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Sheet 1

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.)

$$e^{(A+B)\varepsilon} = \sum_{n=0}^{\infty} \frac{(A+B)^n \varepsilon^n}{n!} \approx 1 + (A+B)\varepsilon + \underbrace{(A+B)^2}_{\substack{= A^2 + AB + BA + B^2 \\ = A^2 + 2AB - [A,B] + B^2}} \varepsilon^2 \frac{1}{2} + \mathcal{O}(\varepsilon^3)$$

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

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

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

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

(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.)

$$e^{A\varepsilon} e^{B\varepsilon} \approx \left(1 + A\varepsilon + A^2 \frac{\varepsilon^2}{2} + \mathcal{O}(\varepsilon^3)\right)\left(1 + B\varepsilon + B^2 \frac{\varepsilon^2}{2} + \mathcal{O}(\varepsilon^3)\right)$$

$$= 1 + A\varepsilon + A^2 \frac{\varepsilon^2}{2} + B\varepsilon + \underbrace{AB}_{= [A,B] + BA} \varepsilon^2 + B^2 \frac{\varepsilon^2}{2} + \mathcal{O}(\varepsilon^3)$$

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

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

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

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

$$e^{A+B} = \lim_{n\to\infty} \left(1 + \frac{(A+B)}{n}\right)^n = \lim_{n\to\infty} \left(1 + \frac{(A+B)}{n} + \underbrace{\mathcal{O}\left(\frac{1}{n^2}\right)}_{\text{goes to zero for } n\to\infty}\right)^n$$

$$= \lim_{n\to\infty} \left(\left(1 + \frac{A}{n} + \mathcal{O}\left(\frac{1}{n^2}\right)\right)\left(1 + \frac{B}{n} + \mathcal{O}\left(\frac{1}{n^2}\right)\right)\right)^n$$

$$= \lim_{n\to\infty} \left(e^{A/n} \cdot e^{B/n}\right)^n$$

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

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

We showed $e^{A\varepsilon} \cdot e^{B\varepsilon} = e^{B\varepsilon} e^{A\varepsilon} e^{[A,B]\varepsilon^2 + \mathcal{O}(\varepsilon^2)}$, we set $\varepsilon = 1$ as part of the perturbation done above where $e^{(A+B)} = e^{(A+B)\varepsilon}\big|_{\varepsilon=1}$, also set $[A,B] = c \cdot \mathbb{1}$

↳ higher order terms can be neglected

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

(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.

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

$$= \left(B + AB\varepsilon + \frac{A^2}{2}B\varepsilon^2 + \mathcal{O}(\varepsilon^3)\right)\left(1 - A\varepsilon + \frac{A^2}{2}\varepsilon^2 + \mathcal{O}(\varepsilon^3)\right)$$

$$= B + AB\varepsilon + \frac{A^2}{2}B\varepsilon^2 - BA\varepsilon - ABA\varepsilon^2 + B\frac{A^2}{2}\varepsilon^2 + \mathcal{O}(\varepsilon^3)$$

$$= B + (AB - BA)\varepsilon + (\underbrace{A^2B - 2ABA + BA^2}) \frac{\varepsilon^2}{2} + \mathcal{O}(\varepsilon^3)$$

$$= ABA - 2ABA + A[A,B] + BA^2$$
$$= A[A,B] - [A,B]A - BA^2 + BA^2$$
$$= [A, [A,B]]$$

$$= [A,B]_0 + [A,B]_1\varepsilon + [A,B]_2 \frac{\varepsilon^2}{2} + \mathcal{O}(\varepsilon^3)$$

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

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.)

$$\langle 1|H|1\rangle = \langle 2|H|2\rangle = \langle 3|H|3\rangle = 0$$

$$\langle 1|H|2\rangle = \langle 2|H|1\rangle = \langle 1|H|3\rangle = \langle 3|H|1\rangle = \langle 2|H|3\rangle = \langle 3|H|2\rangle = -J$$

$$\Rightarrow \quad H = -J \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

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

$$\det(H - E\mathbb{1}) = \det\left(\begin{pmatrix} -E & -J & -J \\ -J & -E & -J \\ -J & -J & -E \end{pmatrix}\right) = 0$$

$$\Rightarrow \quad E(E^2 - J^2) - J(JE - J^2) + J(J^2 - JE) = 0$$

$$\Rightarrow \quad E^3 - J^2E + 2J^3 - 2J^2E = 0$$

$$\Rightarrow \quad E^3 - 3J^2E + 2J^3 = 0 \qquad \Rightarrow \quad E \in \{-2J, J\}$$ ✓ Eigenvalues

(c) Determine the eigenvectors.

$$(H - E\mathbb{1})\vec{x} = 0 \quad , \text{ with } \quad x_1^2 + x_2^2 + x_3^2 = 1$$

$$\text{For } E = -2J : \quad -J\begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}\vec{x} = 0 \quad \Rightarrow \quad \vec{x} \in \left\{ \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \right\}$$

$$E = J : \quad -J\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}\vec{x} = 0 \quad \Rightarrow \quad \vec{x} \in \left\{ \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} \right\}$$

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

$$S = \begin{pmatrix} 1 & -1 & -1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad S^{-1} = \begin{pmatrix} 1 & 1 & 1 \\ -1 & -1 & 2 \\ -1 & 2 & -1 \end{pmatrix} \frac{1}{3} \quad \text{and} \quad D = -J \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$(SDS^{-1})^n = SD^n S^{-1}$$

$$\Rightarrow H = SDS^{-1} \quad \Rightarrow U(t) = e^{-iSDS^{-1}t} = \sum_{n=0}^{\infty} \frac{(-it)^n \overbrace{(SDS^{-1})^n}}{n!}$$

$$= S \sum_{n=0}^{\infty} \begin{pmatrix} (+it2J)^n & 0 & 0 \\ 0 & (-itJ)^n & 0 \\ 0 & 0 & (-itJ)^n \end{pmatrix} \frac{1}{n!} S^{-1}$$

$$= \begin{pmatrix} 1 & -1 & -1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} e^{it2J} & 0 & 0 \\ 0 & e^{-itJ} & 0 \\ 0 & 0 & e^{-itJ} \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ -1 & -1 & 2 \\ -1 & 2 & -1 \end{pmatrix} \frac{1}{3}$$

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

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.)

$L=2$: $H = J\sum_{j=0}^{1}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + S_j^z S_{j+1}^z\right)$

$= J\left(S_0^x S_1^x + S_0^y S_1^y + S_0^z S_1^z + S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z\right)$

States: $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$ accounting for two particles and their spin

$L=3$: $H = J\sum_{j=0}^{2}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + S_j^z S_{j+1}^z\right)$

$= J\left(S_0^x S_1^x + S_0^y S_1^y + S_0^z S_1^z + S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z + S_2^x S_3^x + S_2^y S_3^y + S_2^z S_3^z\right)$

States: $|\uparrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\uparrow\downarrow\downarrow\rangle, |\downarrow\downarrow\downarrow\rangle,$
$|\downarrow\uparrow\uparrow\rangle, |\downarrow\uparrow\downarrow\rangle, |\downarrow\downarrow\uparrow\rangle$

Intepretate $|\uparrow\rangle = |1\rangle$ and $|\downarrow\rangle = |0\rangle$, as vectors $|1\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, $|0\rangle = \begin{pmatrix}0\\1\end{pmatrix}$

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

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

with

$S^x|1\rangle = \frac{1}{2}|0\rangle$ $\quad S^x|0\rangle = \frac{1}{2}|1\rangle$

$S^y|1\rangle = \frac{i}{2}|0\rangle$ $\quad S^y|0\rangle = -\frac{i}{2}|1\rangle$

$S_z|1\rangle = \frac{1}{2}|1\rangle$ $\quad S_z|0\rangle = -1/2\,|0\rangle$

$L = 3:$

$$H = J \begin{pmatrix} 3/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1/4 & 1/2 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 1/2 & -1/4 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1/4 & 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 & 0 & -1/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 & 0 & -1/4 & 1/2 & 0 \\ 0 & 0 & 0 & 1/2 & 0 & 1/2 & -1/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3/4 \end{pmatrix}$$

Calculation done in the same way like for $L = 2$

c) + d) see Jupyter notebook, it should be uploaded, if not contact me