

Homework #1: Brief Solutions

1. $|1\rangle, |2\rangle, |3\rangle$ form a set of complete *non-orthogonal* basis of a Hilbert space, with the following overlaps(inner products), $\langle 1|1\rangle = \langle 2|2\rangle = \langle 3|3\rangle = 1$, $\langle 1|2\rangle = \langle 2|3\rangle = \langle 3|1\rangle = 1/3$.

(a)(2pts). *Show that $|1\rangle, |2\rangle, |3\rangle$ are linearly independent.*

(b)(5pts). Use the “Gram-Schmidt orthogonalization” procedure to find a set of complete orthonormal basis, $|\tilde{1}\rangle, |\tilde{2}\rangle, |\tilde{3}\rangle$, as follows:

find $|\tilde{1}\rangle = c_{1,1}|1\rangle$ normalized; then

find $|\tilde{2}\rangle = c_{2,2}|2\rangle + c_{2,1}|\tilde{1}\rangle$ normalized, and orthogonal to $|\tilde{1}\rangle$; then

find $|\tilde{3}\rangle = c_{3,3}|3\rangle + c_{3,1}|\tilde{1}\rangle + c_{3,2}|\tilde{2}\rangle$ normalized, and orthogonal to both $|\tilde{1}\rangle$ and $|\tilde{2}\rangle$.

Solve these coefficients $c_{j,i}$. And finally represent the original basis $|1\rangle, |2\rangle, |3\rangle$ as linear combinations of the new basis $|\tilde{1}\rangle, |\tilde{2}\rangle, |\tilde{3}\rangle$.

(c)(3pts). *Find the reciprocal basis, $|1'\rangle, |2'\rangle, |3'\rangle$, in terms of $|1\rangle, |2\rangle, |3\rangle$, such that the inner products $(|i'\rangle, |j\rangle) = \delta_{i,j}$. Show that $|1\rangle\langle 1'| + |2\rangle\langle 2'| + |3\rangle\langle 3'|$ is the identity operator.*

(d)(5pts). A linear operator \hat{A} is defined by its action on this basis as follows: $\hat{A}|1\rangle = (-|1\rangle + |2\rangle + |3\rangle)$, $\hat{A}|2\rangle = (-|2\rangle + |3\rangle + |1\rangle)$, $\hat{A}|3\rangle = (-|3\rangle + |1\rangle + |2\rangle)$. *Is \hat{A} a hermitian operator? Is \hat{A} a unitary operator? Solve the eigenvalues and normalized eigenvectors (in terms of $|1\rangle, |2\rangle, |3\rangle$) of \hat{A} .*

Solutions:

(a) the matrix of overlaps (Gram matrix) is $G_{ij} \equiv \langle i|j\rangle = \begin{pmatrix} 1 & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & 1 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & 1 \end{pmatrix}$, and is non-singular

(the Gram determinant $\det(G) = \frac{20}{27} \neq 0$).

Therefore these three states are linearly independent.

(b) We can choose $c_{1,1} = 1$, then $\langle \tilde{1}|2\rangle = \langle \tilde{1}|3\rangle = \frac{1}{3}$.

From $\langle \tilde{1}|\tilde{2}\rangle = 0$, we have $\frac{1}{3}c_{2,2} + c_{2,1} = 0$, namely, $c_{2,1} = -\frac{1}{3}c_{2,2}$.

From $\langle \tilde{2}|\tilde{2}\rangle = 1$, we have $1 = |c_{2,2}|^2 + |c_{2,1}|^2 + \frac{1}{3}(c_{2,2}^*c_{2,1} + c_{2,1}^*c_{2,2}) = \frac{8}{9}|c_{2,2}|^2$.

We can choose $c_{2,2} = \frac{3}{\sqrt{8}}$, $c_{2,1} = -\frac{1}{\sqrt{8}}$, then $\langle \tilde{2}|3\rangle = \frac{1}{3\sqrt{2}}$.

From $\langle \tilde{1} | \tilde{3} \rangle = 0$, we have $\frac{1}{3}c_{3,3} + c_{3,1} = 0$, namely, $c_{3,1} = -\frac{1}{3}c_{3,3}$.

From $\langle \tilde{2} | \tilde{3} \rangle = 0$, we have $\frac{1}{3\sqrt{2}}c_{3,3} + c_{3,2} = 0$, namely, $c_{3,2} = -\frac{1}{3\sqrt{2}}c_{3,3}$.

From $\langle \tilde{3} | \tilde{3} \rangle = 1$, we have $1 = |c_{3,3}|^2 + |c_{3,1}|^2 + |c_{3,2}|^2 + \frac{1}{3}(c_{3,3}^*c_{3,1} + c_{3,1}^*c_{3,3}) + \frac{1}{3\sqrt{2}}(c_{3,3}^*c_{3,2} + c_{3,2}^*c_{3,3}) = (1 + \frac{1}{9} + \frac{1}{18} - \frac{2}{9} - \frac{1}{9}) \cdot |c_{3,3}|^2 = \frac{5}{6}|c_{3,3}|^2$.

We can choose $c_{3,3} = \sqrt{\frac{6}{5}}$, $c_{3,1} = -\sqrt{\frac{2}{15}}$, $c_{3,2} = -\frac{\sqrt{1}}{15}$.

Invert the above relations, $|1\rangle = |\tilde{1}\rangle$, $|2\rangle = \frac{\sqrt{8}}{3}|\tilde{2}\rangle + \frac{1}{3}|\tilde{1}\rangle$, $|3\rangle = \sqrt{\frac{5}{6}}|\tilde{3}\rangle + \frac{1}{3}|\tilde{1}\rangle + \frac{1}{3\sqrt{2}}|\tilde{2}\rangle$.

It should be easy to check the overlaps between $|1\rangle, |2\rangle, |3\rangle$ using the orthonormal relations between $|\tilde{1}\rangle, |\tilde{2}\rangle, |\tilde{3}\rangle$.

(c) suppose the reciprocal basis are related to the original basis by $|i'\rangle = \sum_k S_{ik}|k\rangle$, where S_{ik} are entries of a 3×3 complex matrix.

Then $\langle i' | j \rangle = \sum_k S_{ik}^* \langle k | j \rangle = \sum_k S_{ik}^* G_{kj} = (S^* \cdot G)_{ij}$.

We want $\langle i' | j \rangle$ to be the identity matrix, therefore S^* should be the inverse of the Gram

matrix G [see part (a)], $S^* = \begin{pmatrix} \frac{6}{5} & -\frac{3}{10} & -\frac{3}{10} \\ -\frac{3}{10} & \frac{6}{5} & -\frac{3}{10} \\ -\frac{3}{10} & -\frac{3}{10} & \frac{6}{5} \end{pmatrix}$.

Finally $|1'\rangle = \frac{6}{5}|1\rangle - \frac{3}{10}|2\rangle - \frac{3}{10}|3\rangle$; $|2'\rangle = -\frac{3}{10}|1\rangle + \frac{6}{5}|2\rangle - \frac{3}{10}|3\rangle$; $|3'\rangle = -\frac{3}{10}|1\rangle - \frac{3}{10}|2\rangle + \frac{6}{5}|3\rangle$.

For any state $|\psi\rangle$, it has a unique expansion in terms of the original basis, $|\psi\rangle = \psi_1|1\rangle + \psi_2|2\rangle + \psi_3|3\rangle = \sum_j |j\rangle\psi_j$, where $\psi_{1,2,3}$ are complex numbers.

Act the right-hand-side of resolution of identity on $|\psi\rangle$, we have $\sum_i |i\rangle\langle i'|\psi\rangle = \sum_{i,j} |i\rangle\langle i'|j\rangle\psi_j = \sum_{i,j} |i\rangle\delta_{i,j}\psi_j = \sum_j |j\rangle\psi_j = |\psi\rangle$. Therefore the right-hand-side $\sum_i |i\rangle\langle i'|$ is indeed the identity operator $\mathbb{1}$ in this Hilbert space.

You can also use the orthonormal basis $|\tilde{i}\rangle$ in (b), represent $|1'\rangle = |\tilde{1}\rangle - \frac{1}{\sqrt{8}}|\tilde{2}\rangle - \sqrt{\frac{3}{40}}|\tilde{3}\rangle$, $|2'\rangle = \frac{3}{\sqrt{8}}|\tilde{2}\rangle - \sqrt{\frac{3}{40}}|\tilde{3}\rangle$, $|3'\rangle = \sqrt{\frac{6}{5}}|\tilde{3}\rangle$. and then show that $\sum_i |i\rangle\langle i'| = \sum_i |\tilde{i}\rangle\langle \tilde{i}|$.

(d) the action of \hat{A} is $(|1\rangle, |2\rangle, |3\rangle) \mapsto (|1\rangle, |2\rangle, |3\rangle) \cdot \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$. Denote the last 3×3

matrix by A_{ij} , the action of \hat{A} is thus $\hat{A}|i\rangle = \sum_j |j\rangle A_{ji}$.

It should be noted that $A_{ij} \neq \langle i | \hat{A} | j \rangle$, it is instead $A_{ij} = \langle i' | \hat{A} | j \rangle$.

Consider the definition of hermitian conjugate $(\hat{A}^\dagger|\psi\rangle, |\phi\rangle) = (|\psi\rangle, \hat{A}|\phi\rangle)$. To check whether \hat{A} is hermitian or not, we should compute and compare $(\hat{A}|\psi\rangle, |\phi\rangle)$ and $(|\psi\rangle, \hat{A}|\phi\rangle)$.

Let $|\psi\rangle = \sum_j |j\rangle\psi_j$ and $|\phi\rangle = \sum_j |j\rangle\phi_j$, where ψ_j and ϕ_j are complex numbers. Then $(|\psi\rangle, \hat{A}|\phi\rangle) = \sum_{j,j',k} \psi_j^* \langle j|j'\rangle A_{j'k} \phi_k = \sum_{j,j',k} \psi_j^* G_{jj'} A_{j'k} \phi_k = \sum_{j,k} \psi_j^* (G \cdot A)_{jk} \phi_k$, and $(\hat{A}|\psi\rangle, |\phi\rangle) = \sum_{j,j',k} \psi_j^* A_{j'j}^* \langle j'|k\rangle \phi_k = \sum_{j,j',k} \psi_j^* A_{j'j}^* G_{j'k} \phi_k = \sum_{j,k} \psi_j^* (A^\dagger \cdot G)_{jk} \phi_k$. Here G is the Gram matrix [see part (a)].

One can check that $G \cdot A = A^\dagger \cdot G = \begin{pmatrix} -\frac{1}{3} & 1 & 1 \\ 1 & -\frac{1}{3} & 1 \\ 1 & 1 & -\frac{1}{3} \end{pmatrix}$.

Therefore $(|\psi\rangle, \hat{A}|\phi\rangle) = (\hat{A}|\psi\rangle, |\phi\rangle)$ for any states $|\psi\rangle$ and $|\phi\rangle$, then \hat{A} is a hermitian operator.

A unitary operator \hat{U} should preserve inner products, $(\hat{U}|\psi\rangle, \hat{U}|\phi\rangle) = \langle\psi|\phi\rangle$ for any ψ, ϕ . If \hat{A} is unitary, we should have $A^\dagger \cdot G \cdot A = G$, however $A^\dagger \cdot G \cdot A = \begin{pmatrix} \frac{7}{3} & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{7}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{7}{3} \end{pmatrix} \neq G$.

Therefore \hat{A} is NOT a unitary operator.

Suppose $c_1|1\rangle + c_2|2\rangle + c_3|3\rangle$ is an eigenstate of \hat{A} with eigenvalue λ .

$$\hat{A}(c_1|1\rangle + c_2|2\rangle + c_3|3\rangle) = \lambda \cdot (c_1|1\rangle + c_2|2\rangle + c_3|3\rangle).$$

Then $(|1\rangle, |2\rangle, |3\rangle) \cdot A \cdot \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \lambda \cdot (|1\rangle, |2\rangle, |3\rangle) \cdot \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$. This shows that λ is an eigenvalue

of the 3×3 matrix A on the left-hand-side, and $(c_1, c_2, c_3)^T$ is a right-eigenvector.

This matrix has eigenvalue 1 for eigenvector $(1, 1, 1)^T$; and eigenvalue -2 for eigenvectors $(1, -1, 0)^T$ and $(1, 1, -2)^T$.

The eigenvalues of \hat{A} are 1 with normalized eigenstate $\sqrt{\frac{1}{3}}(|1\rangle + |2\rangle + |3\rangle)$; -2 with normalized eigenstates $\sqrt{\frac{3}{4}}(|1\rangle - |2\rangle)$ and $\frac{1}{2}(|1\rangle + |2\rangle - 2|3\rangle)$.

The choices of the last two degenerate eigenstates are not unique.

NOTE: you can check that the last two degenerate eigenstates are orthogonal to each other, although $|1\rangle, |2\rangle, |3\rangle$ are not orthonormal basis.

2. (5pts) If $[\hat{A}, \hat{B}] = 0$, namely \hat{A} and \hat{B} commute, then $\exp(\hat{A} + \hat{B}) = \exp(\hat{A}) \cdot \exp(\hat{B})$.

Prove this by brute-force expansion: $\exp(\hat{A}) \equiv \sum_{n=0}^{\infty} \frac{1}{n!} (\hat{A})^n$.

Solutions:

$$\exp(\hat{A} + \hat{B}) = \sum_{N=0}^{\infty} \frac{1}{N!} (\hat{A} + \hat{B})^N.$$

By mathematical induction (steps omitted), we can prove that if $[\hat{A}, \hat{B}] = 0$, then

$$(\hat{A} + \hat{B})^N = \sum_{m=0}^N \binom{N}{m} \hat{A}^{N-m} \hat{B}^m = \sum_{m=0}^N \frac{N!}{(N-m)!m!} \hat{A}^{N-m} \hat{B}^m.$$

$$\text{Then } \exp(\hat{A} + \hat{B}) = \sum_{N=0}^{\infty} \frac{1}{N!} (\hat{A} + \hat{B})^N = \sum_{N=0}^{\infty} \sum_{m=0}^N \frac{1}{(N-m)!m!} \hat{A}^{N-m} \hat{B}^m.$$

The summations $\sum_{N=0}^{\infty} \sum_{m=0}^N$ can be replaced by $\sum_{n=0}^{\infty} \sum_{m=0}^{\infty}$, where $n \equiv N - m$.

$$\text{Then this becomes } \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{n!m!} \hat{A}^n \hat{B}^m = \exp(\hat{A}) \cdot \exp(\hat{B}).$$

3. (5pts) Prove the Baker-Hausdorff formula, $e^{\hat{A}} \hat{B} e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + [\hat{A}, [\hat{A}, \hat{B}]]/2! + \dots$, by brute-force: expand both sides into sums of monomials $(\hat{A})^m \hat{B} (\hat{A})^n$, compare coefficients.

Solutions:

$$e^{\hat{A}} \hat{B} e^{-\hat{A}} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{\hat{A}^m}{m!} \hat{B} \frac{(-\hat{A})^n}{n!}, \text{ so the coefficient of } \hat{A}^m \hat{B} \hat{A}^n \text{ on the left-hand-side is } (-1)^n / m! / n!.$$

On the right-hand-side, the only term that can contribute $\hat{A}^m \hat{B} \hat{A}^n$ is the $(m+n)$ -fold commutator $\frac{1}{(m+n)!} [\hat{A}, \dots, [\hat{A}, \hat{B}] \dots]$. Expand the commutators will produce 2^{m+n} terms. Each commutator can provide either a factor \hat{A} in front of \hat{B} , or a factor $(-\hat{A})$ after \hat{B} . Therefore the number of appearance of the term $\hat{A}^m \hat{B} \hat{A}^n$ is the binomial coefficient $\binom{m+n}{n}$, with a sign of $(-1)^n$. So the coefficient of $\hat{A}^m \hat{B} \hat{A}^n$ on the right-hand-side is $\frac{1}{(m+n)!} (-1)^n \binom{m+n}{n} = (-1)^n / m! / n!$, same as that of the left-hand-side.

The above argument about the nested commutators can be made rigorous by proving $\underbrace{[\hat{A}, [\hat{A}, \dots [\hat{A}, \hat{B}] \dots]]}_{n\text{-fold commutator}} = \sum_{m=0}^n \binom{n}{m} \hat{A}^{n-m} \cdot \hat{B} \cdot (-\hat{A})^m$ by mathematical induction (steps omitted).

4. If the commutator $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$ is a c -number (that commutes with everything), prove the following (these formulas may be useful later in this course).

(a)(2pts). $\exp(\hat{A}) \cdot \exp(\hat{B}) = \exp(\hat{B}) \cdot \exp(\hat{A}) \cdot \exp([\hat{A}, \hat{B}])$. [Hint: try to use the Baker-Hausdorff formula]

(b)(3pts). $\exp(\hat{A}) \cdot \exp(\hat{B}) = \exp(\hat{A} + \hat{B}) \cdot \exp(\frac{1}{2}[\hat{A}, \hat{B}])$. [Hint: check the heuristic proof]

of the Baker-Hausdorff formula, try to derive a differential equation.] [Side remark: this is a special case of Baker-Campbell-Hausdorff formula, $e^{\hat{A}}e^{\hat{B}} = \exp(\hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}] + \dots)$.]

Solutions:

(a) $\exp(\hat{A}) \cdot \exp(\hat{B}) = \exp(\hat{A}) \cdot \exp(\hat{B}) \cdot \exp(-\hat{A}) \cdot \exp(\hat{A}) = \exp(e^{\hat{A}} \cdot \hat{B} \cdot e^{-\hat{A}}) \cdot \exp(\hat{A})$.

If $[\hat{A}, \hat{B}]$ is a c -number, then by the Baker-Hausdorff formula $e^{\hat{A}} \cdot \hat{B} \cdot e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}]$, because the 2nd and higher order nested commutators $[\hat{A}, \dots [\hat{A}, \hat{B}] \dots]$ vanish.

Therefore $\exp(\hat{A}) \cdot \exp(\hat{B}) = \exp(\hat{B} + [\hat{A}, \hat{B}]) \cdot \exp(\hat{A}) = \exp(\hat{B}) \cdot \exp([\hat{A}, \hat{B}]) \cdot \exp(\hat{A}) = \exp(\hat{B}) \cdot \exp(\hat{A}) \cdot \exp([\hat{A}, \hat{B}])$.

(b) By the Baker-Hausdorff formula, we have the following lemma [used in (a) already]:

if $[\hat{X}, \hat{Y}]$ is a c -number, then $e^{\hat{X}} \cdot \hat{Y} = e^{\hat{X}} \hat{Y} e^{-\hat{X}} \cdot e^{\hat{X}} = (\hat{Y} + [\hat{X}, \hat{Y}]) \cdot e^{\hat{X}}$.

Consider $\hat{f}(t) = e^{-t(\hat{A}+\hat{B})} e^{t\hat{A}} e^{t\hat{B}}$. Obviously $\hat{f}(t=0) = \mathbb{1}$.

$$\begin{aligned} \text{Then } \frac{d}{dt} \hat{f}(t) &= (-\hat{A} - \hat{B}) e^{-t(\hat{A}+\hat{B})} e^{t\hat{A}} e^{t\hat{B}} + e^{-t(\hat{A}+\hat{B})} \hat{A} \cdot e^{t\hat{A}} e^{t\hat{B}} + e^{-t(\hat{A}+\hat{B})} \cdot e^{t\hat{A}} \hat{B} \cdot e^{t\hat{B}} \\ &= (-\hat{A} - \hat{B}) e^{-t(\hat{A}+\hat{B})} e^{t\hat{A}} e^{t\hat{B}} + (\hat{A} - t[\hat{B}, \hat{A}]) e^{-t(\hat{A}+\hat{B})} e^{t\hat{A}} e^{t\hat{B}} + e^{-t(\hat{A}+\hat{B})} (\hat{B} + t[\hat{A}, \hat{B}]) \cdot e^{t\hat{A}} e^{t\hat{B}} \\ &= (-\hat{A} - \hat{B}) e^{-t(\hat{A}+\hat{B})} e^{t\hat{A}} e^{t\hat{B}} + (\hat{A} - t[\hat{B}, \hat{A}]) e^{-t(\hat{A}+\hat{B})} e^{t\hat{A}} e^{t\hat{B}} + (\hat{B} + t[\hat{A}, \hat{B}] - t[\hat{A}, \hat{B}]) e^{-t(\hat{A}+\hat{B})} e^{t\hat{A}} e^{t\hat{B}} \\ &= t[\hat{A}, \hat{B}] e^{-t(\hat{A}+\hat{B})} e^{t\hat{A}} e^{t\hat{B}} = t[\hat{A}, \hat{B}] \cdot \hat{f}(t) \end{aligned}$$

Note that the factor $t[\hat{A}, \hat{B}]$ in front of $\hat{f}(t)$ in the last expression is a c -number. This differential equation can be formally solved to give $\ln \hat{f}(t) = \ln \hat{f}(t=0) + \frac{t^2}{2}[\hat{A}, \hat{B}]$, then $\hat{f}(t) = e^{(t^2/2)[\hat{A}, \hat{B}]}$. When $t=1$, this is $e^{\frac{1}{2}[\hat{A}, \hat{B}]} = e^{-\hat{A}-\hat{B}} e^{\hat{A}} e^{\hat{B}}$. Left-multiply both sides by $e^{\hat{A}+\hat{B}}$, this becomes the identity to prove.

5.(5pts). Given the commutation relations $[\hat{A}, \hat{B}] = i\hat{C}$, $[\hat{B}, \hat{C}] = i\hat{A}$, and $[\hat{C}, \hat{A}] = i\hat{B}$. Compute $\exp(i\theta\hat{A}) \cdot (a\hat{A} + b\hat{B} + c\hat{C}) \cdot \exp(-i\theta\hat{A})$ where θ, a, b, c are c -numbers (result should be a finite-degree polynomial of $\hat{A}, \hat{B}, \hat{C}$). Hereafter $i \equiv \sqrt{-1}$ denotes the imaginary unit. [Hint: use the Baker-Hausdorff formula, try to write down several terms in the expansion, and find some pattern.]

Solutions:

This is a direct application of the Baker-Hausdorff formula.

$$e^{i\theta\hat{A}} \cdot (a\hat{A} + b\hat{B} + c\hat{C}) \cdot e^{-i\theta\hat{A}} = a e^{i\theta\hat{A}} \hat{A} e^{-i\theta\hat{A}} + b e^{i\theta\hat{A}} \hat{B} e^{-i\theta\hat{A}} + c e^{i\theta\hat{A}} \hat{C} e^{-i\theta\hat{A}}$$

$$= a\hat{A} + b \sum_{n=0}^{\infty} \frac{\theta^n}{n!} \underbrace{[\hat{A}, [\hat{A}, \dots [\hat{A}, \hat{B}] \dots]]}_{n\text{-fold commutator}} + c \sum_{n=0}^{\infty} \frac{\theta^n}{n!} \underbrace{[\hat{A}, [\hat{A}, \dots [\hat{A}, \hat{C}] \dots]]}_{n\text{-fold commutator}}$$

The n -fold commutator results can be obtained by mathematical induction,

$$\underbrace{[\hat{A}, [\hat{A}, \dots [\hat{A}, \hat{B}] \dots]]}_{n\text{-fold commutator}} = \begin{cases} (-1)^m \hat{B}, & n = 2m; \\ -(-1)^m \hat{C}, & n = 2m + 1. \end{cases}$$

$$\underbrace{[\hat{A}, [\hat{A}, \dots [\hat{A}, \hat{C}] \dots]]}_{n\text{-fold commutator}} = \begin{cases} (-1)^m \hat{C}, & n = 2m; \\ (-1)^m \hat{B}, & n = 2m + 1. \end{cases}$$

The result is $a\hat{A} + b\hat{B} \sum_{m=0}^{\infty} \frac{\theta^{2m}}{(2m)!} (-1)^m + b\hat{C} \sum_{m=0}^{\infty} \frac{\theta^{2m+1}}{(2m+1)!} (-1)^{m+1} + c\hat{C} \sum_{m=0}^{\infty} \frac{\theta^{2m}}{(2m)!} (-1)^m + c\hat{B} \sum_{m=0}^{\infty} \frac{\theta^{2m+1}}{(2m+1)!} (-1)^m = a\hat{A} + (b \cos \theta + c \sin \theta) \hat{B} + (-b \sin \theta + c \cos \theta) \hat{C}.$

6. Define the Pauli matrices, $\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. It is easy to check that $\{\sigma_1, \sigma_2\} = \{\sigma_2, \sigma_3\} = \{\sigma_3, \sigma_1\} = 0$, and $(\sigma_i)^2 = \mathbb{1}_{2 \times 2}$, and $[\sigma_1, \sigma_2] = 2i\sigma_3$, $[\sigma_2, \sigma_3] = 2i\sigma_1$, $[\sigma_3, \sigma_1] = 2i\sigma_2$.

(a)(5pts). Consider a 2×2 matrix $M = a_0\sigma_0 + a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3$, where $a_{0,1,2,3}$ are complex numbers. If M is a hermitian matrix, what is the condition on $a_{0,1,2,3}$? Show that $M \cdot M = c_0\mathbb{1}_{2 \times 2} + c_1M$ and solve the numbers c_0 and c_1 in terms of $a_{0,1,2,3}$. Then solve the eigenvalues of M in terms of $a_{0,1,2,3}$. [Hint: you don't really need to diagonalize a 2×2 matrix. This result will be useful later in this course.]

(b)(5pts). Compute $\exp[i(a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3)]$, where $a_{1,2,3}$ are real numbers. The result should be a linear combination of Pauli matrices. [Hint: compute the first few terms in the Taylor expansion and try to find some pattern. This result will be useful later in this course.]

Solution:

(a) Pauli matrices are hermitian ($\sigma_i^\dagger = \sigma_i$) and linearly independent, so for M to be hermitian, all the coefficients $a_{0,1,2,3}$ must be real.

$$M^2 = (a_0^2 + a_1^2 + a_2^2 + a_3^2) + 2a_0(a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3) = (-a_0^2 + a_1^2 + a_2^2 + a_3^2) + 2a_0M.$$

Namely $c_0 = -a_0^2 + a_1^2 + a_2^2 + a_3^2$ and $c_1 = 2a_0$.

The eigenvalues λ of M should also satisfy $\lambda^2 = c_0 + c_1\lambda$ (think about acting M^2 on an eigenvector of M), so the eigenvalues are $a_0 \pm \sqrt{a_1^2 + a_2^2 + a_3^2}$.

(b) denote $A = a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3$, it is easy to check that $A^2 = (a_1^2 + a_2^2 + a_3^2)\mathbb{1}$. Therefore $A^{2m} = (a_1^2 + a_2^2 + a_3^2)^m \mathbb{1}$ and $A^{2m+1} = (a_1^2 + a_2^2 + a_3^2)^m A$ for non-negative integer m .

$$\begin{aligned} \text{Then } \exp(iA) &= \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m)!} A^{2m} + \sum_{m=0}^{\infty} \frac{(-1)^{m+1}}{(2m+1)!} A^{2m+1} \\ &= \cos(\sqrt{a_0^2 + a_1^2 + a_2^2})\mathbb{1} + i \sin(\sqrt{a_0^2 + a_1^2 + a_2^2}) \frac{1}{\sqrt{a_0^2 + a_1^2 + a_2^2}} (a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3). \end{aligned}$$

7. \mathcal{H}_1 and $\hat{\mathcal{H}}_2$ are both 2-dimensional Hilbert spaces. \mathcal{H}_1 has complete orthonormal basis $|e_1\rangle$ and $|e_2\rangle$, \mathcal{H}_2 has complete orthonormal basis $|e'_1\rangle$ and $|e'_2\rangle$.

(a)(4pts). (4pts). Define operators $\hat{\sigma} = |e_1\rangle\langle e_2| + |e_2\rangle\langle e_1|$ in \mathcal{H}_1 , and $\hat{\sigma}' = |e'_1\rangle\langle e'_2| + |e'_2\rangle\langle e'_1|$ in \mathcal{H}_2 . Write down all the eigenvalues and normalized eigenstates of $\hat{\sigma} \otimes \hat{\sigma}'$ in $\mathcal{H}_1 \otimes \mathcal{H}_2$.

(b)(1pt). Define a state $|\varphi\rangle = \frac{1}{\sqrt{2}}(|e_1\rangle \otimes |e'_2\rangle + |e_2\rangle \otimes |e'_1\rangle)$. Show that this state CANNOT be written as a single tensor product, $|\psi\rangle \otimes |\psi'\rangle$, where $|\psi\rangle$ is a state in \mathcal{H}_1 , and $|\psi'\rangle$ is a state in \mathcal{H}_2 . [Hint: assume this is $|\psi\rangle \otimes |\psi'\rangle$, try to solve $|\psi\rangle$ and $|\psi'\rangle$ in terms of basis]

Solution:

(a) the eigenstates of the tensor product operator can be formed by the tensor product of eigenstates of each operator.

Both operators $\hat{\sigma}$ and $\hat{\sigma}'$ are represented by the 2×2 matrix $\sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ under the above mentioned basis for \mathcal{H}_1 and \mathcal{H}_2 . Their eigenvalues and corresponding eigenvectors are listed in the following table,

eigenvalues	eigenvector of $\hat{\sigma}_1$	eigenvector of $\hat{\sigma}'_1$
+1	$\frac{1}{\sqrt{2}}(e_1\rangle + e_2\rangle)$	$\frac{1}{\sqrt{2}}(e'_1\rangle + e'_2\rangle)$
-1	$\frac{1}{\sqrt{2}}(e_1\rangle - e_2\rangle)$	$\frac{1}{\sqrt{2}}(e'_1\rangle - e'_2\rangle)$

Then the eigenvalues and eigenstates of $\hat{\sigma} \otimes \hat{\sigma}'$ are

eigenvalues	eigenvectors
+1 = (+1) · (+1)	$\frac{1}{2}(e_1\rangle + e_2\rangle) \otimes (e'_1\rangle + e'_2\rangle)$
+1 = (-1) · (-1)	$\frac{1}{2}(e_1\rangle - e_2\rangle) \otimes (e'_1\rangle - e'_2\rangle)$
-1 = (+1) · (-1)	$\frac{1}{2}(e_1\rangle + e_2\rangle) \otimes (e'_1\rangle - e'_2\rangle)$
-1 = (-1) · (+1)	$\frac{1}{2}(e_1\rangle - e_2\rangle) \otimes (e'_1\rangle + e'_2\rangle)$

Method#2:

Under the basis $(|e_1 \otimes e'_1\rangle, |e_1 \otimes e'_2\rangle, |e_2 \otimes e'_1\rangle, |e_2 \otimes e'_2\rangle)$, operator $\hat{\sigma} \otimes \hat{\sigma}'$ is the 4×4 matrix

$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$. If we rearrange the basis into $(|e_1 \otimes e'_1\rangle, |e_2 \otimes e'_2\rangle, |e_1 \otimes e'_2\rangle, |e_2 \otimes e'_1\rangle)$, this matrix is obviously block-diagonalized, $\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$. So we only need to diagonalize the top-left and bottom-right 2×2 diagonal blocks, $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, with eigenvalue $+1$ for eigenvector $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, and eigenvalue -1 for eigenvector $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

eigenvalues	eigenvectors
+1	$\frac{1}{\sqrt{2}}(e_1 \otimes e'_1\rangle + e_2 \otimes e'_2\rangle)$
-1	$\frac{1}{\sqrt{2}}(e_1 \otimes e'_1\rangle - e_2 \otimes e'_2\rangle)$
+1	$\frac{1}{\sqrt{2}}(e_1 \otimes e'_2\rangle + e_2 \otimes e'_1\rangle)$
-1	$\frac{1}{\sqrt{2}}(e_1 \otimes e'_2\rangle - e_2 \otimes e'_1\rangle)$

(b) proof by contradiction: suppose $|\varphi\rangle = |\psi\rangle \otimes |\psi'\rangle$, then

method #1: brute-force method,

Suppose $|\psi\rangle = c_1|e_1\rangle + c_2|e_2\rangle$, $|\psi'\rangle = d_1|e'_1\rangle + d_2|e'_2\rangle$, where $c_{1,2}$ and $d_{1,2}$ are complex coefficients. Then we must have $c_1d_1 = 0$, $c_1d_2 = \frac{1}{\sqrt{2}}$, $c_2d_1 = \frac{1}{\sqrt{2}}$, $c_2d_2 = 0$.

However there is no solution to the above equations. The first equation demands that either $c_1 = 0$ (then the second equation cannot be satisfied), or $d_1 = 0$ (then the third equation cannot be satisfied). This contradiction proves that $|\varphi\rangle$ cannot be represented as a single tensor product state.

method #2: (not required) use reduced density matrix,

If $|\varphi\rangle = |\psi\rangle \otimes |\psi'\rangle$, then the density matrix $\hat{\rho}$ of $|\varphi\rangle$ is $\hat{\rho} = \frac{|\varphi\rangle\langle\varphi|}{\langle\varphi|\varphi\rangle} = \frac{|\psi\otimes\psi'\rangle\langle\psi\otimes\psi'|}{\langle\psi|\psi\rangle\langle\psi'|\psi'\rangle}$.

The reduced density matrix on Hilbert space \mathcal{H}_1 will be the density matrix of the pure state $|\psi\rangle$, $\hat{\rho}_1 \equiv \text{Tr}_{\mathcal{H}_2}(\hat{\rho}) = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$. The density matrix $\hat{\rho}$ of $|\varphi\rangle$ under the tensor product basis

$$(|e_1\rangle|\tilde{e}_1\rangle, |e_1\rangle|\tilde{e}_2\rangle, |e_2\rangle|\tilde{e}_1\rangle, |e_2\rangle|\tilde{e}_2\rangle) \text{ is } \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The reduced density matrix $\hat{\rho}_1$ under the $(|e_1\rangle, |e_2\rangle)$ basis is then $\begin{pmatrix} (0 + \frac{1}{2}), & (0 + 0) \\ (0 + 0), & (\frac{1}{2} + 0) \end{pmatrix}$. This is NOT a pure state density matrix [has two nonzero eigenvalues, has nonzero von Neumann entropy $\log(2)$]. This contradiction proves that $|\varphi\rangle$ cannot be represented as a single tensor product state.