Time Evolution of Quantum Systems 2025: Exercise 1

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Baker-Campbell-Hausdorff formula

H.1 In the following, we use the Lie brackets as shorthand notation for the commutator $[A, B] := AB - BA$ 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 $\varepsilon^3, \varepsilon^4, \ldots$ 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. (2 P.)

We can simply truncate the Taylor series after the second order in ε and get

$$\begin{aligned}
e^{(A+B)\varepsilon} &= \mathbb{1} + (A+B)\varepsilon + \frac{1}{2}(A+B)^2\varepsilon^2 + \mathcal{O}(\varepsilon^3) \\
&= \mathbb{1} + A\varepsilon + B\varepsilon + \frac{1}{2}A^2\varepsilon^2 + \frac{1}{2}AB\varepsilon^2 + \frac{1}{2}BA\varepsilon^2 + \frac{1}{2}B^2\varepsilon^2 + \mathcal{O}(\varepsilon^3) \\
&= \mathbb{1} + A\varepsilon + \frac{1}{2}A^2\varepsilon^2 + B\varepsilon + \frac{1}{2}B^2\varepsilon^2 + AB\varepsilon^2 - \frac{1}{2}AB\varepsilon^2 + \frac{1}{2}BA\varepsilon^2 + \mathcal{O}(\varepsilon^3) \\
&= \left(\mathbb{1} + A\varepsilon + \frac{1}{2}A^2\varepsilon^2\right)\left(\mathbb{1} + B\varepsilon + \frac{1}{2}B^2\varepsilon^2\right)\left(\mathbb{1} - \frac{1}{2}[A,B]\varepsilon^2 + \mathcal{O}(\varepsilon^3)\right) \\
&= e^{A\varepsilon} e^{B\varepsilon} e^{-\frac{1}{2}[A,B]\varepsilon^2 + \mathcal{O}(\varepsilon^3)}
\end{aligned}$$

(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.)

A similar calculation as above leads to the correct result. Alternatively, you can also use the well-known BCH formula:

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

The addition of matrices commutes, i.e. $A + B = B + A$. By equating you then get

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

where the antisymmetry of the commutator $[A, B] = -[B, A]$ and the inverse matrix exponential function $\exp(A)^{-1} = \exp(-A)$ were also used.

(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.)

For all $n \in \mathbb{N}$ applies (because $A+B$ commutes with itself)

$$e^{A+B} = \left(e^{\frac{1}{n}(A+B)}\right)^n .$$

If n is large enough, the BCH formula $e^{\frac{1}{n}(A+B)} = e^{\frac{1}{n}A}e^{\frac{1}{n}B}e^{\mathcal{O}\left(n^{-2}\right)}$ also applies. In the limit $n \to \infty$, the term in $\mathcal{O}\left(n^{-2}\right)$ is negligible compared to the leading terms and therefore $e^{A+B} = \lim_{n\to\infty}\left(e^{\frac{1}{n}A}e^{\frac{1}{n}B}\right)^n$.

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

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

(e) Prove the Baker-Campbell-Hausdorff formula 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 $[A,B]_k = [A,[A,B]]_{k-1}$.

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

First, notice that we can expand the k-order nested commutators as follows:

$$\begin{aligned}
k=0 \qquad & [A,B]_0 = B \\
k=1 \qquad & [A,B]_1 = AB - BA \\
k=2 \qquad & [A,B]_2 = [A,[A,B]] = A^2B - 2ABA + BA^2 \\
k=3 \qquad & [A,B]_3 = [A,[A,[A,B]]] = A^3B + 3ABA^2 - 3A^2BA - BA^3 \\
k=4 \qquad & [A,B]_3 = [A,[A,[A,[A,B]]]] = A^4B - 4A^3BA + 6A^2BA^2 - 4ABA^3 + BA^4) \\
\vdots \qquad &
\end{aligned}$$

Let us substitute A with εA, we can expand the above expression as:

$$\begin{aligned}
e^{\varepsilon A}Be^{-\epsilon A} =& \left(\sum_{n=0}^{\infty}\frac{1}{n!}(\epsilon A)^n\right)B\left(\sum_{m=0}^{\infty}\frac{1}{m!}(-\epsilon A)^m\right) \\
=& \left(\mathbb{1} + \varepsilon A + \frac{(\epsilon A)^2}{2} + \frac{(\epsilon A)^3}{6} + \frac{(\epsilon A)^4}{24}\right)B\left(\mathbb{1} - \varepsilon A + \frac{(\epsilon A)^2}{2} - \frac{(\epsilon A)^3}{6} + \frac{(\epsilon A)^4}{24}\right) \\
=& \mathbb{1} + \varepsilon(AB - BA) + \frac{\epsilon^2}{2}(A^2B + BA^2 - 2ABA) + \\
& + \frac{\varepsilon^3}{6}(A^3B + 3ABA^2 - 3A^2BA - BA^3) \\
& + \frac{\varepsilon^4}{24}(A^4B - 4A^3BA + 6A^2BA^2 - 4ABA^3 + BA^4) + \mathcal{O}(\epsilon^5)
\end{aligned}$$

where we recognize the k-order nested commutators

$$e^{\varepsilon A}Be^{-\epsilon A} = \mathbb{1} + \varepsilon[A,B]_1 + \frac{\epsilon^2}{2}[A,B]_2 + \frac{\epsilon^3}{6}[A,B]_3 + \frac{\epsilon^4}{24}[A,B]_4 + \mathcal{O}(\epsilon^5) \equiv \sum_{k=0}^{\infty}\frac{\epsilon^k}{k!}[A,B]_k.$$

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.

> The Hamiltonian in matrix form in the basis $(|1\rangle, |2\rangle, |3\rangle)$ is:
>
> $$H = \begin{pmatrix} 0 & -J & -J \\ -J & 0 & -J \\ -J & -J & 0 \end{pmatrix}$$

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

> The characteristic equation is:
>
> $$\det(H - \lambda I) = \det \begin{pmatrix} -\lambda & -J & -J \\ -J & -\lambda & J \\ -J & -J & -\lambda \end{pmatrix} = 0$$
>
> Expanding the determinant,
>
> $$\begin{aligned} \det(H - \lambda I) =& (-\lambda) \begin{vmatrix} -\lambda & -J \\ -J & -\lambda \end{vmatrix} + J \begin{vmatrix} -J & -J \\ -J & -\lambda \end{vmatrix} - J \begin{vmatrix} -J & -\lambda \\ -J & -J \end{vmatrix} = \\ =& -\lambda(\lambda^2 - J^2) + J(-J\lambda + J^2) - J(-J\lambda + J^2) = -\lambda^3 - 2J^3 + 3\lambda J^2 = 0 \end{aligned}$$
>
> Thus, the eigenvalues are: $\lambda_1 = J, \quad \lambda_2 = J, \quad \lambda_3 = -2J$

(c) Determine the eigenvectors.

> For $\lambda_1 = J$, solving $H\mathbf{v} = J\mathbf{v}$, we find
>
> $$\mathbf{v}_1 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ e^{i2\pi/3} \\ e^{-i2\pi/3} \end{pmatrix} \qquad \mathbf{v}_2 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ e^{-i2\pi/3} \\ e^{i2\pi/3} \end{pmatrix},$$
>
> while, for $\lambda_3 = -2J$, we obtain $\mathbf{v}_3 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$.

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

> The characteristic equation is:
>
> $$U(t) = e^{-iHt} = e^{-iJt}|\mathbf{v}_1\rangle\langle\mathbf{v}_1| + e^{-iJt}|\mathbf{v}_2\rangle\langle\mathbf{v}_2| + e^{+i2Jt}|\mathbf{v}_3\rangle\langle\mathbf{v}_3|$$

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).

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

(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 $L = 3$.

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.