# Computational Tools for Quantum Many-Body Physics 2024/25

- General motivation:
  - Full quantum mechanical understanding of macroscopic objects can be essential for description of their basic physical phenomenology.

  ⇝ Prominent examples: Complex macro-molecules in quantum chemistry, high $T_c$ superconductivity, ......

  ⇝ Revolutionary potential applications enabled by solution to quantum many-body problem

- Better understanding of quantum many-body physics essential for new quantum algorithms

  ⇝ Paradigm shift in computer science towards quantum information theory.

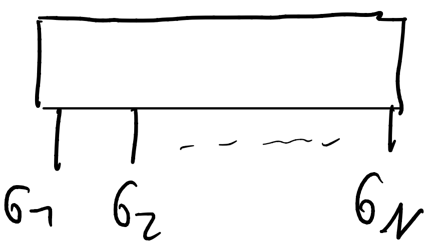
- Fundamental caveat: Exponential complexity of quantum many-body (QMB) systems

  - If a single particle state is defined in a Hilbert space $h$ of dimension $d$, a state of $N$ particles is defined in the ((anti)-symmetrized sub-space of the) space $\mathcal{H} = \underbrace{h \otimes h \otimes \dots h}_{N \text{ factors}}$ of dimension $d^N$.

- Illustration for spins with $d = 2s+1$ on a 1D lattice:

$s = \frac{1}{2}$

$$\Psi(\sigma) = \langle \sigma_1, \sigma_2, \dots, \sigma_N | \Psi \rangle \text{ "="}$$




$\approx$ ?

$\rightsquigarrow$ $|\Psi\rangle$ is a tensor with $N$ a priori independent indices, which illustrates its exponential number of entries.

This course is about computational tools for facing and taming this exponential complexity in order to solve QMB problems.

# Coarse Outline:

A : Independent identical particles and mean field methods

B : Exact diagonalization - Accepting the challenge of exponential complexity

C : Tensor network approach - Taming exponential complexity with a clever ansatz

D : Quantum Monte Carlo methods - Stochastic solution of QMB problems

# Computational Complexity in a Nutshell