Karlsruhe Institute of Technology
Institute for Theoretical Condensed Matter physics (TKM)
Institute of Nanotechnology (INT)
Prof. Dr. Jörg Schmalian, Dr. Peter Schmitteckert, Dr. Andreas Poenicke, Benedikt Schönauer

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Exercise Sheet No. 6
"Computational Condensed Matter Theory"

14 Density Matrix Renormalization Group method (DMRG) [40 points]

Consider a 1D chain of spinless hard-core bosons with nearest-neighbor hopping t and nearest-neighbor-interaction U:

$$\hat{\mathrm{H}} = -t \sum_{<i,j>} (\hat{\mathrm{c}}_i^\dagger \hat{\mathrm{c}}_j + \mathrm{h.c.}) + U \sum_{<i,j>} \hat{\mathrm{n}}_i \hat{\mathrm{n}}_j - U \sum_i \hat{\mathrm{n}}_i, \tag{1}$$

where $\hat{\mathrm{c}}_i^\dagger$ denotes the creation operator at site i, $\hat{\mathrm{n}}_i$ the density at site i. The last term in the Hamiltonian is included to make the interaction particle-hole symmetric. The creation and annihilation operators $\hat{\mathrm{c}}^\dagger$ and $\hat{\mathrm{c}}$ for hard-core bosons obey bosonic commutation relations, but only the single occupation of a state is allowed, i.e. $\hat{\mathrm{c}}^\dagger |1\rangle = 0$ and thus a suitable basis for a single site is given by $\{|0\rangle, |1\rangle\}$.

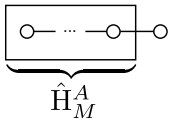
a) Initial System: Two Sites

At first consider a system of 2 sites with hard wall boundary conditions. Write the operators $\hat{\mathrm{c}}_1$, $\hat{\mathrm{c}}_2$, $\hat{\mathrm{n}}_1$ and $\hat{\mathrm{n}}_2$, which in this case are represented as 4×4 matrices.

Using these operators, construct the Hamiltonian (Eq. 1) for the 2-site system. This Hamiltonian describing the initial block A shall be denoted by $\hat{\mathrm{H}}_2^A$.

b) DMRG Iteration Step 1: Add a Site

Now increase the size of the block A by adding an additional site, which results in a larger basis $\left\{ |\tilde{\lambda}\rangle_{M+1}^A \right\} = \left\{ |\lambda\rangle_M^A \right\} \otimes \left\{ |n\rangle \right\}$. Given the Hamiltonian $\hat{\mathrm{H}}_M^A$ (for M sites) the new Hamiltonian in this basis, $\tilde{\mathrm{H}}_{M+1}^A$, is obtained by



$$\tilde{\mathrm{H}}_{M+1}^A = \hat{\mathrm{H}}_M^A \otimes \mathbb{1} - t(\hat{\mathrm{c}}_M^\dagger \otimes \hat{\mathrm{c}} + \hat{\mathrm{c}}_M \otimes \hat{\mathrm{c}}^\dagger) + U(\hat{\mathrm{n}}_M \otimes \hat{\mathrm{n}}) - U(\mathbb{1} \otimes \hat{\mathrm{n}}). \tag{2}$$

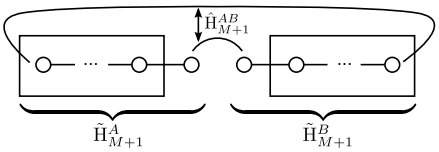
Save the operators $\hat{\mathrm{n}}_{M+1} = \mathbb{1} \otimes \hat{\mathrm{n}}$ and $\hat{\mathrm{c}}_{M+1} = \mathbb{1} \otimes \hat{\mathrm{c}}$.

c) DMRG Step 2: Double the System

Consider a block B, which in our case is a copy of block A, thus $\hat{\mathrm{H}}_{M+1}^B = \hat{\mathrm{H}}_{M+1}^A$.

The combined system of both blocks may be described in a basis $\left\{ |\tilde{\lambda}\rangle_{M+1}^{AB} \right\} = \left\{ |\tilde{\lambda}\rangle_{M+1}^A \right\} \otimes \left\{ |\tilde{\lambda}\rangle_{M+1}^B \right\}$. Construct the Hamiltonian $\hat{\mathrm{H}}_{M+1}^{AB}$, which connects both blocks at the respective sites $M+1$, and for periodic boundary conditions also at the respective sites 1. Thus,

$$\hat{\mathrm{H}}_{M+1}^{AB} = -t(\hat{\mathrm{c}}_{M+1}^\dagger \otimes \hat{\mathrm{c}}_{M+1} + \hat{\mathrm{c}}_{M+1} \otimes \hat{\mathrm{c}}_{M+1}^\dagger) - t(\hat{\mathrm{c}}_1^\dagger \otimes \hat{\mathrm{c}}_1 + \hat{\mathrm{c}}_1 \otimes \hat{\mathrm{c}}_1^\dagger) + U(\hat{\mathrm{n}}_1 \otimes \hat{\mathrm{n}}_1 + \hat{\mathrm{n}}_{M+1} \otimes \hat{\mathrm{n}}_{M+1}). \tag{3}$$



The total Hamiltonian for the combined system of $2M+2$ sites is therefore given by

$$\bar{\mathrm{H}}_{2M+2} = \tilde{\mathrm{H}}_{M+1}^A \otimes \mathbb{1} + \mathbb{1} \otimes \tilde{\mathrm{H}}_{M+1}^B + \hat{\mathrm{H}}_{M+1}^{AB}. \tag{4}$$

Hint: Use `kron(sparse(mat1), sparse(mat2))` to create a sparse Kronecker product.

d) DMRG Step 3: Diagonalize the Total Hamiltonian

Calculate the ground state energy $E_0(2M+2)$ and wavefunction Ψ_0 of the Hamiltonian $\bar{\mathrm{H}}_{2M+2}$.

Hint: Matlab's `eigs` function can be used to efficiently calculate only one eigenvector with the lowest eigenvalue. (Use the option "smallest real part" to achieve this.)

e) DMRG Step 4: Calculate the Reduced Density Matrix

Consider the density matrix for this ground state, $\hat{\rho} = |\Psi_0\rangle\langle\Psi_0|$. Trace out all degrees of freedom from block B to obtain the reduced density matrix ρ^A,

$$\hat{\rho}^A_{il} = \left(\mathrm{tr}^B \hat{\rho}\right)_{il} = \sum_{j\in B} \hat{\rho}_{(i,j),(l,j)},$$

where the notation (i,j) denotes a single index of the density matrix ρ, where i is the index belonging to the subspace of block A and j the index belonging to the subspace B.

Hint: An efficient way to calculate the reduced density matrix in Matlab without first constructing the full density matrix is given by the following code:

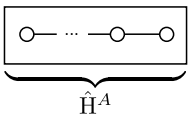
```
psi_R = reshape(psi_0, dim_B, dim_A); rho_A = psi_R' * psi_R;
```

Here `dim_A` is the dimension of the subspace A and `dim_B` the dimension of subspace B.

f) DMRG Step 5: Projection on Subspace

Fully diagonalize the reduced density matrix ρ^A. Now use the eigenvectors corresponding to the largest N_{states} eigenvalues as a new basis. Project and store the operators (for block A) $\hat{\mathrm{c}}_1$, $\hat{\mathrm{c}}_{M+1}$, $\hat{\mathrm{n}}_1$, $\hat{\mathrm{n}}_{M+1}$.

As a final step project $\tilde{\mathrm{H}}^A_{M+1}$ to obtain a new $\hat{\mathrm{H}}^A_M$ as input for the next iteration. Repeat DMRG steps 1 to 5 until the system size $2M+2$ reaches a chosen value.



f) Luttinger-Liquid Behavior

For three different values of $U = 0, -\sqrt{3}t, \sqrt{3}t$, perform a DMRG calculation up to a system size of $L_{\max}$. Extract the system-size dependence of the ground state energy $E(L)$. Choose $N_{\mathrm{states}} = 50$ and $L_{\max} = 70$.

As can be shown analytically the lowest-order finite size corrections for the ground state energy per site e_L for this model are given by

$$e_L = \frac{E(L)}{L} = e_\infty(U) - v(U)\frac{\pi}{6}\frac{1}{L^2}, \tag{5}$$

where v is the velocity of lowest-lying excitations in the system. By analyzing your data, extract e_∞ and v for the given values of U and plot $E(L)/L$ versus $1/L^2$. Discuss the behavior of $v(U)$ with decreasing U. **Hint:** For $U = 0$ the analytics yield $v = 2$ and $e_\infty = -2/\pi$.

15* Performance Optimization

The use of the full Hamiltonian $\bar{\mathrm{H}}_{2M+2}$ can become very expensive. But for Krylov methods it is sufficient to know the result of the application of the operator to a given vector. `eigs` uses a Krylov space method, so it is possible to forego the explicit construction of $\bar{\mathrm{H}}_{2M+2}$. With the help of `psi_mat = reshape(psi, dim_B, dim_A);` one can rewrite any vector in the full tensor product space as a matrix. Then, the following relation holds for the application of operators on this vector:

$$\Phi = (O^A \otimes O^B)\Psi \qquad \Leftrightarrow \qquad \Phi_{\mathrm{Mat}} = O^B \Psi_{\mathrm{Mat}} (O^A)^{\mathrm{T}}$$

Write a function that takes a column vector Ψ as input and returns $\bar{\mathrm{H}}_{2M+2}\Psi$ without explicitly constructing the full Hamiltonian. Use this function to optimize DMRG step 3. Repeat the calculation of exercise 14f) for larger N_{states} and $L_{\max}$. Compare your results.

Hint: `eigs(matrix, ...)` $\Leftrightarrow$ `eigs(@function, dim_A * dim_B, ...)`.