

# **Quantum Computation and Quantum Information**

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## **Chapter 2. Introduction to Quantum Mechanics**

### **Selected Problems**

#### **Set-I**

**2.16)** Show that any linear operator  $P$  defined on a vector space  $V$  is a projector if and only if  $P^2 = P$ .

**Solution:**

$$P \text{ is a projector} \Rightarrow P^2 = P$$

Suppose  $W$  is the  $k$ -dimensional vector subspace of the  $d$ -dimensional vector space  $V$ . Using the Gram-Schmidt procedure it is possible to construct an orthonormal basis  $|1\rangle, |2\rangle, \dots, |d\rangle$  for  $V$  such that  $|1\rangle, |2\rangle, \dots, |k\rangle$  is an orthonormal basis for  $W$ . By definition,

$$P \equiv \sum_{i=1}^k |i\rangle \langle i| \quad (1)$$

is a projector onto the subspace  $W$ .

$$\begin{aligned} P^2 &= \left( \sum_{i=1}^k |i\rangle \langle i| \right) \left( \sum_{j=1}^k |j\rangle \langle j| \right) \\ \Rightarrow P^2 &= \sum_{i,j=1}^k |i\rangle \underbrace{\langle i|j\rangle}_{\substack{0 \text{ for } i \neq j \\ 1 \text{ for } i = j}} \langle j| \end{aligned}$$

We see that  $|i\rangle$  and  $|j\rangle$  being orthonormal results to  $\langle i|j\rangle = 0$  for  $i \neq j$  and  $\langle i|j\rangle = 1$  for  $i = j$ . Hence,

$$\Rightarrow P^2 = \sum_{i,j=1}^k |i\rangle \langle i|j\rangle \langle j| = \sum_{i,j=1}^k |i\rangle \langle j| \delta_{ij} = \sum_{i=1}^k |i\rangle \langle i| = P \Rightarrow P^2 = P$$

$$P^2 = P \Rightarrow P \text{ is a projector}$$

It is given that  $P : V \rightarrow V$  is a linear operator defined on the vector space  $V$  such that  $P = P^2$ . We show that  $P$  is a projector by showing:

- $P$  is the identity operator on the subspace  $U = \text{im}(P)$ , i.e.  $\forall |u\rangle \in U, P|u\rangle = |u\rangle$ .
- $V = U \oplus W$ , where the subspace  $W = \ker(P)$ , i.e.  $\forall |v\rangle \in V, |v\rangle = |u\rangle + |w\rangle$ , where  $|u\rangle = P|v\rangle$  and  $|w\rangle = (I - P)|v\rangle$  and  $|u\rangle \in U, |w\rangle \in W$ .

a) First, we show that the operator  $P$  is an identity matrix on the subspace  $U$ .

$U$  is the image of  $P$  which is defined as

$$\text{im}(P) = U = \left\{ |u\rangle \in V \mid P|v\rangle = |u\rangle \text{ for some } |v\rangle \in V \right\}$$

Suppose the vector space  $V$  is spanned by the orthonormal basis  $\{|v_1\rangle, |v_2\rangle, \dots, |v_d\rangle\}$ . Using the Gram-Schmidt procedure we can produce the orthonormal basis  $\{|x_1\rangle, |x_2\rangle, \dots, |x_k\rangle\}$  that

spans the subspace  $U$ . It is given that  $P = P^2$ . So, for some  $|u\rangle \in U$  (and some  $|v\rangle \in V$ ) we have  $P|u\rangle = P(P|v\rangle) = P^2|v\rangle = P|v\rangle = |u\rangle$ .

Hence

$$\begin{aligned} P|u\rangle = |u\rangle &\Rightarrow P|u\rangle = \sum_{i=1}^k \langle x_i|u\rangle |x_i\rangle = \sum_{i=1}^k |x_i\rangle \langle x_i|u\rangle \\ P|u\rangle = \left( \sum_{i=1}^k |x_i\rangle \langle x_i| \right) |u\rangle &\Rightarrow P \equiv \sum_{i=1}^k |x_i\rangle \langle x_i| \underbrace{=}_{\text{Completeness Relation}} I \end{aligned}$$

Hence,  $P$  is an identity matrix on the subspace  $U$ .

b) Next, we show that any vector  $|v\rangle \in V$  can be uniquely decomposed into a sum of the vector  $|u\rangle \in U$  and a vector  $|w\rangle \in W$ . We also show that the set of vectors in the intersection  $U \cap W$  is  $\{0\}$ .  $W$  is the kernel of  $P$  which is defined as

$$\ker(P) = W = \left\{ |w\rangle \in V \mid P|w\rangle = 0 \right\}$$

Consider a vector  $|x\rangle \in V$ . Since it is given that  $P^2 = P$ , we note that  $P|x\rangle = P^2|x\rangle \Rightarrow P(I|x\rangle - P|x\rangle) = |0\rangle \Rightarrow P(|x\rangle - P|x\rangle) = |0\rangle$ . Hence, we can define a vector  $|w\rangle \in V$  as  $|w\rangle = |x\rangle - P|x\rangle$  where  $|x\rangle \in V$ . Clearly,  $|w\rangle$  satisfies  $P|w\rangle = 0$ . And so we can redefine the subspace  $W = \ker(P)$  as

$$\ker(P) = W = \left\{ |w\rangle \in V \mid |w\rangle = |x\rangle - P|x\rangle \text{ for some } |x\rangle \in V \right\} \quad (2)$$

Therefore, every vector  $|x\rangle \in V$  can be decomposed as  $|x\rangle = P|x\rangle + |x\rangle - P|x\rangle$ . By definition of  $U$  and  $W$ ,  $P|x\rangle \in U$  and  $(|x\rangle - P|x\rangle) \in W$ . Next, we show that such a decomposition is unique by showing that  $U \cap W = \{0\}$ . Consider some  $|z\rangle \in U \cap W$ . Because  $|z\rangle \in U$ ,  $|z\rangle = P|v\rangle$  for some  $|v\rangle \in V$ . Applying  $P$  on both sides we get  $P|z\rangle = P^2|v\rangle$ . Also,  $|z\rangle \in W$ . So,  $0 = P|z\rangle = P^2|v\rangle = P|v\rangle = |z\rangle$ . Hence for some  $|z\rangle \in U \cap W$  we have  $|z\rangle = 0$ . So,  $U \cap W = \{0\}$ . Hence,

$$V = U \oplus W \quad \text{i.e.} \quad V = \text{im}(P) \oplus \ker(P) \quad (3)$$

Therefore,  $P : V \rightarrow V$  with  $P = P^2$  is a projector.

**2.60)** Show that  $\vec{v} \cdot \vec{\sigma}$  has eigenvalues  $\pm 1$ , and that the projectors on the corresponding eigenspaces are given by  $P_{\pm} = (I \pm \vec{v} \cdot \vec{\sigma})/2$ .

**Solution:**

We use the definition of the Pauli matrices,  $\sigma_1, \sigma_2, \sigma_3$ . Also,  $\vec{v}$  is a unit vector which means  $\sqrt{v_1^2 + v_2^2 + v_3^2} = 1$ . Let  $\lambda$  be the eigenvalue of  $\vec{v} \cdot \vec{\sigma}$ .

$$\begin{aligned}
\vec{v} \cdot \vec{\sigma} &= v_1 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + v_2 \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + v_3 \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} v_3 & v_1 - iv_2 \\ v_1 + iv_2 & -v_3 \end{bmatrix} \\
|\lambda - \vec{v} \cdot \vec{\sigma}| &= 0 \\
\Rightarrow (\lambda - v_3)(\lambda + v_3) + (iv_2 - v_1)(iv_2 + v_1) &= 0 \\
\Rightarrow \lambda^2 - v_3^2 - v_2^2 - v_1^2 &= 0 \\
\Rightarrow \lambda &= \pm 1
\end{aligned}$$

Let  $\lambda_+ = 1$  and  $\lambda_- = -1$ . And,  $P_+$  be the projector onto the eigenspace of  $\vec{v} \cdot \vec{\sigma}$  corresponding to  $\lambda_+ = 1$  and  $P_-$  be the projector onto the eigenspace of  $\vec{v} \cdot \vec{\sigma}$  corresponding to  $\lambda_- = -1$ . We can see that the observable  $\vec{v} \cdot \vec{\sigma}$  is Hermitian.

$$(\vec{v} \cdot \vec{\sigma})^\dagger = \left( \begin{bmatrix} v_3 & v_1 - iv_2 \\ v_1 + iv_2 & -v_3 \end{bmatrix} \right)^\dagger = \begin{bmatrix} v_3 & v_1 + iv_2 \\ v_1 - iv_2 & -v_3 \end{bmatrix} = \begin{bmatrix} v_3 & v_1 - iv_2 \\ v_1 + iv_2 & -v_3 \end{bmatrix} = \vec{v} \cdot \vec{\sigma}$$

Then, we have

$$\vec{v} \cdot \vec{\sigma} = \lambda_+ P_+ + \lambda_- P_- = P_+ - P_- \quad (4)$$

Also, projectors are Hermitian operators, which means they are self adjoint, i.e.  $P^\dagger = P$ . Also,  $P^2 = P$ . Hence from the completeness relation  $\sum P^\dagger P = \sum P P = \sum P^2 = \sum P = I$ , we have the following.

$$P_+ + P_- = I \quad (5)$$

Solving (2) and (3) we get  $P_+ = (I + \vec{v} \cdot \vec{\sigma})/2$  and  $P_- = (I - \vec{v} \cdot \vec{\sigma})/2$ .

**2.67)** Suppose  $V$  is a Hilbert space with a subspace  $W$ . Suppose  $U : W \rightarrow V$  is a linear operator which preserves inner products, i.e. for any  $|w_1\rangle$  and  $|w_2\rangle$  in  $W$  we have

$$\langle w_1 | U^\dagger U | w_2 \rangle = \langle w_1 | w_2 \rangle$$

Prove that there exists a Unitary operator  $U' : V \rightarrow V$  which extends  $U$ , i.e.  $U' |w\rangle = U |w\rangle$  for all  $|w\rangle \in W$ , where  $U'$  is defined in the entire space  $V$ .

**Solution:**

It is given that  $W \subset V$  is a subspace of  $V$ . Then  $V = W \oplus W^\perp$ , where  $W^\perp \subset V$  is the orthogonal complement of  $W$ . Any vector in  $W \subset V$  is orthogonal to a vector in  $W^\perp \subset V$ . Let, the dimension of  $W$ ,  $\dim W = k$ , i.e. the subspace  $W$  has basis vectors, say  $\{|w_1\rangle, |w_2\rangle, \dots, |w_k\rangle\}$ . Then by Gram-Schmidt procedure we can add basis vectors  $\{|w'_{k+1}\rangle, |w'_{k+2}\rangle, \dots, |w'_{k+m}\rangle\} \in W^\perp$ , such that the basis vectors in the entire space  $V$  are  $\{|w_1\rangle, |w_2\rangle, \dots, |w_k\rangle, |w'_{k+1}\rangle, |w'_{k+2}\rangle, \dots, |w'_{k+m}\rangle\}$ . (Note that  $\dim V = \dim W + \dim W^\perp$ ).

Now, by definition a vector in  $W$  is orthogonal to a vector in  $W^\perp$ . So, we have

$$\langle w_i | w'_j \rangle = 0 \quad \text{for} \quad \begin{cases} i = 1, 2, \dots, k \\ j = k+1, k+2, \dots, k+m \end{cases}$$

Next, we see that

$$\text{image}(U) = \{U|w\rangle = |u\rangle \in V \mid |w\rangle \in W\}$$

Hence,  $|u_i\rangle = U|w_i\rangle \in \text{image}(U), i = 1, \dots, k$ . Now, the problem tells us that such a  $U$  is a linear operator that preserves inner products, i.e. for any  $|w_1\rangle$  and  $|w_2\rangle \in W$ , we have  $\langle u_1 | u_2 \rangle = \langle w_1 | U^\dagger U | w_2 \rangle = \langle w_1 | w_2 \rangle$ . Hence,  $U$  preserves orthogonality.

Therefore, using Gram-Schmidt we can extend this for  $i = k+1, \dots, k+m$ . We can add vectors  $|u'_{k+1}\rangle, |u'_{k+2}\rangle, \dots, |u'_{k+m}\rangle$  such that  $|u'_i\rangle \in (\text{image}(U))^\perp \subset V, i = k+1, \dots, k+m$ . Also,  $\langle u_i | u'_j \rangle = 0$  for  $i = 1, \dots, k$  and  $j = k+1, \dots, k+m$ . There is a linear map defined in  $W^\perp$  that maps vectors  $|w'_i\rangle \in W^\perp$  to vectors  $|u'_i\rangle \in V$ .

Next, using  $|w_i\rangle, |u_i\rangle, |w'_i\rangle, |u'_i\rangle$  we construct the following matrix.

$$\sum_{i=1}^k |u_i\rangle \langle w_i| + \sum_{i=k+1}^{k+m} |u'_i\rangle \langle w'_i| \quad (6)$$

We operate the matrix constructed above on a vector  $|v\rangle \in V$ . We want to see if the matrix defined in (4) sends vectors defined in  $V$  to  $V$  itself. Since we have considered  $V = W \oplus W^\perp$ , any vector  $|v\rangle \in V$  can be uniquely represented as  $|v\rangle = \sum_{i=1}^k \alpha_i |w_i\rangle + \sum_{i=k+1}^{k+m} \beta_i |w'_i\rangle$ .

$$\begin{aligned} & \left( \sum_{i=1}^k |u_i\rangle \langle w_i| + \sum_{i=k+1}^{k+m} |u'_i\rangle \langle w'_i| \right) |v\rangle \\ &= \left( \sum_{i=1}^k |u_i\rangle \langle w_i| + \sum_{i=k+1}^{k+m} |u'_i\rangle \langle w'_i| \right) \left( \sum_{i=1}^k \alpha_i |w_i\rangle + \sum_{i=k+1}^{k+m} \beta_i |w'_i\rangle \right) \\ &= \sum_{i=1}^k \sum_{j=1}^k \alpha_j |u_i\rangle \langle w_i | w_j \rangle + \sum_{i=1}^k \sum_{j=k+1}^{k+m} \beta_j |u_i\rangle \langle w_i | w'_j \rangle + \sum_{i=k+1}^{k+m} \sum_{j=1}^k \alpha_j |u'_i\rangle \langle w'_i | w_j \rangle + \sum_{i=k+1}^{k+m} \sum_{j=k+1}^{k+m} \beta_j |u'_i\rangle \langle w'_i | w'_j \rangle \\ &= \sum_{i=1}^k \sum_{j=1}^k \alpha_j |u_i\rangle \delta_{ij} + \sum_{i=k+1}^{k+m} \sum_{j=k+1}^{k+m} \beta_j |u'_i\rangle \delta_{ij} \\ &= \sum_{i=1}^k \alpha_i |u_i\rangle + \sum_{i=k+1}^{k+m} \beta_i |u'_i\rangle \in V \end{aligned}$$

We see that in the four double summation terms above, the second and the third double summation terms vanish because of the fact that  $|w_i\rangle \in W$  is orthogonal to  $|w'_j\rangle \in W^\perp$ . So, the matrix  $\sum_{i=1}^k |u_i\rangle \langle w_i| + \sum_{i=k+1}^{k+m} |u'_i\rangle \langle w'_i|$  maps a  $|v\rangle \in V$  to  $V$ . Next, we define this matrix as

$$U' = \sum_{i=1}^k |u_i\rangle \langle w_i| + \sum_{i=k+1}^{k+m} |u'_i\rangle \langle w'_i|. \quad (7)$$

So, there exists a linear map  $U'$  that sends  $|v\rangle \in V$  to  $V$ .

Next, we want to show that such a linear map defined in the entire space  $V$  agrees with

$U$  defined in  $W$  on any  $|w\rangle \in W$ , i.e.,  $U|w\rangle = U'|w\rangle$ .

$$\begin{aligned} U'|w\rangle &= \left( \sum_{i=1}^k |u_i\rangle \langle w_i| + \sum_{i=k+1}^{k+m} |u'_i\rangle \langle w'_i| \right) |w\rangle \\ &= \sum_{i=1}^k |u_i\rangle \langle w_i|w\rangle + \sum_{i=k+1}^{k+m} |u'_i\rangle \langle w'_i|w\rangle \end{aligned}$$

Now, any  $|w\rangle \in W$  can be written in terms of its basis vectors  $|w_i\rangle$ . And because  $|w'_i\rangle \in W^\perp$  is orthogonal to  $|w_i\rangle \in W$ , the terms in the second summation evaluate to zero. Hence, we have

$$U'|w\rangle = \sum_{i=1}^k |u_i\rangle \langle w_i|w\rangle = \left( \sum_{i=1}^k |u_i\rangle \langle w_i| \right) |w\rangle = U|w\rangle \quad (8)$$

where  $\sum_{i=1}^k |u_i\rangle \langle w_i|$  is the outer product expression for the matrix  $U$  defined in the subspace  $W$ .

Next, we check that such a  $U'$  as defined above is unitary. We want to show that  $U'^\dagger U' = I$ .

$$U'^\dagger U' = \left( \sum_{i=1}^k |w_i\rangle \langle u_i| + \sum_{i=k+1}^{k+m} |w'_i\rangle \langle u'_i| \right) \left( \sum_{i=1}^k |u_i\rangle \langle w_i| + \sum_{i=k+1}^{k+m} |u'_i\rangle \langle w'_i| \right)$$

There are double summation terms that involve inner products  $\langle u_i|u'_i\rangle$  and  $\langle w_i|w'_i\rangle$  which are zero by virtue of orthogonality. The reduced expression reads

$$\begin{aligned} U'^\dagger U' &= \sum_{i=1}^k \sum_{j=1}^k |w_i\rangle \langle u_i|u_j\rangle \langle w_j| + \sum_{i=k+1}^{k+m} \sum_{j=k+1}^{k+m} |w'_i\rangle \langle u'_i|u'_j\rangle \langle w'_j| \\ &= \sum_{i=1}^k |w_i\rangle \langle u_i|u_i\rangle \langle w_i| + \sum_{i=k+1}^{k+m} |w'_i\rangle \langle u'_i|u'_i\rangle \langle w'_i| \\ &= \sum_{i=1}^k |w_i\rangle \langle w_i| + \sum_{i=k+1}^{k+m} |w'_i\rangle \langle w'_i| \\ &= I \end{aligned}$$

Hence,  $U'^\dagger U' = I$ . Similarly, we can show that  $U'U'^\dagger = I$ . Hence,  $U'$  is unitary.

**2.73)** Let  $\rho$  be a density operator. A minimum ensemble is an ensemble  $\{p_i, |\psi_i\rangle\}$  containing a number of elements equal to the rank of  $\rho$ . Let  $|\psi\rangle$  be any vector in the support of  $\rho$ . A support for a Hermitian operator is the space spanned by the eigenvectors with non-zero eigenvalues. Show that there is a minimum ensemble for  $\rho$  containing  $|\psi\rangle$ . In any such ensemble  $|\psi\rangle$  may appear with a probability

$$p_i = \frac{1}{\langle \psi_i | \rho^{-1} | \psi_i \rangle}$$

**Solution:**

Let the dimension for the state space of the entire system be  $d$ . Since the density opera-

tor,  $\rho$  is positive, it has a spectral decomposition. So,  $\rho = \sum_{j=1}^d \lambda_j |x_j\rangle\langle x_j|$ , where  $\lambda_j$ 's are the eigenvalues and  $|x_j\rangle$ 's are the corresponding eigenvectors. The support of  $\rho$  is the space spanned by the eigenvectors corresponding to the non-zero eigenvalues. Let the dimension of the support be  $k$  ( $\leq d$ ), i.e. the number of  $|x_j\rangle$ 's spanning the support is  $k$ . Hence, the spectral decomposition can be rewritten as  $\rho = \sum_{j=1}^k \lambda_j |x_j\rangle\langle x_j|$ .

Next, consider a state vector  $|\psi_i\rangle$  in the support of  $\rho$ . We can write  $|\psi_i\rangle$  as a linear combination of  $|x_j\rangle$ 's since the  $|x_j\rangle$ 's span the support of  $\rho$ . So,  $|\psi_i\rangle = \sum_{j=1}^k c_{ij} |x_j\rangle$ .

In order to show that there exists a minimal ensemble containing any such  $|\psi_i\rangle$  we create an ensemble of states  $\{|\psi_i\rangle\}_{i=1}^k$  and show that the density matrix obtained from such a set is equal to the density  $\rho = \sum_{j=1}^k \lambda_j |x_j\rangle\langle x_j|$ .

Next,  $\rho$  when considered as an operator acting on its own support is full rank. This can be inferred from the diagonal representation of  $\rho = \sum_{i=1}^k \lambda_i |x_i\rangle\langle x_i|$ , where all the  $|x_i\rangle$ 's are the eigenvectors corresponding to non-zero  $\lambda_i$ 's. Consider a density matrix  $\sum_{i=1}^k p_i |\psi_i\rangle\langle \psi_i|$  where  $p_i$  is the probability of the states  $|\psi_i\rangle$  in the support of  $\rho$ . Define a unitary relationship between  $|\psi_i\rangle$  and  $|\lambda_j\rangle$  as follows:

$$\sqrt{p_i} |\psi_i\rangle = \sum_{j=1}^k \sqrt{\lambda_j} u_{ij} |x_j\rangle$$

where  $u_{ij}$  is a unitary matrix of complex numbers with indices  $i$  and  $j$ . Plugging in the expression for  $|\psi_i\rangle$ , i.e.  $|\psi_i\rangle = \sum_{j=1}^k c_{ij} |x_j\rangle$  in the above expression and comparing term-by-term we have

$$\sqrt{p_i} \sum_{j=1}^k c_{ij} |x_j\rangle = \sum_{j=1}^k \sqrt{\lambda_j} u_{ij} |x_j\rangle \Rightarrow \sqrt{p_i} c_{ij} = \sqrt{\lambda_j} u_{ij} \Rightarrow u_{ij} = \frac{\sqrt{p_i} c_{ij}}{\sqrt{\lambda_j}}$$

Since  $u_{ij}$  are the elements of a unitary matrix, it must satisfy  $\sum_{j=1}^k |u_{ij}|^2 = 1$ . Plugging in the expression for  $u_{ij}$  obtained above we have

$$\sum_{j=1}^k \frac{p_i |c_{ij}|^2}{\lambda_j} = 1 \Rightarrow p_i \sum_{j=1}^k \frac{|c_{ij}|^2}{\lambda_j} = 1 \Rightarrow p_i = \frac{1}{\sum_{j=1}^k \frac{|c_{ij}|^2}{\lambda_j}} = \left( \sum_{j=1}^k \frac{|c_{ij}|^2}{\lambda_j} \right)^{-1} \quad (\star)$$

Now, we show that the density matrix  $\sum_{i=1}^k p_i |\psi_i\rangle\langle \psi_i|$  refer to the same density matrix  $\rho = \sum_{j=1}^k \lambda_j |x_j\rangle\langle x_j|$ .

$$\begin{aligned} \sum_{i=1}^k p_i |\psi_i\rangle\langle \psi_i| &= \sum_{i=1}^k \sqrt{p_i} |\psi_i\rangle \sqrt{p_i} \langle \psi_i| = \sum_{i=1}^k \sum_{j=1}^k \sqrt{\lambda_j} u_{ij} |x_j\rangle \sum_{l=1}^k \sqrt{\lambda_l} u_{il}^* \langle x_l| \\ &= \sum_{i=1}^k \sum_{jl} \sqrt{\lambda_j \lambda_l} u_{ij} u_{il}^* |x_j\rangle\langle x_l| = \sum_{jl} \sqrt{\lambda_j \lambda_l} \underbrace{\sum_{i=1}^k u_{ij} u_{il}^*}_{\delta_{jl}} |x_j\rangle\langle x_l| = \sum_{j=1}^k \lambda_j |x_j\rangle\langle x_j| = \rho \end{aligned}$$

where  $\sum_{i=1}^k u_{ij} u_{il}^* = \delta_{jl}$  since  $u_{ij}$  is a unitary matrix.

Hence we have shown that  $\sum_{i=1}^k p_i |\psi_i\rangle\langle \psi_i| = \rho = \sum_{j=1}^k \lambda_j |x_j\rangle\langle x_j|$ . So the sets  $\{p_i, |\psi_i\rangle\}_{i=1}^k$  and  $\{\lambda_j, |x_j\rangle\}_{j=1}^k$  generate the same density matrix. Therefore, we have shown that we can construct a minimal ensemble  $\{p_i, |\psi_i\rangle\}_{i=1}^k$  containing the state  $|\psi_i\rangle$  in the support of  $\rho$ .

Now, we want to obtain the expression of the probability  $p_i$  of the state  $|\psi_i\rangle$  in the minimal ensemble we just constructed.

Since  $\rho$  is full rank (when acting on its own support), it is invertible, i.e.  $\rho^{-1}$  exists. We can also see this from the eigen-decomposition of  $\rho$  which is  $\sum_{j=1}^k \lambda_j |x_j\rangle\langle x_j|$ . Since  $\det(\rho) = \lambda_1 \lambda_2 \cdots \lambda_k$  and all the  $\lambda_j$ 's are non-zero, we can see that  $\rho^{-1}$  exists. In fact,  $\rho^{-1}$  is also Hermitian. This is due to one of the properties of Hermitian matrices which states that the inverse of an invertible Hermitian matrix is Hermitian. Indeed, suppose if  $A$  is Hermitian and invertible then  $A^{-1}A = AA^{-1} = I$ .

Then  $I^\dagger = I \Rightarrow (AA^{-1})^\dagger = AA^{-1} \Rightarrow (A^{-1})^\dagger A^\dagger = AA^{-1} \Rightarrow (A^{-1})^\dagger A^\dagger = A^{-1}A \Rightarrow (A^{-1})^\dagger A = A^{-1}A$  and hence  $(A^{-1})^\dagger = A^{-1}$ .

Next, the eigenvalues of  $\rho^{-1}$  are  $\lambda_j^{-1}$  for  $j = 1, \dots, k$  and the eigen-decomposition is  $\rho^{-1} = \sum_{j=1}^k \lambda_j^{-1} |x_j\rangle\langle x_j|$ . So,  $\rho^{-1}$  can be considered as an observable with outcomes  $\lambda_j^{-1}$  in the support of  $\rho$ .

Therefore, the probability of  $|\psi_i\rangle$  in the minimal ensemble can be obtained as shown below.

$$\langle \psi_i | \rho^{-1} | \psi_i \rangle = \langle \psi_i | \left( \sum_{j=1}^k \lambda_j^{-1} |x_j\rangle\langle x_j| \right) | \psi_i \rangle = \sum_{j=1}^k \lambda_j^{-1} \langle \psi_i | x_j \rangle \langle x_j | \psi_i \rangle = \sum_{j=1}^k \lambda_j^{-1} |\langle \psi_i | x_j \rangle|^2$$

Now, from  $\psi_i = \sum_{j=1}^k c_{ij} |x_j\rangle$  we have  $\langle \psi_i | x_j \rangle = c_{ij}$  and hence

$$\begin{aligned} \langle \psi_i | \rho^{-1} | \psi_i \rangle &= \sum_{j=1}^k \lambda_j^{-1} |\langle \psi_i | x_j \rangle|^2 = \sum_{j=1}^k \lambda_j^{-1} |c_{ij}|^2 = \sum_{j=1}^k \frac{|c_{ij}|^2}{\lambda_j} \stackrel{\text{From } (*)}{=} p_i^{-1} \\ \Rightarrow p_i &= (\langle \psi_i | \rho^{-1} | \psi_i \rangle)^{-1} = \frac{1}{\langle \psi_i | \rho^{-1} | \psi_i \rangle} \end{aligned}$$

**2.78)** a) Prove that a state  $|\psi\rangle$  of a composite system AB is a product state if and only if it has a Schmidt number 1. b) Prove that  $|\psi\rangle$  is a product state if and only if  $\rho_A$  (and thus  $\rho_B$ ) are pure states.

**Solution:**

a) Schmidt Number = 1  $\Rightarrow |\psi\rangle$  is a product state:

It is given that the Schmidt number is 1. So, there exists only one non-zero  $\lambda_i$  such that  $|\psi\rangle = \sum_i \lambda_i |i_A\rangle |i_B\rangle = \lambda |i_A\rangle |i_B\rangle$ . The condition  $\sum_i \lambda_i^2 = 1$  and the fact that there is only one such  $\lambda_i$  implies that  $\lambda_i = \lambda = 1$ . Hence,  $|\psi\rangle = \lambda |i_A\rangle |i_B\rangle = |i_A\rangle |i_B\rangle = |i_A\rangle \otimes |i_B\rangle$ .

In addition, we see that

$$\rho_{AB} = |\psi\rangle\langle\psi| = |i_A\rangle |i_B\rangle \langle i_A| \langle i_B|. \quad (9)$$

Now,  $\rho_A = \text{tr}_B(\rho_{AB}) = \text{tr}_B |i_A\rangle |i_B\rangle \langle i_A| \langle i_B| = |i_A\rangle \langle i_A| \langle i_B | i_B \rangle = |i_A\rangle \langle i_A|$ .

Similarly,  $\rho_B = \text{tr}_A(\rho_{AB}) = |i_B\rangle \langle i_B|$ . We take the (tensor) product of the two density matrices  $\rho_A$  and  $\rho_B$ .



$$\rho_A \otimes \rho_B = |i_A\rangle\langle i_A| \otimes |i_B\rangle\langle i_B| = |i_A\rangle\langle i_A| \otimes |i_B\rangle\langle i_B| = |i_A\rangle\langle i_A| |i_B\rangle\langle i_B| = \rho_{AB} \quad (10)$$

where we have used the property of tensor products:  $(S_1 T_1) \otimes (S_2 T_2) = (S_1 \otimes S_2)(T_1 \otimes T_2)$ .

$|\psi\rangle$  is a product state  $\Rightarrow$  Schmidt number = 1:

The Schmidt number is always greater than or equal to 1.

Now, we are given that  $|\psi_{AB}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$ . We assume that the states  $|\psi_A\rangle$  and  $|\psi_B\rangle$  are normalized, i.e. they are of unit length. We claim that  $|\psi_{AB}\rangle$  is already in the Schmidt decomposed form. This is because  $|\psi_A\rangle$  and  $|\psi_B\rangle$  are unit vectors (by assumption). And we can find normalized states  $\{|\psi'_A\rangle\}$  and  $\{|\psi'_B\rangle\}$  that are orthogonal to  $|\psi_A\rangle$  and  $|\psi_B\rangle$  respectively and write the decomposition as  $|\psi_{AB}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle + \sum 0 \cdot |\psi'_A\rangle \otimes |\psi'_B\rangle$ .

This shows that the Schmidt number of  $|\psi_{AB}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$  is 1.

Next, we show that  $|\psi\rangle$  is a product state if and only if  $\rho_A$  and  $\rho_B$  are pure states.

b)  $|\psi\rangle$  is a product state  $\Rightarrow \rho_A$  and  $\rho_B$  are pure states:

$|\psi\rangle$  is a product state. As shown in part a) of the problem the Schmidt number is equal to 1. Hence, the Schmidt decomposition of  $|\psi\rangle$  is  $|\psi\rangle = \lambda |i_A\rangle |i_B\rangle$  and because  $\lambda$  must satisfy the condition  $\lambda^2 = 1$  and  $\lambda \geq 0$ , we have  $\lambda = 1$ . So,  $|\psi\rangle = |i_A\rangle |i_B\rangle$ . Therefore, the density matrix for  $|\psi\rangle$  is  $\rho_{AB} = |\psi\rangle\langle\psi| = |i_A i_B\rangle\langle i_A i_B|$ . Taking the partial trace with respect to  $A$  and  $B$  respectively gives us  $\rho_A$  and  $\rho_B$ .

$$\rho_A = \text{tr}_B \rho_{AB} = \text{tr}_B (|i_A i_B\rangle\langle i_A i_B|) = |i_A\rangle\langle i_A| \text{tr}(|i_B\rangle\langle i_B|) = |i_A\rangle\langle i_A| \langle i_B | i_B \rangle = |i_A\rangle\langle i_A|$$

Taking the trace of  $\rho_A^2$  gives us the following:

$$\text{tr}(\rho_A^2) = \text{tr}(|i_A\rangle\langle i_A| |i_A\rangle\langle i_A|) = \text{tr}(|i_A\rangle\langle i_A|) = \text{tr} \rho_A = 1$$

Similarly, obtaining  $\rho_B$  using  $\text{tr}_A \rho_{AB}$  and taking the trace  $\text{tr}(\rho_B^2)$  we get  $\text{tr}(\rho_B^2) = 1$ . Hence,  $\rho_A$  and  $\rho_B$  are pure states.

$\rho_A$  and  $\rho_B$  are pure states  $\Rightarrow |\psi\rangle$  is a product state:

Consider the Schmidt decomposition:  $|\psi\rangle = \sum_i \lambda_i |i_A\rangle |i_B\rangle$ .

Given that  $\rho_A$  and  $\rho_B$  are pure states, we show that  $|\psi\rangle$  is a product state, i.e. the Schmidt decomposition turns out to be  $|\psi\rangle = |i_A\rangle |i_B\rangle$ . It suffices to show that the Schmidt number of  $|\psi\rangle$  is equal to 1. Now, we have  $\rho_A = \sum_i \lambda_i^2 |i_A\rangle\langle i_A|$  and  $\rho_B = \sum_i \lambda_i^2 |i_B\rangle\langle i_B|$  by taking the partial trace of  $\rho_{AB}$  with respect to  $B$  and  $A$  respectively.

Also,

$$\rho_A^2 = \sum_i \lambda_i^2 |i_A\rangle \langle i_A| \sum_i \lambda_i^2 |i_A\rangle \langle i_A| = \sum_{ij} \lambda_i^2 \lambda_j^2 |i_A\rangle \underbrace{\langle i_A | j_A \rangle}_{=\delta_{ij}} \langle j_A| = \sum_i \lambda_i^4 |i_A\rangle \langle i_A|$$

Similarly,  $\rho_B^2 = \sum_i \lambda_i^4 |i_B\rangle \langle i_B|$ . Since  $\rho_A$  and  $\rho_B$  are pure states,

$$\begin{aligned} \text{tr}(\rho_A^2) &= \text{tr}\left(\sum_i \lambda_i^4 |i_A\rangle \langle i_A|\right) = 1 \\ \text{tr}(\rho_B^2) &= \text{tr}\left(\sum_i \lambda_i^4 |i_B\rangle \langle i_B|\right) = 1 \end{aligned}$$

Note that  $\{|i_A\rangle\}$  and  $\{|i_B\rangle\}$  are respectively sets of orthonormal states. By Gram-Schmidt procedure we can extend them to orthonormal basis sets. And hence  $\sum_i \lambda_i^4 |i_A\rangle \langle i_A|$  and  $\sum_i \lambda_i^4 |i_B\rangle \langle i_B|$  are the diagonal representations of  $\rho_A^2$  and  $\rho_B^2$  respectively. The trace conditions (obtained above) for both of them show that  $\sum_i \lambda_i^4 = 1$ . Also, since  $\rho_A$  and  $\rho_B$  are densities, by their expressions obtained from the partial trace of  $\rho_{AB}$  we must have  $\text{tr}\rho_A = \text{tr}\rho_B = \sum_i \lambda_i^2 = 1$ . Hence,  $\lambda_i$ 's must satisfy:  $\sum_i \lambda_i^4 = \sum_i \lambda_i^2 = 1$  with the constraint  $\lambda_i \geq 0$  (with at least one  $\lambda_i > 0$ ). The only permissible solution is:  $\lambda_i = 1$  for some index  $i$  and the rest  $\lambda_{\neq i} = 0$ .

Hence, we have shown that the Schmidt number is 1 and therefore, the Schmidt decomposition of  $|\psi\rangle$  turns out to be  $|i_A\rangle |i_B\rangle$  which shows that it is a product state.

**2.80)** Suppose  $|\psi\rangle$  and  $|\phi\rangle$  are two pure states of a composite quantum system with components  $A$  and  $B$ , with identical Schmidt coefficients. Show that there are unitary transformations  $U$  on system  $A$  and  $V$  on system  $B$  such that  $|\psi\rangle = (U \otimes V)|\phi\rangle$ .

**Solution:**

We represent the pure states of the composite quantum system  $AB$  in their Schmidt decomposition form. The states  $|\psi\rangle$  and  $|\phi\rangle$  can be written as

$$\begin{aligned} |\psi\rangle &= \sum_i \lambda_i |x_i^A\rangle |x_i^B\rangle \\ |\phi\rangle &= \sum_i \lambda_i |y_i^A\rangle |y_i^B\rangle \end{aligned}$$

The vectors  $|x_i^A\rangle, |x_i^B\rangle, |y_i^A\rangle, |y_i^B\rangle$  are orthonormal bases.  $\lambda_i$  is the Schmidt coefficient.

**Note:** In *Nielsen and Chuang*  $|x_i^A\rangle, |x_i^B\rangle, |y_i^A\rangle, |y_i^B\rangle$  have been referred to as orthonormal states. However, it depends on how we choose to see it. If we allow  $\lambda_i = 0$  in the expression for Schmidt decomposition, we can refer  $|x_i^A\rangle, |x_i^B\rangle, |y_i^A\rangle, |y_i^B\rangle$  as orthonormal bases. The following example explains it further.

For the state  $|\psi\rangle = \frac{1}{2}(|00\rangle - |01\rangle - |10\rangle + |11\rangle)$  in the composite system  $AB$  we can write  $|\psi\rangle$  in the Schmidt decomposition formula as  $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = |-\rangle |-\rangle$  with a Schmidt coefficient of  $\lambda_1 = 1$ . However, we can also see it as  $|\psi\rangle = 1 \times |-\rangle |-\rangle + 0 \times |+\rangle |+\rangle$ . And  $|-\rangle = \left(\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)\right)$  and  $|+\rangle = \left(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right)$  are orthonormal bases for the state space of both  $A$  and  $B$ .

Next, we define linear maps  $U : A \rightarrow A$  and  $V : B \rightarrow B$  as follows.

$$U = \sum_i |x_i^A\rangle\langle y_i^A| \quad V = \sum_i |x_i^B\rangle\langle y_i^B|$$

We can check that they are unitary, i.e. they satisfy  $U^\dagger U = U U^\dagger = I$  and  $V^\dagger V = V V^\dagger = I$ .

$$U^\dagger U = \left( \sum_i |x_i^A\rangle\langle y_i^A| \right)^\dagger \left( \sum_i |x_i^A\rangle\langle y_i^A| \right) = \left( \sum_i |y_i^A\rangle\langle x_i^A| \right) \left( \sum_i |x_i^A\rangle\langle y_i^A| \right) = \sum_{ij} |y_i^A\rangle\langle x_i^A| \underbrace{|x_i^A\rangle\langle x_j^A|}_{=\delta_{ij}} \langle y_j^A| = \sum_i |y_i^A\rangle\langle y_i^A| = I$$

Since  $|y_i^A\rangle$ 's are orthonormal  $|y_i^A\rangle\langle y_i^A|$ 's are projective measurements and they follow the completeness relation, i.e.  $\sum_i |y_i^A\rangle\langle y_i^A| = I$ . The same is true for  $|x_i^A\rangle$ 's.

$$U U^\dagger = \left( \sum_i |x_i^A\rangle\langle y_i^A| \right) \left( \sum_i |y_i^A\rangle\langle x_i^A| \right)^\dagger = \left( \sum_i |x_i^A\rangle\langle y_i^A| \right) \left( \sum_i |y_i^A\rangle\langle x_i^A| \right) = \sum_{ij} |x_i^A\rangle\langle y_i^A| \underbrace{|y_i^A\rangle\langle y_j^A|}_{=\delta_{ij}} \langle x_j^A| = \sum_i |x_i^A\rangle\langle x_i^A| = I$$

Similarly, we can show that  $V = \sum_i |x_i^B\rangle\langle y_i^B|$  satisfies  $V^\dagger V = V V^\dagger = I$ . Hence, both  $U$  and  $V$  are unitary.

Next, we do the following.

$$\begin{aligned} (U \otimes V)|\phi\rangle &= (U \otimes V) \sum_i \lambda_i |y_i^A\rangle |y_i^B\rangle = \sum_i \lambda_i U |y_i^A\rangle \otimes V |y_i^B\rangle \\ &= \sum_i \lambda_i \underbrace{\left( \sum_i |x_i^A\rangle\langle y_i^A| \right) |y_i^A\rangle}_{=|x_i^A\rangle} \otimes \underbrace{\left( \sum_i |x_i^B\rangle\langle y_i^B| \right) |y_i^B\rangle}_{=|x_i^B\rangle} = \sum_i \lambda_i |x_i^A\rangle |x_i^B\rangle = |\psi\rangle \end{aligned}$$

Note that  $\left( \sum_i |x_i^A\rangle\langle y_i^A| \right) |y_i^A\rangle = \sum_k |x_k^A\rangle\langle y_k^A| y_i^A\rangle \delta_{ik} = |x_i^A\rangle$  and  $\left( \sum_i |x_i^B\rangle\langle y_i^B| \right) |y_i^B\rangle = \sum_k |x_k^B\rangle\langle y_k^B| y_i^B\rangle \delta_{ik} = |x_i^B\rangle$ . Hence, we have shown that there exists unitary transformations  $U$  on system  $A$  and  $V$  on system  $B$  such that  $|\psi\rangle = (U \otimes V)|\phi\rangle$ .

**2.81) (Freedom in purifications)** Let  $|AR_1\rangle$  and  $|AR_2\rangle$  be two purifications of a state  $\rho^A$  to a composite system  $AR$ . Prove that there exists a unitary transformation  $U_R$  acting on system  $R$  such that  $|AR_1\rangle = (I_A \otimes U_R)|AR_2\rangle$ .

**Solution:**

It is given that both pure states  $|AR_1\rangle$  and  $|AR_2\rangle$  are purifications of the impure state  $\rho^A$  (in system  $A$ ). Hence, it must be that

$$\rho^A = \text{tr}_R |AR_1\rangle\langle AR_1| = \text{tr}_R |AR_2\rangle\langle AR_2| \quad (11)$$

Suppose the pure states  $|AR_1\rangle$  and  $|AR_2\rangle$  have Schmidt decomposition:  $|AR_1\rangle = \sum_i \lambda_i |u_i^A\rangle |u_i^R\rangle$  and  $|AR_2\rangle = \sum_j \mu_j |v_j^A\rangle |v_j^R\rangle$ . We consider the states  $|u_i^A\rangle, |u_i^R\rangle, |v_j^A\rangle, |v_j^R\rangle$  to be orthonormal basis in systems  $A$  and  $R$ . Then the Schmidt number or Schmidt rank is the number of

non-zero  $\lambda_i$  (and  $\mu_j$ ) in the Schmidt decomposition of  $|AR_1\rangle$  (and  $|AR_2\rangle$ ). From (11) we have

$$\rho^A = \sum_i \lambda_i^2 |u_i^A\rangle\langle u_i^A| = \sum_j \mu_j^2 |v_j^A\rangle\langle v_j^A| \quad (12)$$

The Schmidt coefficients  $\lambda_i$  (and  $\mu_j$ ) are the square root of the eigenvalues of the reduced density matrix (impure state)  $\rho^A$ . The eigenvalues (and hence the coefficients) are unique, so for (2) we must have  $\lambda_i = \mu_j$ . With the assumption that the eigenvalues are non-degenerate, the eigenvectors  $|u_i^A\rangle$  and  $|v_j^A\rangle$  associated with  $\lambda_i$  and  $\mu_j$  respectively are also uniquely determined. If  $\lambda_i = \mu_j$ , then it must be that  $|u_i^A\rangle = |v_j^A\rangle$ .

Next, we define  $U_R = \sum_{i=1}^k |u_i^R\rangle\langle v_i^R|$  where  $k = \text{Sch}(AR_1) = \text{Sch}(AR_2)$ .

$$(I_A \otimes U_R)|AR_2\rangle = (I_A \otimes U_R) \sum_{j=1}^k \mu_j |v_j^A\rangle \otimes |v_j^R\rangle = \sum_{j=1}^k \mu_j I |v_j^A\rangle \otimes U_R |v_j^R\rangle = \sum_{j=1}^k \lambda_j |u_j^A\rangle |u_j^R\rangle = |AR_1\rangle$$

Hence,  $|AR_1\rangle = (I_A \otimes U_R)|AR_2\rangle$ .

*Note:*  $U_R |v_j^R\rangle = \left( \sum_{i=1}^k |u_i^R\rangle\langle v_i^R| \right) |v_j^R\rangle = \sum_{i=1}^k |u_i^R\rangle \langle v_i^R | v_j^R \rangle \delta_{ij} = |u_j^R\rangle$ .

**2.82)** Suppose  $\{p_i, |\psi_i\rangle\}$  is an ensemble of states generating a density matrix  $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$  for a quantum system  $A$ . Introduce a system  $R$  with an orthonormal basis  $|i\rangle$ .

(1) Show that  $\sum_i \sqrt{p_i} |\psi_i\rangle |i\rangle$  is a purification of  $\rho$ .

(2) Suppose we measure  $R$  in the basis  $|i\rangle$ , obtaining outcome  $i$ . With what probability do we obtain the result  $i$ , and what is the corresponding state of system  $A$ ?

(3) Let  $|AR\rangle$  be any purification of  $\rho$  to the system  $AR$ . Show that there exists an orthonormal basis  $|i\rangle$  in which  $R$  can be measured such that the corresponding post-measurement state for system  $A$  is  $|\psi_i\rangle$  with probability  $p_i$ .

**Solution:**

(1) We denote  $\sum_i \sqrt{p_i} |\psi_i\rangle |i\rangle$  as  $|AR\rangle$ .  $|\psi_i\rangle$  is any state in the system  $A$  (not necessarily orthonormal).  $|AR\rangle = \sum_i \sqrt{p_i} |\psi_i\rangle |i\rangle$

$$\begin{aligned} |AR\rangle\langle AR| &= \left( \sum_i \sqrt{p_i} |\psi_i\rangle |i\rangle \right) \left( \sum_j \sqrt{p_j} \langle\psi_j| \langle j| \right) \\ &\Rightarrow |AR\rangle\langle AR| = \sum_{ij} \sqrt{p_i p_j} |\psi_i\rangle |i\rangle \langle\psi_j| \langle j| \end{aligned}$$

$$\begin{aligned} \text{tr}_R(|AR\rangle\langle AR|) &= \sum_{ij} \sqrt{p_i p_j} |\psi_i\rangle \langle\psi_j| \text{tr}_R(|i\rangle\langle j|) = \sum_{ij} \sqrt{p_i p_j} |\psi_i\rangle \langle\psi_j| \langle j|i\rangle = \sum_{ij} \sqrt{p_i p_j} |\psi_i\rangle \langle\psi_j| \delta_{ij} \\ &\Rightarrow \text{tr}_R(|AR\rangle\langle AR|) = \sum_i p_i |\psi_i\rangle \langle\psi_i| = \rho \end{aligned}$$

Hence  $\sum_i p_i |\psi_i\rangle |i\rangle$  is a purification of  $\rho$  since the partial trace  $\text{tr}_R(|AR\rangle\langle AR|)$  gives the density matrix  $\rho$  generated by the ensemble of states  $\{p_i, |\psi_i\rangle\}$ .

(2) We want to obtain the outcome  $i$  by measuring system  $R$  in the basis  $|i\rangle$ . *To measure in basis  $|i\rangle$*  means to perform projective measurement using the projectors  $|i\rangle\langle i|$ . We use the projective operator  $I \otimes |i\rangle\langle i|$  in the space of system  $AR$  on the state  $|AR\rangle = \sum_j \sqrt{p_j} |\psi_j\rangle |j\rangle$  to measure  $R$ . The probability of obtaining the outcome  $i$  is

$$\begin{aligned} & \left( \sum_j \sqrt{p_j} |\psi_j\rangle |j\rangle \right)^\dagger \left( I \otimes |i\rangle\langle i| \right) \left( \sum_j \sqrt{p_j} |\psi_j\rangle |j\rangle \right) \\ &= \left( \sum_j \sqrt{p_j} \langle \psi_j | \langle j | \right) \left( I \otimes |i\rangle\langle i| \right) \left( \sum_j \sqrt{p_j} |\psi_j\rangle |j\rangle \right) \\ &= \left( \sum_j \sqrt{p_j} \langle \psi_j | \langle j | \right) \left( \sum_j \sqrt{p_j} I |\psi_j\rangle \otimes |i\rangle\langle i| j \right) \delta_{ij} \\ &= \left( \sum_j \sqrt{p_j} \langle \psi_j | \langle j | \right) \sqrt{p_i} |\psi_i\rangle \otimes |i\rangle = \sum_j \sqrt{p_j} \sqrt{p_i} \langle \psi_j | \psi_i \rangle \delta_{ij} = p_i \langle \psi_i | \psi_i \rangle = p_i \end{aligned}$$

Hence, the probability of obtaining the outcome  $i$  by measuring  $R$  in the basis  $|i\rangle$  is  $p_i$ . The post measurement state of the system  $AR$  is

$$\frac{(I \otimes |i\rangle\langle i|) |AR\rangle}{\sqrt{p_i}} = \frac{(I \otimes |i\rangle\langle i|) \sum_j \sqrt{p_j} |\psi_j\rangle |j\rangle}{\sqrt{p_i}} = \frac{\sqrt{p_i} |\psi_i\rangle |i\rangle}{\sqrt{p_i}} = |\psi_i\rangle |i\rangle$$

We see that the corresponding state of system  $A$  is  $|\psi_i\rangle$ .

(3) The density matrix generated by the ensemble of states  $\{p_i, |\psi_i\rangle\}$  is  $\sum_i p_i |\psi_i\rangle\langle \psi_i|$ . We assume the states  $|\psi_i\rangle$  to be normalized. However, they are not necessarily orthogonal.  $|AR\rangle$  is a purification of  $\rho$  to the system  $AR$ . Let the orthonormal decomposition of  $\rho$  be  $\sum_k \mu_k |u_k^A\rangle\langle u_k^A|$ . As a consequence of Theorem 2.6 (unitary freedom in the ensemble of density matrices) we can say that  $\rho = \sum_k \mu_k |u_k^A\rangle\langle u_k^A| = \sum_i p_i |\psi_i\rangle\langle \psi_i|$  for normalized states  $|u_k^A\rangle$  and  $|\psi_i\rangle$  if and only if

$$\sqrt{\mu_k} |u_k^A\rangle = \sum_i v_{ik} \sqrt{p_i} |\psi_i\rangle$$

where  $v_{ik}$  are the entries of a unitary matrix and we can pad the smaller ensemble with zeroes to make the two ensembles the same size.

The Schmidt representation for the pure state  $|AR\rangle$  is  $\sum_k \sqrt{\mu_k} |u_k^A\rangle |k^R\rangle$  where  $|k^R\rangle$  are a set of orthonormal states in system  $R$ . Substituting the expression for  $\sqrt{\mu_k} |u_k^A\rangle$  we have the following

$$|AR\rangle = \sum_k \sqrt{\mu_k} |u_k^A\rangle |k^R\rangle = \sum_k \left( \sum_i \sqrt{p_i} v_{ik} |\psi_i\rangle \right) |k^R\rangle = \sum_i \sum_k \sqrt{p_i} v_{ik} |\psi_i\rangle \otimes |k^R\rangle = \sum_i \sqrt{p_i} |\psi_i\rangle \otimes \sum_k v_{ik} |k^R\rangle$$

Next, we define  $|i\rangle = \sum_k v_{ik} |k^R\rangle$ . We can check if  $|i\rangle$  (as defined) is orthonormal.

$$\langle j | i \rangle = \left( \sum_k v_{jk}^* \langle k^R | \right) \left( \sum_k v_{ik} |k^R\rangle \right) = \sum_{lk} v_{jl}^* v_{ik} \underbrace{\langle l^R | k^R \rangle}_{=\delta_{lk}} = \underbrace{\sum_l v_{jl}^* v_{il}}_{\text{due to unitarity of } v_{ik}} = \delta_{ij}$$

We see that  $|i\rangle = \sum_k v_{ik} |k^R\rangle$  is orthonormal. But it might not be a basis of system  $R$ . We can use Gram Schmidt method to extend it to an orthonormal basis for system  $R$ . So, there exists an orthonormal basis to measure  $R$  such that the corresponding post-measurement state for system  $A$  is  $|\psi_i\rangle$  with probability  $p_i$ .

**Problem 2.1: (Functions of Pauli Matrices)** Let  $f(\cdot)$  be any function from complex numbers to complex numbers. Let  $\vec{n}$  be a normalized vector in three dimensions, and let  $\theta$  be real. Show that

$$f(\theta \vec{n} \cdot \vec{\sigma}) = \frac{f(\theta) + f(-\theta)}{2} I + \frac{f(\theta) - f(-\theta)}{2} \vec{n} \cdot \vec{\sigma} \quad (13)$$

**Solution:**  $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$  are the Pauli matrices. In Problem 2.60 it was already shown that  $\vec{n} \cdot \vec{\sigma} = n_1 \sigma_1 + n_2 \sigma_2 + n_3 \sigma_3$  has eigenvalues  $\pm 1$ . Suppose  $|v_+\rangle$  and  $|v_-\rangle$  are the eigenvectors corresponding to the eigenvalues  $+1$  and  $-1$ . Then we can write  $\vec{n} \cdot \vec{\sigma}$  as

$$\vec{n} \cdot \vec{\sigma} = |v_+\rangle \langle v_+| - |v_-\rangle \langle v_-| \quad (14)$$

Also, because  $|v_+\rangle \langle v_+|$  and  $|v_-\rangle \langle v_-|$  are measurement operators they add up to  $I$ .

$$|v_+\rangle \langle v_+| + |v_-\rangle \langle v_-| = I \quad (15)$$

Given a function from complex numbers to complex numbers it is possible to define a corresponding operator function. If  $A = \sum_a a |a\rangle \langle a|$  is the spectral decomposition of the operator  $A$  then  $f(A) = \sum_a f(a) |a\rangle \langle a|$ . Using this we can proceed with the given problem as shown below.

$$\begin{aligned} \theta \vec{n} \cdot \vec{\sigma} &= \theta |v_+\rangle \langle v_+| + (-\theta) |v_-\rangle \langle v_-| \\ f(\theta \vec{n} \cdot \vec{\sigma}) &= f(\theta) |v_+\rangle \langle v_+| + f(-\theta) |v_-\rangle \langle v_-| \\ f(\theta \vec{n} \cdot \vec{\sigma}) &= \frac{f(\theta) + f(-\theta) - f(-\theta) + f(\theta)}{2} |v_+\rangle \langle v_+| + \frac{f(-\theta) + f(\theta) - f(\theta) + f(-\theta)}{2} |v_-\rangle \langle v_-| \\ &= \frac{f(\theta) + f(-\theta)}{2} |v_+\rangle \langle v_+| + \frac{f(\theta) - f(-\theta)}{2} |v_+\rangle \langle v_+| + \frac{f(\theta) + f(-\theta)}{2} |v_-\rangle \langle v_-| + \frac{f(-\theta) - f(\theta)}{2} |v_-\rangle \langle v_-| \\ &= \frac{f(\theta) + f(-\theta)}{2} (|v_+\rangle \langle v_+| + |v_-\rangle \langle v_-|) + \frac{f(\theta) - f(-\theta)}{2} (|v_+\rangle \langle v_+| - |v_-\rangle \langle v_-|) \\ &\Rightarrow f(\theta \vec{n} \cdot \vec{\sigma}) = \frac{f(\theta) + f(-\theta)}{2} I + \frac{f(\theta) - f(-\theta)}{2} \vec{n} \cdot \vec{\sigma} \quad \text{from (4) and (5)} \end{aligned}$$

**Problem 2.2: (Properties of the Schmidt Number)** Suppose  $|\psi\rangle$  is a pure state of a composite system with components  $A$  and  $B$ .

(1) Prove that the Schmidt number of  $|\psi\rangle$  is the rank of the reduced density matrix  $\rho_A = \text{tr}_B |\psi\rangle\langle\psi|$ . (Note that the rank of a Hermitian operator is equal to the dimension of its support).

(2) Suppose  $\sum_j |\alpha_j\rangle |\beta_j\rangle$  is a representation for  $|\psi\rangle$ , where  $|\alpha_j\rangle$  and  $|\beta_j\rangle$  are (un-normalized) states for systems  $A$  and  $B$ , respectively. Prove that the number of terms in such a decomposition is greater than or equal to the Schmidt number of  $|\psi\rangle$ ,  $\text{Sch}(\psi)$ .

(3) Suppose  $|\psi\rangle = \alpha |\phi\rangle + \beta |\gamma\rangle$ . Prove that

$$\text{Sch}(\psi) \geq |\text{Sch}(\phi) - \text{Sch}(\gamma)| \quad (16)$$

**Solution:**

1) Let the Schmidt decomposition of  $|\psi\rangle$  be  $\sum_i \lambda_i |u_i\rangle |v_i\rangle$ , where we consider  $|u_i\rangle$  and  $|v_i\rangle$  as the orthonormal basis of systems  $A$  and  $B$  respectively. The Schmidt number is the number of non-zero  $\lambda_i$ 's in the Schmidt decomposition of  $|\psi\rangle$ . The reduced density matrix obtained by taking the partial trace of  $|\psi\rangle\langle\psi|$  with respect to  $B$  is  $\text{tr}_B |\psi\rangle\langle\psi| = \rho_A = \sum_i \lambda_i^2 |u_i\rangle\langle u_i|$ . This is the diagonal representation of  $\rho_A$  since  $|u_i\rangle$  is an orthonormal basis set in  $A$ .

Next, by the Rank-Nullity theorem we see that the rank of  $\rho_A$  is the number of non-zero  $\lambda_i$ 's in the expression  $\sum_i \lambda_i^2 |u_i\rangle\langle u_i|$ . Since this expression is obtained by taking the partial trace of  $|\psi\rangle\langle\psi|$  wrt  $B$ , it follows that the Schmidt number of  $|\psi\rangle$  is the rank of the reduced density matrix  $\rho_A = \text{tr}_B |\psi\rangle\langle\psi|$ . And since the support of  $\rho_A$  (a Hermitian operator) is the space spanned by its eigenvectors corresponding to non-zero eigenvalues, it follows that the rank of  $\rho_A$  is the dimension of its support.

(2) We start with the Schmidt decomposition of  $|\psi\rangle$ .

$|\psi\rangle = \sum_{i=1}^I \lambda_i |i_A\rangle |i_B\rangle$ , where  $I = \text{Sch}(\psi) \leq \min(d_A, d_B)$  and  $d_A = \dim(A)$ ,  $d_B = \dim(B)$ . We know the states  $|i_A\rangle$  and  $|i_B\rangle$  are orthonormal.

Rewriting the Schmidt decomposition as  $|\psi\rangle = \sum_{i=1}^I \sqrt{\lambda_i} |i_A\rangle \sqrt{\lambda_i} |i_B\rangle = \sum_{i=1}^I |\tilde{i}_A\rangle |\tilde{i}_B\rangle$ , we see that the states  $|\tilde{i}_A\rangle = \sqrt{\lambda_i} |i_A\rangle$  and  $|\tilde{i}_B\rangle = \sqrt{\lambda_i} |i_B\rangle$  are un-normalized states.

Next, we write  $|\tilde{i}_B\rangle$  in the standard basis  $|k\rangle$  of  $B$ :  $|\tilde{i}_B\rangle = \sum_{k=1}^{d_B} c_{ik} |k\rangle$ . Plugging this in the expression of  $|\psi\rangle$  we have

$$|\psi\rangle = \sum_{i=1}^I |\tilde{i}_A\rangle |\tilde{i}_B\rangle = \sum_{i=1}^I |\tilde{i}_A\rangle \left( \sum_{k=1}^{d_B} c_{ik} |k\rangle \right) = \underbrace{\sum_{i=1}^I \sum_{k=1}^{d_B}}_{\text{Re-index } j=1 \text{ to } Id_B} \underbrace{|\tilde{i}_A\rangle c_{ik}}_{|\alpha_j\rangle} \underbrace{|k\rangle}_{|\beta_j\rangle} = \sum_{j=1}^{Id_B} |\alpha_j\rangle |\beta_j\rangle$$

where  $|\alpha_j\rangle$  and  $|\beta_j\rangle$  are un-normalized.

In the expression  $\sum_j |\alpha_j\rangle |\beta_j\rangle$  the number of terms  $Id_B$  is greater than or equal to  $I = \text{Sch}(\psi)$ .

(3)  $|\psi\rangle = \alpha |\phi\rangle + \beta |\gamma\rangle$ . Expressing  $|\psi\rangle$ ,  $|\phi\rangle$  and  $|\gamma\rangle$  in the standard basis we have

$$\begin{aligned}
|\psi\rangle &= \alpha|\phi\rangle + \beta|\gamma\rangle \\
\Rightarrow \sum_{jk} a_{jk} |j\rangle |k\rangle &= \alpha \sum_{jk} b_{jk} |j\rangle |k\rangle + \beta \sum_{jk} c_{jk} |j\rangle |k\rangle = \sum_{jk} (\alpha b_{jk} + \beta c_{jk}) |j\rangle |k\rangle
\end{aligned}$$

Comparing term by term we have  $a_{jk} = \alpha b_{jk} + \beta c_{jk}$ . Each of the terms  $a_{jk}, b_{jk}, c_{jk}$  are entries of matrices  $\mathbf{A}, \mathbf{B}$  and  $\mathbf{C}$  respectively. Using singular value decomposition (svd) we have  $\mathbf{A} = \mathbf{U}_\mathbf{A} \mathbf{D}_\mathbf{A} \mathbf{V}_\mathbf{A}$  where  $\mathbf{D}_\mathbf{A}$  is a diagonal matrix with non-negative entries and  $\mathbf{U}_\mathbf{A}$  and  $\mathbf{V}_\mathbf{A}$  are unitary matrices. The rank of  $\mathbf{A}$  is the number of non-zero entries of  $\mathbf{D}_\mathbf{A}$ . Likewise, we can use svd on  $\mathbf{B}$  and  $\mathbf{C}$ . From  $a_{jk} = \alpha b_{jk} + \beta c_{jk}$  we have  $\mathbf{A} = \alpha \mathbf{B} + \beta \mathbf{C}$ . One of the classical inequalities in Linear Algebra is the rank-sum inequality that states

$$|\text{rank}(\mathbf{B}) - \text{rank}(\mathbf{C})| \leq \text{rank}(\mathbf{B} + \mathbf{C}) \leq \text{rank}(\mathbf{B}) + \text{rank}(\mathbf{C})$$

Hence for  $\mathbf{A} = \alpha \mathbf{B} + \beta \mathbf{C}$  we have

$$\text{rank}(\mathbf{A}) \geq |\text{rank}(\mathbf{B}) - \text{rank}(\mathbf{C})| \quad (17)$$

Now  $\text{rank}(\mathbf{A})$  is equal to the rank of  $\mathbf{D}_\mathbf{A}$ , i.e. the diagonal matrix in its singular value decomposition, which in turn is equal to the number of non-zero entries along the diagonal. Hence,  $\text{rank}(\mathbf{A}) = \text{rank}(\mathbf{D}_\mathbf{A}) = \text{Sch}(\psi)$ . Likewise,  $\text{rank}(\mathbf{B}) = \text{Sch}(\phi)$  and  $\text{rank}(\mathbf{C}) = \text{Sch}(\gamma)$ . Therefore, from (7) we have

$$\text{Sch}(\psi) \geq |\text{Sch}(\phi) - \text{Sch}(\gamma)|$$

**Problem 2.3: (Tsirelson's Inequality)** Suppose  $\vec{Q} = \vec{q} \cdot \vec{\sigma}$ ,  $\vec{R} = \vec{r} \cdot \vec{\sigma}$ ,  $\vec{S} = \vec{s} \cdot \vec{\sigma}$ ,  $\vec{T} = \vec{t} \cdot \vec{\sigma}$  where  $\vec{q}, \vec{r}, \vec{s}, \vec{t}$  are real unit vectors in three dimensions. Show that

$$(\vec{Q} \otimes \vec{S} + \vec{R} \otimes \vec{S} + \vec{R} \otimes \vec{T} - \vec{Q} \otimes \vec{T})^2 = 4I + [\vec{Q}, \vec{R}] \otimes [\vec{S}, \vec{T}] \quad (18)$$

Use this result to prove that

$$\langle \vec{Q} \otimes \vec{S} \rangle + \langle \vec{R} \otimes \vec{S} \rangle + \langle \vec{R} \otimes \vec{T} \rangle - \langle \vec{Q} \otimes \vec{T} \rangle \leq 2\sqrt{2} \quad (19)$$

so the violation of the Bell inequality is the maximum possible in quantum mechanics.

**Solution:**

In problem 2.60 we showed that the observable  $Q = \vec{q} \cdot \vec{\sigma}$  has eigenvalues  $\pm 1$  and the corresponding eigenspaces have projectors  $P_\pm = (I \pm \vec{q} \cdot \vec{\sigma})/2$ . Hence,  $Q$  can be written as  $Q = \vec{q} \cdot \vec{\sigma} = (+1)P_+ + (-1)P_-$ . Note that  $P_\pm^2 = P_\pm$ .



We see that

$$\begin{aligned}
Q^2 &= (\vec{q} \cdot \vec{\sigma})^2 = ((+1)P_+ + (-1)P_-)^2 \\
\Rightarrow Q^2 &= P_+P_+ - P_+P_- - P_-P_+ + P_-P_- = P_+ - P_+P_- - P_-P_+ + P_- \quad \underbrace{\quad}_{\text{Completeness Relation}} = I - P_+P_- - P_-P_+ \\
\Rightarrow Q^2 &= I - \frac{1}{2}(I + \vec{q} \cdot \vec{\sigma})\frac{1}{2}(I - \vec{q} \cdot \vec{\sigma}) - \frac{1}{2}(I - \vec{q} \cdot \vec{\sigma})\frac{1}{2}(I + \vec{q} \cdot \vec{\sigma}) = I - \frac{1}{4}(I - (\vec{q} \cdot \vec{\sigma})^2) - \frac{1}{4}(I - (\vec{q} \cdot \vec{\sigma})^2) \\
\Rightarrow Q^2 &= I - \frac{1}{2}(I - (\vec{q} \cdot \vec{\sigma})^2) = I - \frac{1}{2}(I - Q^2) = \frac{1}{2}I + \frac{1}{2}Q^2 \\
\Rightarrow \frac{1}{2}Q^2 &= \frac{1}{2}I \Rightarrow Q^2 = I
\end{aligned}$$

This can be shown for  $R, S$  and  $T$ . Hence,  $Q^2 = R^2 = S^2 = T^2 = I$ .

Next, we show that  $\left(Q \otimes S + R \otimes S + R \otimes T - Q \otimes T\right)^2 = 4I + [Q, R] \otimes [S, T]$ .

$$\begin{aligned}
&\left(Q \otimes S + R \otimes S + R \otimes T - Q \otimes T\right)^2 = \left(Q \otimes (S - T) + R \otimes (S + T)\right)^2 \\
&= (Q \otimes (S - T))(Q \otimes (S - T)) + (R \otimes (S + T))(R \otimes (S + T)) + (Q \otimes (S - T))(R \otimes (S + T)) + (R \otimes (S + T))(Q \otimes (S - T)) \\
&= Q^2 \otimes (S - T)^2 + R^2 \otimes (S + T)^2 + QR \otimes (S - T)(S + T) + RQ \otimes (S + T)(S - T) \\
&= I \otimes (S^2 + T^2 - ST - TS) + I \otimes (S^2 + T^2 + ST + TS) + QR \otimes ((S^2 + ST - TS - T^2) + RQ \otimes (S^2 - ST + TS - T^2)) \\
&= I \otimes (2I - ST - TS) + I \otimes (2I + ST + TS) + QR \otimes (I + ST - TS - I) + RQ \otimes (I - ST + TS - I) \\
&= 2I \otimes I + 2I \otimes I - I \otimes ST - I \otimes TS + I \otimes ST + I \otimes TS + QR \otimes (ST - TS) + RQ \otimes (TS - ST) \\
&= 4I \otimes I + QR \otimes (ST - TS) + RQ \otimes (TS - ST) = 4I + QR \otimes (ST - TS) - RQ \otimes (ST - TS) \\
&\Rightarrow \left(Q \otimes S + R \otimes S + R \otimes T - Q \otimes T\right)^2 = 4I + (QR - RQ) \otimes (ST - TS) = 4I + [Q, R] \otimes [S, T]
\end{aligned}$$

The sup-norm of a tensor product satisfies  $\|[Q, R] \otimes [S, T]\|_\infty \leq \|[Q, R]\|_\infty \|[S, T]\|_\infty$ . Next,  $\|[Q, R]\|_\infty = \|QR - RQ\|_\infty \leq \|QR\|_\infty + \|RQ\|_\infty \leq \|Q\|_\infty \|R\|_\infty + \|R\|_\infty \|Q\|_\infty \leq 2\|Q\|_\infty \|R\|_\infty$ .

Next, we show that  $\|Q\|_\infty \leq 1$ .

$$\|Q\|_\infty = \max_{\|\psi\|=1} \langle \psi | Q | \psi \rangle = \max_{\|\psi\|=1} \text{tr}(Q |\psi\rangle \langle \psi|) = \max_{\|\psi\|=1} \text{tr}(Q \rho) = \max_{\|\psi\|=1} \text{tr}(\vec{q} \cdot \vec{\sigma} \frac{1}{2}(I + \vec{n} \cdot \vec{\sigma}))$$

$$\text{tr}(\vec{q} \cdot \vec{\sigma} \frac{1}{2}(I + \vec{n} \cdot \vec{\sigma})) = \frac{1}{2} \text{tr}(\vec{q} \cdot \vec{\sigma} + (\vec{q} \cdot \vec{\sigma})(\vec{n} \cdot \vec{\sigma})) = \frac{1}{2} (\text{tr}(\vec{q} \cdot \vec{\sigma}) + \text{tr}(\vec{q} \cdot \vec{\sigma})(\vec{n} \cdot \vec{\sigma})) \quad \underbrace{\quad}_{\text{tr}(\sigma_i \sigma_j)} = \frac{1}{2} \text{tr}(\vec{q} \cdot \vec{\sigma})(\vec{n} \cdot \vec{\sigma}) = \frac{1}{2} \text{tr} \sum_{ij} q_i n_j \sigma_i \sigma_j =$$

$\frac{1}{2} \sum_{ij} q_i n_j \text{tr}(\sigma_i \sigma_j)$ . We know that  $\text{tr}(\sigma_i \sigma_j) = 2\delta_{ij}$ . So,  $\frac{1}{2} \sum_{ij} q_i n_j \text{tr}(\sigma_i \sigma_j) = \frac{1}{2} \sum_{ij} q_i n_j 2\delta_{ij} = \sum_i q_i n_i$ .

Next,  $\sum_{ij} q_i n_i = \langle \vec{q} | \vec{n} \rangle \leq |\langle \vec{q} | \vec{n} \rangle| \leq \underbrace{\|\vec{q}\| \|\vec{n}\|}_{C-S} = 1 \cdot 1 = 1$ . Therefore,  $\text{tr}(Q \rho) \leq 1$  for all  $|\psi\rangle$  satisfying

$\|\psi\| = 1$ . Hence,  $\max_{\|\psi\|=1} \text{tr}(Q \rho) \leq 1$ . And so  $\|Q\|_\infty \leq 1$ .

Similarly, we can show that  $\|R\|_\infty \leq 1$ ,  $\|S\|_\infty \leq 1$ ,  $\|T\|_\infty \leq 1$ .

Previously we had shown  $\|[Q, R]\|_\infty \leq 2\|Q\|_\infty \|R\|_\infty$ . Hence,  $\|[Q, R]\|_\infty \leq 2 \cdot 1 \cdot 1 = 2$ .

Also,  $\|[S, T]\|_\infty \leq 2$ .

So,  $\|[Q, R] \otimes [S, T]\|_\infty \leq \|[Q, R]\|_\infty \|[S, T]\|_\infty \leq 2 \cdot 2 = 4$ . Putting these results together we have

$$\left\| \left( Q \otimes (S - T) + R \otimes (S + T) \right)^2 \right\|_\infty = \|4I + [Q, R] \otimes [S, T]\|_\infty \leq 4 + \|[Q, R]\|_\infty \|[S, T]\|_\infty \leq 4 + 4 = 8$$

Hence,

$$\begin{aligned} & \|Q \otimes (S - T) + R \otimes (S + T)\|_{\infty} \leq \sqrt{8} = 2\sqrt{2} \\ \Rightarrow & \langle Q \otimes (S - T) + R \otimes (S + T) \rangle \leq \|Q \otimes (S - T) + R \otimes (S + T)\|_{\infty} \leq \sqrt{8} = 2\sqrt{2} \\ \text{i.e. } & \langle Q \otimes S \rangle + \langle R \otimes S \rangle + \langle R \otimes T \rangle - \langle Q \otimes T \rangle \leq 2\sqrt{2} \end{aligned}$$

# **Quantum Computation and Quantum Information**

-Michael A. Nielsen and Isaac L. Chuang

## **Chapter 2. Introduction to Quantum Mechanics**

### **Selected Problems**

#### **Set-II**

**2.20) (Basis changes)** Suppose  $A'$  and  $A''$  are matrix representations of an operator  $A$  on a vector space  $V$  with respect to two different orthonormal bases,  $|v_i\rangle$  and  $|w_i\rangle$ . Then the elements of  $A'$  and  $A''$  are  $A'_{ij} = \langle v_i | A | v_j \rangle$  and  $A''_{ij} = \langle w_i | A'' | w_j \rangle$ . Characterize the relationship between  $A'$  and  $A''$ .

It is given that the vectors  $|v_i\rangle$  and  $|w_i\rangle$  are each a set of orthonormal bases on the vector space  $V$ . We define the matrix  $U = \sum_i |v_i\rangle \langle w_i|$ . We can check that the matrix  $U$  is a unitary matrix.  $U^\dagger U = \sum_{ij} |w_i\rangle \langle v_i | v_j \rangle \langle w_j| = \sum_{ij} |w_i\rangle \delta_{ij} \langle w_j| = \sum_i |w_i\rangle \langle w_i|$ . Each  $|w_i\rangle \langle w_i|$  is a projection operator and hence by the completeness relation  $\sum_i |w_i\rangle \langle w_i| = I$ . Therefore,  $U^\dagger U = I$ . Similarly, we can check that  $UU^\dagger = I$ .

Next, with respect to the orthonormal bases  $|v_i\rangle$ , each entry for the matrix  $A'$  is

$$\begin{aligned} A'_{ij} &= \langle v_i | A | v_j \rangle = \langle v_i | U^\dagger U A U^\dagger U | v_j \rangle = \sum_{\alpha\beta\gamma\theta} \langle v_i | w_\alpha \rangle \langle v_\alpha | v_\beta \rangle \langle w_\beta | A | w_\gamma \rangle \langle v_\gamma | v_\theta \rangle \langle w_\theta | v_j \rangle \\ &\Rightarrow A'_{ij} = \sum_{\alpha\beta\gamma\theta} \langle v_i | w_\alpha \rangle \delta_{\alpha\beta} \langle w_\beta | A | w_\gamma \rangle \delta_{\gamma\theta} \langle w_\theta | v_j \rangle = \sum_{\alpha\gamma} \langle v_i | w_\alpha \rangle \underbrace{\langle w_\alpha | A | w_\gamma \rangle}_{=A''_{\alpha\gamma}} \langle w_\gamma | v_j \rangle \end{aligned}$$

Therefore, we can characterize the relationship between each entry of the matrices  $A'$  and  $A''$  as:

$$A'_{ij} = \sum_{\alpha\gamma} A''_{\alpha\gamma} \langle v_i | w_\alpha \rangle \langle w_\gamma | v_j \rangle \quad \text{for all } i, j$$

where  $A'_{ij}$  and  $A''_{\alpha\gamma}$  are the entries of the matrices  $A'$  and  $A''$  respectively.

**2.21)** Repeat the proof of spectral decomposition in Box 2.2 for the case when  $M$  is Hermitian, simplifying the proof wherever possible.

When  $M$  is Hermitian the spectral decomposition theorem reads: *Any Hermitian operator  $M$  on a vector space  $V$  is diagonal with respect to some orthonormal basis for  $V$ .*  
..... (Incomplete).

**2.22)** Prove that two eigenvectors of a Hermitian operator with different eigenvalues are necessarily orthogonal.

Let  $|v_1\rangle$  be the eigenvector with respect to the eigenvalue  $\lambda_1$  and  $|v_2\rangle$  be the eigenvector with respect to the eigenvalue  $\lambda_2$ . And  $\lambda_1 \neq \lambda_2$ . Then we have  $H|v_1\rangle = \lambda_1|v_1\rangle$  and  $H|v_2\rangle = \lambda_2|v_2\rangle$ . Taking the adjoint of  $H|v_1\rangle = \lambda_1|v_1\rangle$  we get  $\langle v_1 | H^\dagger = \lambda_1 \langle v_1 |$ . Taking the inner product with  $|v_2\rangle$  gives  $\langle v_1 | H^\dagger | v_2 \rangle = \lambda_1 \langle v_1 | v_2 \rangle$ . Next  $H^\dagger = H$ , so  $\langle v_1 | H^\dagger | v_2 \rangle = \langle v_1 | H | v_2 \rangle$  which is equal to  $\lambda_2 \langle v_1 | v_2 \rangle$ . So we have  $\lambda_1 \langle v_1 | v_2 \rangle = \lambda_2 \langle v_1 | v_2 \rangle$  which implies that  $\langle v_1 | v_2 \rangle$  must necessarily be equal to 0 (and hence  $|v_1\rangle$  and  $|v_2\rangle$  are orthogonal) since  $\lambda_1 \neq \lambda_2$ .

**2.23)** Show that the eigenvalues of the projector  $P$  are all either 0 or 1.

Let  $P$  be a projector and  $|v\rangle$  be an eigenvector with respect to the eigenvalue  $\lambda$ . Then we have  $P^2|v\rangle = P|v\rangle$  which implies  $P(P|v\rangle) = \lambda|v\rangle \Rightarrow P(\lambda|v\rangle) = \lambda|v\rangle \Rightarrow \lambda^2|v\rangle = \lambda|v\rangle$ . Hence  $(\lambda^2 - \lambda)|v\rangle = 0$ . So,  $\lambda(\lambda - 1) = 0$  which means  $\lambda$  is either 0 or 1. This is true for all such  $\lambda$ 's. Hence, the eigenvalues of the projector  $P$  are all either 0 or 1.

**2.24 (Hermiticity of positive operators)** Show that a positive operator is necessarily Hermitian. (Hint: Show that an arbitrary operator  $A$  can be written  $A = B + iC$  where  $B$  and  $C$  are Hermitian).

The book defines a positive operator  $A$  as an operator such that for any vector  $|v\rangle$ ,  $\langle v|A|v\rangle$  is real and non-negative. Next, we define  $A = \frac{A+A^\dagger}{2} + i\frac{A-A^\dagger}{2i}$ . So,  $A = B + iC$  where  $B = \frac{A+A^\dagger}{2}$  and  $C = \frac{A-A^\dagger}{2i}$ . We can check that  $B$  and  $C$  are both Hermitian.  $B^\dagger = \frac{1}{2}(A+A^\dagger)^\dagger = \frac{1}{2}(A^\dagger + A) = B$ . And  $C^\dagger = -\frac{1}{2i}(A-A^\dagger)^\dagger = -\frac{1}{2i}(A^\dagger - A) = \frac{1}{2i}(A - A^\dagger) = C$ . Next, we see that  $\langle v|A|v\rangle = \langle v|B|v\rangle + i\langle v|C|v\rangle$ . But it is given that  $A$  is a positive operator which means  $\langle v|A|v\rangle \geq 0$  and real. This implies that  $\langle v|C|v\rangle$  must vanish for all  $|v\rangle$ . And hence  $\langle v|A|v\rangle = \langle v|B|v\rangle$  for all  $|v\rangle$ . So,  $A = B = \frac{A+A^\dagger}{2} \Rightarrow 2A = A + A^\dagger \Rightarrow A = A^\dagger$  and hence  $A$  is Hermitian.

**2.35) (Exponential of the Pauli matrices)** Let  $\vec{v}$  be any real, three dimensional unit vector and  $\theta$  be a real number. Prove that  $\exp\{i\theta\vec{v}\cdot\vec{\sigma}\} = \cos(\theta)I + i\sin(\theta)(\vec{v}\cdot\vec{\sigma})$  where  $\vec{v}\cdot\vec{\sigma} = \sum_{i=1}^3 v_i\sigma_i$ .

In the process of solving Problem 2.60 (in Set-I) we found that for a unit vector in  $\vec{v} \in \mathbb{R}^3$ ,  $\vec{v}\cdot\vec{\sigma}$  has eigenvalues 1 and -1 and we can write  $\vec{v}\cdot\vec{\sigma}$  in the form  $\vec{v}\cdot\vec{\sigma} = |v_+\rangle\langle v_+| - |v_-\rangle\langle v_-|$  where  $|v_+\rangle$  and  $|v_-\rangle$  are the eigenvectors corresponding to the eigenvalues 1 and -1 respectively. Hence we have

$$i\theta\vec{v}\cdot\vec{\sigma} = i\theta(|v_+\rangle\langle v_+| - |v_-\rangle\langle v_-|) \Rightarrow \exp(i\theta\vec{v}\cdot\vec{\sigma}) = e^{i\theta}|v_+\rangle\langle v_+| + e^{-i\theta}|v_-\rangle\langle v_-|$$

Also,  $|v_+\rangle\langle v_+|$  and  $|v_-\rangle\langle v_-|$  are projection operators that satisfy the completeness relation  $|v_+\rangle\langle v_+| + |v_-\rangle\langle v_-| = I$ . Solving the two equations  $\vec{v}\cdot\vec{\sigma} = |v_+\rangle\langle v_+| - |v_-\rangle\langle v_-|$  and  $|v_+\rangle\langle v_+| + |v_-\rangle\langle v_-| = I$  we get  $|v_\pm\rangle\langle v_\pm| = \frac{1}{2}(I \pm \vec{v}\cdot\vec{\sigma})$ . Hence we have

$$\begin{aligned} \exp(i\theta\vec{v}\cdot\vec{\sigma}) &= e^{i\theta}|v_+\rangle\langle v_+| + e^{-i\theta}|v_-\rangle\langle v_-| \\ \Rightarrow \exp(i\theta\vec{v}\cdot\vec{\sigma}) &= e^{i\theta}\left(\frac{I + \vec{v}\cdot\vec{\sigma}}{2}\right) + e^{-i\theta}\left(\frac{I - \vec{v}\cdot\vec{\sigma}}{2}\right) = \frac{e^{i\theta} + e^{-i\theta}}{2}I + \frac{e^{i\theta} - e^{-i\theta}}{2}\vec{v}\cdot\vec{\sigma} = \cos(\theta)I + i\sin(\theta)\vec{v}\cdot\vec{\sigma} \end{aligned}$$

where  $\cos(\theta) = \frac{e^{i\theta} + e^{-i\theta}}{2}$  and  $\sin(\theta) = \frac{e^{i\theta} - e^{-i\theta}}{2i}$ .

**2.39) (Hilbert-Schmidt inner product on operators)** The set  $L_V$  of linear operators on a Hilbert space  $V$  is obviously a vector space – the sum of two linear operators is a linear operator,  $zA$  is a linear operator if  $A$  is a linear operator and  $z$  is a complex number, and there is a zero element 0. An important additional result is that the vector space  $L_V$  can be given a natural inner product structure, turning it into a Hilbert space.

(1) Show that the function  $(\cdot, \cdot)$  on  $L_V \times L_V$  defined by  $(A, B) \equiv \text{tr}(A^\dagger B)$  is an inner product function. This inner product is known as the Hilbert-Schmidt inner product or trace inner product.

(2) If  $V$  has  $d$  dimensions show that  $L_V$  has dimension  $d^2$ .

(3) Find an orthonormal basis of Hermitian matrices for the Hilbert space  $L_V$ .

**(1)** In order to show that the function  $(\cdot, \cdot)$  on  $L_V \times L_V$  defined by  $(A, B) \equiv \text{tr}(A^\dagger B)$  is an inner product function we need to show a) Symmetry, b) Linearity and c) Positive-Definite.

a) **Symmetry:**

We have  $A, B \in L_V$ . Let  $A = \sum_{ij} a_{ij} |i\rangle \langle j|$  and  $B = \sum_{ij} b_{ij} |i\rangle \langle j|$  be the expansion of  $A$  and  $B$  in the standard basis. We show that  $(A, B) = \overline{(B, A)}$ . Using the definition of  $(\cdot, \cdot)$  we have

$$(A, B) = \text{tr}(A^\dagger B) = \text{tr} \left( \sum_{ij} a_{ij}^* |j\rangle \langle i| \sum_{kl} b_{kl} |k\rangle \langle l| \right) = \text{tr} \left( \sum_{ijkl} a_{ij}^* b_{kl} |j\rangle \underbrace{\langle i|k\rangle}_{=\delta_{ik}} \langle l| \right) = \text{tr} \left( \sum_{ijl} a_{ij}^* b_{il} |j\rangle \langle l| \right) = \sum_{ij} a_{ij}^* b_{ij} \quad (20)$$

$$(B, A) = \text{tr}(B^\dagger A) = \text{tr} \left( \sum_{ij} b_{ij}^* |j\rangle \langle i| \sum_{kl} a_{kl} |k\rangle \langle l| \right) = \text{tr} \left( \sum_{ijkl} b_{ij}^* a_{kl} |j\rangle \underbrace{\langle i|k\rangle}_{=\delta_{ik}} \langle l| \right) = \text{tr} \left( \sum_{ijl} b_{ij}^* a_{il} |j\rangle \langle l| \right) = \sum_{ij} b_{ij}^* a_{ij} \quad (21)$$

$$\Rightarrow (B, A) = \sum_{ij} b_{ij}^* a_{ij} = \left( \sum_{ij} a_{ij}^* b_{ij} \right)^* = \overline{(A, B)} \quad (22)$$

b) **Linearity:**

For some  $\alpha \in \mathbb{C}$  we have

$$(\alpha A, B) = \text{tr}((\alpha A)^\dagger B) = \text{tr}(\alpha^* A^\dagger B) = \alpha^* \text{tr}(A^\dagger B) = \alpha^* (A, B) \quad (23)$$

$$(A, \alpha B) = \text{tr}(A^\dagger (\alpha B)) = \text{tr}(\alpha A^\dagger B) = \alpha \text{tr}(A^\dagger B) = \alpha (A, B) \quad (24)$$

Next, for some  $A, B, C \in L_V$  we have

$$(A + C, B) = \text{tr}((A + C)^\dagger B) = \text{tr}(A^\dagger B + C^\dagger B) = \text{tr}(A^\dagger B) + \text{tr}(C^\dagger B) = (A, B) + (C, B) \quad (25)$$

c) **Positive-Definite:**

$$(A, A) = \text{tr}(A^\dagger A) = \text{tr}\left(\sum_{ij} a_{ij}^* |j\rangle\langle i| \sum_{ij} a_{ij} |i\rangle\langle j|\right) = \text{tr}\left(\sum_{ijkl} a_{ij}^* a_{kl} |j\rangle\langle i| \underbrace{|k\rangle\langle l|}_{=\delta_{ik}}\right) = \text{tr}\left(\sum_{ijl} a_{ij}^* a_{il} |j\rangle\langle l|\right) = \sum_{ij} a_{ij}^* a_{ij}$$

Hence  $(A, A) = \sum_{ij} a_{ij}^* a_{ij} = \sum_{ij} |a_{ij}|^2 \geq 0$  with equality iff  $a_{ij} = 0$  i.e.  $A = 0$

**(2)** Suppose  $\{|1\rangle, |2\rangle, \dots, |d\rangle\}$  is the set of orthonormal basis for the vector space  $V$ . Then the dimension of  $V$  is the cardinality of the basis of  $V$ , i.e.  $d$ .  $L_V$  is the set of linear operators  $T$  on  $V$  such that  $T: V \rightarrow V$ . We want to show that the cardinality of the basis of  $L_V$  is  $d^2$ . By the completeness relation we have  $I_V = \sum_{i=1}^d |i\rangle\langle i|$ . One application of the completeness relation is to give a means for representing an operator in the outer product notation. For  $T: V \rightarrow V$  and  $\{|i\rangle\}_{i=1}^d$ , an orthonormal basis for  $V$ , using the completeness relation twice gives

$$T = I_V T I_V = \sum_{i=1}^d |i\rangle\langle i| T \sum_{i=1}^d |i\rangle\langle i| = \sum_{i=1}^d \sum_{j=1}^d |i\rangle\langle i| T |j\rangle\langle j| = \sum_{i=1}^d \sum_{j=1}^d \langle i| T |j\rangle |i\rangle\langle j| \quad (26)$$

which is the outer product representation for  $T$ .  $T$  has matrix element  $\langle i| T |j\rangle$  in the  $i$ th row and the  $j$ th column, with respect to the input basis  $|j\rangle$  and the output basis  $|i\rangle$  (where  $i, j = 1, 2, \dots, d$ ). In (26) we have shown that the elements  $|i\rangle\langle j|$  span the space of  $L_V$  since the matrix representation of any linear operator  $T: V \rightarrow V$  can be obtained by the linear combination of  $|i\rangle\langle j|$ . In order to show that the elements  $|i\rangle\langle j|$  are indeed basis elements of  $L_V$  we need to also show that they are mutually linearly independent. From the matrix representation of any linear operator  $T: V \rightarrow V$  as obtained in (26) we see that  $\langle i| T |j\rangle$  are the weights (real/complex) for  $|i\rangle\langle j|$  for all  $i, j = 1, \dots, d$ . And  $\sum_{i=1}^d \sum_{j=1}^d \langle i| T |j\rangle |i\rangle\langle j| = 0$  if and only if  $\langle i| T |j\rangle = 0$  for all  $i, j = 1, \dots, d$ . This shows that  $\{|i\rangle\langle j|\}_{i,j=1}^d$  are linearly independent. So, (26) shows that there are  $d^2$  such elements in the representation of a linear operator  $T$ . Hence the cardinality of the basis  $\{|i\rangle\langle j|\}_{i,j=1}^d$  of  $L_V$  is  $d^2$ , i.e.  $\dim(L_V)$  is  $d^2$ .

**(3)** Assuming a dimension of 2 the Pauli matrices  $\sigma_1, \sigma_2, \sigma_3$  form an orthonormal basis of Hermitian matrices for the Hilbert space  $L_V$ . For higher dimensions we need some generalization of the Pauli matrices. Suppose we have the standard basis  $\{|j\rangle\}_{j=1}^n$  (and  $n > 2$ ) in the Hilbert space  $V$ . We define the following three types of matrices:

$$(1) \text{ Symmetric } \left(\frac{d(d-1)}{2} \text{ matrices}\right): \Lambda_s^{jk} = |j\rangle\langle k| + |k\rangle\langle j|, \quad \text{for } 1 \leq j < k \leq n \quad (27)$$

$$(2) \text{ Asymmetric } \left(\frac{d(d-1)}{2} \text{ matrices}\right): \Lambda_a^{jk} = -i|j\rangle\langle k| + i|k\rangle\langle j|, \quad \text{for } 1 \leq j < k \leq n \quad (28)$$

$$(3) \text{ Diagonal } (d-1 \text{ matrices}): \Lambda_d^l = \sqrt{\frac{2}{l(l+1)}} \left( \sum_{j=1}^l |j\rangle\langle j| - l|l+1\rangle\langle l+1| \right), \quad \text{for } 1 \leq l \leq n-1 \quad (29)$$

The  $\frac{n(n-1)}{2} + \frac{n(n-1)}{2} + n-1 = n^2-1$  matrices in (27), (28) and (29) are the so-called *generalized Gell-Mann matrices*. They are a generalization of the Pauli matrices to dimensions greater than 2. By definition the matrices  $\{\Lambda_s^{jk}, \Lambda_a^{jk}, \Lambda_d^l\}$  are Hermitian. Also, each of them have a trace equal to zero. They are orthogonal in the Hilbert-Schmidt sense, i.e.  $\text{tr}(\Lambda_i^\dagger \Lambda_j) = 2\delta_{ij}$ .

For  $n = 2$  and  $n = 3$  the collection of matrices defined above recover the Pauli and Gell-Mann matrices respectively.

**2.54)** Suppose  $A$  and  $B$  are commuting Hermitian operators. Prove that  $\exp(A)\exp(B) = \exp(A + B)$ . (Hint: Use the results of section 2.1.9).

Given that  $A$  and  $B$  are commuting Hermitian operators, i.e.  $A^\dagger = A$ ,  $B^\dagger = B$  and  $[A, B] = AB - BA = 0$  we can use the *simultaneous diagonalization theorem* given in section 2.1.9 which says: *If  $A$  and  $B$  are Hermitian. Then  $[A, B] = 0$  if and only if there exists an orthonormal basis such that both  $A$  and  $B$  are diagonal with respect to that basis. We say that  $A$  and  $B$  are simultaneously diagonalizable in that case.*

Since  $[A, B] = 0$ ,  $A$  and  $B$  can be simultaneously diagonalized as  $A = \sum_i \lambda_i |i\rangle \langle i|$  and  $B = \sum_i \mu_i |i\rangle \langle i|$  where  $\lambda_i$  and  $\mu_i$  are reals since  $A$  and  $B$  are Hermitian. Hence

$$\begin{aligned}\exp(A)\exp(B) &= \left( \sum_i \exp(\lambda_i) |i\rangle \langle i| \right) \left( \sum_i \exp(\mu_i) |i\rangle \langle i| \right) = \sum_{ij} \exp(\lambda_i) \exp(\mu_j) |i\rangle \underbrace{\langle i|j\rangle}_{=\delta_{ij}} \langle j| \\ \Rightarrow \exp(A)\exp(B) &= \sum_i \exp(\lambda_i) \exp(\mu_i) |i\rangle \langle i| = \sum_i \exp(\lambda_i + \mu_i) |i\rangle \langle i| = \exp \left( \sum_i (\lambda_i + \mu_i) |i\rangle \langle i| \right) \\ &\Rightarrow \exp(A)\exp(B) = \exp \left( \sum_i \lambda_i |i\rangle \langle i| + \sum_i \mu_i |i\rangle \langle i| \right) = \exp(A + B)\end{aligned}$$

**2.55)** Prove that  $U(t_1, t_2)$  defined in Equation (2.91) is unitary.

$U(t_1, t_2)$  is defined in Equation (2.91) as

$$U(t_1, t_2) = \exp \left( \frac{-iH(t_2 - t_1)}{\hbar} \right)$$

Using the spectral decomposition of the Hamiltonian  $H = \sum_E E |E\rangle \langle E|$  and  $\sum_E |E\rangle \langle E| = I$

$$\begin{aligned}U^\dagger(t_1, t_2)U(t_1, t_2) &= \exp \left( \frac{iH(t_2 - t_1)}{\hbar} \right) \exp \left( \frac{-iH(t_2 - t_1)}{\hbar} \right) \\ &= \exp \left( \frac{i(t_2 - t_1)}{\hbar} \sum_E E |E\rangle \langle E| \right) \exp \left( -\frac{i(t_2 - t_1)}{\hbar} \sum_E E |E\rangle \langle E| \right) \\ \Rightarrow U^\dagger(t_1, t_2)U(t_1, t_2) &= \left( \sum_E \exp \left( \frac{i(t_2 - t_1)}{\hbar} E \right) |E\rangle \langle E| \right) \left( \sum_E \exp \left( -\frac{i(t_2 - t_1)}{\hbar} E \right) |E\rangle \langle E| \right) \\ \Rightarrow U^\dagger(t_1, t_2)U(t_1, t_2) &= \sum_{E, E'} \exp \left( \frac{i(t_2 - t_1)}{\hbar} E \right) \exp \left( -\frac{i(t_2 - t_1)}{\hbar} E' \right) |E\rangle \underbrace{\langle E|E'\rangle}_{=\delta_{E, E'}} \langle E'| \\ \Rightarrow U^\dagger(t_1, t_2)U(t_1, t_2) &= \sum_{E, E'} \exp \left( \frac{i(t_2 - t_1)}{\hbar} E - \frac{i(t_2 - t_1)}{\hbar} E' \right) |E\rangle \underbrace{\langle E|E'\rangle}_{=\delta_{E, E'}} \langle E'| = \sum_E \exp \left( \frac{i(t_2 - t_1)}{\hbar} E - \frac{i(t_2 - t_1)}{\hbar} E \right) |E\rangle \langle E| \\ &\Rightarrow U^\dagger(t_1, t_2)U(t_1, t_2) = \sum_E \exp(0) |E\rangle \langle E| = \sum_E |E\rangle \langle E| = I\end{aligned}$$

With a similar approach we can show that  $U(t_1, t_2)U^\dagger(t_1, t_2) = I$ . Hence  $U^\dagger(t_1, t_2)U(t_1, t_2) = U(t_1, t_2)U^\dagger(t_1, t_2) = I$ . Hence  $U(t_1, t_2)$  is unitary.

Note: In the expression  $H = \sum_E E |E\rangle \langle E|$  of the Hamiltonian (a Hermitian operator),  $|E\rangle$  is the



energy eigenstate or sometimes referred to as *stationary state* and  $E$  is the *energy* of the state  $|E\rangle$ . The lowest energy is known as the *ground state energy* for the system and the corresponding energy eigenstate (or eigenspace) is known as the *ground state*.

**2.56)** Use the spectral decomposition to show that  $K \equiv -i \log(U)$  is Hermitian for any unitary  $U$ , and thus  $U = \exp(iK)$  for some Hermitian  $K$ .

The unitary operator  $U$  satisfies  $U^\dagger U = U U^\dagger = I$ . Hence,  $U$  is normal and by the spectral decomposition theorem we have  $U = \sum_j \lambda_j |j\rangle \langle j|$ , where  $\lambda_j$  is the eigenvalue corresponding to the eigenvector  $|j\rangle$ . So,  $\log(U) = \sum_j \log(\lambda_j) |j\rangle \langle j|$ . Also,  $|\lambda_j| = 1$ . Let  $\lambda_j = e^{i\theta_j}$  for  $\theta_j \in \mathbb{R}$ . Then  $\log(U) = \sum_j \log(\lambda_j) |j\rangle \langle j| = \sum_j \log(e^{i\theta_j}) |j\rangle \langle j| = \sum_j i\theta_j |j\rangle \langle j|$ . Hence,  $K = -i \log(U) = -i \sum_j i\theta_j |j\rangle \langle j| = \sum_j \theta_j |j\rangle \langle j|$ . We can check that  $K$  is Hermitian.  $K^\dagger = (\sum_j \theta_j |j\rangle \langle j|)^\dagger = \sum_j \theta_j^* |j\rangle \langle j| = \sum_j \theta_j |j\rangle \langle j| = K$  since  $\theta_j \in \mathbb{R}$ . Hence,  $U = \exp(iK)$  for some Hermitian  $K$ . This shows that the exponential of  $i$  times a Hermitian operator is unitary. And so there is a one-to-one correspondence between the discrete-time description of dynamics using unitary operators, and the continuous time description using Hamiltonians.

**2.57) (Cascaded measurements are single measurements)** Suppose  $\{L_l\}$  and  $\{M_m\}$  are two sets of measurement operators. Show that a measurement defined by the measurement operators  $\{L_l\}$  followed by a measurement defined by the measurement operators  $\{M_m\}$  is physically equivalent to a single measurement defined by measurement operators  $\{N_{lm}\}$  with the representation  $N_{lm} \equiv M_m L_l$ .

Suppose the state of the system immediately before the measurement is  $|\psi\rangle$ . Then the probability of obtaining the result  $l$  using the operator  $L_l$  is  $p(l) = \langle \psi | L_l^\dagger L_l | \psi \rangle$  and the state of the system after the measurement is  $|\phi\rangle = \frac{L_l |\psi\rangle}{\sqrt{\langle \psi | L_l^\dagger L_l | \psi \rangle}}$ . Next, we use the operator  $M_m$  on the state  $|\phi\rangle$ . The state of the system after the measurement is

$$\begin{aligned} \frac{M_m |\phi\rangle}{\sqrt{\langle \phi | M_m^\dagger M_m | \phi \rangle}} &= \frac{\frac{M_m L_l |\psi\rangle}{\sqrt{\langle \psi | L_l^\dagger L_l | \psi \rangle}}}{\sqrt{\frac{\langle \psi | L_l^\dagger M_m^\dagger M_m L_l | \psi \rangle}{\langle \psi | L_l^\dagger L_l | \psi \rangle}}} = \frac{M_m L_l |\psi\rangle}{\sqrt{\langle \psi | L_l^\dagger L_l | \psi \rangle}} \sqrt{\frac{\langle \psi | L_l^\dagger L_l | \psi \rangle}{\langle \psi | L_l^\dagger M_m^\dagger M_m L_l | \psi \rangle}} = \frac{M_m L_l |\psi\rangle}{\sqrt{\langle \psi | L_l^\dagger M_m^\dagger M_m L_l | \psi \rangle}} \\ &= \frac{M_m L_l |\psi\rangle}{\sqrt{\langle \psi | (M_m L_l)^\dagger (M_m L_l) | \psi \rangle}} = \frac{N_{lm} |\psi\rangle}{\sqrt{\langle \psi | N_{lm}^\dagger N_{lm} | \psi \rangle}} \end{aligned}$$

Hence the measurement using the operator  $L_l$  followed by the measurement using the operator  $M_m$  is physically equivalent to a single measurement using the operator  $N_{lm} \equiv M_m L_l$ . Next, we show that the probability of obtaining the outcome  $lm$  using the operator  $N_{lm}$  is the same as that of the cascaded measurement  $L_l$  followed by  $M_m$ .

The probability of obtaining  $lm$  using  $N_{lm}$  is  $p(lm) = \langle \psi | N_{lm}^\dagger N_{lm} | \psi \rangle$ . In the cascaded measurement we first use the operator  $L_l$  on the initial state  $|\psi\rangle$  and obtain the outcome  $l$  with probability  $p(l) = \langle \psi | L_l^\dagger L_l | \psi \rangle$  and obtain the post-measurement state  $|\phi\rangle = \frac{L_l |\psi\rangle}{\sqrt{\langle \psi | L_l^\dagger L_l | \psi \rangle}}$ . Next, we use the operator  $M_m$  on the state  $|\phi\rangle$  and obtain the outcome  $m$  with probability

$$p(m) = \langle \phi | M_m^\dagger M_m | \phi \rangle = \frac{\langle \psi | L_i^\dagger M_m^\dagger M_m L_i | \psi \rangle}{\sqrt{\langle \psi | L_i^\dagger L_i | \psi \rangle} \sqrt{\langle \psi | L_i^\dagger L_i | \psi \rangle}} = \frac{\langle \psi | L_i^\dagger M_m^\dagger M_m L_i | \psi \rangle}{\langle \psi | L_i^\dagger L_i | \psi \rangle} = \frac{\langle \psi | N_{lm}^\dagger N_{lm} | \psi \rangle}{\langle \psi | L_i^\dagger L_i | \psi \rangle}.$$

Hence, the probability of observing the outcome  $lm$  in the cascaded scenario is  $p(l)p(m) = \langle \psi | L_i^\dagger L_i | \psi \rangle \times \frac{\langle \psi | N_{lm}^\dagger N_{lm} | \psi \rangle}{\langle \psi | L_i^\dagger L_i | \psi \rangle} = \langle \psi | N_{lm}^\dagger N_{lm} | \psi \rangle$  which is equal to the probability  $p(lm)$  of obtaining the outcome  $lm$  using the operator  $N_{lm}$ .

**2.76)** Extend the proof of Schmidt decomposition to the case where  $A$  and  $B$  may have state spaces of different dimensionality.

We begin by stating the Schmidt decomposition theorem.

Suppose  $H_A$  and  $H_B$  are the Hilbert spaces of dimensions  $d_A$  and  $d_B$  respectively (with  $d_A \geq d_B$ ). For any state  $|\psi\rangle$  in the state space of  $H_A \otimes H_B$  there exist orthonormal sets  $|i_A\rangle$  and  $|i_B\rangle$  such that  $|\psi\rangle = \sum_{i=1} \lambda_i |i_A\rangle |i_B\rangle$  where  $\lambda_i$  is real, non-negative and satisfies  $\sum_i \lambda_i^2 = 1$ . Note that the orthonormal sets  $|i_A\rangle$  and  $|i_B\rangle$  can be extended to orthonormal basis by the Gram-Schmidt procedure.

*Proof:* Any state in the state space of  $H_A \otimes H_B$  can be viewed as  $|\psi\rangle = \sum_{j=1}^{d_A} \sum_{k=1}^{d_B} c_{jk} |j\rangle |k\rangle$ , where  $\{|j\rangle\}_{j=1}^{d_A}$  and  $\{|k\rangle\}_{k=1}^{d_B}$  are the standard basis in the state space of  $H_A$  and  $H_B$  respectively. Then  $c_{jk}$  are the elements of a  $d_A \times d_B$  matrix  $C$ . By the singular value decomposition theorem of a (real/complex) matrix we can find  $d_A \times d_A$  unitary  $U$ , a  $d_B \times d_B$  unitary  $V$  and a  $d_B \times d_B$  positive semi-definite diagonal matrix  $D$  such that  $C = UDV^\dagger$ . Note that since we have assumed  $d_A \geq d_B$  we can write  $C$  as  $C = U \begin{pmatrix} D \\ 0 \end{pmatrix} V^\dagger$ , where we have appended  $d_A - d_B$  rows of 0's to the diagonal matrix  $D$ .