(40)] # S=1 chain
sc = spinchain.Spin_Chain(spins) # create spin chain object
h = 0 # initialize Hamiltonian
for i in range(len(spins)-1):
    h = h + sc.Sx[i]*sc.Sx[i+1]
    h = h + sc.Sy[i]*sc.Sy[i+1]
    h = h + sc.Sz[i]*sc.Sz[i+1]
sc.set_hamiltonian(h)
sc.get_dynamical_correlator(name=(sc.Sz[0], sc.Sz[0]))
```

Generic Python library for tensor-network kernel polynomial algorithms for spins, fermions, parafermions, with static and dynamical solvers

https://github.com/joselado/dmrgpy

Some paradigmatic problems solved with matrix product states

Solving the 2D Hubbard model at finite doping



Science, 365(6460), 1424-1428 (2019)

Solving the 2D Heisenberg model in frustrated lattices



 $\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$

Phys. Rev. Lett. 123, 207203 (2019)

Many-body state compression

Matrix-product states

Projected entangled pair-states

Neural-network quantum states







Phys. Rev. Lett. 69, 2863 (1992)

Annals of Physics 326, 96 (2011)

Science 355.6325 (2017): 602-606.

Other compressed many-body states could be potentially used for noisy quantum circuit simulation

Plan for today

• Emulating quantum circuits with tensor-networks

Phys. Rev. Research 6, 033325 (2024)

• Computing topological invariants in a superconducting quantum computer

Phys. Rev. Research 6, 043288 (2024)

Marcel Niedermeier

Marc Nairn







Tensor-networks for noisy quantum circuits

What is a quantum computer

Time evolution of quantum systems are described by $-i \frac{\partial}{\partial t} |\Psi\rangle = H(t) |\Psi
angle$

Whose solution is
$$|\Psi(t)
angle = e^{i\int_{t=0}^{t}H(t')dt'}|\Psi(t=0)
angle$$

A quantum computer is a controllable quantum system where $|\Psi(t=0)
angle$ and ~H(t)~ can be controlled

The results of the computation consist on observables $\langle A
angle = \langle \Psi(t) | A | \Psi(t)
angle$

Quantum computers enabling simulating dynamics that may require exponentially large resources

A method to simulate large quantum many-body dynamics (tensor networks) also allows to simulate large quantum computers

How much entanglement do we need

Qubit fidelity limits which states we can create in a quantum circuit

Tensor-network bond dimension limits which states we parametrize



Both constrains put bounds to the entanglement of accessible states

Do we need the whole Hilbert space to successfully run a quantum algorithm? Could we get meaningful results even if we can only access part of the Hilbert space?

Phys. Rev. X 10, 041038 (2020)

What is the relation between a noisy qubit and a tensor network?



The finite tensor-network bond dimension can be understood as a finite qubit fidelity

Applying a single qubit gate to a tensor network



Applying a multi-qubit gate to a tensor network



Original MPS

Multi-qubit gate

Higher dimension updated MPS

Compressed updated MPS

Three quantum algorithms with tensor-network quantum circuits

- **Quantum Fourier transform:** quantum analogue of the discrete Fourier transform
- Grover's algorithm: find elements in a database
- *Quantum counting algorithm:* counting the number of solutions for a given search problem

The quantum Fourier transform

N is the number of qubits

Circuit architecture



Grover's search algorithm

N is the number of qubits



Circuit architecture

Grover operator G, repeat r times



Grover fidelity (m marked elements) $f_r = \frac{1}{m} \sum_{i}^{m} |\langle \omega_i | \Psi_r \rangle|^2$

Quantum counting algorithm

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Circuit architecture



Phases of marked elements (correct in red)



Entanglement propagation in the quantum-circuit

Quantum Fourier transform

Grover's algorithm

Quantum counting algorithm



Entanglement builds up in concrete locations and steps of the quantum circuit

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Quantum circuits for topological quantum materials

Topological invariant in a Hamiltonian

We can classify Hamiltonians according to topological invariants



Berry phase with a quantum circuit

Take the eigenstates of the Hamiltonian

 $H(\mathbf{k}) |n(\mathbf{k})\rangle = E_n(\mathbf{k}) |n(\mathbf{k})\rangle$

Evolve them in reciprocal space

$$U(T,0) |n(\mathbf{k})\rangle = e^{i(\Theta_B - \Theta_D)} |n(\mathbf{k})\rangle$$

Geometric phase

Dynamical phase

$$\Theta_B = i \int_0^T dt \langle n(\mathbf{k}(t)) | \partial_t | n(\mathbf{k}(t)) \rangle \qquad \Theta_D = \int_0^T dt E_n(\mathbf{k}(t))$$

We want to cancel out the dynamical phase, so we can evolve first forward and then backwards in time

$$\overline{U}(T,0)U(T,0)|n(\boldsymbol{k})\rangle = e^{i2\Theta_B}|n(\boldsymbol{k})\rangle$$
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Quantum circuits to compute topological invariants

Berry phase with quantum phase estimation (based on QFT)



Berry flux (based on Hadamard test)



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Two ways of computing a Chern number

Method 1: Integrate the Berry Curvature $C = \frac{1}{2\pi} \int_{RZ} d^2 \mathbf{k} \Omega(\mathbf{k})$

Method 2: Pumping of the Wannier charge centers

$$X_W(k_y) = i \int_{-\pi}^{\pi} dk_x \left\langle n(\boldsymbol{k}) | \partial_{k_x} | n(\boldsymbol{k}) \right\rangle / 2\pi$$

(and count how many times they wind)

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Five implementations of the topological invariant

- Helmi quantum computer
- Exact quantum circuit emulator
- Noisy quantum circuit emulator
- Tensor-network quantum circuit emulator
- Exact classical algorithm

Helmi quantum computer



"Helmi, the first Finnish quantum computer, co-developed by VTT and IQM Quantum Computers, is operated by VTT in Espoo, Finland. Helmi is based on superconducting technology, and presently provides five qubits. Upgrades to 20, then 50 qubits is planned for the near future."

https://fiqci.fi/

Chern number from Wannier winding



Exact classical simulation

Tensor network simulator

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Chern number from Wannier winding



Low bond dimension

Tiny part of the Hilbert space

High bond dimension

Most of the Hilbert space

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Chern number from Berry curvature integration



 $-\pi$

 $-3\pi/2$

Noisy simulation



max min

C = 1



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3erry flux

Topological phase diagram

QWZ model

Haldane model



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Topological phase diagram



Haldane model

Noisy calculations provide qualitatively correct topological phase diagrams

Phys. Rev. Research 6, 043288 (2024)

Future steps in topology on quantum computers

- Next FiQCI quantum computers (20 and 50 qubits) would allow tackling many-body topological models
 - One dimensional topological spin liquids (S=1 Haldane)
 - Two dimensional topological spin liquids (S=1/2)
Take home

Currently available quantum computers allow computing topological invariants, and can be effectively benchmarked with tensor-networks





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Thank you

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