Tensor Network Simulation of Quantum Systems

Class 1 — Spring semester ‘26

Lecturers:

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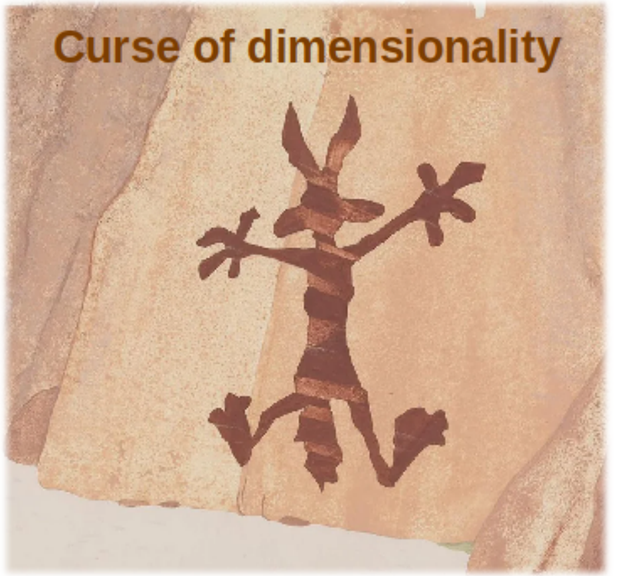
Tensor Network State Simulation of Quantum Systems – Semester overview

- **12-13 lectures – attendance requirement 70% (max 4 absences)**
- **Extra consultation with the lecturers: on request (via email)**
- **Exam:**
  - Grade can be earned by homework projects and their presentation.
  - Grade can also be earned by digesting literature (will be provided by lecturers), and presenting it.
  - One can also earn a grade by passing a conventional oral exam.
- **Literature:**
  - DMRG reviews of Prof. Ulrich Schollwöck:
    - U. Schollwöck, Rev. Mod. Phys. 77, 259-315 (2005)
    - U. Schollwöck Annals of Physics 326, 96-192 (2011)
  - References to time-dependent simulations:
    - G. Vidal Phys. Rev. Lett., 93, 040502 (2004)
    - J. Haegeman et al., Phys. Rev. B 94, 165116 (2016)
  - Review of Szilárd Szalay et al.:
    - Szilárd Szalay et al. Int. J. Q. Chem. 115, 1342-1391 (2015)
  - Class materials will be available at: https://github.com/wernermiklos/TNSClass

Tensor Network State Simulation of Quantum Systems – Semester overview

- **Many-body Hamiltonians:**
  - from atomistic description to universal model systems
- **“Exact diagonalization” and its limits of applicability**
- **Renormalization group-based dimension reduction**
  - Block-RG, Numerical RG, Density Matrix RG.
- **The Density Matrix Renormalization Group algorithm**
- **Matrix Product States**
  - generalized correlations and connection to QIT
- **Symmetries and conservation laws for MPS**
- **Long-ranged & higher-dimensional models:**
  - Matrix Product Operator formalism
- **Time-dependent simulations: TEBD, BUG, TDVP**
- **More complex networks (PEPS, MERA, TTNS)**
- **Advanced topics**
  - open systems
  - fermionic mode optimization
  - parallelization



The many-body Hamiltonian (brief overview)

Non-relativistic Hamiltonian of matter

$$H = -\frac{1}{2m}\sum_i \frac{\partial^2}{\partial \mathbf{r}_i^2} - \sum_\alpha \frac{1}{2M_\alpha}\frac{\partial^2}{\partial \mathbf{R}_\alpha^2} - \sum_{i,\alpha}\frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \sum_{\alpha\neq\beta}\frac{Z_\alpha Z_\beta}{2|\mathbf{R}_\alpha - \mathbf{R}_\beta|} + \sum_{i\neq j}\frac{1}{2|\mathbf{r}_i - \mathbf{r_j}|}$$

kinetic energy of electrons | kinetic energy of nuclei | Coulomb int. el-nuc | Coulomb int. nuc-nuc | Coulomb int. el-el

Many-body wavefunction $\Psi(\mathbf{r}_1, \sigma_1, \mathbf{r}_2, \sigma_2, \ldots, \mathbf{R}_1, \Sigma_1, \mathbf{R}_2, \Sigma_2, \ldots)$

electron spins | nuclear spins

The Born-Oppenheimer approximation $\frac{M_\alpha}{m} \sim 10^4 - 10^5$

Nuclei are slow and heavy – *0'th order approx:* fixed position

- Nucleus-nucleus interaction: constant
- Kinetic energy of nucleons: constant (0)
- Electron-nucleus interaction: external potential

$$U(\mathbf{r}) = -\sum_\alpha \frac{Z_\alpha}{|\mathbf{r} - \mathbf{R}_\alpha|}$$

The electronic Hamiltonian

$$H_e = -\frac{1}{2m}\sum_i \frac{\partial^2}{\partial \mathbf{r}_i^2} + \sum_i U(\mathbf{r}_i) + \sum_{i\neq j}\frac{1}{2|\mathbf{r}_i - \mathbf{r_j}|}$$

The many-body Hamiltonian - second quantization

$$H_e = \underbrace{-\frac{1}{2m}\sum_i \frac{\partial^2}{\partial \mathbf{r}_i^2} + \sum_i U(\mathbf{r}_i)}_{H_{1b}} + \underbrace{\sum_{i\neq j} \frac{1}{2|\mathbf{r}_i - \mathbf{r_j}|}}_{H_{2b}}$$

- **1-electron basis (spin-independent):** $\phi_\alpha(\mathbf{r})$
- **fermionic operators** $\{c_{\alpha\sigma}, c_{\beta\sigma'}\} = 0 \quad \{c_{\alpha\sigma}, c^\dagger_{\beta\sigma'}\} = \delta_{\alpha\beta}\delta_{\sigma\sigma'}$

$$\sigma, \sigma' \longleftrightarrow \text{spin}$$

- **basis states (configurations)**

$$|n_{1\uparrow}, n_{1\downarrow}, n_{2\uparrow}, n_{2\downarrow} \ldots\rangle = (c^\dagger_{1\uparrow})^{n_{1\uparrow}}(c^\dagger_{1\downarrow})^{n_{1\downarrow}}(c^\dagger_{2\uparrow})^{n_{2\uparrow}}(c^\dagger_{2\downarrow})^{n_{2\downarrow}} \ldots |0\rangle \longleftrightarrow \text{occupation number representation}$$

- **1-body Hamiltonian**

$$H_{1b} = \sum_{\alpha,\beta=1}^{\infty} \sum_{\sigma\in\{\uparrow,\downarrow\}} T_{\alpha\beta}\, c^\dagger_{\alpha\sigma} c_{\beta\sigma} \longleftrightarrow T_{\alpha\beta} = \int d^3\mathbf{r}\, \phi^*_\alpha(\mathbf{r}) \left(-\frac{1}{2m}\frac{\partial^2}{\partial \mathbf{r}^2} + U(\mathbf{r})\right)\phi_\beta(\mathbf{r})$$

- **2-body Hamiltonian**

$$H_{2b} = \sum_{\alpha,\beta,\gamma,\delta}^{\infty} \sum_{\sigma,\sigma'} V_{\alpha\beta\gamma\delta}\, c^\dagger_{\alpha\sigma} c^\dagger_{\beta\sigma'} c_{\gamma\sigma'} c_{\delta\sigma} \longleftrightarrow V_{\alpha\beta\gamma\delta} = \int d^3\mathbf{r} d^3\mathbf{r}'\, \phi^*_\alpha(\mathbf{r})\phi^*_\beta(\mathbf{r}') \frac{1}{|\mathbf{r}-\mathbf{r}'|}\phi_\gamma(\mathbf{r}')\phi_\delta(\mathbf{r})$$

Problem: Exact (over-)representation, but infinite number of orbitals

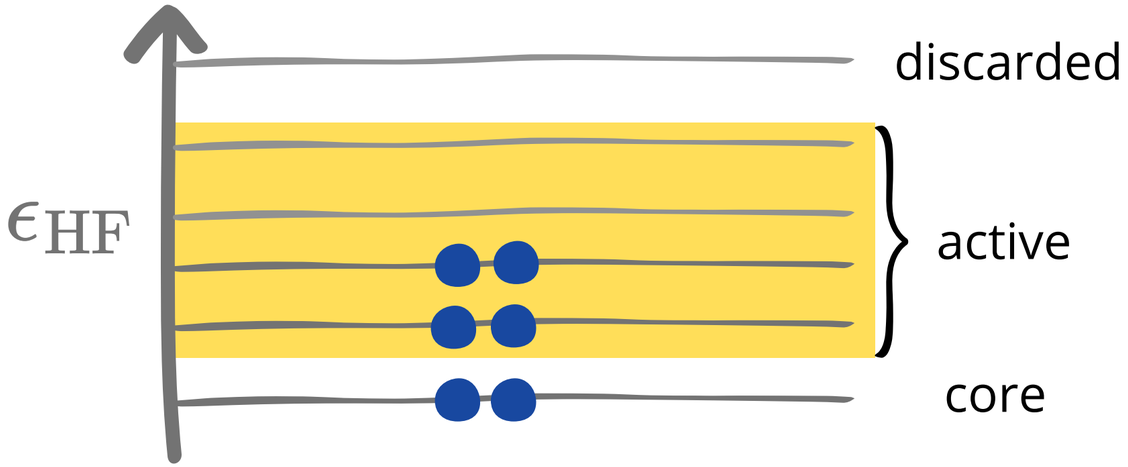
“Quantum chemistry style” approximation: active space selection

- **General idea:**
  - Search 1-particle basis, in which the ground state is simple
  - Restriction to ‘important’ 1-particle orbitals
- **Hartree-Fock Theory**
  - Ground state ansatz $\left|\Psi_0^{\mathrm{HF}}\right\rangle = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger \cdots c_{N_e/2\uparrow}^\dagger c_{N_e/2\downarrow}^\dagger \left|0\right\rangle$
  - Variational search of optimal 1-particle basis

$$\phi_\alpha(\mathbf{r}) = ? \quad \longleftrightarrow \quad \left\langle \Psi_0^{\mathrm{HF}} \right| H \left| \Psi_0^{\mathrm{HF}} \right\rangle = \min$$

- Leads to the Hartree-Fock equations
- Results in the Hartree-Fock orbitals and energies
- **Remark:** virtual (unoccupied) orbitals

  - **Active space selection**



$$H = E_{\mathrm{core}} + \sum_{\alpha,\beta}^{\mathrm{act.}} \sum_{\sigma} \tilde{T}_{\alpha\beta} c_{\alpha\sigma}^\dagger c_{\alpha\sigma} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta}^{\mathrm{act.}} \sum_{\sigma\sigma'} V_{\alpha\beta\gamma\delta} c_{\alpha\sigma}^\dagger c_{\beta\sigma'}^\dagger c_{\gamma\sigma'} c_{\delta\sigma}$$

core orbitals’ correction

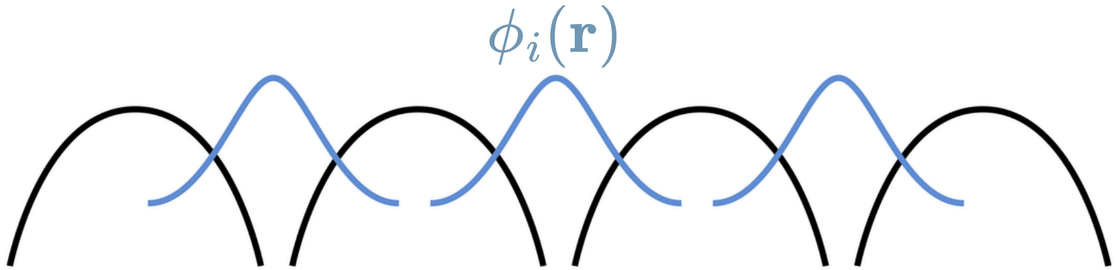
“Physicist style” approximation: universal model Hamiltonians

Huge number of particles ⇨ **Precise microscopic modelling is too hard**

- **Build a simple ‘toy’-model**
- **Fix the model parameters to**
  - exhibit experimentally observed behavior
  - realize interesting quantum states

Example 1: The Hubbard model

1 orbital / lattice site



$$H = -\sum_{\langle i,j\rangle,\sigma} \left(t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + h.c.\right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

⟷ occupation number operator: $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$

Example 2: Spin models

1 particle / lattice site: only the spin freedom remains

$$H = \sum_{\langle i,j\rangle} \left(J^x_{ij} S^x_i S^x_j + J^y_{ij} S^y_i S^y_j + J^z_{ij} S^z_i S^z_j \right)$$

Rest of the class: blackboard, code samples (lecture notes will be provided)

Class materials are available at: https://github.com/wernermiklos/TNSClass

What software / language to use?

Provided ‘toy-codes’ will be in MatLab

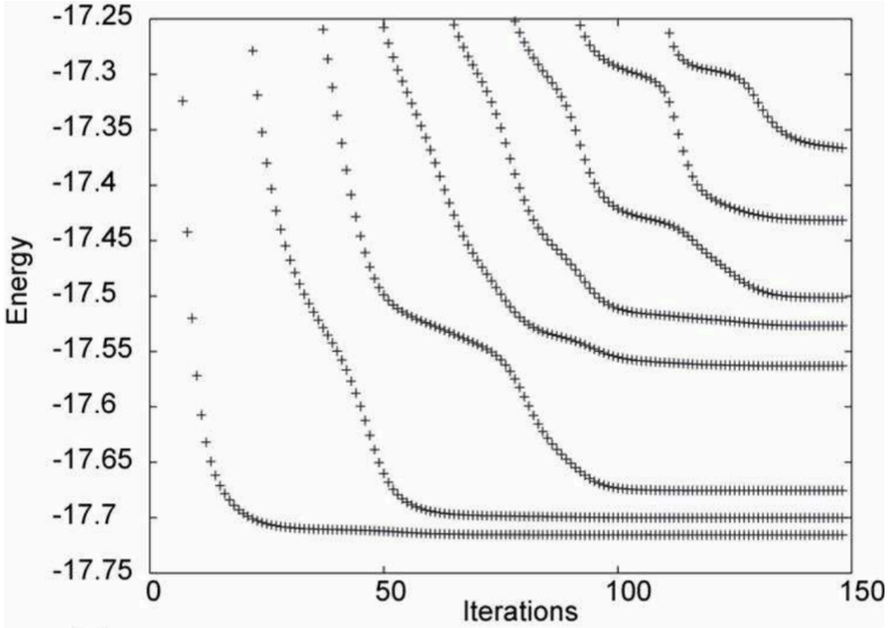
https://math.bme.hu/matlab – BME licence (with edu.bme.hu email address)

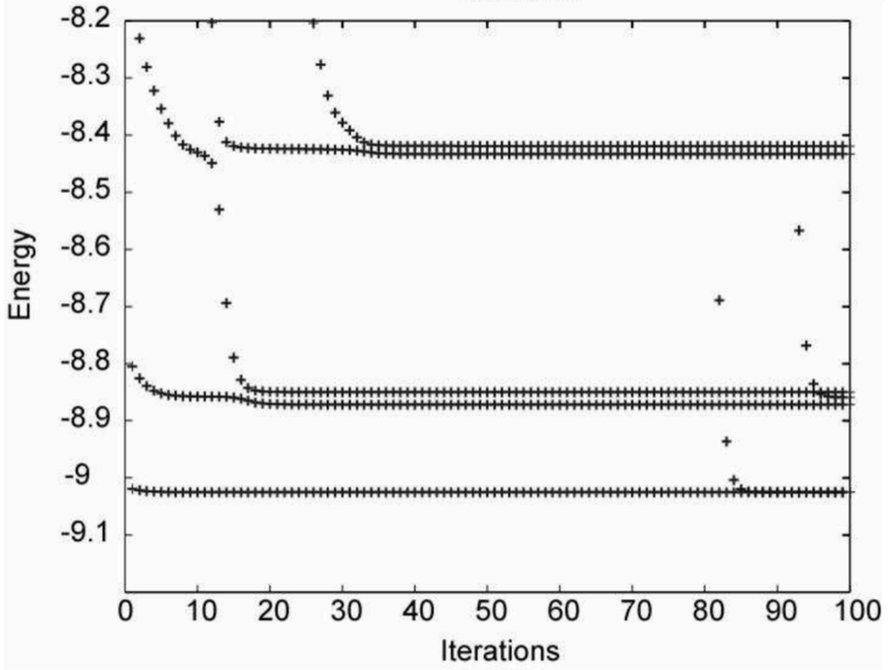
https://matlab.mathworks.com – for online use (no need for desktop app)

Other similar languages:

python with numpy/scipy	**https://www.anaconda.com/download**
julia	**https://julialang.org**

Lánczos algorithm – issues

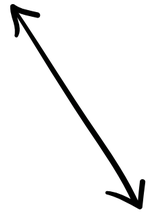




- **eigenvalues converge starting with extremal ones**
- **excited states can get “stuck” for a while**

at longer times:

- **true eigenvalues converged**
- **spurious or “ghost” eigenvalues produced**
- **multiplicity of eigenstates increases**



Orthogonality is lost

Lánczos is very efficient for the ground state