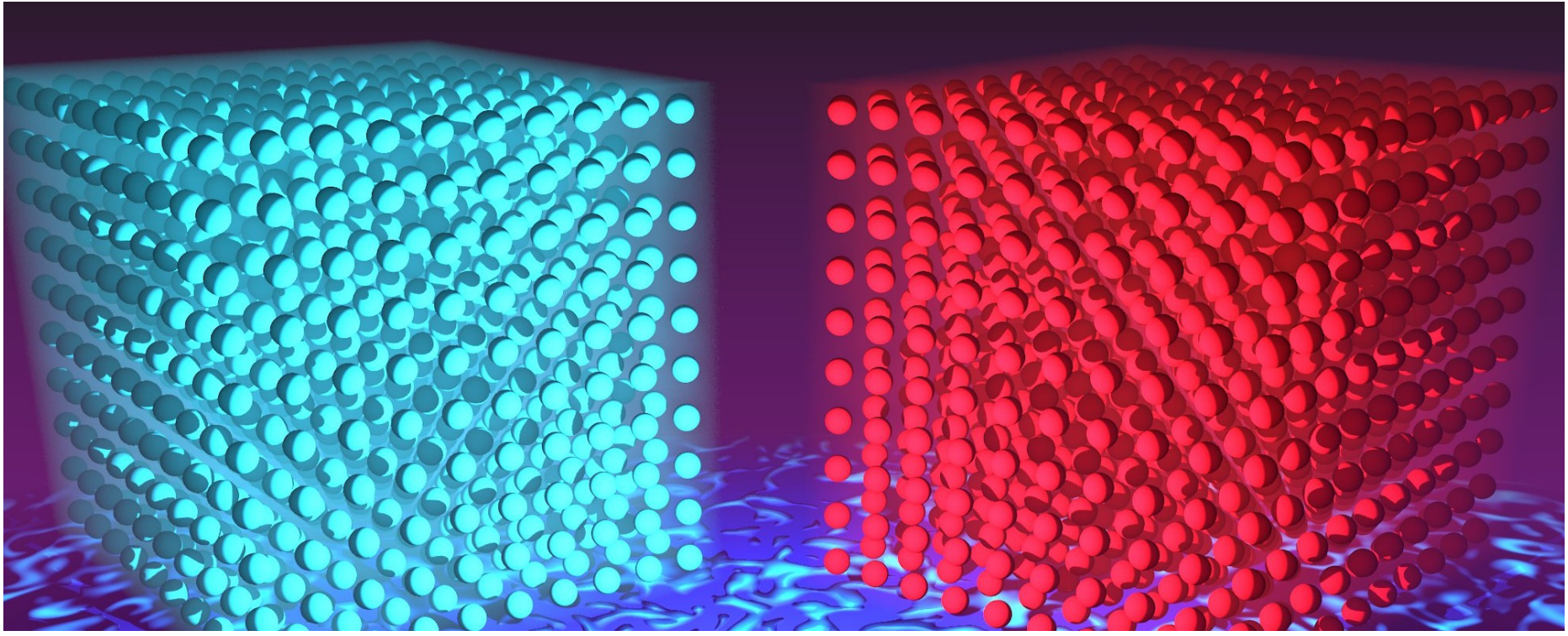
Numerical methods: Density functional theory and tensor network formalism



May 8th 2023

Today's focus

Which highly advanced methods do we have to tackle?

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} V_{ijkl} c_i^\dagger c_j c_k^\dagger c_l$$

With a mean field description

$$H \approx \sum_{ij} \bar{t}_{ij} c_i^\dagger c_j + \sum_{ij} \Delta_{ij} c_i c_j$$

Approximate quadratic Hamiltonian
Effective single particle description

Weakly correlated matter

Without a mean field description

????

No good quadratic approximation
Requires exact solutions or numerical

Strongly correlated matter

Today’s learning outcomes

- Density functional theory allows to study the electronic structure of real materials
- Tensor networks provide a method to tackle quantum many-body problems

Density functional theory

A reminder about the mean-field approximation

Free Hamiltonian ***Interactions (Hubbard term)***

$$H = \sum_{ij} t_{ij} [c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}] + \sum_i U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

Mean field: *Approximate four fermions by two fermions times expectation values*

Four fermions (not exactly solvable) ***Two fermions (exactly solvable)***

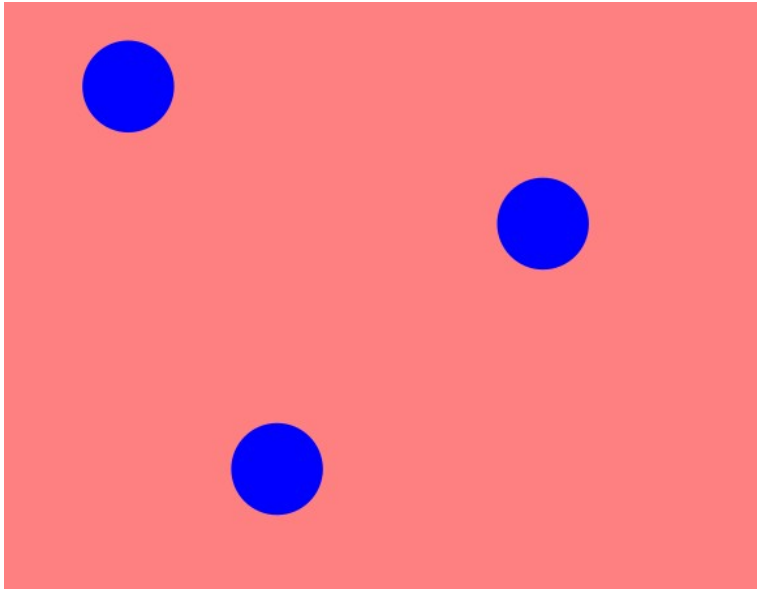
$$U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \approx U \langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle c^\dagger_{i\downarrow} c_{i\downarrow} + ... + h.c.$$

Density functional theory applies an effective “mean-field theory” for complete basis

(for an imaginary electron gas)

The fundamental idea of density functional theory

Take the positions of all the atoms



And find an “accurate” single-particle effective Hamiltonian

The many-electron problem

The Hamiltonian for electrons in a solid

$$H_{\mathrm{el}} = -\frac{1}{2}\sum_{j=1}^{N}\nabla_j^2 - \sum_{j=1}^{N}\sum_{l=1}^{M}\frac{Z_l}{\tilde{r}_{jl}} + \sum_{j=1}^{N}\sum_{k>j}^{N}\frac{1}{r_{jk}}$$

Has an associated electronic density

$$\rho(\boldsymbol{r}) = N\int \mathrm{d}^3\boldsymbol{r}_2 \cdots \int \mathrm{d}^3\boldsymbol{r}_N \left|\Psi\left(\boldsymbol{r}, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_N\right)\right|$$

The Hohenberg-Kohn theorem

For the ground state of a system, there is a one-to-one relation between the electronic density and the many-body wavefunction (Hohenberg-Kohn theorem)

$$\rho_0 \leftrightarrow \left|\Psi\right\rangle$$

The total energy can be written as a functional of the electronic-density

$$E(\rho_0)$$

The ground state energy can be computed if we know the functional (which we do not)

The Kohn-Sham equations

We do not know the “true” functional for density-functional theory

Let us take an “imaginary” non-interacting electron gas, with the same density as the real one

For this “imaginary” system, we can write the functional as

$$F_{\mathrm{HK}}[\rho] = T_{\mathrm{S}}[\rho] + J[\rho] + E_{\mathrm{XC}}[\rho]$$

where

$$T_{\mathrm{S}} = -\frac{1}{2}\sum_{j=1}^{N}\left\langle \psi_j \left| \boldsymbol{\nabla}^2 \right| \psi_j \right\rangle$$

Mean-field electronic interaction

And this is approximated (LDA, GGA, metaGGA, etc)

The Kohn-Sham equations

Given a certain density-functional $F_{KS}(\rho)$

An effective single-particle Hamiltonian must be solved, taking the form

$$H_{KS}|\psi_n\rangle = \epsilon_n|\psi_n\rangle$$

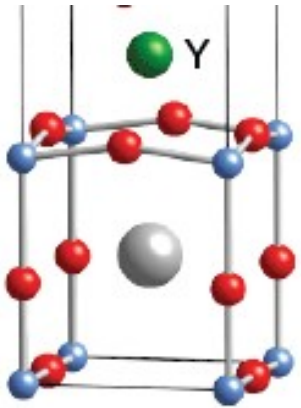
Where the Hamiltonian is obtained as a functional derivative

$$(H_{KS} - \epsilon_n)|\psi_n\rangle = \frac{\delta F_{KS}}{\delta|\psi_n\rangle} = 0$$

The Kohn-Sham equations

Define your crystal
(atomic positions)

$$V(\mathbf{r})$$



Electronic density

$$\rho(\mathbf{r})$$

Hamiltonian

$$H_{KS}(\rho)$$

KS eigenvectors

$$|\psi_n\rangle$$

Solved selfconsistently in a certain basis (plane-waves, LAPW, etc)

Density-functional theory spectra

DFT maps the many-body electron problem to a new non-interacting problem

$$H_{KS}|\psi\rangle = \epsilon_n|\psi_n\rangle$$

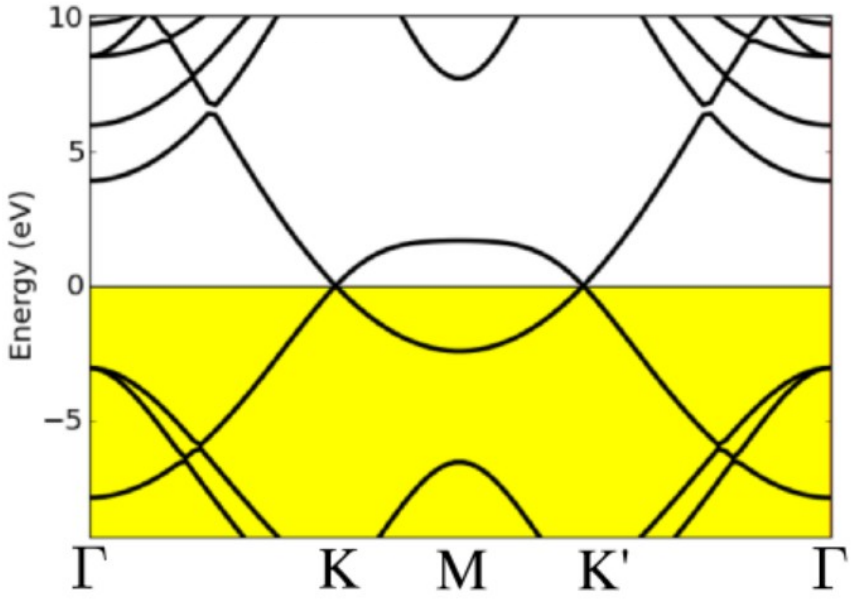
DFT eigenvalues

Effectively, the DFT procedure requires solving a selfconsistent set of equations, similar to those of mean-field methods (yet with additional terms)

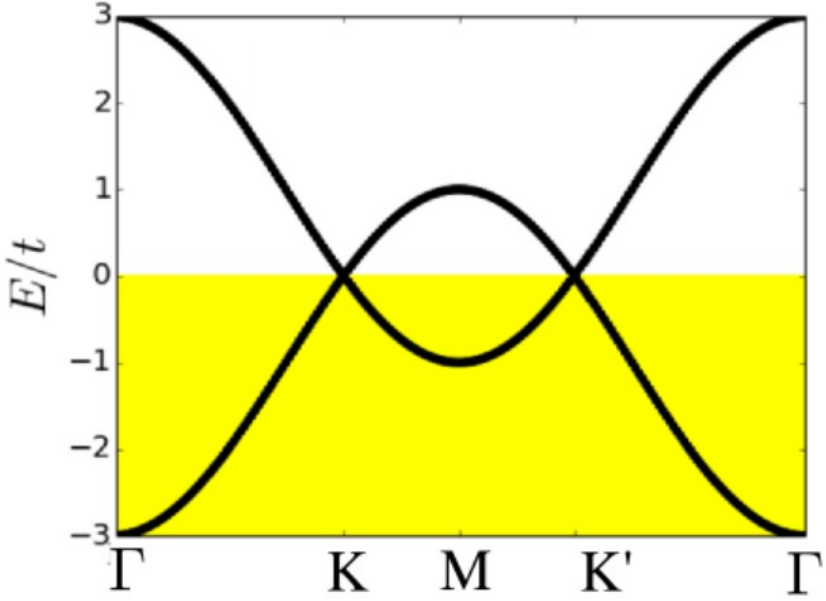
The eigenvalues obtained in DFT are understood as the effective single-particle energies of the true electronic state

DFT VS tight binding

DFT



Tight binding



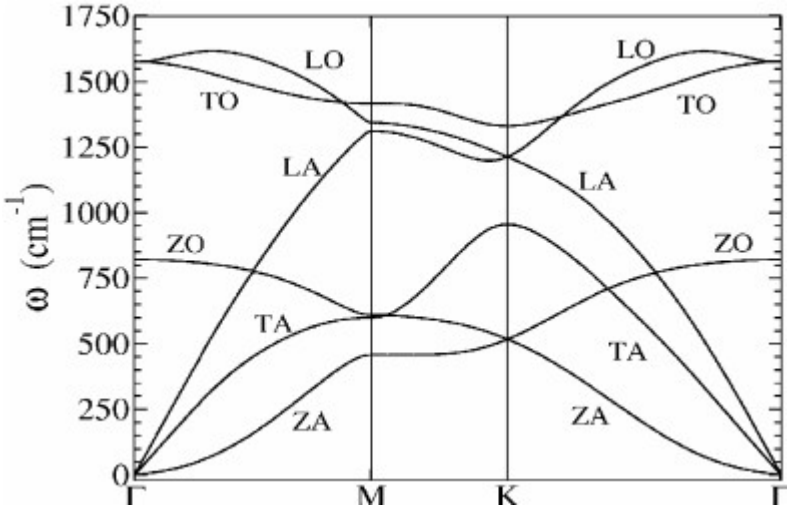
Graphene electronic structure

What can we study with density-functional theory?

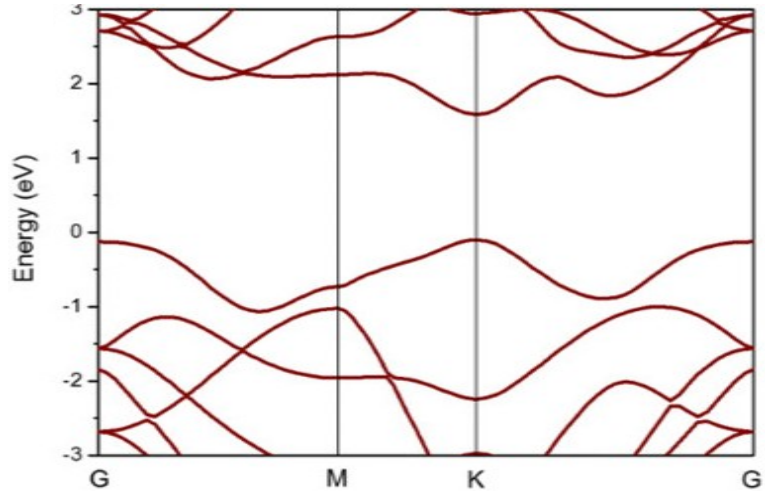
- Structural, magnetic and optical properties
  - Anything related to the structure of the material
  - Anything related with the single-particle eigenvalues
- Topological properties
  - Single-particle eigenstates can be accessed
- Starting point for many-body methods and effective models
  - Low-energy models can be extracted (Wannierization)

What can we study with density-functional theory?

Phonon dispersions



Electronic dispersions



When does density-functional theory fail?

Make groups of 2-3 people, which of these states can be captured with DFT?

Hint: remember, DFT works as a mean-field theory

Chern insulators	Metals	Superconductivity
Fractional quantum Hall	Ferromagnets	Quantum spin liquids

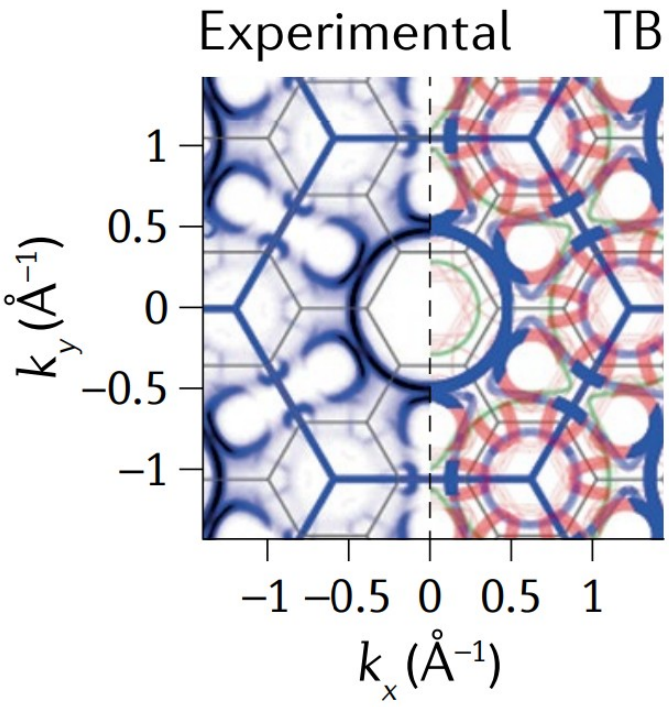
When does density-functional theory fail?

- Strongly correlated systems
  - Mott insulators, rare earth compounds
- Many-body states that cannot be captured at the single particle level
- Other situations, as a result of the approximate nature of the XC functional

Fermi surfaces

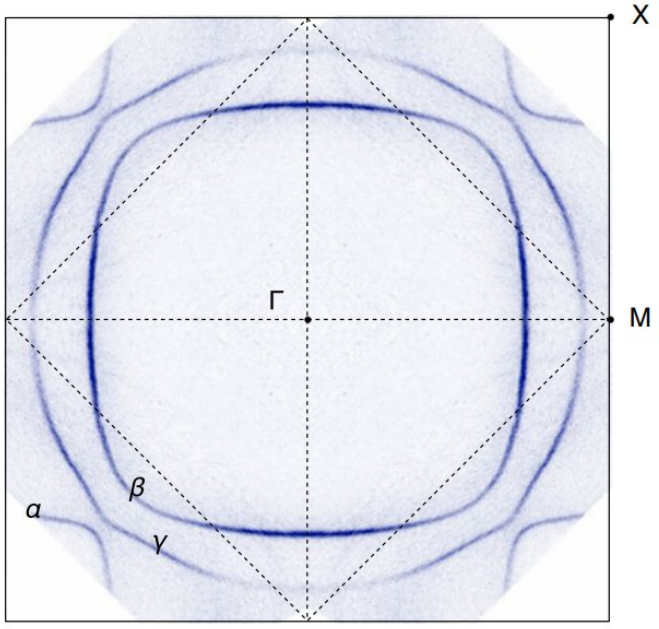
$TaSe_2$

Theory & experiment



Sr_2RuO_4

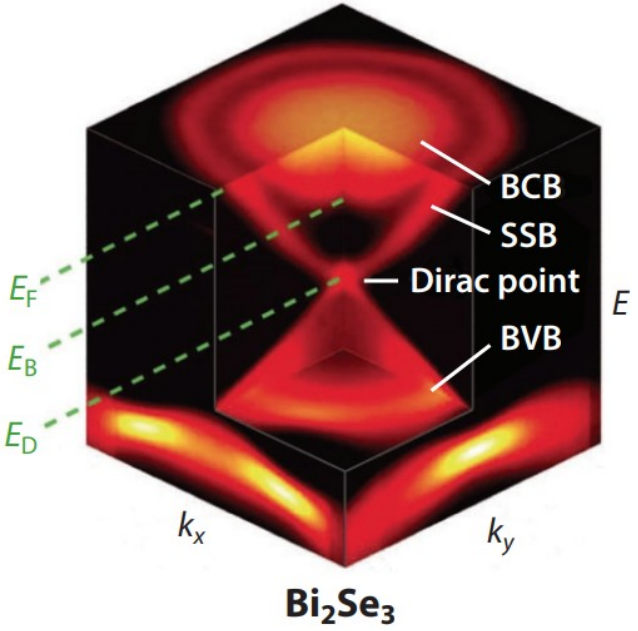
Experiment



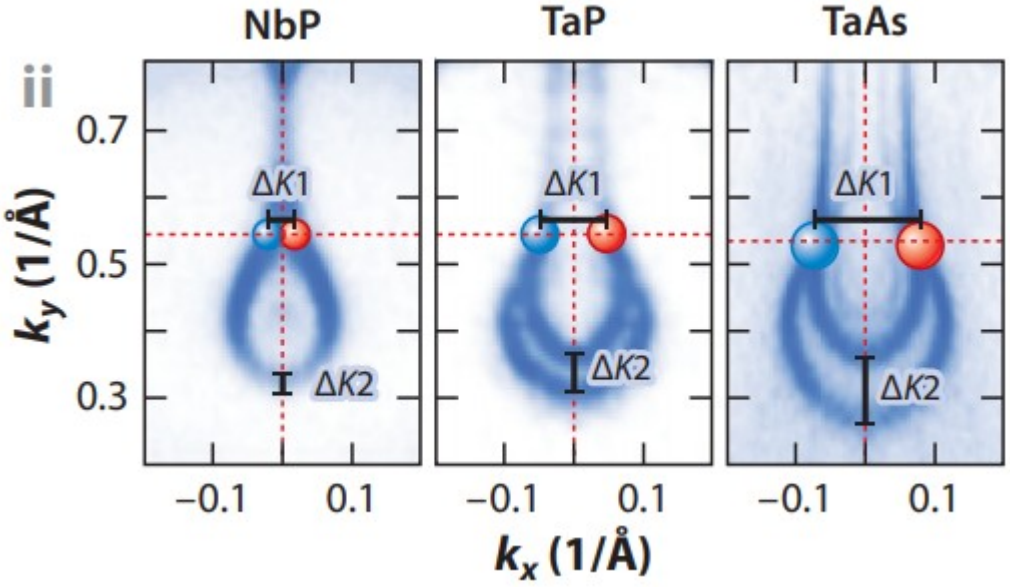
Topological surface states

Bi_2Se_3

Quantum spin-Hall insulators



Topological semi-metals



Open-source software for density-functional theory

Quantum Espresso

https://www.quantum-espresso.org/

Pseudopotentials

Elk

https://elk.sourceforge.io/

All-electron

(and many others)

Beyond density-functional theory

- DFT-DMFT
  - Using DFT as a starting point for DMFT (dynamical mean-field theory), suitable for Mott insulators
- GW
  - Many-body corrections to the DFT eigenenergies
- Bethe-Salpenter equation
  - To compute excitons from DFT

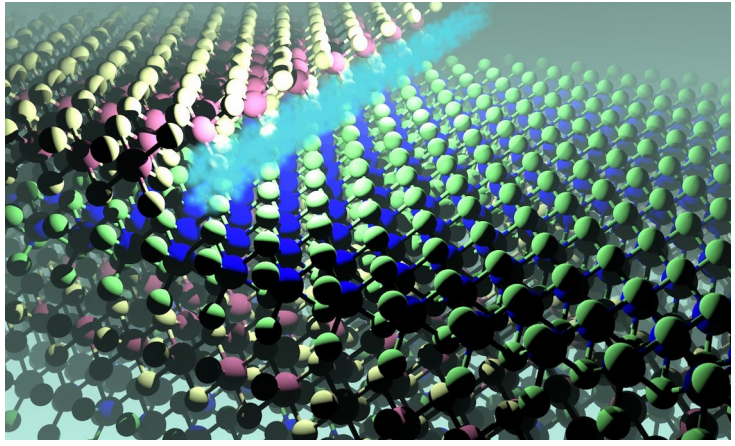
Tensor networks

The fundamental idea of tensor-networks

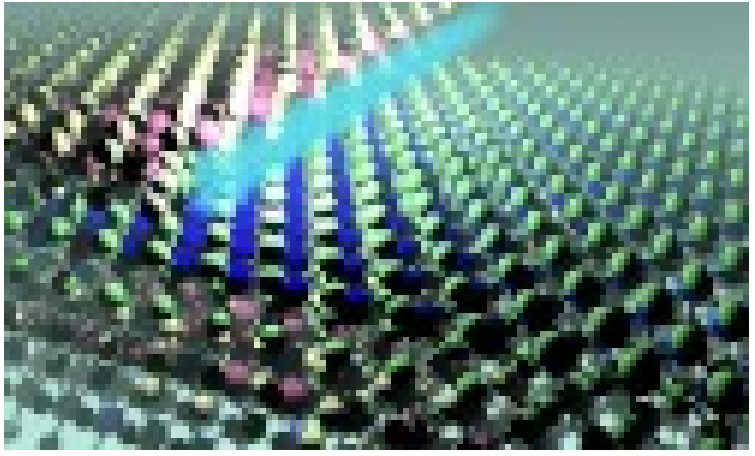
A many-body wavefunction a is a very high dimensional object

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

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



“True wavefunction”



“Tensor-network wavefunction”

The quantum many-body problem

Let us go back to 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

What is the dimension of the Hilbert space?

The quantum many-body problem

Let us go back to 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

What is the dimension of the Hilbert space?

$$d = 2^L$$

The quantum many-body problem

Let us go back to 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 matrix-product state ansatz

For this wavefunction $\left|\Psi\right\rangle = \sum c_{s_1,s_2,\ldots,s_L} \left|s_1, s_2, \ldots s_L\right\rangle$

Let us imagine to propose a parametrization in this form

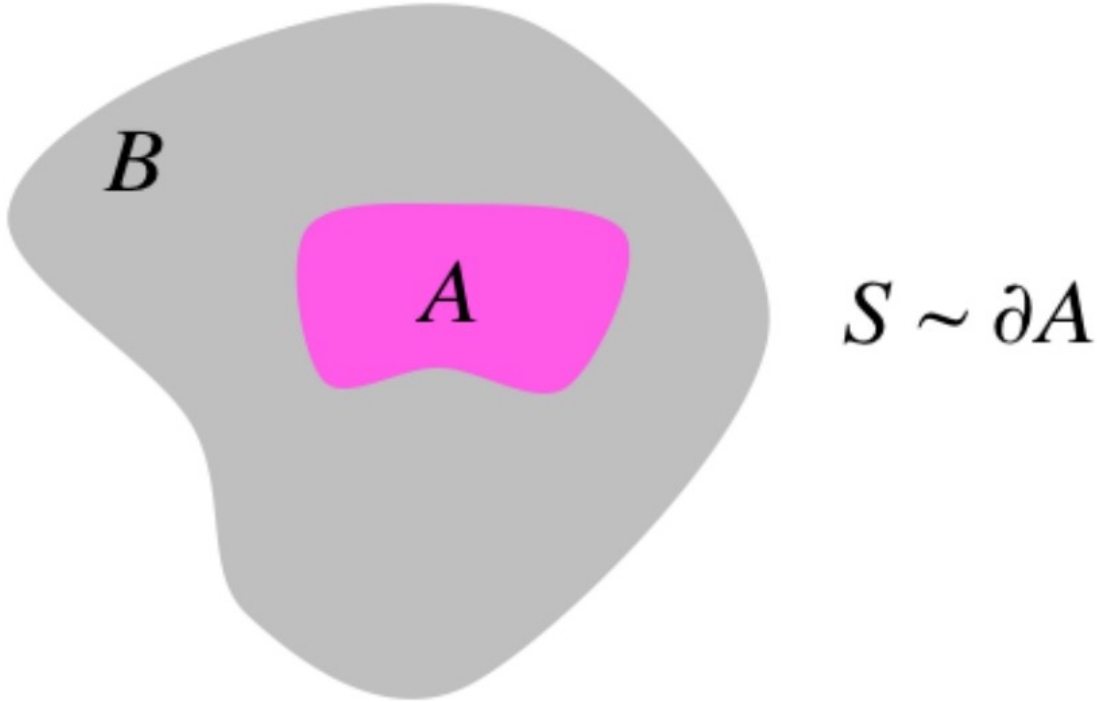
$$c_{s_1,s_2,\ldots,s_L} = M_1^{s_1} M_2^{s_2} \ldots . M_L^{s_3}$$

dimension 2^L

dimension $\sim Lm^2$

(m dimension of the matrix)

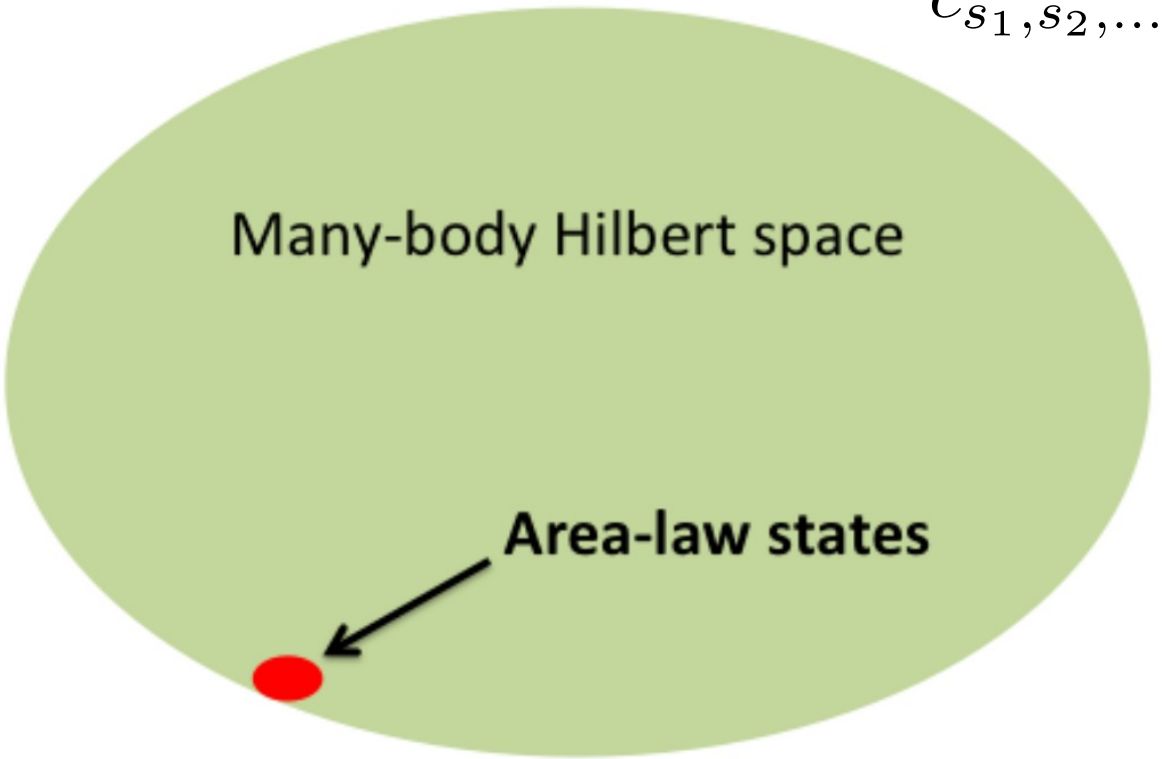
The many-body entanglement entropy



The MPS representation is successful thanks to the area law

Area law states

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



The matrix-product state ansatz

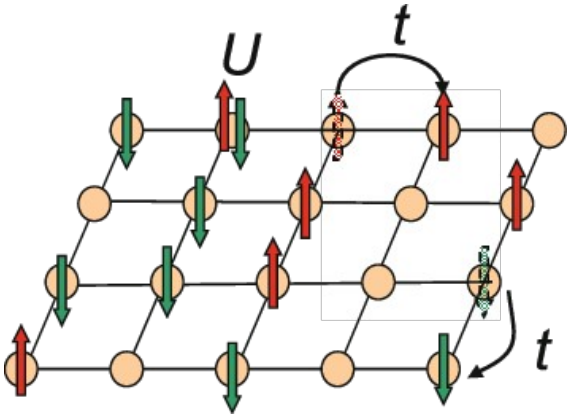
- This ansatz enforces a maximum amount of entanglement entropy in the state $S \sim \log m$
- One-dimensional problems, have ground states that can be captured with this ansatz

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

This ansatz can be generalized for time-evolution, excited states, open systems, etc...

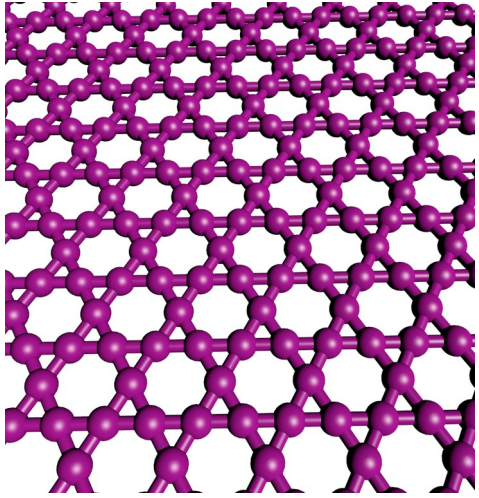
Some (non-trivial) problems tackled with MPS

Solving the 2D Hubbard model at finite doping



$$H = \sum_{ij,s} t_{ij} c^{\dagger}_{is} c_{js} + \sum_{i} U c^{\dagger}_{i\uparrow} c_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow}$$

Solving the 2D Heisenberg model in frustrated lattices



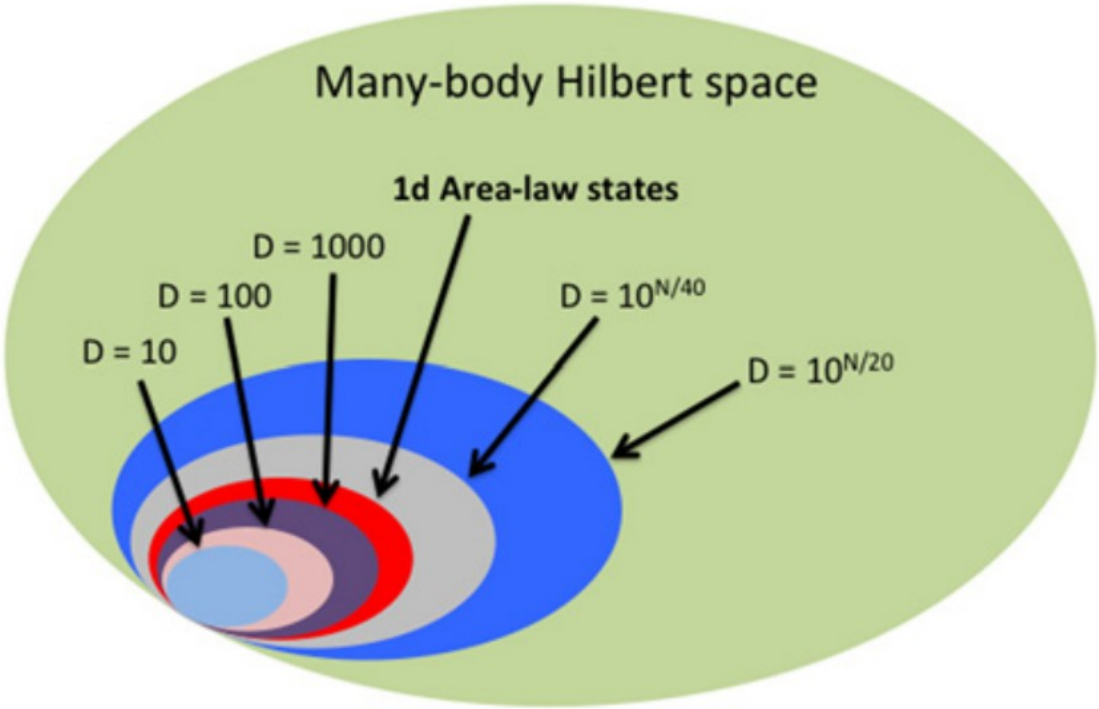
$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

When do MPS fail?

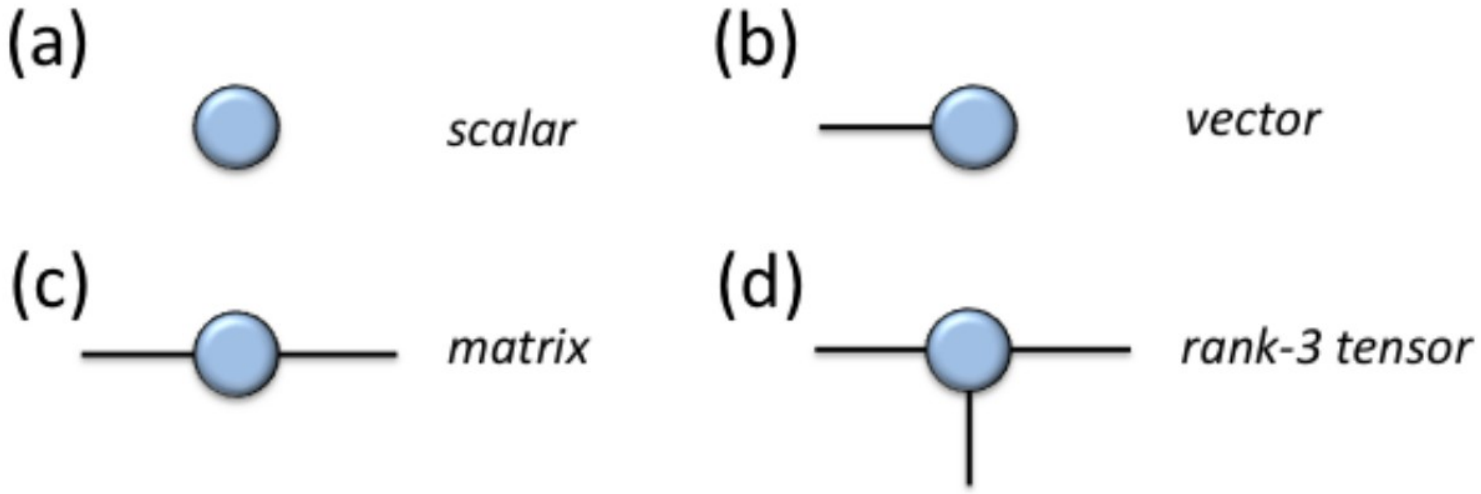
- This ansatz enforces a maximum amount of entanglement entropy in the state $S \sim \log m$
- If the states have too much entanglement, MPS do not capture the state properly
  - Time-evolution to long times
  - Many-body problems above 1D
  - Highly excited states
  - Far from equilibrium states

When do MPS fail?

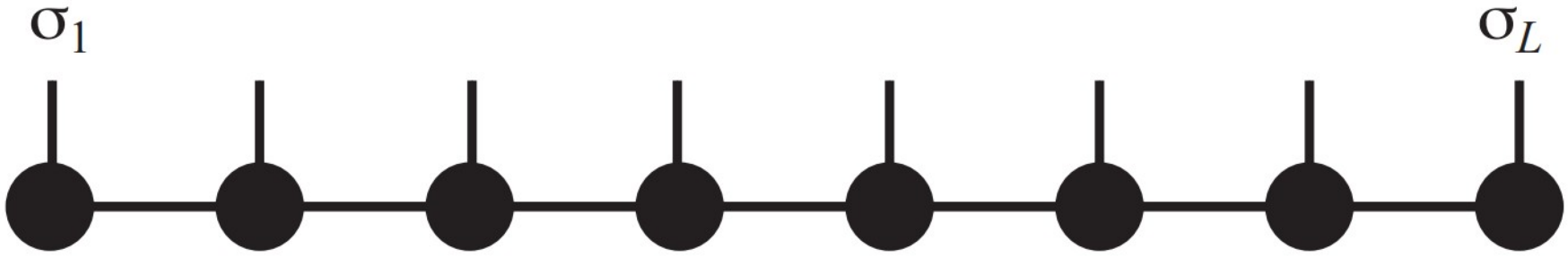
Sketch of the space parametrized with bond dimension D



The graphical representation of matrix product states



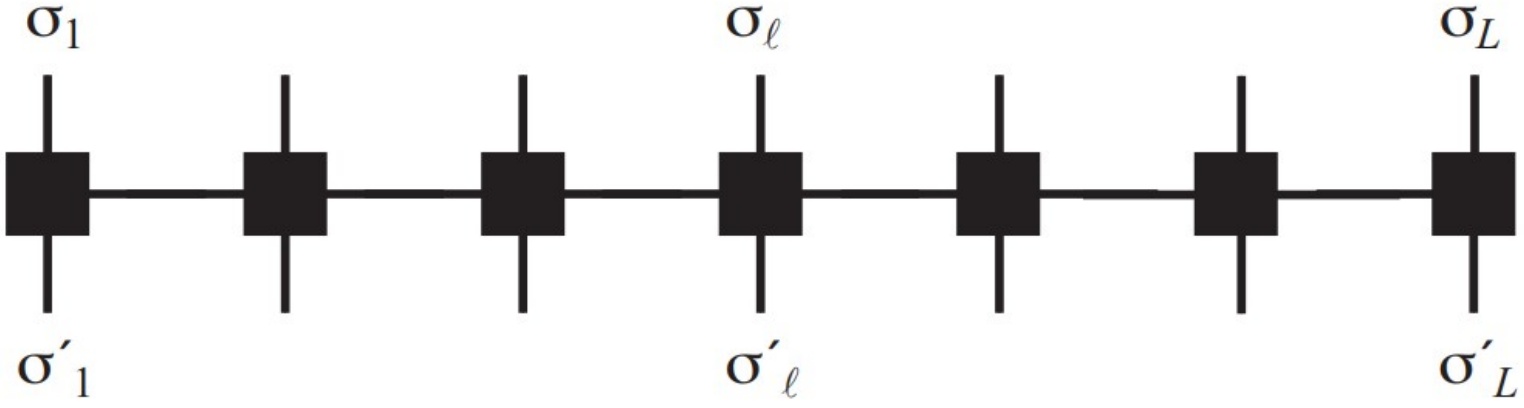
The matrix product state representation



$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} M^{\sigma_1} \dots M^{\sigma_L} |\boldsymbol{\sigma}\rangle$$

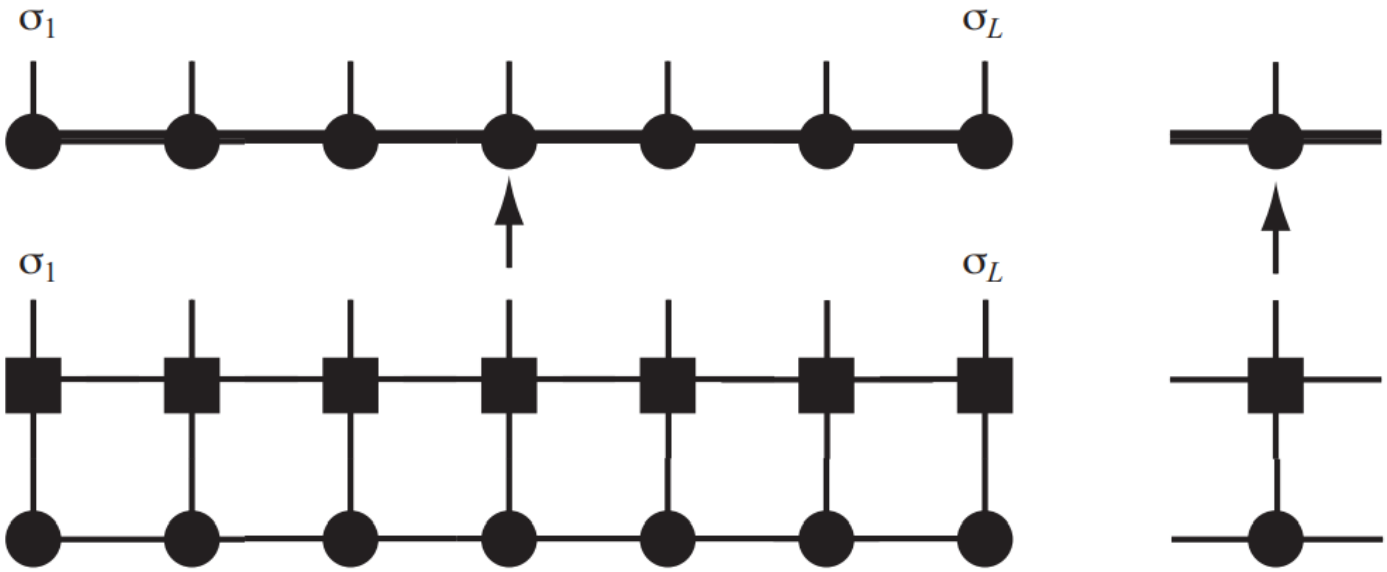
Matrix product operators

Operators can be represented in an analogous form



Operator state product

Products of operators and states can be represented graphically



Ground state calculations

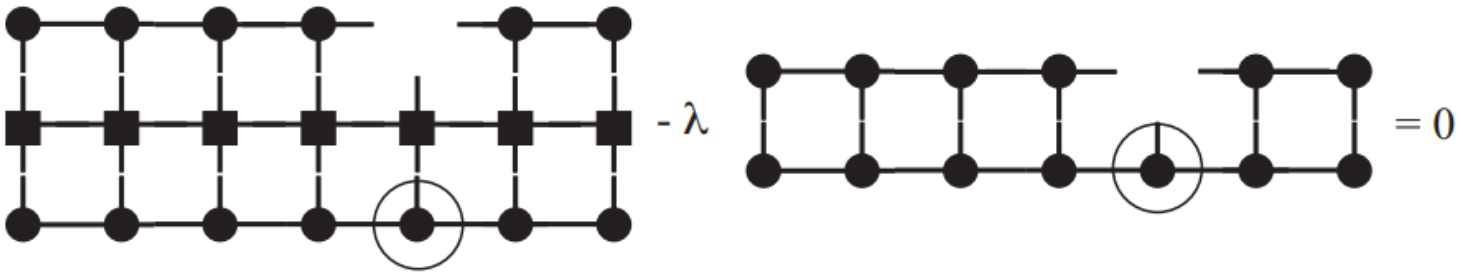
To compute a ground state, we just have to minimize

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

$$E = \langle \Psi | H | \Psi \rangle - \lambda \langle \Psi | \Psi \rangle$$

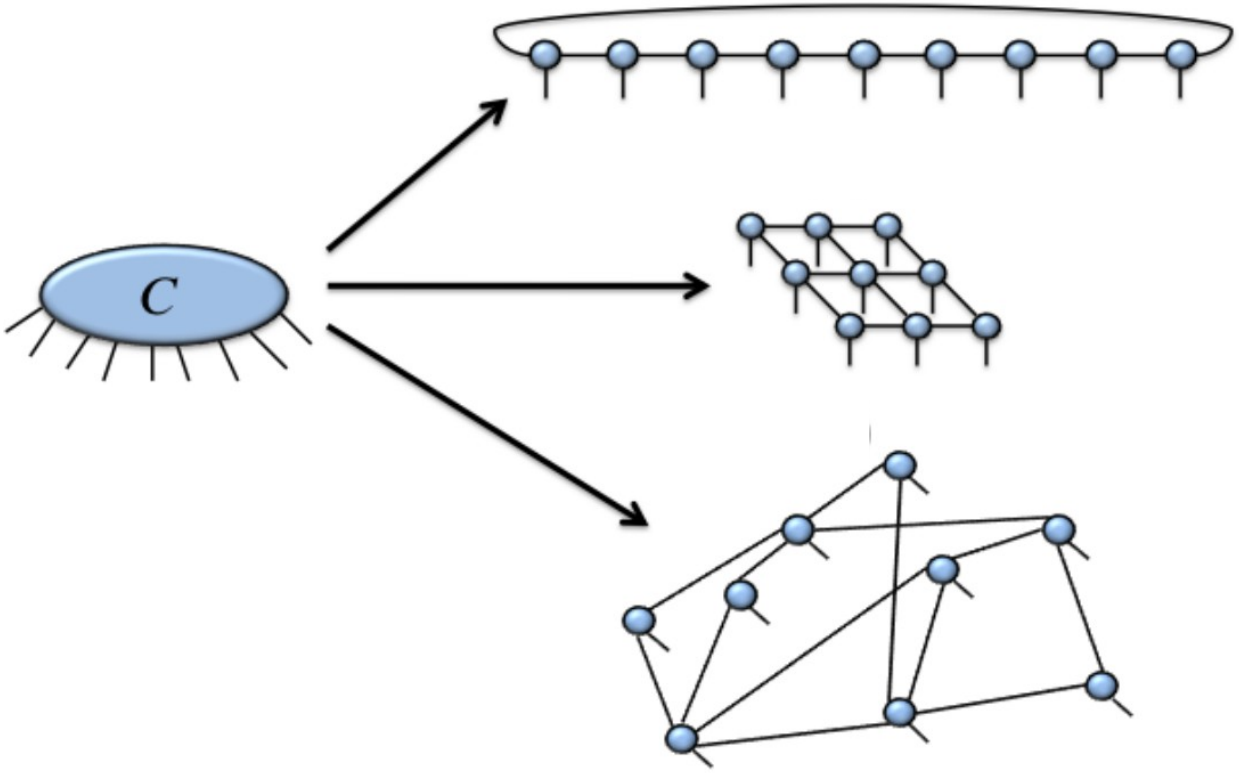
This can be done by minimizing the energy with respect to each matrix

$$\frac{\delta E}{\delta M} = 0$$



This algorithm is known as the density-matrix renormalization group

Beyond matrix-product states

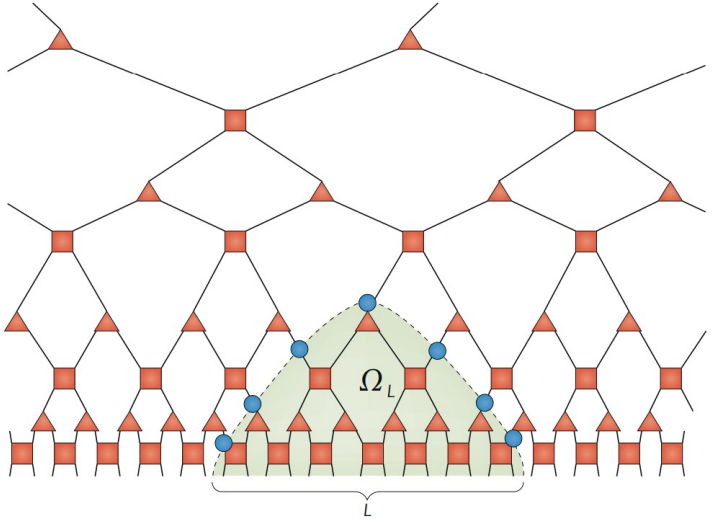


The same tensor can be represented with widely different tensor networks

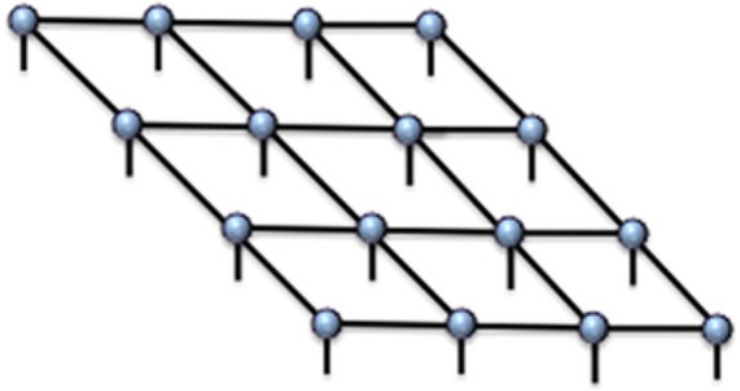
Beyond matrix-product states

Tensor networks can be extended to deal with higher dimensional/critical systems

Multiscale renormalization ansatz



Projected-entangled pair states



Software for generic tensor-network calculations

ITensor

https://itensor.org/

Take home

- Density-functional theory allows to compute electronic spectra of real materials
- Tensor-network methods allow solving 1D quantum many-body problems