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. (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.)

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H.1 – Baker–Campbell–Hausdorff formula

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

$$e^{(A+B)\varepsilon} = \mathbb{1} + (A+B)\varepsilon + \tfrac{1}{2}(A+B)^2\varepsilon^2 + \mathcal{O}(\varepsilon^3)$$

$$= \mathbb{1} + A\varepsilon + B\varepsilon + \tfrac{1}{2}A^2\varepsilon^2 + \tfrac{1}{2}B^2\varepsilon^2 + \tfrac{1}{2}(AB+BA)\varepsilon^2 + \mathcal{O}(\varepsilon^3) \quad - AB\varepsilon^2 + AB\varepsilon^2$$

$$= \mathbb{1} + A\varepsilon + B\varepsilon + \tfrac{1}{2}A^2\varepsilon^2 + \tfrac{1}{2}B^2\varepsilon^2 - \tfrac{1}{2}(AB-BA)\varepsilon^2 + AB\varepsilon^2 + \mathcal{O}(\varepsilon^3)$$

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

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

b) BCH – formula II $e^{A\varepsilon} e^{B\varepsilon} = e^{B\varepsilon} e^{A\varepsilon} e^{[A,B]\varepsilon^2} + \mathcal{O}(\varepsilon^3)$

$$e^{A\varepsilon} e^{B\varepsilon} = (\mathbb{1} + A\varepsilon + \tfrac{1}{2}A^2\varepsilon^2 + \dots)(\mathbb{1} + B\varepsilon + \tfrac{1}{2}B^2\varepsilon^2 + \dots) \qquad \mathcal{O}(\varepsilon^3) \mapsto \dots$$

$$= \mathbb{1} + B\varepsilon + \tfrac{1}{2}B^2\varepsilon^2 + A\varepsilon + \underbrace{AB\varepsilon^2}_{=[A,B]\varepsilon^2 + BA\varepsilon^2} + \tfrac{1}{2}A^2\varepsilon^2 + \dots$$

$$= \mathbb{1} + A\varepsilon + \tfrac{1}{2}A^2\varepsilon^2 + B\varepsilon + \tfrac{1}{2}B^2\varepsilon^2 + BA\varepsilon^2 + [A,B]\varepsilon^2 + \dots$$

$$= (\mathbb{1} + B\varepsilon + \tfrac{1}{2}B^2\varepsilon^2 + \dots)(\mathbb{1} + A\varepsilon + \tfrac{1}{2}A^2\varepsilon^2 + \dots)(\mathbb{1} + [A,B]\varepsilon^2 + \dots)$$

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

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

write $e^{\frac{1}{n}A} e^{\frac{1}{n}B} = e^{\frac{1}{n}A + \frac{1}{n}B} e^{\frac{1}{2n^2}[A,B]}$

$$\left(e^{\frac{1}{n}A} e^{\frac{1}{n}B}\right)^n = \Big(\underbrace{e^{\frac{1}{n}(A+B)} \cdot e^{\frac{1}{2n^2}[A,B]}}_{\overset{(*)}{\simeq}\, e^{\frac{1}{n}(A+B) + \frac{1}{2n^2}[A,B]}}\Big)^n = e^{A+B} e^{\frac{1}{2n}[A,B]}$$

$$\Rightarrow \lim_{n\to\infty} \left(e^{\frac{1}{n}A} e^{\frac{1}{n}B}\right)^n = \lim_{n\to\infty} \left(e^{A+B} e^{\frac{1}{2n}[A,B]}\right) = e^{A+B}$$

$$(*) \quad e^{(A+B)\varepsilon} e^{\frac{1}{2}[A,B]\varepsilon^2} = (\mathbb{1} + A\varepsilon + B\varepsilon + \tfrac{1}{2}(A+B)^2\varepsilon^2 + \dots)(\mathbb{1} + \tfrac{1}{2}[A,B]\varepsilon^2 + \dots)$$

$$= \mathbb{1} + \tfrac{1}{2}[A,B]\varepsilon^2 + (A+B)\varepsilon + \tfrac{1}{2}(A+B)^2\varepsilon^2 + \dots$$

$$e^{(A+B)\varepsilon + \frac{1}{2}[A,B]\varepsilon^2} = \mathbb{1} + (A+B)\varepsilon + \tfrac{1}{2}[A,B]\varepsilon^2 + \tfrac{1}{2}(A+B)^2\varepsilon^2 + \dots$$

d) $[A,B] = c\mathbb{1}$ w/ $c \in \mathbb{C}$

[note: easiest to set $\varepsilon = 1$ and use BCH – formula, all nested commutators vanish; but we only considered the validity up to second order for small ε]

def. $f(x) = e^{Ax} e^{Bx}$

$$\frac{df(x)}{dx} = Ae^{Ax}e^{Bx} + e^{Ax}Be^{Bx} = (A + e^{Ax}Be^{-Ax}) f(x)$$

· $[B, A^n] = BA^n - A^nB = BA \cdot A^{n-1} - A^nB = [B,A]A^{n-1} + ABA^{n-1} - A^nB$

$$= [B,A]A^{n-1} + A[B,A]A^{n-2} + A^2BA^{n-2} - A^nB$$

since $[A,[A,B]] = 0$

$$= (n-1)[B,A]A^{n-1} + \underbrace{A^{n-1}BA - A^{n-1}AB}_{= A^{n-1}[B,A]}$$

$$= nA^{n-1}[B,A]$$

· $[B, e^{-Ax}] = [B, \sum_{n=0}^{\infty} \frac{(-Ax)^n}{n!}] = \sum_{n=0}^{\infty} \frac{(-1)^n x^n}{n!} [B,A^n]$

$$= \sum_{n=1}^{\infty} \frac{(-1)^n x^n}{n!} nA^{n-1}[B,A] = \underbrace{\sum_{n=1}^{\infty} \frac{(-1)^{n-1} x^{n-1}}{(n-1)!} A^{n-1}}_{= e^{Ax}} \cdot (-x)[B,A]$$

$$= -xe^{Ax}[B,A]$$

↳ $[B, e^{-Ax}] = Be^{-Ax} - e^{-Ax}B = -xe^{Ax}[B,A]$

$\Rightarrow$ $e^{Ax}Be^{-Ax} = B - x[B,A] = B + x[A,B]$

$\Rightarrow$ $\frac{d}{dx} f(x) = (A + B + x[A,B]) f(x)$

$\Rightarrow$ $f(x) = e^{Ax + Bx + \frac{1}{2}[A,B]x^2} = e^{(A+B)x} e^{\frac{1}{2}[A,B]x^2}$ (const. = 0)

↳ since $[A,[A,B]] = [B,[A,B]] = 0$

$x = 1$: $\boxed{f(x) = e^A e^B = e^{A+B} e^{\frac{1}{2}[A,B]}}$

Now $[A,B] = c\mathbb{1}$:

$$\left.\begin{aligned} e^A e^B = e^{A+B} e^{c/2\,\mathbb{1}} &\to e^{A+B} = e^A e^B e^{-c/2\,\mathbb{1}} \\ e^B e^A = e^{B+A} e^{-c/2\,\mathbb{1}} = e^{A+B} e^{-c/2\,\mathbb{1}} &\to e^{A+B} = e^B e^A e^{c/2\,\mathbb{1}} \end{aligned}\right\} e^A e^B = e^B e^A e^{c\mathbb{1}}$$

e) <u>Campbell identity</u> $e^A B e^{-A} = \sum_{k=0}^{\infty} \frac{1}{k!} [A,B]_k$ w/ $[A,B]_k = [A,[A,B]]_{k-1}$, $[A,B]_0 = B$

$$f(\varepsilon) = e^{A\varepsilon} B e^{-A\varepsilon} = \sum_k \frac{f^{(k)}(0)}{k!} \varepsilon^k$$

$$f^{(1)}(\varepsilon) = Ae^{A\varepsilon}Be^{-A\varepsilon} + e^{A\varepsilon}B(-A)e^{-A\varepsilon} = e^{A\varepsilon}[A,B]e^{-A\varepsilon} \to f^{(1)}(0) = [A,B]$$

shown for n=1

$$f^{(n+1)}(\varepsilon) = \frac{d^n}{d\varepsilon^n}\left(e^{A\varepsilon}[A,B]e^{-A\varepsilon}\right) \overset{\downarrow}{=} e^{A\varepsilon}[A,[A,\ldots,[A,B]..]e^{-A\varepsilon} = e^{A\varepsilon}[A,B]_n e^{-A\varepsilon}$$

$\Rightarrow$ $f(\varepsilon) = \sum_k \frac{f^{(k)}(0)}{k!} \varepsilon^k \Rightarrow f(1) = \sum_k \frac{1}{k!} [A,B]_k$

H.2 - Analytic Exact Diagonalization

Tight-binding Hamiltonian: $H = -J \sum_{\langle ij \rangle} (c_i^+ c_j + c_j^+ c_i)$

Consider a 3-site 1D chain w/ periodic boundary conditions

$$\begin{array}{c|ccc} & |1\rangle & |2\rangle & |3\rangle \\ \hline |1\rangle & & & \\ |2\rangle & & & \\ |3\rangle & & & \end{array}$$

a) Hamiltonian matrix in basis $\{|1\rangle, |2\rangle, |3\rangle\}$

$$H = -J \left\{ c_1^+ c_2 + c_2^+ c_1 + c_1^+ c_3 + c_3^+ c_1 + c_2^+ c_3 + c_3^+ c_2 \right\}$$

$$= -J \left\{ \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \right\}$$

$$= -J \underbrace{\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}}_{=M}$$

b) $\det(M - E\mathbb{1}) = -E(E^2 - 1) - 1 \cdot (-E - 1) + 1 \cdot (1 + E)$

$$= -E^3 + E + 2 + 2E = -E^3 + 3E + 2 = 0$$

$\Leftrightarrow E^3 - 3E - 2 = (E+1)(E^2 - E - 2) = (E+1)(E+1)(E-2)$

$\Rightarrow E_1 = E_2 = -1, \; E_3 = 2$

$\Rightarrow H_{diag} = -J \begin{pmatrix} -1 & & \\ & -1 & \\ & & 2 \end{pmatrix}$

c) w/ $M\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} y+z \\ x+z \\ x+y \end{pmatrix}$

I. $M\vec{v}_1 = E_1 \vec{v}_1 = -\vec{v}_1 \Rightarrow \vec{v}_1 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$

II. $M\vec{v}_2 = E_2 \vec{v}_2 = -\vec{v}_2 \Rightarrow \vec{v}_2 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$

III. $M\vec{v}_3 = E_3 \vec{v}_3 = 2\vec{v}_3 \Rightarrow \vec{v}_3 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$

d) $T = (\vec{v}_1 | \vec{v}_2 | \vec{v}_3) \rightarrow HT = TH_{diag} \Rightarrow H = TH_{diag}T^{-1}$

$\Rightarrow U(t) = e^{-iHt} = \sum_k \frac{(iHt)^k}{k!} = \sum_k \frac{(-it)^k}{k!} \underbrace{(TH_{diag}T^{-1})^k}_{= T H_{diag}^k T^{-1}} = T e^{-iH_{diag}t} T^{-1}$

$$= T \begin{pmatrix} e^{-iJt} & & \\ & e^{-iJt} & \\ & & e^{2iJt} \end{pmatrix} T^{-1}$$

w/ $T = \begin{pmatrix} 1 & 1 & 1 \\ 0 & -1 & 1 \\ -1 & 0 & 1 \end{pmatrix} \rightarrow T^{-1} = \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 1 & -2 & 1 \\ -2 & 1 & 1 \end{pmatrix}$

$$= \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 0 & -1 & 1 \\ -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} e^{-iJt} & & \\ & e^{-iJt} & \\ & & e^{2iJt} \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ 1 & -2 & 1 \\ -2 & 1 & 1 \end{pmatrix}$$

$$= \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 0 & -1 & 1 \\ -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} e^{-iJt} & e^{-iJt} & e^{-iJt} \\ e^{-iJt} & -2e^{-iJt} & e^{-iJt} \\ -2e^{2iJt} & e^{2iJt} & e^{2iJt} \end{pmatrix}$$

$$= \frac{1}{3}\begin{pmatrix} 2(e^{-iJt}-e^{2iJt}) & e^{2iJt}-e^{-iJt} & 2e^{-iJt}+e^{2iJt} \\ -e^{-iJt}-2e^{2iJt} & 2e^{-iJt}+e^{2iJt} & e^{2iJt}-e^{-iJt} \\ -e^{-iJt}-2e^{2iJt} & e^{2iJt}-e^{-iJt} & e^{2iJt}-e^{-iJt} \end{pmatrix}$$

$$= \frac{1}{3}e^{-iJt}\begin{pmatrix} 2(1-e^{3iJt}) & e^{3iJt}-1 & 2+e^{3iJt} \\ -1-2e^{3iJt} & 2+e^{3iJt} & e^{3iJt}-1 \\ -1-2e^{3iJt} & e^{3iJt}-1 & e^{3iJt}-1 \end{pmatrix}$$

H.3 – Numerical Exact Diagonalization

One-dimensional Heisenberg XXZ model, L spin-$1/2$ particles, NN interactions

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

w/ $S_x = \frac{1}{2}\sigma_x = \frac{1}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}$, $S_y = \frac{1}{2}\sigma_y = \frac{1}{2}\begin{pmatrix}0&-i\\i&0\end{pmatrix}$, $S_z = \frac{1}{2}\sigma_z = \frac{1}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}$

a) Computational basis states $\qquad (S_i^x \equiv S_{x,i})$

$L=2$: $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$

$L=3$: $|\uparrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\uparrow\downarrow\downarrow\rangle, |\downarrow\uparrow\uparrow\rangle, |\downarrow\uparrow\downarrow\rangle, |\downarrow\downarrow\uparrow\rangle, |\downarrow\downarrow\downarrow\rangle$

b) $S_x|\uparrow\rangle = \frac{1}{2}|\downarrow\rangle$, $S_x|\downarrow\rangle = \frac{1}{2}|\uparrow\rangle$

$S_y|\uparrow\rangle = \frac{i}{2}|\downarrow\rangle$, $S_y|\downarrow\rangle = \frac{-i}{2}|\uparrow\rangle$

$S_z|\uparrow\rangle = \frac{1}{2}|\uparrow\rangle$, $S_z|\downarrow\rangle = -\frac{1}{2}|\downarrow\rangle$

$\underline{L=2}$: $S_{x,0}S_{x,1}|\uparrow\uparrow\rangle = \frac{1}{4}|\downarrow\downarrow\rangle \qquad S_{x,0}S_{x,1}|\downarrow\uparrow\rangle = \frac{1}{4}|\uparrow\downarrow\rangle$

$S_{x,0}S_{x,1}|\uparrow\downarrow\rangle = \frac{1}{4}|\downarrow\uparrow\rangle \qquad S_{x,0}S_{x,1}|\downarrow\downarrow\rangle = \frac{1}{4}|\uparrow\uparrow\rangle$

$S_{y,0}S_{y,1}|\uparrow\uparrow\rangle = -\frac{1}{4}|\downarrow\downarrow\rangle \qquad S_{y,0}S_{y,1}|\downarrow\uparrow\rangle = \frac{1}{4}|\uparrow\downarrow\rangle$

$S_{y,0}S_{y,1}|\uparrow\downarrow\rangle = \frac{1}{4}|\downarrow\uparrow\rangle \qquad S_{y,0}S_{y,1}|\downarrow\downarrow\rangle = -\frac{1}{4}|\uparrow\uparrow\rangle$

$S_{z,0}S_{z,1}|\uparrow\uparrow\rangle = \frac{1}{4}|\uparrow\uparrow\rangle \qquad S_{z,0}S_{z,1}|\downarrow\uparrow\rangle = -\frac{1}{4}|\uparrow\downarrow\rangle$

$S_{z,0}S_{z,1}|\uparrow\downarrow\rangle = -\frac{1}{4}|\uparrow\downarrow\rangle \qquad S_{z,0}S_{z,1}|\downarrow\downarrow\rangle = \frac{1}{4}$

$$\Rightarrow H = -J\left\{\begin{array}{c c} & \begin{array}{cccc}\uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow\downarrow\end{array} \\ & \begin{pmatrix} 0&0&0&1/4 \\ 0&0&1/4&0 \\ 0&1/4&0&0 \\ 1/4&0&0&0 \end{pmatrix}\begin{array}{c}\uparrow\uparrow\\ \uparrow\downarrow\\ \downarrow\uparrow\\ \downarrow\downarrow\end{array}\end{array} + \begin{pmatrix} 0&0&0&-1/4 \\ 0&0&1/4&0 \\ 0&1/4&0&0 \\ -1/4&0&0&0 \end{pmatrix} + \begin{pmatrix} 1/4&&& \\ &-1/4&& \\ &&-1/4& \\ &&&1/4 \end{pmatrix}\right\}$$

$$= -\frac{J}{4}\begin{pmatrix} 1&0&0&0 \\ 0&-1&2&0 \\ 0&2&-1&0 \\ 0&0&0&1 \end{pmatrix}$$

L = 3:

$$S_{x,0} S_{x,1} |\uparrow\uparrow\uparrow\rangle = \frac{1}{4} |\downarrow\downarrow\uparrow\rangle \qquad S_{x,1} S_{x,2} |\uparrow\uparrow\uparrow\rangle = \frac{1}{4} |\uparrow\downarrow\downarrow\rangle$$

$$H = -J\Bigg\{ \begin{array}{c} \begin{array}{cccccccc} \uparrow\uparrow\uparrow & \uparrow\uparrow\downarrow & \uparrow\downarrow\uparrow & \uparrow\downarrow\downarrow & \downarrow\uparrow\uparrow & \downarrow\uparrow\downarrow & \downarrow\downarrow\uparrow & \downarrow\downarrow\downarrow \end{array} \\ \begin{pmatrix} & & & & & & 1/4 & 0 \\ & & & & & & 0 & 1/4 \\ & & & & 1/4 & 0 & & \\ & & & & 0 & 1/4 & & \\ & & 1/4 & 0 & & & & \\ & & 0 & 1/4 & & & & \\ 1/4 & 0 & & & & & & \\ 0 & 1/4 & & & & & & \end{pmatrix} \end{array} + \begin{array}{c} \begin{array}{cccccccc} \uparrow\uparrow\uparrow & \uparrow\uparrow\downarrow & \uparrow\downarrow\uparrow & \uparrow\downarrow\downarrow & \downarrow\uparrow\uparrow & \downarrow\uparrow\downarrow & \downarrow\downarrow\uparrow & \downarrow\downarrow\downarrow \end{array} \\ \begin{pmatrix} & & 0 & 1/4 & & & & \\ & & 1/4 & 0 & & & & \\ 0 & 1/4 & & & & & & \\ 1/4 & 0 & & & & & & \\ & & & & & & 0 & 1/4 \\ & & & & & & 1/4 & 0 \\ & & & & 0 & 1/4 & & \\ & & & & 1/4 & 0 & & \end{pmatrix} \end{array}$$

$$+ \begin{array}{c} \begin{array}{cccccccc} \uparrow\uparrow\uparrow & \uparrow\uparrow\downarrow & \uparrow\downarrow\uparrow & \uparrow\downarrow\downarrow & \downarrow\uparrow\uparrow & \downarrow\uparrow\downarrow & \downarrow\downarrow\uparrow & \downarrow\downarrow\downarrow \end{array} \\ \begin{pmatrix} & & & & & & -1/4 & 0 \\ & & & & & & 0 & -1/4 \\ & & & & 1/4 & 0 & & \\ & & & & 0 & 1/4 & & \\ & & 1/4 & 0 & & & & \\ & & 0 & 1/4 & & & & \\ -1/4 & 0 & & & & & & \\ 0 & -1/4 & & & & & & \end{pmatrix} \end{array} + \begin{array}{c} \begin{array}{cccccccc} \uparrow\uparrow\uparrow & \uparrow\uparrow\downarrow & \uparrow\downarrow\uparrow & \uparrow\downarrow\downarrow & \downarrow\uparrow\uparrow & \downarrow\uparrow\downarrow & \downarrow\downarrow\uparrow & \downarrow\downarrow\downarrow \end{array} \\ \begin{pmatrix} & & 0 & -1/4 & & & & \\ & & 1/4 & 0 & & & & \\ 0 & 1/4 & & & & & & \\ -1/4 & 0 & & & & & & \\ & & & & & & 0 & -1/4 \\ & & & & & & 1/4 & 0 \\ & & & & 0 & 1/4 & & \\ & & & & -1/4 & 0 & & \end{pmatrix} \end{array}$$

$$+ \begin{array}{c} \begin{array}{cccccccc} \uparrow\uparrow\uparrow & \uparrow\uparrow\downarrow & \uparrow\downarrow\uparrow & \uparrow\downarrow\downarrow & \downarrow\uparrow\uparrow & \downarrow\uparrow\downarrow & \downarrow\downarrow\uparrow & \downarrow\downarrow\downarrow \end{array} \\ \begin{pmatrix} 1/4 & & & & & & & \\ & 1/4 & & & & & & \\ & & -1/4 & & & & & \\ & & & -1/4 & & & & \\ & & & & -1/4 & & & \\ & & & & & -1/4 & & \\ & & & & & & 1/4 & \\ & & & & & & & 1/4 \end{pmatrix} \end{array} + \begin{array}{c} \begin{array}{cccccccc} \uparrow\uparrow\uparrow & \uparrow\uparrow\downarrow & \uparrow\downarrow\uparrow & \uparrow\downarrow\downarrow & \downarrow\uparrow\uparrow & \downarrow\uparrow\downarrow & \downarrow\downarrow\uparrow & \downarrow\downarrow\downarrow \end{array} \\ \begin{pmatrix} 1/4 & & & & & & & \\ & -1/4 & & & & & & \\ & & -1/4 & & & & & \\ & & & 1/4 & & & & \\ & & & & 1/4 & & & \\ & & & & & -1/4 & & \\ & & & & & & -1/4 & \\ & & & & & & & 1/4 \end{pmatrix} \end{array} \Bigg\}$$

$$= -J \begin{array}{c} \begin{array}{cccccccc} \uparrow\uparrow\uparrow & \uparrow\uparrow\downarrow & \uparrow\downarrow\uparrow & \uparrow\downarrow\downarrow & \downarrow\uparrow\uparrow & \downarrow\uparrow\downarrow & \downarrow\downarrow\uparrow & \downarrow\downarrow\downarrow \end{array} \\ \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & -1/2 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/2 & 0 & 0 \\ 0 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 & 0 & -1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 \end{pmatrix} \end{array}$$

TEQS_Exercise_01

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[1]:
```
import numpy as np
```

1 H.3 a)

[13]:
```
# L = 2

H_2 = -1/4 * np.matrix([
    [1, 0, 0, 0],
    [0, -1, 2, 0],
    [0, 2, -1, 0],
    [0, 0, 0, 1]
])

eigenvals2, eigenvecs2 = np.linalg.eig(H_2)

print("Eigenvalues:", eigenvals2, '\n')
print("Eigenvectors:\n", eigenvecs2, '\n')
```

```
Eigenvalues: [ 0.75 -0.25 -0.25 -0.25]

Eigenvectors:
 [[ 0.          0.          1.          0.        ]
 [-0.70710678  0.70710678  0.          0.        ]
 [ 0.70710678  0.70710678  0.          0.        ]
 [ 0.          0.          0.          1.        ]]
```

[14]:
```
# L = 3

H_3 = -1/2 * np.matrix([
    [1, 0, 0, 0, 0, 0, 0, 0],
    [0, 0, 1, 0, 0, 0, 0, 0],
    [0, 1, -1, 0, 1, 0, 0, 0],
    [0, 0, 0, 0, 0, 1, 0, 0],
    [0, 0, 1, 0, 0, 0, 0, 0],
    [0, 0, 0, 1, 0, -1, 1, 0],
    [0, 0, 0, 0, 0, 1, 0, 0],
```

```
    [0, 0, 0, 0, 0, 0, 0, 1]
])

eigenvals3, eigenvecs3 = np.linalg.eig(H_3)

print("Eigenvalues:", np.round(eigenvals3, 5), '\n')
print("Eigenvectors:\n", np.round(eigenvecs3, 5), '\n')
```

```
Eigenvalues: [ 1.  -0.  -0.5  1.  -0.5  0.  -0.5 -0.5]

Eigenvectors:
 [[ 0.        0.        0.        0.        0.        0.        1.        0.      ]
 [ 0.        0.        0.       -0.40825 -0.57735  0.70711  0.        0.      ]
 [ 0.        0.        0.        0.8165  -0.57735 -0.        0.        0.      ]
 [-0.40825  0.70711  0.57735  0.        0.        0.        0.        0.      ]
 [ 0.        0.        0.       -0.40825 -0.57735 -0.70711  0.        0.      ]
 [ 0.8165   0.        0.57735  0.        0.        0.        0.        0.      ]
 [-0.40825 -0.70711  0.57735  0.        0.        0.        0.        0.      ]
 [ 0.        0.        0.        0.        0.        0.        0.        1.      ]]
```

2 H.3 b)

[19]:
```
# transformation matrix P

P = [np.matrix(eigenvecs2), np.matrix(eigenvecs3)]
H_diag = [np.diag(eigenvals2), np.diag(eigenvals3)]



# time evolution operator

def U(t, L):
    PL = P[L%2]
    HL = H_diag[L%2]

    return PL * np.exp(-1j * HL * t) * PL.T
```

[22]:
```
# test call

np.round(U(1, 2), 4)
```

[22]:
```
matrix([[ 0.9689+0.2474j,  0.    +0.j    ,  1.4142+0.j    ,
          1.    +0.j    ],
        [ 0.    +0.j    , -0.1497-0.2171j,  0.1186+0.4645j,
          0.    +0.j    ],
        [ 1.4142+0.j    ,  0.1186+0.4645j,  1.8503-0.2171j,
          1.4142+0.j    ],
```

```
 [ 1.      +0.j     ,  0.      +0.j     ,  1.4142+0.j     ,
   0.9689+0.2474j]])
```

```
[ ]:
```

Calculations (ignore)

H.1

a)

II. $e^{A\varepsilon} = \mathbb{1} + A\varepsilon + \frac{1}{2}A^2\varepsilon^2 + \dots$

III. $e^{B\varepsilon} = \mathbb{1} + B\varepsilon + \frac{1}{2}B^2\varepsilon^2 + \dots$

$\hookrightarrow e^{A\varepsilon}e^{B\varepsilon} = \mathbb{1} + B\varepsilon + \frac{1}{2}B^2\varepsilon^2 + A\varepsilon + AB\varepsilon + \frac{1}{2}A^2\varepsilon^2 + \dots$

$= \mathbb{1} + A\varepsilon + B\varepsilon + \frac{1}{2}A^2\varepsilon^2 + \frac{1}{2}B^2\varepsilon^2 + AB\varepsilon^2$

IV. $e^{-\frac{1}{2}[A,B]\varepsilon^2} = \mathbb{1} - \frac{1}{2}[A,B]\varepsilon^2 + \dots$

$\hookrightarrow e^{A\varepsilon}e^{B\varepsilon}e^{-\frac{1}{2}[A,B]\varepsilon^2} = (\mathbb{1} + A\varepsilon + B\varepsilon + \frac{1}{2}A^2\varepsilon^2 + \frac{1}{2}B^2\varepsilon^2 + AB\varepsilon^2)(\mathbb{1} - \frac{1}{2}[A,B]\varepsilon^2)$

$= \mathbb{1} - \frac{1}{2}[A,B]\varepsilon^2 + A\varepsilon + B\varepsilon + \frac{1}{2}A^2\varepsilon^2 + \frac{1}{2}B^2\varepsilon^2 + AB\varepsilon^2$