Time Evolution of Quantum Systems 2025: Exercise 1

M. Gisti, T. Luu, M. Maležič, J. Ostmeyer Hand in: 23.04.2025

Baker-Campbell-Hausdorff formula

H.1 In the following, we use the Lie brackets as shorthand notation for the commutator $[A, B] \coloneqq AB - BA$ of two matrices A, B. Furthermore, we use Landau's big-O-notation. In particular, the Landau symbol $\mathcal{O}(g)$ in O-notation means that a considered function f grows at most as fast as g. In our case, $\mathcal{O}(\varepsilon^3)$ means that we can neglect all terms of orders $\varepsilon^3, \varepsilon^4, \dots$ because we assume ε to be small.

(a) Show the Baker-Campbell-Hausdorff formula (BCH formula)

$$e^{(A+B)\varepsilon} = e^{A\varepsilon} e^{B\varepsilon} e^{-\frac{1}{2}[A,B]\varepsilon^2 + \mathcal{O}(\varepsilon^3)}$$

up to the second order. (1 P.)

(b) Now show $e^{A\varepsilon} e^{B\varepsilon} = e^{B\varepsilon} e^{A\varepsilon} e^{[A,B]\varepsilon^2 + \mathcal{O}(\varepsilon^3)}$. This variant is sometimes also referred to as the BCH formula. (1 P.)

(c) Finally, show the Lie product formula $e^{A+B} = \lim_{n\to\infty} \left(e^{\frac{1}{n}A} e^{\frac{1}{n}B}\right)^n$. (1 P.)

(d) Suppose that $[A, B] = c\mathbb{1}$ with $c \in \mathbb{C}$. Show that

$$e^A \cdot e^B = e^B \cdot e^A \cdot e^{c\mathbb{1}}.$$

(1 P.)

(e) Prove the Campbell identity for a linear operator on Hilbert space,

$$e^A B e^{-A} = \sum_{k=0}^{\infty} \frac{1}{k!} [A, B]_k$$

where $[A, B]_0 = B$ and $[A, B]_k = [A, [A, B]]_{k-1}$. (2 P.)

Hint: Replace the operator A by εA with $\epsilon \in \mathbb{R}$, and do a Taylor expansion in ϵ.

Analytic Exact Diagonalization

H.2 Consider a particle in a 3-site 1D chain with periodic boundary conditions. The system is described by the following tight-binding Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} (c_i^\dagger c_j + c_j^\dagger c_i)$$

where $c_i^\dagger$ and c_i are creation and annihilation operators at site i, and J is the hopping amplitude. Assume periodic boundary conditions, meaning site 3 connects back to site 1.

(a) Construct the Hamiltonian matrix in the basis $|1\rangle, |2\rangle, |3\rangle$, where $|i\rangle$ represents the particle localized at site i in the chain. (1 P.)

(b) Find the eigenvalues of the system by diagonalizing H. (1 P.)

(c) Determine the eigenvectors. (1 P.)

(d) Calculate the time evolution operator $U(t) = e^{-iHt}$, expressing it terms of the Hamiltonian eigenvectors. (1 P.)

Numerical Exact Diagonalization

H.3 In this exercise, you will write a small exact diagonalization code to solve a fundamental problem of quantum mechanics: the one-dimensional Heisenberg XXZ model. Consider a system of L spin-$\frac{1}{2}$ particles, subjected to nearest-neighbor interactions, the system is described by the following Hamiltonian,

$$H = J \sum_{j=0}^{L-1} \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + S_j^z S_{j+1}^z \right),$$

with

$$S^x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^y = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S^z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and J being the interaction strength.

(a) Write down the computational basis states for $L = 2$ ($2^2 = 4$ states) and $L = 3$ ($2^3 = 8$ states). (2 P.)

(b) Construct the Hamiltonian explicitly as a matrix using the basis from part (a), for both $L = 2$ and $L = 3$. (2 P.)

(c) Compute the eigenvalues and eigenvectors by numerically diagonalizing the Hamiltonian with $J = 1$ (e.g. `numpy.linalg.eigh()` or an equivalent function in your preferred programming language), for both $L = 2$ and $L = 3$. (4 P.)

Note: This dense matrix approach is computationally inefficient and becomes impractical for larger system sizes.

(d) Implement a function that takes a time t and returns the complete time evolution operator and returns the full time evolution operator matrix $U(t) = e^{-iHt}$ for $L = 2, 3$ using the previously determined eigenvalues and -vectors. (2 P.)