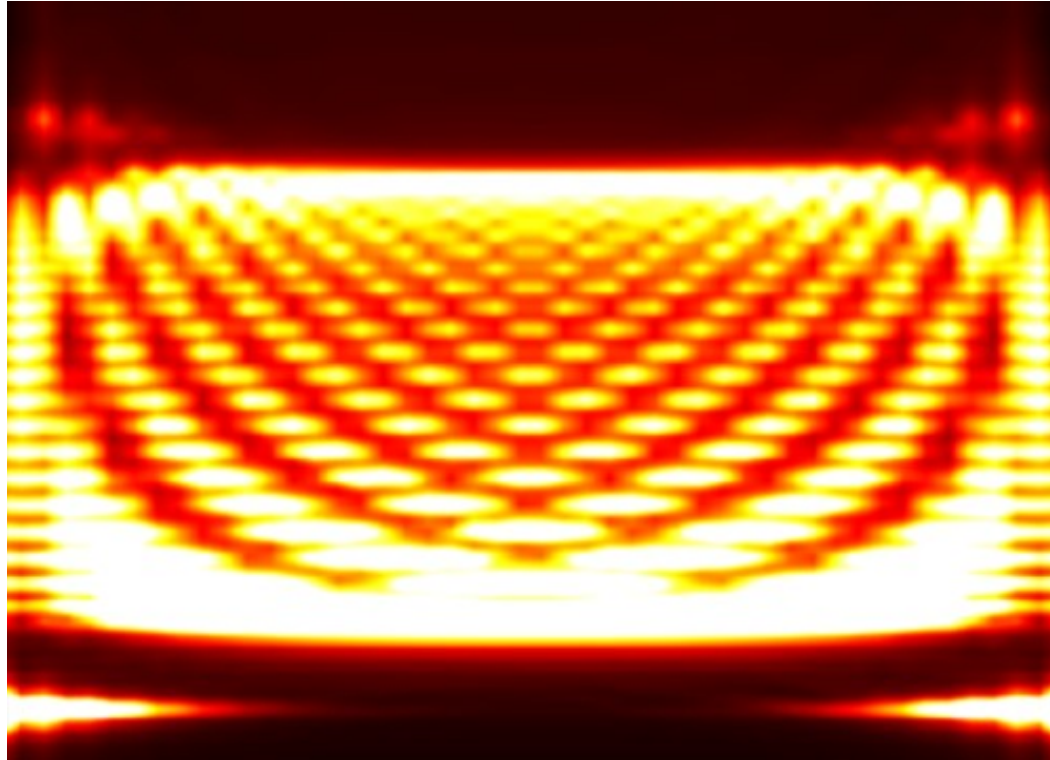# Numerical methods: Density functional theory and tensor network formalism

May 17th 2021

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

A reminder from previous lectures

We can consider two broad groups of interacting quantum matter

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

With a mean field description

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

Approximate quadratic Hamiltonian
Effective single particle description

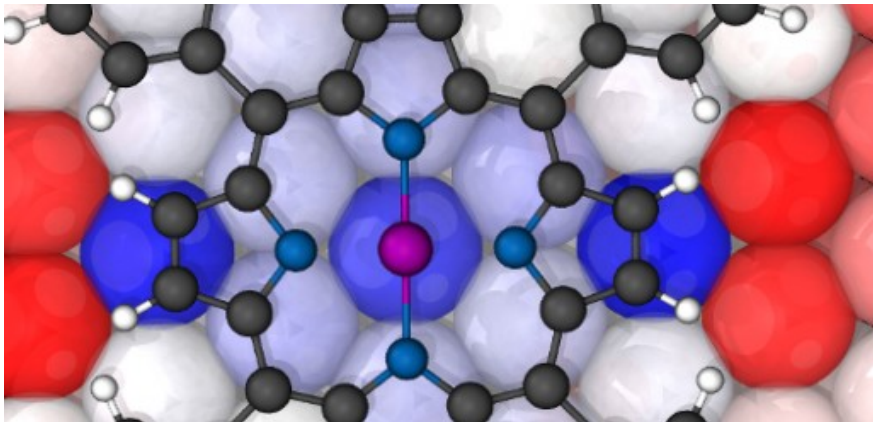*Weakly correlated matter*

Without a mean field description

$$?????$$

No good quadratic approximation
Requires exact solutions or numerical
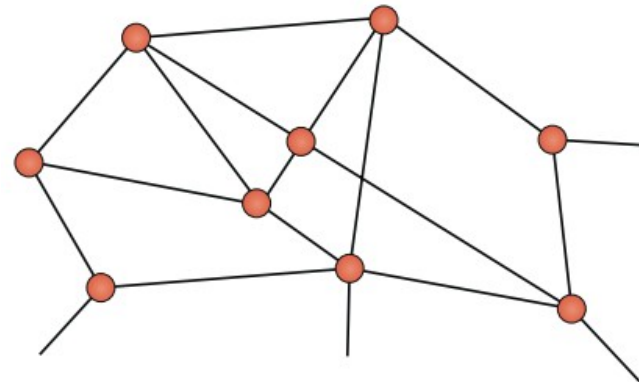
Strongly correlated matter

Computational methods for quantum materials

Density functional theory

Tensor-networks

Real quantum materials
Especially in the weakly
interacting limit

To solve effective models
Captures many-body
entangled states

Density functional theory

The many-electron problem

The Hamiltonian for electrons in a solid

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

Has an associated electronic density

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

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)

$$\rho_0 \leftrightarrow |\Psi\rangle$$

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

$$T_{\mathrm{S}} = -\frac{1}{2}\sum_{j=1}^{N}\langle\psi_j|\boldsymbol{\nabla}^2|\psi_j\rangle, \qquad \rho_{\mathrm{S}}(\boldsymbol{r})\sum_{j=1}^{N}|\psi_j(\boldsymbol{r})|^2 \overset{!}{=} \rho(\boldsymbol{r}), \qquad E_{\mathrm{XC}}[\rho]$$

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

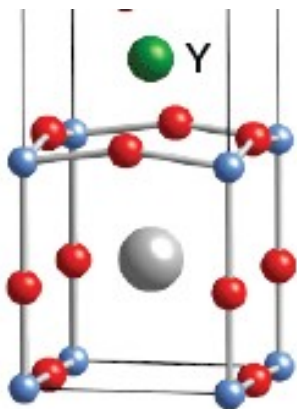$$H_{KS}|\psi\rangle = \epsilon_n|\psi_n\rangle$$

Where the Hamiltonian is obtained as a functional derivative

$$H_{KS} = \frac{\delta F_{KS}}{\delta|\psi_n\rangle}$$

The Kohn-Sham equations

Define your crystal
(atomic positions)

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

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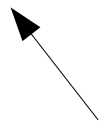
$$\rho(\mathbf{r})$$

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

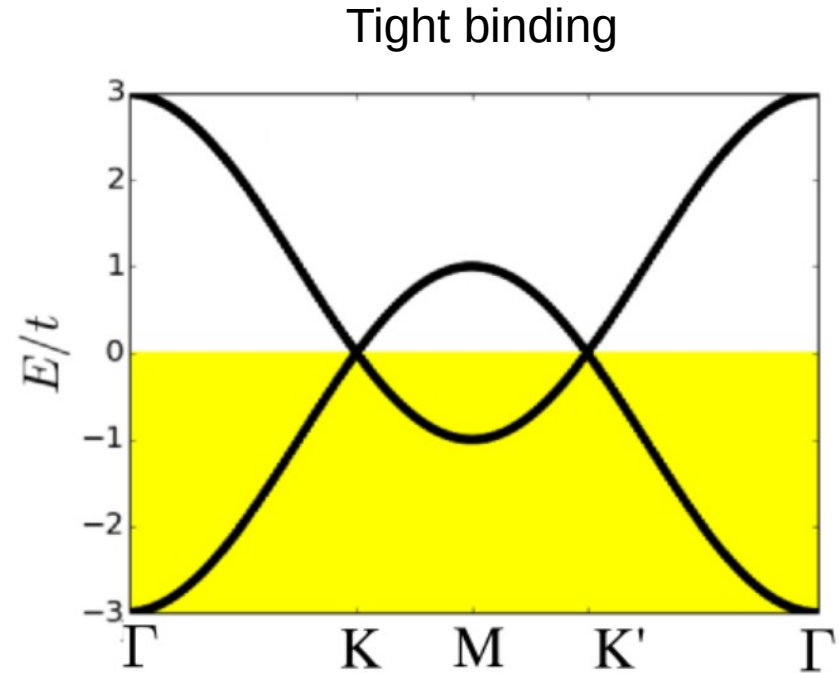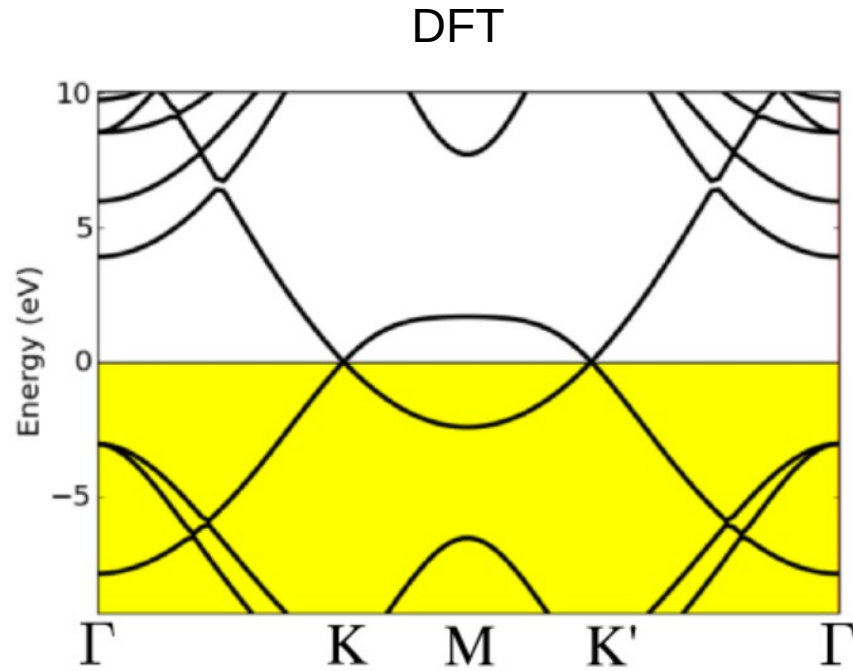$$H_{KS}|\psi\rangle = \epsilon_n|\psi_n\rangle$$

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
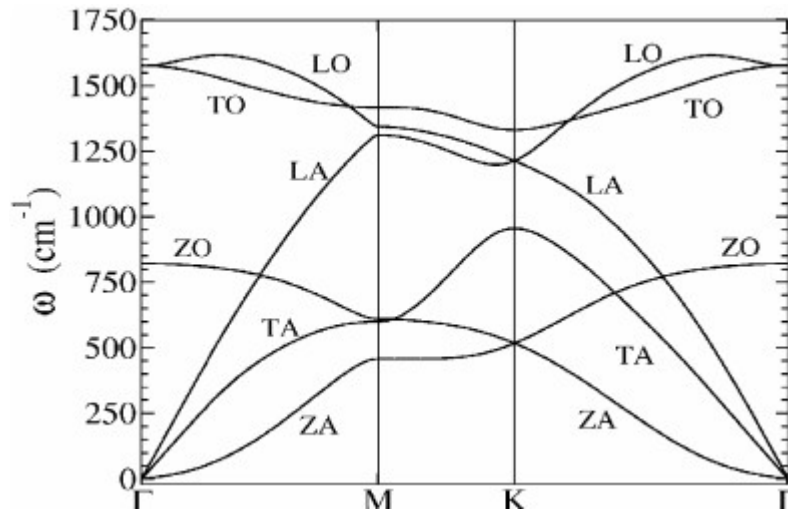
Electronic dispersions
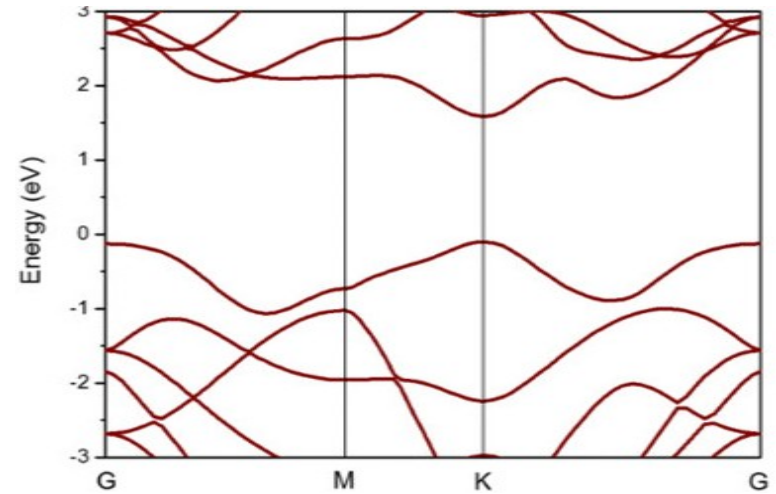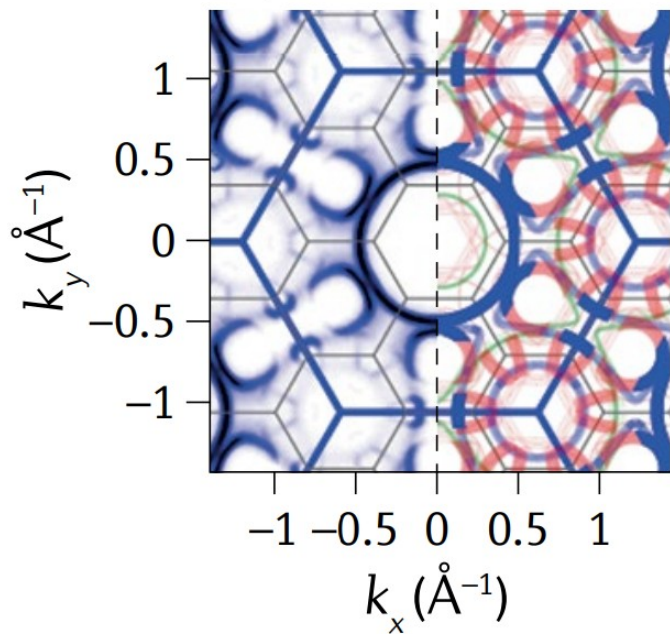
When does density-functional theory fail?

- 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
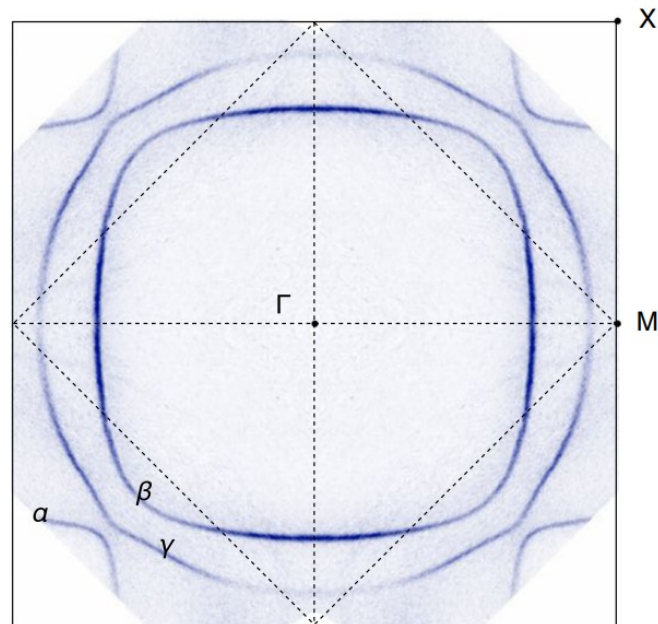
Fermi surfaces

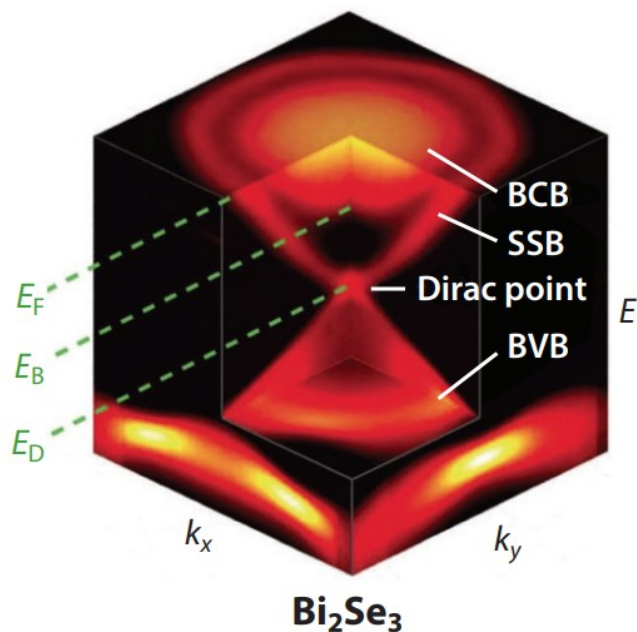**TaSe$_2$**

Theory & experiment
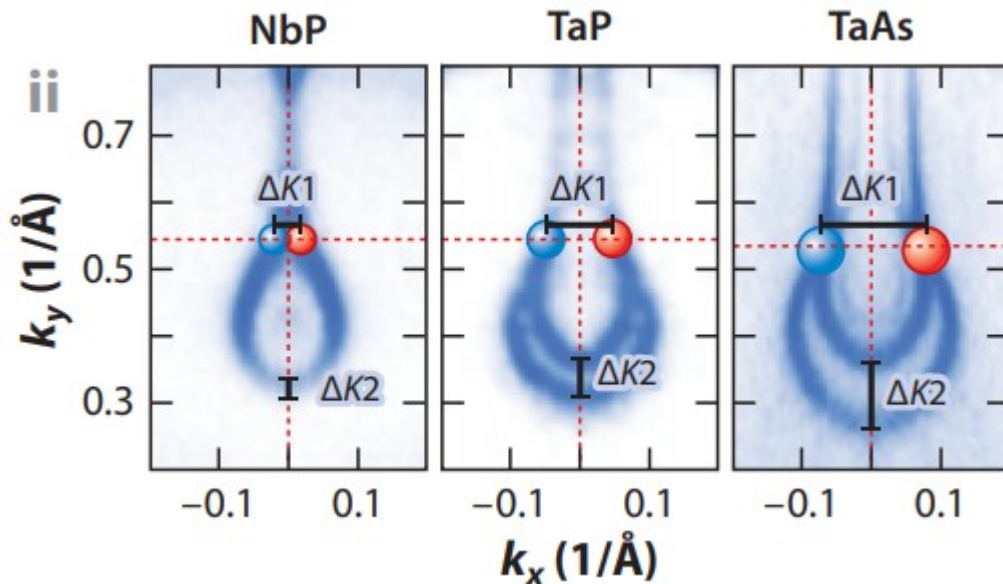
Sr$_2$RuO$_4$

Experiment

Topological surface states

Bi$_2$Se$_3$

Quantum spin-Hall insulators

Topological semi-metals

Open-source software
for density-functional theory

Quantum Espresso

Elk

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

https://elk.sourceforge.io/

Pseudopotentials

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

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 $\sim L m^2$

(m dimension of the matrix)
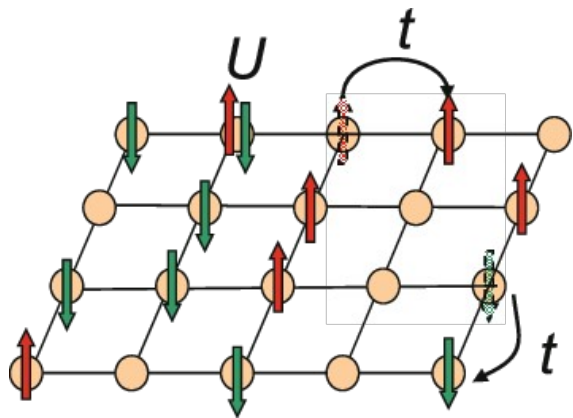
The matrix-product state ansatz

- 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

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

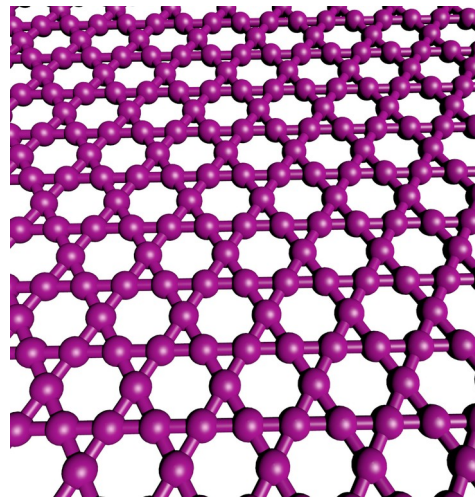This ansatz can be generalized for time-evolution, excited states, open systems, etc...

Some (non-trivial) problems tackled with MPS

Solving the 2D Hubbard model at finite doping

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

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?

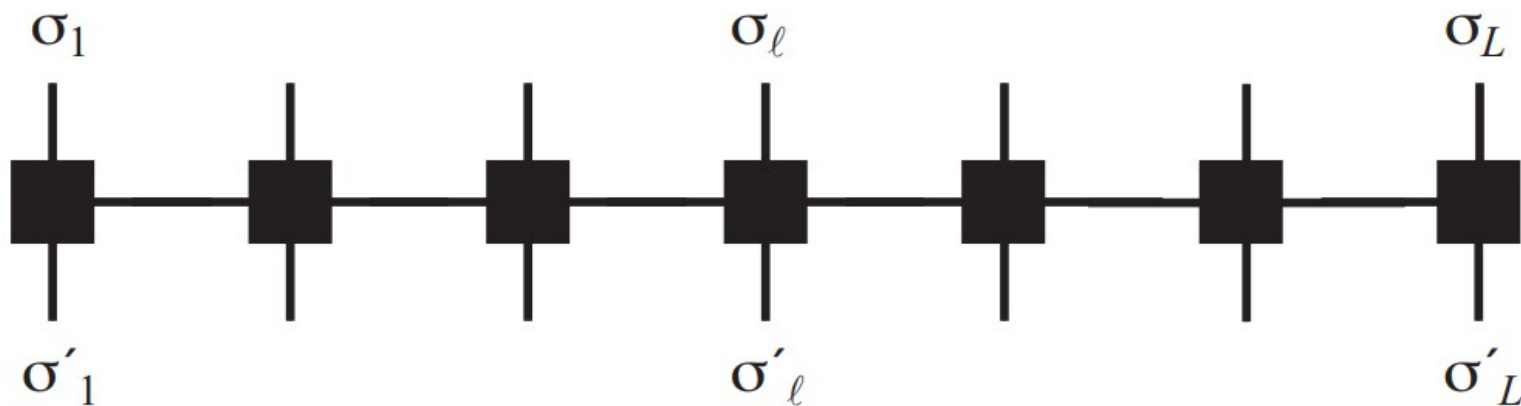Sketch of the space parametrized with bond dimension D
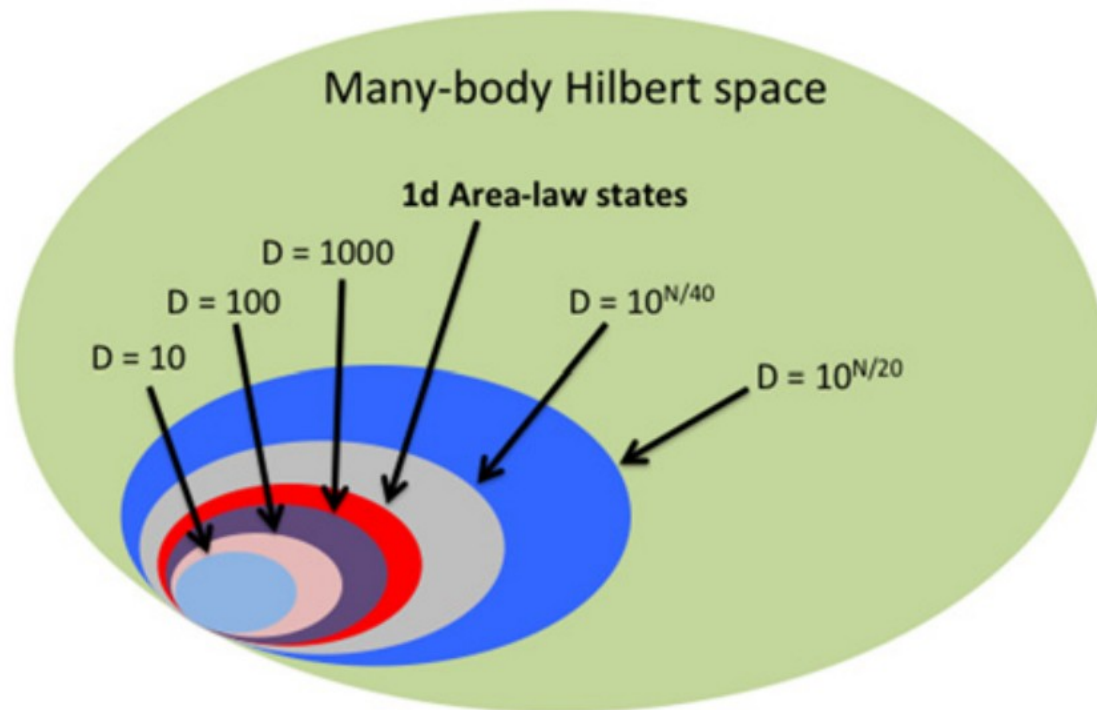
The matrix product state representation
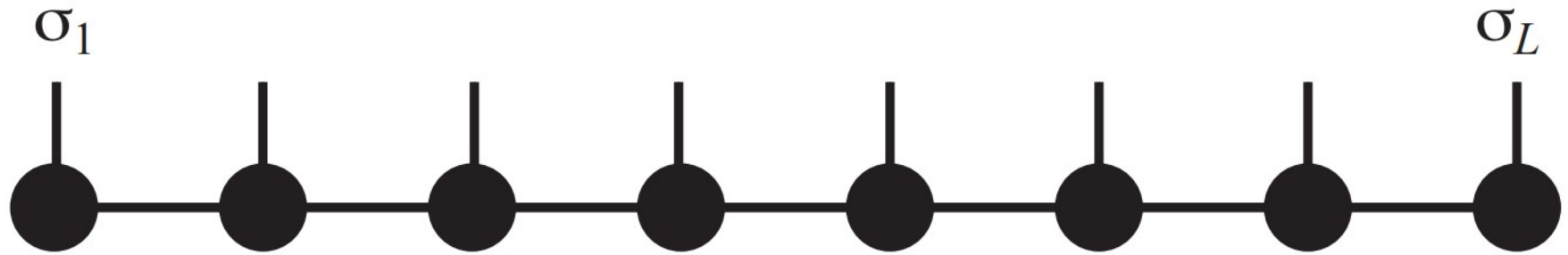
$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} M^{\sigma_1} \dots M^{\sigma_L} |\boldsymbol{\sigma}\rangle$$
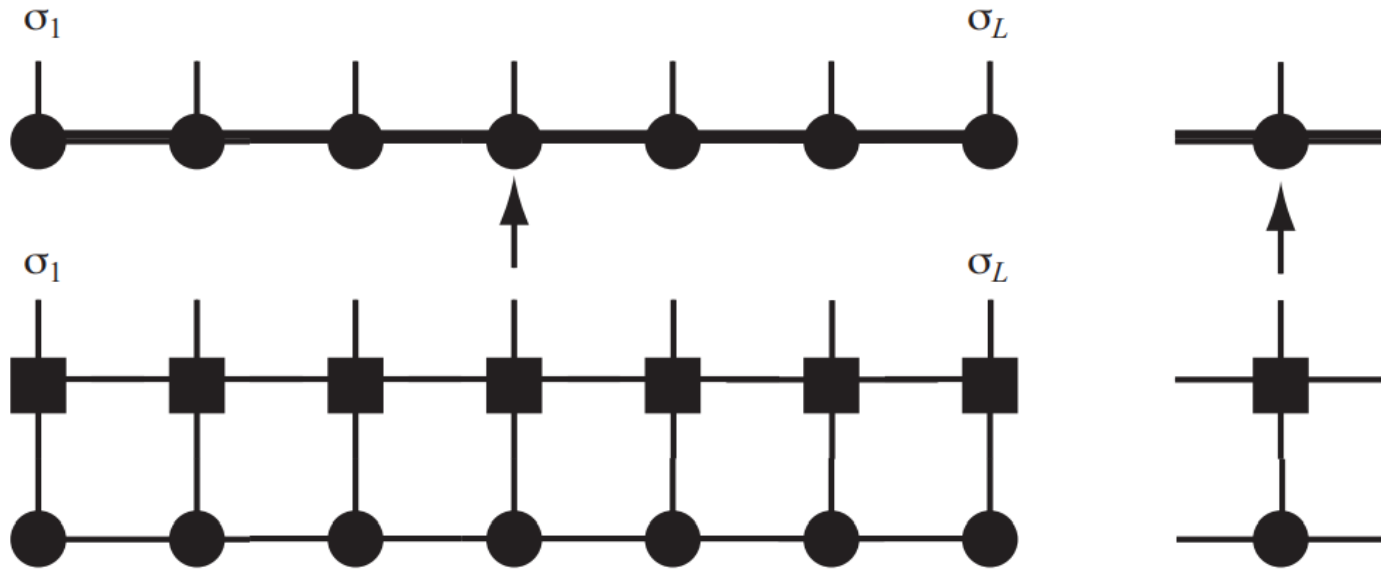
Matrix product operators

Operators can be represented in an analogous form

Operator state product

Products of operators and states can be represented graphically
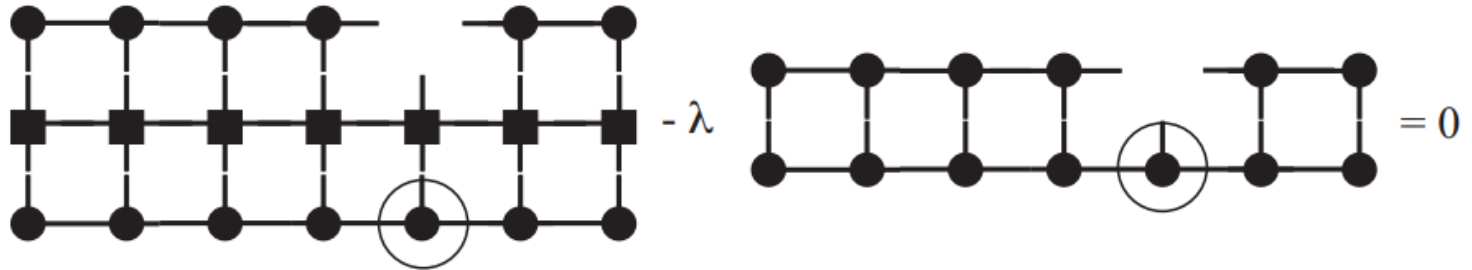
Ground state calculations

To compute a ground state, we just have to minimize

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

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

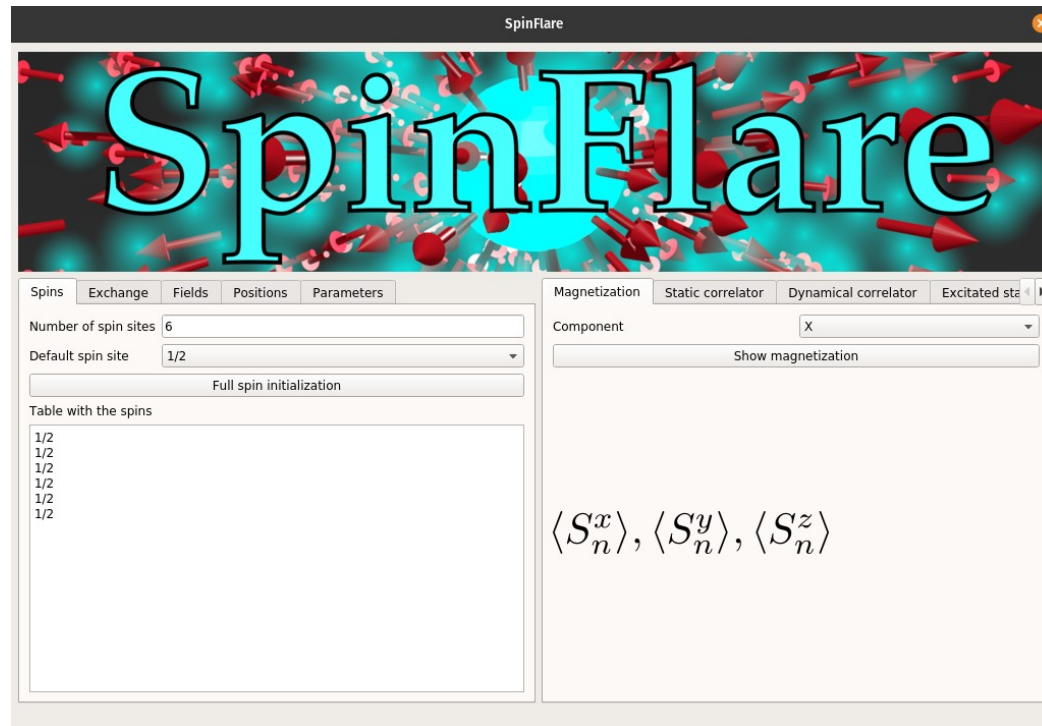This can be done by minimizing the energy with respect to each matrix

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

This algorithm is known as the density-matrix renormalization group
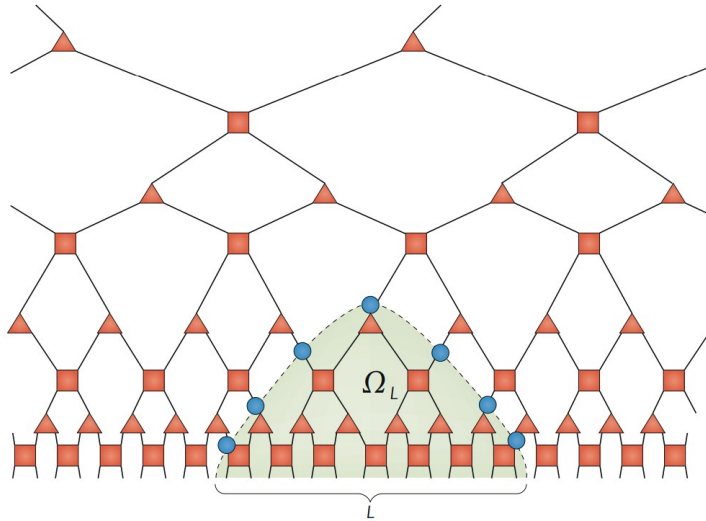
Tensor-networks, interactively

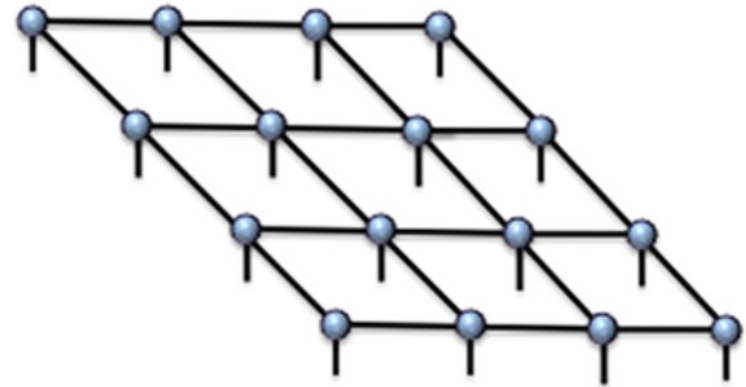A user interface to solve many-body problems with tensor-networks

https://github.com/joselado/spinflare

Beyond matrix-product states

Tensor networks can be extended to deal with higher dimensional/critical systems
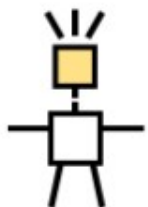
Multiscale renormalization ansatz
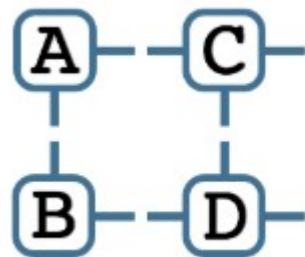
Projected-entangled pair states

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

Reading material

- Titus Neupert lecture notes, pages 148-154

- Roman Orus practical guide on tensor networks, pages 118-136