0.1 Homework 1

0.1.1 Hermitian operators

1. **Prove theorem 1: If A is Hermitian operator, then all its eigenvalues are real numbers, and the eigenvectors corresponding to different eigenvalues are orthogonal.**

   (a) Since A is Hermitian, we have $A^\dagger = A$. Let λ be an eigenvalue of A and v the corresponding eigenvector, so

   $$Av = \lambda v.$$

   Consider the inner product

   $$\langle v, Av\rangle = \langle v, \lambda v\rangle = \lambda\langle v, v\rangle = \lambda||v||^2.$$
   $$\langle Av, v\rangle = \langle \lambda v, v\rangle = \lambda^*\langle v, v\rangle = \lambda^*||v||^2.$$

   So we have $\lambda||v||^2 = \lambda^*||v||^2$, which implies $\lambda = \lambda^*$, so λ is real(since $||v||^2$ is not zero, as $v \neq 0$).

   (b) Let λ_1 and λ_2 be two different eigenvalues of A, and v_1 and v_2 the corresponding eigenvectors, so we have

   $$Av_1 = \lambda_1 v_1, \quad Av_2 = \lambda_2 v_2.$$

   Consider the inner product

   $$\langle v_1, Av_2\rangle = \langle v_1, \lambda_2 v_2\rangle = \lambda_2\langle v_1, v_2\rangle,$$
   $$\langle Av_1, v_2\rangle = \langle \lambda_1 v_1, v_2\rangle = \lambda_1\langle v_1, v_2\rangle.$$

   Since A is Hermitian, we have $\langle v_1, Av_2\rangle = \langle Av_1, v_2\rangle$, so we have $(\lambda_1 - \lambda_2)\langle v_1, v_2\rangle = 0$, which implies $\langle v_1, v_2\rangle = 0$(since $\lambda_1 \neq \lambda_2$).□

2. **Prove theorem 2: If A is Hermitian operator, then it can be always diagonalized by unitary transformation.**

   (a) Non-degenerate.

   Let $\{\lambda_1, \lambda_2, \cdots, \lambda_n\}$ be the eigenvalues of A, and $\{v_1, v_2, \cdots, v_n\}$ the corresponding eigenvectors.

   By theorem 1, we have $\langle v_1, v_2\rangle = \delta_{ij}$.

   We define the unitary matrix as $U = [v_1, v_2, \cdots, v_n]$, so we have $U^\dagger U = \mathbb{I}$. Now we compute $U^\dagger AU$. Since $Av_i = \lambda_i v_i$, we have

   $$U^\dagger AU = \begin{pmatrix} v_1^\dagger \\ v_2^\dagger \\ \vdots \\ v_n^\dagger \end{pmatrix} A \begin{pmatrix} v_1 & v_2 & \cdots & v_n \end{pmatrix} = \begin{pmatrix} v_1^\dagger Av_1 & v_1^\dagger Av_2 & \cdots & v_1^\dagger Av_n \\ v_2^\dagger Av_1 & v_2^\dagger Av_2 & \cdots & v_2^\dagger Av_n \\ \vdots & \vdots & \ddots & \vdots \\ v_n^\dagger Av_1 & v_n^\dagger Av_2 & \cdots & v_n^\dagger Av_n \end{pmatrix}$$
   $$= \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} = \Lambda.$$

   (b) 简并.

   令 m 重简并 λ_1 的本征矢为 $\{v_1^{(1)}, v_1^{(2)}, \cdots, v_1^{(m)}\}$. 那么新的 U 矩阵将为 $U = \left[v_1^{(1)}, v_1^{(2)}, \cdots, v_1^{(m)}, v_{m+1}, \cdots, v_n\right]$. 那

么计算

$$U^\dagger AU = \begin{pmatrix} v_1^{(1)\dagger} \\ v_1^{(2)\dagger} \\ \vdots \\ v_1^{(m)\dagger} \\ v_{m+1}^\dagger \\ \vdots \\ v_n^\dagger \end{pmatrix} A \begin{pmatrix} v_1^{(1)} & v_1^{(2)} & \cdots & v_1^{(m)} & v_{m+1} & \cdots & v_n \end{pmatrix}$$

$$= \begin{pmatrix} v_1^{(1)\dagger} \\ v_1^{(2)\dagger} \\ \vdots \\ v_1^{(m)\dagger} \\ v_{m+1}^\dagger \\ \vdots \\ v_n^\dagger \end{pmatrix} \begin{pmatrix} \lambda_1 v_1^{(1)} & \lambda_1 v_1^{(2)} & \cdots & \lambda_1 v_1^{(m)} & \lambda_{m+1} v_{m+1} & \cdots & \lambda_n v_n \end{pmatrix}$$

$$= \begin{pmatrix} \lambda_1 & v_1^{(1)\dagger} v_1^{(2)} & \cdots & v_1^{(1)\dagger} v_1^{(m)} & v_1^{(1)\dagger} v_{m+1} & \cdots & v_1^{(1)\dagger} v_n \\ v_1^{(2)\dagger} v_1^{(1)} & \lambda_1 & \cdots & v_1^{(2)\dagger} v_1^{(m)} & v_1^{(2)\dagger} v_{m+1} & \cdots & v_1^{(2)\dagger} v_n \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ v_1^{(m)\dagger} v_1^{(1)} & v_1^{(m)\dagger} v_1^{(2)} & \cdots & \lambda_1 & v_1^{(m)\dagger} v_{m+1} & \cdots & v_1^{(m)\dagger} v_n \\ v_{m+1}^\dagger v_1^{(1)} & v_{m+1}^\dagger v_1^{(2)} & \cdots & v_{m+1}^\dagger v_1^{(m)} & \lambda_{m+1} & \cdots & v_{m+1}^\dagger v_n \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ v_n^\dagger v_1^{(1)} & v_n^\dagger v_1^{(2)} & \cdots & v_n^\dagger v_1^{(m)} & v_n^\dagger v_{m+1} & \cdots & \lambda_n \end{pmatrix}$$

我们并不清楚 λ_1 简并子空间内各基矢是否相互正交, 但是可确定的是 $v_1^{(j)\dagger} v_k, \quad k > m$ 和 $v_j^\dagger v_k, \quad j, k > m$ 是必定为 0 的. 那么上述矩阵将化为

$$U^\dagger AU = \begin{pmatrix} \lambda_1 & v_1^{(1)\dagger} v_1^{(2)} & \cdots & v_1^{(1)\dagger} v_1^{(m)} & & & \\ v_1^{(2)\dagger} v_1^{(1)} & \lambda_1 & \cdots & v_1^{(2)\dagger} v_1^{(m)} & & & \\ \vdots & \vdots & \ddots & \vdots & & & \\ v_1^{(m)\dagger} v_1^{(1)} & v_1^{(m)\dagger} v_1^{(2)} & \cdots & \lambda_1 & & & \\ & & & & \lambda_{m+1} & & \\ & & & & & \ddots & \\ & & & & & & \lambda_n \end{pmatrix}$$

使用 Gram-Schmidt 正交化方法, 使得 $\{v_1^{(1)}, v_1^{(2)}, \cdots, v_1^{(m)}\}$ 化为正交归一的基矢 $\{\phi_1, \phi_2, \cdots, \phi_m\}$:

$$v_1^{(1)\prime} = v_1^{(1)}, \quad \phi_1 = \frac{v_1^{(1)\prime}}{||v_1^{(1)\prime}||},$$

$$v_1^{(2)\prime} = v_1^{(2)} - \langle v_1^{(2)}, \phi_1 \rangle \phi_1, \quad \phi_2 = \frac{v_1^{(2)\prime}}{||v_1^{(2)\prime}||},$$

$$v_1^{(3)\prime} = v_1^{(3)} - \langle v_1^{(3)}, \phi_1 \rangle \phi_1 - \langle v_1^{(3)}, \phi_2 \rangle \phi_2, \quad \phi_3 = \frac{v_1^{(3)\prime}}{||v_1^{(3)\prime}||}, \cdots$$

以此类推, 我们可以得到 $\{\phi_1, \phi_2, \cdots, \phi_m\}$, 那么我们可以构造新的 $U = \left[\phi_1, \phi_2, \cdots, \phi_m, v_{m+1}, \cdots, v_n\right]$, 并且存在关系 $\phi_i^\dagger A \phi_j = \lambda_1 \delta_{ij}$, 使得 $U^\dagger AU$ 为对角矩阵 Λ.□

3. **Prove theorem 3: Two diagonalizable operators A and B can be simultaneously diagonalized if, and only if, $[A, B] = 0$.**

(a) Let's say

$$A|v\rangle = \lambda|v\rangle, \quad B|v\rangle = \mu|v\rangle.$$

where $|v\rangle$ is the eigenvector of A and B, λ and μ are the corresponding eigenvalues.

So

$$[A,B]|v\rangle = (AB-BA)|v\rangle = (AB|v\rangle - BA|v\rangle) = (\lambda\mu - \mu\lambda)|v\rangle = 0.$$

for all $|v\rangle$, which means $[A,B]=0$.

(b) Let's say $[A,B]=0$.

$$\begin{gathered} A|v\rangle = \lambda|v\rangle, \\ AB|v\rangle = BA|v\rangle = B\lambda|v\rangle = \lambda\left(B|v\rangle\right), \end{gathered}$$

i. 非简并. 那么 $B|v_i\rangle = \mu_i|v_i\rangle$.

ii. 简并. 假设 A 的本征值 λ_1 存在 m 重简并, 对应的本征矢为 $\{|v_1^{(1)}\rangle, |v_1^{(2)}\rangle, \cdots, |v_1^{(m)}\rangle\}$. 设 $B|v_1^{(i)}\rangle = \displaystyle\sum_j b_{ij}|v_1^{(j)}\rangle$. 而其余本征矢则维持非简并形式 $B|v_j\rangle = \mu_j|v_j\rangle$. 令幺正矩阵 $U = \left[|v_1^{(1)}\rangle, |v_1^{(2)}\rangle, \cdots, |v_1^{(m)}\rangle, |v_{m+1}\rangle, \cdots, |v_n\rangle\right]$ 尝试使 B 对角化:

$$\begin{aligned}
U^\dagger B U &= \begin{pmatrix} \langle v_1^{(1)}| \\ \langle v_1^{(2)}| \\ \vdots \\ \langle v_1^{(m)}| \\ \langle v_{m+1}| \\ \vdots \\ \langle v_n| \end{pmatrix} B \begin{pmatrix} |v_1^{(1)}\rangle & |v_1^{(2)}\rangle & \cdots & |v_1^{(m)}\rangle & |v_{m+1}\rangle & \cdots & |v_n\rangle \end{pmatrix} \\
&= \begin{pmatrix} \langle v_1^{(1)}| \\ \langle v_1^{(2)}| \\ \vdots \\ \langle v_1^{(m)}| \\ \langle v_{m+1}| \\ \vdots \\ \langle v_n| \end{pmatrix} \begin{pmatrix} \sum_j b_{1j}|v_1^{(j)}\rangle & \sum_j b_{2j}|v_1^{(j)}\rangle & \cdots & \sum_j b_{mj}|v_1^{(j)}\rangle & \mu_{m+1}|v_{m+1}\rangle & \cdots & \mu_n|v_n\rangle \end{pmatrix} \\
&= \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1m} & & & \\ b_{21} & b_{22} & \cdots & b_{2m} & & & \\ \vdots & \vdots & \ddots & \vdots & & & \\ b_{m1} & b_{m2} & \cdots & b_{mm} & & & \\ & & & & \mu_{m+1} & & \\ & & & & & \ddots & \\ & & & & & & \mu_n \end{pmatrix} = \begin{pmatrix} b & 0 \\ 0 & \Lambda_\mu \end{pmatrix}
\end{aligned}$$

所以问题就在于要使分块矩阵 $b = \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1m} \\ b_{21} & b_{22} & \cdots & b_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ b_{m1} & b_{m2} & \cdots & b_{mm} \end{pmatrix}$ 对角化. 构造 $b = U_b^\dagger \Lambda_b U_b$, 于是

$$
\begin{aligned}
U^\dagger B U = \begin{pmatrix} U_b^\dagger \Lambda_b U_b & \\ & \Lambda_\mu \end{pmatrix} &= \begin{pmatrix} U_b^\dagger & \\ & \mathbb{I} \end{pmatrix} \begin{pmatrix} \Lambda_b & \\ & \Lambda_\mu \end{pmatrix} \begin{pmatrix} U_b & \\ & \mathbb{I} \end{pmatrix} \\
\Rightarrow \underbrace{\begin{pmatrix} U_b^\dagger & \\ & \mathbb{I} \end{pmatrix}^{-1} U^\dagger}_{U'^\dagger} B \underbrace{U \begin{pmatrix} U_b & \\ & \mathbb{I} \end{pmatrix}^{-1}}_{U'} &= \begin{pmatrix} \Lambda_b & \\ & \Lambda_\mu \end{pmatrix} = \Lambda.
\end{aligned}
$$

于是通过构造 U' 和 $U'^\dagger$, 我们可以将 B 对角化. □

0.1.2 Matrix diagonalization and unitary transformation

1. **Diagonalizing a matrix L corresponds to finding a unitary transformation V such that $L = V\Lambda V^\dagger$, where Λ is a diagonal matrix whose diagonal elements are eigenvalues, V is an unitary matrix whose column vectors are the corresponding eigenstates. Find a unitary matrix V that can diagonalize the Pauli matrix $\sigma^x_{(z)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and find the eigenvalues of $\sigma^x_{(z)}$.**

   Find the eigenvalues of $\sigma^x_{(z)}$ by solving the characteristic equation

$$
\det(\sigma^x_{(z)} - \lambda I) = \det \begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix} = \lambda^2 - 1 = 0,
$$

   So we have $\boxed{\lambda = \pm 1}$. For $\lambda_+ = 1$, we have

$$
\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = 1 \cdot \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \Rightarrow v_1 = v_2.
$$

   So the eigenvector corresponding to λ_+ is $|+\rangle^x_{(z)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$. For $\lambda_- = -1$, we have

$$
\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = -1 \cdot \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \Rightarrow v_1 = -v_2.
$$

   So the eigenvector corresponding to λ_- is $|-\rangle^x_{(z)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$. The eigenvectors have been normalized, so the unitary matrix V is $[|+\rangle^x_{(z)}, |-\rangle^x_{(z)}] = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$. The diagonal matrix Λ contains the eigenvalues on the diagonal, which means

$$
\Lambda = \mathrm{diag}\{\lambda_+, \lambda_-\} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma^z_{(z)}
$$

   Thus we diagonalized the Pauli matrix $\sigma^x_{(z)}$ by the unitary transformation V:

$$
\sigma^x_{(z)} = V^\dagger \Lambda V = V^\dagger \sigma^z_{(z)} V
$$

   We notice that the diagnosed matrix Λ is just the Pauli matrix $\sigma^z_{(z)}$, which means we can transform the representation of the Pauli matrix σ^z to the σ^x representation by the unitary transformation V:

$$
\sigma^x_{(z)} = V^\dagger \sigma^z_{(z)} V = V^\dagger \sigma^x_{(x)} V \Rightarrow \sigma^x_{(x)} = \left(V^\dagger\right)^{-1} \sigma^x_{(z)} (V)^{-1}
$$

   $\sigma^x_{(z)}$ is the matrix of σ^x in the σ^z representation. Noticed that $V = V^\dagger = V^{-1}$, so

$$
\sigma^x_{(x)} = V \sigma^x_{(z)} V
$$

2. **The three components of the spin angular momentum operator $\vec{S}$ for spin-$1/2$ are S^x, S^y, and S^z. If we use the S^z representation, their matrix representations are given by $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, where the three components of $\vec{\sigma}$ are the Pauli matrices σ^x, σ^y, and σ^z.**

   Now consider using the S^x representation. Please list the order of basis vectors you have chosen in the S^x representation, and calculate the matrix representations of the three components of the operator $\vec{S}$ in this representation.

   Within S^z representation, we have

$$S^x_{(z)} = \frac{\hbar}{2}\sigma^x_{(z)} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

   From the previous question, we have found the eigenvalues and corresponding eigenvectors:

$$|+\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |-\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

   The matrix V that transforms the S^z representation to the S^x representation is

$$V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

   In the S^z representation, we have

$$S^x_{(z)} = \frac{\hbar}{2}\sigma^x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^y_{(z)} = \frac{\hbar}{2}\sigma^y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S^z_{(z)} = \frac{\hbar}{2}\sigma^z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

   So

$$\begin{aligned} S^x_{(x)} &= V S^x_{(z)} V = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \\ S^y_{(x)} &= V S^y_{(z)} V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \\ S^z_{(x)} &= V S^z_{(z)} V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \end{aligned}$$

   So the basis vectors in the S^x representation are

$$|+\rangle^x_{(x)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle^x_{(x)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$