ETH
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Computational Quantum Physics
Exercise 2

FS 09
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Submitting Block A You should now submit your results to Block A, i.e. the solutions to Problem 1.1 and 1.2, to one of the assistants. We expect you to write a short summary of the algorithm and your results and send it along with the source code. All results should be handed in by Wednesday, March 11th.

Problem 2.1 Tensor product

As a preparation for writing a DMRG code for the Heisenberg chain, you should implement a routine that returns the matrix representation of the tensor product of two operators acting in a tensor product Hilbert space, i.e. for two operators $\mathcal{A} : \mathcal{H}_1 \to \mathcal{H}_1$ and $\mathcal{B} : \mathcal{H}_2 \to \mathcal{H}_2$ we would like to find a matrix representation of $\mathcal{A}\otimes\mathcal{B} : \mathcal{H}_1\otimes\mathcal{H}_2 \to \mathcal{H}_1\otimes\mathcal{H}_2$. To give you an example: a typical operator occuring in the Hamiltonian for a spin-$\frac{1}{2}$ system would be the Ising coupling, $H = \sigma_z^1\sigma_z^2$, where σ_z denotes the Pauli matrix for the z-component of the spin operator. In more precise notation, this corresponds to an operator acting on the product Hilbert space of two spin-$\frac{1}{2}$ particles, $\mathcal{H} = \mathcal{H}_{1/2} \otimes \mathcal{H}_{1/2}$,

$$H = \left(\sigma_z^1 \otimes \mathbb{I}^2\right) \cdot \left(\mathbb{I}^1 \otimes \sigma_z^2\right), \tag{1}$$

where the superscript indicates which particle the operator acts on, $\mathcal{I}$ denotes the identity and $\cdot$ denotes the standard matrix product. In order to find a matrix representation of this, we need to express the tensor products $(\sigma_z^1 \otimes \mathbb{I}^2)$ and $(\mathbb{I}^1 \otimes \sigma_z^2)$ in the product basis for $\mathcal{H}$. The result would be

$$H = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{2}$$

Confirm this result and write a general routine to implement the tensor product.

Problem 2.2 Exact diagonalization

Based on this, we can now proceed to write an exact diagonalization program. We want to solve the eigenvalue problem

$$H|\Psi\rangle = E|\Psi\rangle, \tag{3}$$

where in this example we take H as the Heisenberg Hamiltonian on a one-dimensional chain of spin-$\frac{1}{2}$ sites with open boundary conditions,

$$H = \sum_{\langle i,j\rangle} \vec{\sigma^i}\vec{\sigma^j}. \tag{4}$$

The sum runs over pairs of nearest neighbours and $\vec{\sigma^j} = (\sigma_x^j, \sigma_y^j, \sigma_z^j)$ are the Pauli matrices. Since the dimension of the Hilbert space grows exponentially in the number of sites on the chain, we will only be able to tackle small problems. Start by constructing the Hamiltonian matrix for a very small number of lattice sites (using the result from problem 2.1) and diagonalize this to find the ground state energy.

You can check your results against the following:

L	**Energy per site**
2	-1.5
3	$-\frac{4}{3}$
4	-1.61
$\vdots$	$\vdots$
∞	-1.773

(5)