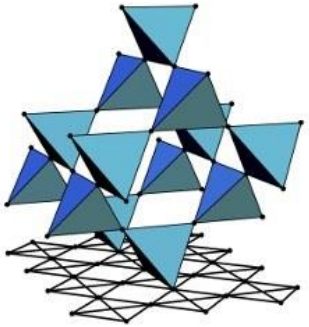

SFB 1143

Tensor Networks (SS2021)

Lecture 1: General introduction + Tensor Network Basics

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April 12th, 2021

Time and format

- Lecture/tutorial: Monday + Thursday, 14:50 – 16:20
- Office hours: Friday 13:00 – 14:00 (with appointment)

Course webpage: https://tu-dresden.de/mn/physik/itp/ket/studium/lehre/tn_ss21
(slides, videos, information sheet…)

OPAL link:
https://bildungsportal.sachsen.de/opal/auth/RepositoryEntry/29985308674/CourseNode/1618108323446632005 (forum, code sharing…)

Exercise and oral exam

Exercise:

- There will be 6-7 exercises. We will discuss them during the tutorials.
- There is no written exam. For Bachelor and Master students who need a grade, it's required to give a short presentation (10+5 minutes).

I will provide some sample Matlab codes, but you could certainly use your own favorite programming language (Python, Julia, C++, ….) and/or libraries (iTensor, TeNPy, …).

You are encouraged to pair up in teams to solve the exercise problems!

Exercise and oral exam

Exercise:

- There will be 6-7 exercises. We will discuss them during the tutorials.
- There is no written exam. For Bachelor and Master students who need a grade, it's required to give a short presentation (10+5 minutes).

Oral exam:

- For Master students, this course can be chosen as one of the two oral exam subjects for "Vertiefung: Theoretische Physik".
- Doctoral candidates may take the oral exam in replacement for the Rigorosum or choose this course to be examined in the Rigorosum.

Covered topics

Tensor networks for many-body physics:

- Matrix product state
- Density matrix renormalization group
- Projected entangled pair state
- Tensor network contractions
- …

Theory + algorithms + implementation

Reference

- F. Verstraete, V. Murg & J. I. Cirac, “Matrix product states, projected entangled pair states, and variational renormalization group methods for quantum spin systems”, Adv. Phys. 57,143 (2008).
- U. Schollwöck, “The density-matrix renormalization group in the age of matrix product states”, Ann. Phys. 326, 96 (2011).
- R. Orús, “A practical introduction to tensor networks: matrix product states and projected tntangled pair states”, Ann. Phys. 349, 117 (2014).
- J. I. Cirac, D. Perez-Garcia, N. Schuch & F. Verstraete, “Matrix product states and projected entangled pair states: concepts, symmetries, and theorems”, arXiv:2011.12127.
- J. von Delft, Lecture on Tensor Networks (SS2020); see link.
- …

§ 0. Tensor Network Basics

Example: single quantum spin-1/2

- States: $|0\rangle \equiv |\uparrow\rangle,\ |1\rangle \equiv |\downarrow\rangle$ $\quad |\psi\rangle \in \mathbb{C}^2$

$$|\psi\rangle = \psi(0)|0\rangle + \psi(1)|1\rangle = \sum_{s=0,1} \psi(s)|s\rangle$$

- Operators: $\sigma^0 \equiv I,\ \sigma^x,\ \sigma^y,\ \sigma^z$

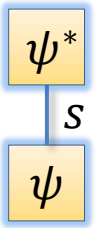
$$O = \sum_{s,s'=0,1} O_{s's}|s'\rangle\langle s|$$

§ 0. Tensor Network Basics

Example: single quantum spin-1/2

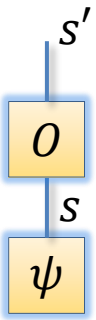
- Norm: $\langle\psi|\psi\rangle$

$$\langle\psi|\psi\rangle = \sum_{s',s=0,1} \psi^*(s')\psi(s)\langle s'|s\rangle = \sum_{s=0,1} \psi^*(s)\psi(s)$$



- Acting operator on state: $O|\psi\rangle$

$$O|\psi\rangle = \sum_{s',s,s''=0,1} O_{s's}\psi(s'')|s'\rangle\langle s|s''\rangle = \sum_{s'=0,1}\left[\sum_{s=0,1} O_{s's}\psi(s)\right]|s'\rangle$$



§ 0. Tensor Network Basics

Example: single quantum spin-1/2

- Expectation value: $\langle\psi|O|\psi\rangle$

$$\langle\psi|O|\psi\rangle = \sum_{s',s=0,1} \psi^*(s')O_{s's}\psi(s)$$

- Matrix element: $\langle\psi'|O|\psi\rangle$

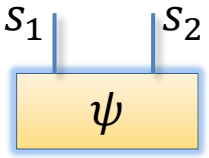
$$\langle\psi'|O|\psi\rangle = \sum_{s',s=0,1} \psi'^*(s')O_{s's}\psi(s)$$

§ 0. Tensor Network Basics

Example: two spin-1/2's $\quad |\psi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$

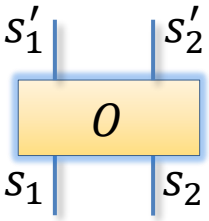
- States: $|0,0\rangle \equiv |0\rangle \otimes |0\rangle,\ |0,1\rangle,\ |1,0\rangle,\ |1,1\rangle$

$$|\psi\rangle = \sum_{s_1,s_2=0,1} \psi(s_1,s_2)|s_1,s_2\rangle$$



- Operators: $\sigma^a \otimes \sigma^b \quad (a,b = 0,x,y,z)$

$$O = \sum_{s_1,s_2\,,s_1's_2'=0,1} O_{s_1's_2';s_1s_2}|s_1',s_2'\rangle\langle s_1,s_2|$$

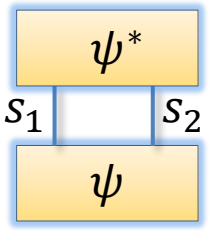


§ 0. Tensor Network Basics

Example: two spin-1/2's

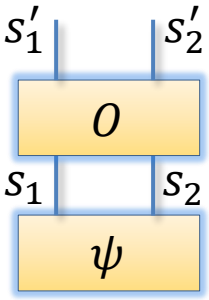
- Norm: $\langle\psi|\psi\rangle$

$$\langle\psi|\psi\rangle = \sum_{s_1,s_2=0,1} \psi^*(s_1,s_2)\psi(s_1,s_2)$$



- Acting operator on state: $O|\psi\rangle$

$$O|\psi\rangle = \sum_{s_1's_2'=0,1} \left[\sum_{s_1,s_2=0,1} O_{s_1's_2';s_1s_2}\, \psi(s_1,s_2) \right] |s_1', s_2'\rangle$$

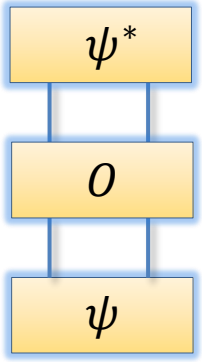


§ 0. Tensor Network Basics

Example: two spin-1/2's

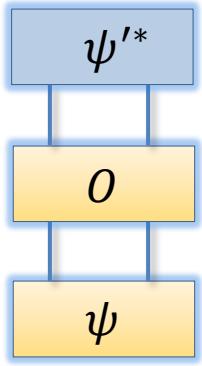
- Expectation value: $\langle\psi|O|\psi\rangle$

$$\langle\psi|O|\psi\rangle = \sum_{s_1' s_2', s_1 s_2} \psi^*(s_1', s_2') O_{s_1' s_2'; s_1 s_2} \psi(s_1, s_2)$$



- Matrix element: $\langle\psi'|O|\psi\rangle$

$$\langle\psi'|O|\psi\rangle = \sum_{s_1' s_2', s_1 s_2} \psi'^*(s_1', s_2') O_{s_1' s_2'; s_1 s_2} \psi(s_1, s_2)$$

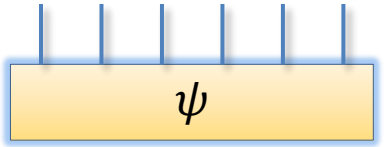


§ 0. Tensor Network Basics

Example: N spin-1/2's $\quad |\psi\rangle \in (\mathbb{C}^2)^{\otimes N}$

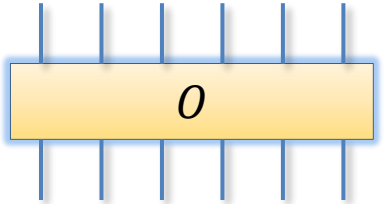
- States: $|s_1, s_2, \dots, s_N\rangle \equiv |s_1\rangle \otimes |s_2\rangle \otimes \cdots \otimes |s_N\rangle$

$$|\psi\rangle = \sum_{s_1,\dots,s_N} \psi(s_1, \dots, s_N)|s_1, \dots, s_N\rangle$$



- Operators: $\sigma^{a_1} \otimes \cdots \otimes \sigma^{a_N}$

$$O = \sum_{\{s'\},\{s\}} O_{s'_1,\dots,s'_N;s_1,\dots,s_N} |s'_1, \dots, s'_N\rangle\langle s_1, \dots, s_N|$$

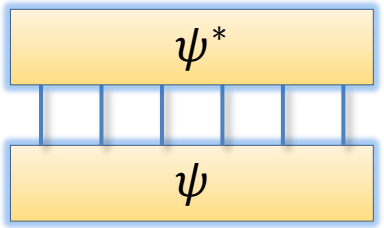


§ 0. Tensor Network Basics

Example: N spin-1/2's

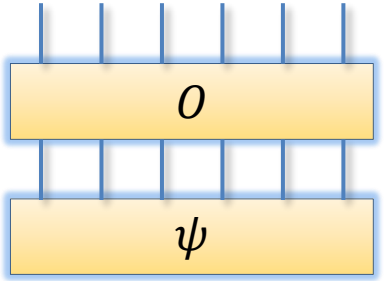
- Norm: $\langle\psi|\psi\rangle$

$$\langle\psi|\psi\rangle = \sum_{\{s\}} \psi^*(s_1, \ldots, s_N)\psi(s_1, \ldots, s_N)$$



- Acting operator on state: $O|\psi\rangle$

$$O|\psi\rangle = \sum_{\{s'\}} \left[\sum_{\{s\}} O_{\{s'\};\{s\}} \psi(\{s\}) \right] |\{s'\}\rangle$$

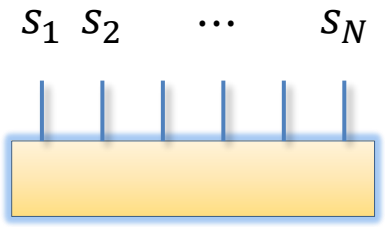


§ 0. Tensor Network Basics

Example: spin-$1/2$ Heisenberg chain with N sites

$$H = \sum_{i=1}^{N-1} \vec{\sigma}_i \cdot \vec{\sigma}_{i+1} \qquad \vec{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$$

Eigenstate: $|\psi\rangle = \sum_{s_1,\ldots,s_N=0,1} \psi(s_1, \ldots, s_N)\, |s_1, \ldots, s_N\rangle$



- # of parameters scales exponentially with # of spins.

$\rightarrow 2^N$

§ 0. Tensor Network Basics

Example: spin-$1/2$ Heisenberg chain with N sites

$$H = \sum_{i=1}^{N-1} \vec{\sigma}_i \cdot \vec{\sigma}_{i+1} \qquad \vec{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$$

Eigenstate: $|\psi\rangle = \sum_{s_1,\ldots,s_N=0,1} \psi(s_1, \ldots, s_N)\, |s_1, \ldots, s_N\rangle$

Analytical methods:

- Exact solution (very few)
- Mean-field theory + perturbation (often no good starting point)

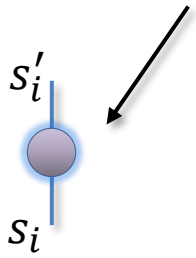
Numerical methods:

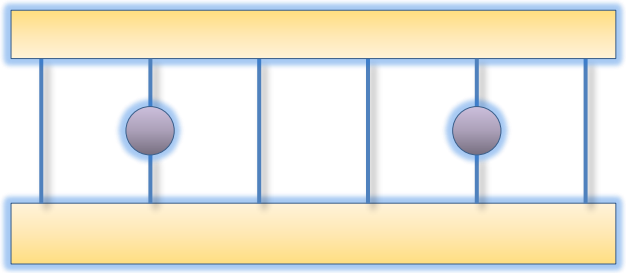
- Exact diagonalization (limited to small system size, $N \sim 50$)
- Quantum Monte Carlo (sign problem)

§ 0. Tensor Network Basics

Two-point correlation function:

$$\langle\psi|\sigma_i^z\sigma_j^z|\psi\rangle = \sum_{s_i',s_j',s_1,\ldots,s_N} \psi^*(s_1 \ldots s_i' \ldots s_j' \ldots s_N)\psi(s_1 \ldots s_i \ldots s_j \ldots s_N)\,\langle s_i'|\sigma_i^z|s_i\rangle\langle s_j'|\sigma_j^z|s_j\rangle$$





$$\psi^\dagger O\psi$$

1×2^N $\quad 2^N \times 2^N$ $\quad 2^N \times 1$

Impossible when N is large!

§ 0. Tensor Network Basics

Two exponential walls:

- Representing many-body wave functions requires exponentially many parameters.

- The computational cost for calculating physical observables grows exponentially.

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.