Chapter 2

Basic Principles in Quantum Mechanics

The purpose of this chapter is to offer a glimpse into some basic quantum mechanics. We shall introduce concepts on

- Copenhagen interpretation
- Density matrix and its statistical meaning
- Entanglements
- Separability
- Partial trace
- Purification

Only some fundamental ideas are outlined as this subject has been and will continue to be extended into much deeper research across multiple academic fields. On the other hand, we do not need all these notions per se when coming down to quantum computation.

2.1 Copenhagen Interpretation

- There are many ways to interpret quantum mechanism.
    - ◇ These are different ways of relating the wave functions to experimental results and our fundamental "belief" of nature.
    - ◇ Some of the interpretations even conflict with others.
    - ◇ All are attempts to explain mathematically three revolutionary principles:
        - ▷ Quantized properties.
        - ▷ Particles of light.
        - ▷ Waves of matter.
- According to the Copenhagen interpretation,
    - ◇ Physical systems generally do not have definite properties prior to being measured.
    - ◇ Quantum mechanics can only predict the probability distribution of a given measurement's possible results.
    - ◇ The act of measurement affects the system, causing the set of probabilities to reduce to only one of the possible values immediately after the measurement. This feature is known as *wave function collapse*.

Postulate 1 – Pure and Mixed States

- To each quantum mechanical system is associated a complex Hilbert space $\mathscr{H}$.
  - ◇ A pure state in quantum mechanics is represented in terms of a unit vector $|\psi\rangle$ in $\mathscr{H}$. (wave function)
    - ▷ Will consider $|\psi\rangle \equiv |\phi\rangle$ if $|\psi\rangle = c\,|\phi\rangle$ and $|c| = 1$.
  - ◇ Mixed states are described by density matrices.
    - ▷ A *density matrix* is a positive operator of unit trace on the Hilbert space $\mathscr{H}$.
      - ✓ If the space has a basis consisting of eigenvectors, then the sum of eigenvalues is 1.
    - ▷ The density matrix for a pure state $|\psi\rangle$ is the rank-1 matrix $|\psi\rangle\langle\psi|$.
      - ✓ The notion of a "matrix" should be interpreted as a linear operator in the sense of a projector

$$(|\psi\rangle\langle\psi|)\,|\mathbf{z}\rangle = \langle\psi|\mathbf{z}\rangle\,|\psi\rangle\,. \tag{2.1}$$

      - ✓ The value of the phase c disappears from density matrix representation.
  - ◇ Why do we need the notion of density matrices?

Postulate 2 – Observables

- Every measurable physical quantity, say, of $\mathfrak{a}$, is called an *observable* and is described by a Hermitian operator $\mathcal{A}$ acting on the Hilbert space $\mathscr{H}$.
  - ◇ $\mathcal{A}$ acts like a statistical operator.
  - ◇ When making a measurement of the associated physical quantity $\mathfrak{a}$, we obtain one of the eigenvalues λ_j of $\mathcal{A}$.
  - ◇ Immediately after the measurement the state undergoes an abrupt change to the eigenstate $|\boldsymbol{\phi}_j\rangle$ of the observed eigenvalue.
- Suppose that the system is in state $|\boldsymbol{\psi}\rangle$ and $\mathcal{A}$ is measured.
  - ◇ Expand $|\boldsymbol{\psi}\rangle$ in terms of eigenstate basis of $\mathcal{A}$,

$$|\boldsymbol{\psi}\rangle = \sum_j c_j |\boldsymbol{\phi}_j\rangle .$$

    - ▷ Assume that the probability of collapsing to the eigenstate $|\boldsymbol{\phi}_j\rangle$ is given by $|c_j|^2$.
  - ◇ Therefore, the expectation value of $\mathfrak{a}$ after many measurements is

$$\langle A\rangle := \sum_j \lambda_j |c_j|^2 = \langle\boldsymbol{\psi}| A |\boldsymbol{\psi}\rangle . \tag{2.2}$$

- How are these measurements realized on a quantum machine?

Postulate 3 – Schröndinger Equation

- The evolution of a state $|\boldsymbol{\psi}\rangle$ in time is governed by the (general) Schrödinger equation

$$\imath\hbar\frac{\partial\,|\boldsymbol{\psi}\rangle}{\partial t} = H\,|\boldsymbol{\psi}\rangle\,, \tag{2.3}$$

  - ◇ $\hbar$ is a physical constant known as the *Planck constant*.
  - ◇ H is a Hermitian operator (matrix) corresponding to the energy of the system and is called the *Hamiltonian*.

- In the overly simplified case when H is time independent, then

$$|\boldsymbol{\psi}(t)\rangle = e^{\frac{-\imath Ht}{\hbar}}\,|\boldsymbol{\psi}(0)\rangle\,. \tag{2.4}$$

  In general,

  - ◇ $|\boldsymbol{\psi}\rangle = |\boldsymbol{\psi}(\mathbf{r},t)\rangle$.
  - ◇ $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)$.

- Solving the Schröndinger equation together with its interpretation and its other applications, say, in the electronmagnatism theory is beyond the scope of this course.

- Suffice to say that the most important concept is that

$$|\boldsymbol{\psi}(t)\rangle = U(t)\,|\boldsymbol{\psi}(0)\rangle\,. \tag{2.5}$$

  - ◇ $U(t)$ is unitary.
    - ▷ Show that if H is Hermitian, then $-\imath H$ is skew-Hermitian and $e^{-\imath H}$ is unitary.
  - ◇ The length of $|\boldsymbol{\psi}(t)\rangle$ is invariant.

2.2 Density Matrix and Its Statistical Meaning

- Convex hull of pure states
- Single qubit and Bloch sphere
- Statistical Ensembles

Convex Hull of Pure States

- The set Ω of density matrices over a Hilbert space $\mathscr{H}$ is convex.
  - ⋄ A convex combination of density matrices remains positive with unit trace.
- The extreme points of Ω are the pure states.
  - ⋄ Recall that $\rho \in \Omega$ is an extreme point if a strict convex combination $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$ with $\rho_1, \rho_2 \in \Omega$ and $0 < \lambda < 1$ is possibly only if $\rho_1 = \rho_2 = \rho$.
  - ⋄ The Schmidt decomposition shows that an extreme point must be a pure state.
  - ⋄ Remains to argue that a pure state is an extreme point.
    - ▷ Assume $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$ with $\rho_1, \rho_2 \in \Omega$.
    - ▷ Since $\rho = |\boldsymbol{\psi}\rangle\langle\boldsymbol{\psi}|$, $\rho^2 = \rho$.
    - ▷ Can write
      $$\rho = \lambda\rho\rho_1\rho + (1-\lambda)\rho\rho_2\rho.$$
      and, hence, $\mathrm{Tr}(\rho\rho_i\rho) = 1$ for $i = 1, 2$.
    - ▷ By the Cauchy-Schwartz inequality, we should have
      $$\mathrm{Tr}(\rho\rho_i\rho) =< \rho, \rho_i\rho >=< \rho, \rho_i >\leq \|\rho\|_F\|\rho_i\|_F \leq 1.$$
    - ▷ The equality holds if and only if $\rho = c_i\rho_i$ for some scalars c_i. Together, we see that $c_i = 1$ and $\rho = \rho_1 = \rho_2$.
- Any density matrix ρ can be written as a convex combination
  $$\rho = \sum_i \mu_i |\boldsymbol{\psi}_i\rangle\langle\boldsymbol{\psi}_i|; \quad \sum_i \mu_i = 1; \quad \mu_i \geq 0, \tag{2.6}$$
  of some pure states $|\boldsymbol{\psi}_i\rangle$.

Bloch Sphere

- Consider the Hilbert space $\mathbb{C}^2$.
  - ◇ Denote the standard basis $\mathbf{e}_1$ and $\mathbf{e}_2$ by $|0\rangle$ and $|1\rangle$, or $|\downarrow\rangle$ and $|\uparrow\rangle$, respectively.
  - ◇ A *qubit* is a quantum superposition of $|0\rangle$ and $|1\rangle$, i.e.,

$$|\boldsymbol{\psi}\rangle = x_1 |1\rangle + z |0\rangle \tag{2.7}$$

    where $x_1 \in \mathbb{R}$, $z \in \mathbb{C}$, and $x_1^2 + |z|^2 = 1$. (Why is $x_1 \in \mathbb{R}$?)
  - ◇ Write $z = x_2 + \imath x_3$. The set of all pure states of a qubit is conveniently visualized as the sphere in $\mathbb{R}^3$, called the *Bloch sphere*.

Pauli Matrices

- Define the Pauli matrices

$$\sigma_x := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad \sigma_y := \begin{bmatrix} 0 & -\imath \\ \imath & 0 \end{bmatrix}; \quad \sigma_z := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}; \quad (2.8)$$

  Then any 2×2 density matrix ρ can be expressed as

$$\rho = \frac{1}{2}(I_2 + \mathbf{x} \cdot \boldsymbol{\sigma}) = \frac{1}{2}\begin{bmatrix} 1 + x_3 & x_1 - \imath x_2 \\ x_1 + \imath x_2 & 1 - x_3 \end{bmatrix} \quad (2.9)$$

  with some $\mathbf{x} \in \mathbb{R}^3$ and $\|\mathbf{x}\| \leq 1$.

  ◇ Rewrite $|\boldsymbol{\psi}\rangle \langle\boldsymbol{\psi}|$ in (2.7) in the form of (2.9).

- Therefore, in the case of $\mathbb{C}^2$, all pure states are on the Bloch sphere, whereas all density matrices are in the *Bloch ball*.

  ◇ What is this to do with the previous theory?

Statistical Ensembles

- Describing a quantum state by its density matrix is a fully general alternative formalism to describing a quantum state by its state vector (its "ket") or by a statistical ensemble of kets.
  - ◇ Use density matrices for calculations involving mixed states.
  - ◇ Use kets for calculations involving only pure states.
- Suppose that a physical quantity $\mathcal{A}$ is measured at a mixed state where the probability of appearing at the state $|\boldsymbol{\psi}_i\rangle$ is μ_i.
  - ◇ $|\boldsymbol{\psi}_i\rangle$ are not necessarily orthogonal.
  - ◇ The portion of the observable $\mathfrak{a}$ at state $|\boldsymbol{\psi}_i\rangle$ is the projection component $\langle\boldsymbol{\psi}_i| A |\boldsymbol{\psi}_i\rangle$.
  - ◇ The expected value of the observable $\mathfrak{a}$ is

$$\langle A\rangle = \sum_i \mu_i \langle\boldsymbol{\psi}_i| A |\boldsymbol{\psi}_i\rangle \tag{2.10}$$

- Thus we are motivated to represent that mixed state by the density matrix

$$\rho = \sum_i \mu_i |\boldsymbol{\psi}_i\rangle \langle\boldsymbol{\psi}_i| ; \quad \sum_i \mu_i = 1; \quad \mu_i \geq 0. \tag{2.11}$$

  - ◇ Can write $\langle A\rangle = \mathrm{Tr}(A\rho)$. (Compare with (2.2))
- The density matrix representation (2.11) does not need $|\boldsymbol{\psi}_i\rangle$ to be mutually orthonormal.

2.3 Entanglement

- Composite systems
- Entanglement of density matrices

Composite Systems

- A bipartite system is described by the tensor product Hilbert space $\mathscr{H}_1 \otimes \mathscr{H}_2$.
  - ◇ Recall from (1.33) that a state in $\mathscr{H}_1 \otimes \mathscr{H}_2$ can be represented by a matrix D. (In lexicographically ordered basis)
  - ◇ A pure state $|\boldsymbol{\psi}\rangle$ is where $\|D\|_F = \sum_{i,j} |d_{ij}|^2 = 1$.
- If a pure state $|\boldsymbol{\psi}\rangle$ is expressible as

$$|\boldsymbol{\psi}\rangle = |\boldsymbol{\psi}_1\rangle \otimes |\boldsymbol{\psi}_2\rangle\,, \tag{2.12}$$

with pure states $|\boldsymbol{\psi}_i\rangle \in \mathscr{H}_i$, $i = 1, 2$, respectively, then the pure state $|\boldsymbol{\psi}\rangle$ is said to be *separable*; otherwise, it is called *entangled*.

  - ◇ A pure state in the composite system can be entangled.
  - ◇ A finite dimensional pure state can always be decomposed as a linear combination of separable states.
    - ▷ Recall the Schmidt decomposition in Section 1.4.

A 2-Qubit System: $\mathbb{C}^2 \otimes \mathbb{C}^2$

- A natural (binary) basis is $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$.
  - ◇ The corresponding matrix representations are:
$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$
- Consider the state
$$|\boldsymbol{\psi}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$
  - ◇ Can consider $|\boldsymbol{\psi}\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix}$. (Not a density matrix!)
  - ◇ Is $|\boldsymbol{\psi}\rangle$ separable?
$$\begin{aligned} |\boldsymbol{\psi}\rangle &= (c_1|0\rangle + c_2|1\rangle) \otimes (d_1|0\rangle + d_2|1\rangle) \\ &= c_1 d_1 |00\rangle + c_1 d_2 |01\rangle + c_2 d_1 |10\rangle + c_2 d_2 |11\rangle . \end{aligned}$$
    - ▷ Find the coefficients.
- Bell basis:
$$\begin{cases} |\Phi^+\rangle := \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \\ |\Phi^-\rangle := \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle), \\ |\Psi^+\rangle := \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle), \\ |\Psi^-\rangle := \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle). \end{cases}$$
  - ◇ Is an orthonormal basis.
  - ◇ The Bell basis can be obtained from the binary basis via a unitary transformation. Find the unitary transformation explicitly.

Bipartite Density Matrices

- Density matrices in a bipartite system are order-4 tensor operators.
- Do not confuse the density matrix of a mixed state with the matrix representation of a state.

Representing a Bipartite Density Matrix

- Consider finite dimensional cases, so $\mathscr{H}_1 \equiv \mathbb{C}^m$ and $\mathscr{H}_2 \equiv \mathbb{C}^n$.
  - ◇ Identify states $|\boldsymbol{\psi}\rangle \in \mathbb{C}^m \otimes \mathbb{C}^n$ by matrices $D \in \mathbb{C}^{m\times n}$.
  - ◇ The density matrix corresponding to a pure state D is a linear operator $\mathcal{T} \in \mathfrak{B}(\mathbb{C}^{m\times n})$ satisfying the relationship

$$\mathcal{T}(Z) = \langle D, Z\rangle D. \tag{2.13}$$

- The linear operator $\mathcal{T}$ should be regarded as an order-4 tensor in $\mathbb{C}^{n\times m\times n\times m}$ whose matrix representation is in $\mathbb{C}^{nm\times nm}$.
  - ◇ With respect to the basis $\{\mathbf{e}_i \otimes \mathbf{f}_j\}$ in lexicographic order, the density matrix of a pure state D is of the form

$$T = \begin{bmatrix} \overline{d}_{11}d_{11} & \overline{d}_{12}d_{11} & \ldots & \overline{d}_{1n}d_{11} & \ldots & \overline{d}_{mn}d_{11} \\ \overline{d}_{11}d_{12} & \overline{d}_{12}d_{12} & \ldots & \overline{d}_{1n}d_{12} & \ldots & \overline{d}_{mn}d_{12} \\ \vdots & \vdots & & & & \\ \overline{d}_{11}d_{1n} & & & & & \\ \overline{d}_{11}d_{21} & & & & & \\ \vdots & & & & & \\ \overline{d}_{11}d_{mn} & \overline{d}_{12}d_{mn} & & & \ldots & \overline{d}_{mn}d_{mn} \end{bmatrix} \in \mathbb{C}^{mn\times mn}, \tag{2.14}$$

    - ▷ Obviously $\mathcal{T}(\mathbf{e}_i \otimes \mathbf{f}_j) = \overline{d}_{ij}D$.
    - ▷ Place $\overline{d}_{ij}D$ at the (i,j)-column in the matrix representation T according to the lexicographical order.
    - ▷ Can write $T = \left|\mathbf{vec}(D^\top)\right\rangle \left\langle\mathbf{vec}(D^\top)\right|$ or, more confusingly, $T = \mathbf{vec}(C) \circ \mathbf{vec}(C)$, where $\circ$ is the complex outer product.

Density Matrices of Mixed States

- As expected, $\mathrm{Tr}(T) = 1$ and that T is positve.
- The mixed state ρ in the bipartite system is an order-4 density matrix that can be written in the form

$$\rho = \sum_i \mu_i \mathbf{vec}(C_i) \circ \mathbf{vec}(C_i); \quad \sum_i \mu_i = 1; \quad \mu_i \geq 0, \quad (2.15)$$

  where each C_i represents a pure state.

  - ◇ Since $\rho \in \mathbb{C}^{mn \times mn}$,(2.15) can be cast as a spectral decomposition of ρ.
  - ◇ A total of mn terms in the summation is sufficient.
  - ◇ This decomposition is doable, but it is not the meaning of separability.

Separability

- We have talked about the separability of a unit state in a bipartite system.
- We have also talked about the Schmidt decomposition that a unit state in a bipartite system can always be expressed as a linear combination of separable unit states.
- The real challenge in the separability problem is to determine whether a given mixed state density matrix ρ.

Separation of General Operators

- In Section 1.3, we have already talked about a special operator $\mathcal{A} \otimes \mathcal{B} \in \mathfrak{B}(\mathbb{C}^m \otimes \mathbb{C}^n)$, i.e.,

$$(\mathcal{A} \otimes \mathcal{B})(\mathbf{e}_i \otimes \mathbf{f}_j) := (\mathcal{A}\mathbf{e}_i) \otimes (\mathcal{B}\mathbf{f}_j),$$

  - ◇ Suppose A and B are the matrix representations of $\mathcal{A}$ and $\mathcal{B}$, respectively.
  - ◇ With respect to the lexicographical ordering, the matrix representation of $\mathcal{A} \otimes \mathcal{B}$ is simply the Kronecker product $A \otimes B$.

- Given a general matrix $X \in \mathbb{C}^{mn \times mn}$, when is it possible that

$$X = A \otimes B$$

  for some $A \in \mathbb{C}^{m \times m}$ and $B \in \mathbb{C}^{n \times n}$?

  - ◇ Partition $X = [H_{ij}]$ as $m \times m$ blocks. Each H_{ij} is of block size $n \times n$.
  - ◇ Introduce the notion of partial traces:

$$\begin{cases} \mathrm{Tr}_1(X) & := & \sum_{j=1}^{m} H_{jj}, \\ \mathrm{Tr}_2(X) & := & [\mathrm{Tr} H_{ij}]. \end{cases} \tag{2.16}$$

  - ◇ Can check
    - ▷ $\mathrm{Tr}_1(A \otimes B) = \mathrm{Tr}(A)B$.
    - ▷ $\mathrm{Tr}_2(A \otimes B) = \mathrm{Tr}(B)A$.
    - ▷ $\mathrm{Tr}(A \otimes B) = \mathrm{Tr}(A)\mathrm{Tr}(B)$.
  - ◇ The necessary condition is

$$\mathrm{Tr}(X)X = \mathrm{Tr}_2(X) \otimes \mathrm{Tr}_1(X).$$

    - ▷ Check to see if the matrix $\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$ separable?

Separation of Positive Operators

- If $\mathcal{A}_i \in \mathfrak{B}(\mathbb{C}^m)$ and $\mathcal{B}_i \in \mathfrak{B}(\mathbb{C}^n)$ are positive operators, then so is

$$\mathcal{X} := \sum_{i=1}^{R} \mathcal{A}_i \otimes \mathcal{B}_i. \tag{2.17}$$

- Given a positive $\mathcal{X} \in \mathfrak{B}(\mathbb{C}^m \otimes \mathbb{C}^n)$, when is it possible that $\mathcal{X}$ can be separated as the sum in (2.17)?
  - ◇ There is no procedure to decide if X in the tensor product space is separable or entangled. (This is an open research problem.)
  - ◇ Part of the difficulty lies at the determination of the minimum value R.
- If a separation is not possible, what is the best approximation to the problem

$$\min_{A_i \geq 0; B_i \geq 0} \|X - \sum_{i=1}^{R} A_i \otimes B_i\|_F^2. \tag{2.18}$$

Structured Kronecker Product Approximation

- The Kronecker product often inherits structures from its factors [397].

$$\text{If } B \text{ and } C \text{ are } \left\{\begin{array}{l}\text{nonsingular}\\ \text{lower(upper) triangular}\\ \text{banded}\\ \text{symmetric}\\ \text{positive definite}\\ \text{stochastic}\\ \text{Toeplitz}\\ \text{permutations}\\ \text{orthogonal}\end{array}\right\}, \text{ then } B\otimes C \text{ is } \left\{\begin{array}{l}\text{nonsingular}\\ \text{lower(upper) triangular}\\ \text{banded}\\ \text{symmetric}\\ \text{positive definite}\\ \text{stochastic}\\ \text{Toeplitz}\\ \text{permutations}\\ \text{orthogonal}\end{array}\right\}.$$

  - ◇ Also, the LU, Cholesky, and QR factorizations of $B \otimes C$ can easily be achieved from the corresponding factorizations of B and C.

- Consider the converse problem:
  - ◇ Let $\Omega_B \subset \mathbb{R}^{m_1\times n_1}$ and $\Omega_C \subset \mathbb{R}^{m_2\times n_2}$ denote the subsets of desired structures of factors, respectively.
  - ◇ Solve the constrained optimization problem:

$$\min_{B^{(\ell)}\in\Omega_B; C^{(\ell)}\in\Omega_C} \|A - \sum_{\ell=1}^{R} B^{(\ell)} \otimes C^{(\ell)}\|_F^2, \tag{2.19}$$

  - ◇ Many interesting applications [220, 399], but hardly studied.

Separation of Density Matrices

- Determine whether a given mixed state density matrix ρ in the bipartite system can be decomposed as

$$\rho = \sum_i p_i \mathcal{D}_i^{(1)} \otimes \mathcal{D}_i^{(2)}, \tag{2.20}$$

  - ◇ $\{\mathcal{D}_i^{(1)}\}$ and $\{\mathcal{D}_i^{(2)}\}$ are density matrices of the subsystems $\mathbb{C}^m$ and $\mathbb{C}^n$, respectively
  - ◇ $p_i \geq 0$, and $\sum_i p_i = 1$.

- A density matrix ρ is separable if and only if it can be decomposed as

$$\rho = \sum_k \theta_i (\mathbf{x}_k \mathbf{x}_k^*) \otimes (\mathbf{y}_k \mathbf{y}_k^*) \tag{2.21}$$

  - ◇ $\mathbf{x}_k \in \mathbb{C}^m$ and $\mathbf{y}_k \in \mathbb{C}^n$ are unit vectors.
  - ◇ $\sum_k \theta_k = 1$, $\theta_k \geq 0$.

- Need to argue the equivalence of (2.20) and (2.21).

Convex Hull of Separable States

- A summation in the form of (2.21) is certainly separable because $\mathbf{x}_i\mathbf{x}_i^*$ and $\mathbf{y}_i\mathbf{y}_i^*$ are density matrices of pure states.
- Rewrite

$$\begin{aligned}\mathcal{D}_i^{(1)} &= \sum_{s=1}^{m} \lambda_s^{(i)} \mathbf{x}_s^{(i)} \mathbf{x}_s^{(i)*}, \\ \mathcal{D}_i^{(2)} &= \sum_{t=1}^{n} \xi_t^{(i)} \mathbf{y}_t^{(i)} \mathbf{y}_t^{(i)*}.\end{aligned}$$

  ◇ $\|\mathbf{x}_s^{(i)}\| = \|\mathbf{y}_t^{(i)}\| = 1.$

  ◇ $\lambda_s^{(i)}, \xi_t^{(i)} \geq 0$

  ◇ $\sum_s \lambda_s^{(i)} = \sum_t \xi_t^{(i)} = 1.$

- Upon substitution,

$$\rho = \sum_i p_i \sum_{s=1}^{m} \lambda_s^{(i)} \sum_{t=1}^{n} \xi_t^{(i)} (\mathbf{x}_s^{(i)} \mathbf{x}_s^{(i)*}) \otimes (\mathbf{y}_t^{(i)} \mathbf{y}_t^{(i)*}). \tag{2.22}$$

  ◇ $p_i \lambda_s^{(i)} \xi_t^{(i)} \geq 0.$

  ◇ Check to see that

$$\sum_{i,s,t} p_i \lambda_s^{(i)} \xi_t^{(i)} = 1. \tag{2.23}$$

  ◇ Check to see that the terms in the summation can be renamed in a serial order.

- Note that the convex hull is of the operators, not of the states.

Entangled Bipartite Low Rank Approximation

- Given positive definite (PD) matrix $\rho \in \mathbb{C}^{mn \times mn}$ with unit trace,
  - ◇ Find
    - ▷ Complex unit vectors $\mathbf{x}_r \in \mathbb{C}^m$, $\mathbf{y}_r \in \mathbb{C}^n$
    - ▷ Nonnegative real number $\lambda_r \in \mathbb{R}_+$ with unit sum
  - ◇ Such that

$$\|\rho - \sum_{r=1}^{R} \lambda_r (\mathbf{x}_r \mathbf{x}_r^*) \otimes (\mathbf{y}_r \mathbf{y}_r^*)\|_F^2, \tag{2.24}$$

    is minimized.

- This is an optimization of real-valued functions over complex variables.
  - ◇ Conventional calculus is not enough to address the derivative information.
  - ◇ Employ the so called Wirtinger calculus. (Another research problem!)

2.4 Purification

- This is an important process, but we have to be brief to stay focused on this course.

Partial Traces

- The notion of partial traces can be defined over an abstract $\mathfrak{B}(\mathscr{H}_1 \otimes \mathscr{H}_2)$ without making references to bases.
  - ◇ Consider the "inclusion" map

$$\begin{aligned} \mathfrak{i} : \mathfrak{B}(\mathscr{H}_1) &\hookrightarrow \mathfrak{B}(\mathscr{H}_1 \otimes \mathscr{H}_2), \\ \mathfrak{i}(\mathcal{A}) &= \mathcal{A} \otimes I. \end{aligned}$$

    - ▷ The map $\mathfrak{i}$ has an adjoint

$$\begin{aligned} \mathfrak{i}^* : \mathfrak{B}(\mathscr{H}_1 \otimes \mathscr{H}_2) &\rightarrow \mathfrak{B}(\mathscr{H}_1) \\ \langle \mathcal{A} \otimes I, X \rangle &= \langle \mathcal{A}, \mathfrak{i}^*(X) \rangle. \end{aligned}$$

    - ▷ $\mathrm{Tr}_2(X) := \mathfrak{i}^*(X)$.
  - ◇ Likewise, $\mathrm{Tr}_1(X) := \mathfrak{j}^*(X)$ with the relationships:

$$\begin{aligned} \mathfrak{j} : \mathfrak{B}(\mathscr{H}_2) &\hookrightarrow \mathfrak{B}(\mathscr{H}_1 \otimes \mathscr{H}_2), \\ \mathfrak{j}(\mathcal{B}) &= I \otimes \mathcal{B}, \\ \langle I \otimes \mathcal{B}, X \rangle &= \langle \mathcal{B}, \mathfrak{j}^*(X) \rangle. \end{aligned}$$

- With respect to basis, show that the above abstract definitions can be realized via (2.16).
- If ρ is a density matrix in $\mathfrak{B}(\mathscr{H}_1 \otimes \mathscr{H}_2)$, it is conventional to write $\rho_1 = \mathrm{Tr}_2(\rho)$. Then

$$\mathrm{Tr}(A\rho_1) = \mathrm{Tr}((A \otimes I)\rho). \tag{2.25}$$

Overlook an Unknown System

- Suppose we are interested only in one system and have no access to the other system.
  - ⋄ The partial trace allows us to forget the other system.
  - ⋄ The partial traces quantify the action on only the known system.
- Let a pure state $|\boldsymbol{\psi}\rangle \in \mathbb{C}^m \otimes \mathbb{C}^n$ be represented by the matrix $D \in \mathbb{C}^{m\times n}$.
  - ⋄ Its density matrix is $\rho = \mathbf{vec}(D^\top)\mathbf{vec}(D^\top)^*$.
  - ⋄ Write $D^\top = [\mathbf{d}_1, \ldots \mathbf{d}_m]$, $\mathbf{d}_j \in \mathbb{C}^n$. Then

$$\begin{aligned} \mathrm{Tr}_1(\rho) &:= \sum_{j=1}^{m} \mathbf{d}_j \mathbf{d}_j^*, \\ \mathrm{Tr}_2(\rho) &:= [\sum_{s=1}^{n} d_{is}\overline{d}_{js}]. \end{aligned}$$

▷ Do the partial traces of a density matrix remain to be density matrices?

Purifying a Mixed State

- Given a mixed state density matrix
$$\rho_1 = \sum_i \mu_i \left|\boldsymbol{\psi}_i\right\rangle \left\langle\boldsymbol{\psi}_i\right|; \quad \sum_i \mu_i = 1; \quad \mu_i \geq 0$$
in $\mathscr{H}_1$, is it always possible to find a pure state density matrix $\rho \in \mathfrak{B}(\mathscr{H}_1 \otimes \mathscr{H}_2)$ whose partial trace over the extra Hilbert space yields the given ρ_1?
  - ◇ Let $\mathscr{H}_2$ be a Hilbert space with the same dimension as $\mathscr{H}_1$.
  - ◇ Let $\{\left|\boldsymbol{\phi}_j\right\rangle\}$ be an orthonormal basis of $\mathscr{H}_2$.
  - ◇ Define
$$\left|\boldsymbol{\Psi}\right\rangle := \sum_i \sqrt{\mu_i} \left|\boldsymbol{\psi}_i\right\rangle \otimes \left|\boldsymbol{\phi}_i\right\rangle .$$
    - ▷ $\left|\boldsymbol{\Psi}\right\rangle$ is a unit vector in $\mathscr{H}_1 \otimes \mathscr{H}_2$.
    - ▷ The density matrix of $\mathscr{H}_1 \otimes \mathscr{H}_2$ is given by
$$\rho := \left|\boldsymbol{\Psi}\right\rangle \left\langle\boldsymbol{\Psi}\right| = \sum_{i,j} \sqrt{\mu_i \mu_j} \left|\boldsymbol{\psi}_i \boldsymbol{\phi}_i\right\rangle \left\langle\boldsymbol{\psi}_j \boldsymbol{\phi}_j\right| .$$
    - ▷ Compute $\mathrm{Tr}_2(\rho)$
$$\begin{aligned}\mathrm{Tr}_2(\rho) &= \sum_k (I \otimes \left\langle\boldsymbol{\phi}_k\right|)(\sum_{i,j} \sqrt{\mu_i \mu_j} \left|\boldsymbol{\psi}_i \boldsymbol{\phi}_i\right\rangle \left\langle\boldsymbol{\psi}_j \boldsymbol{\phi}_j\right|)(I \otimes \left|\boldsymbol{\phi}_k\right\rangle) \\ &= \sum_{i,j,k} \sqrt{\mu_i \mu_j} \left|\boldsymbol{\psi}_i\right\rangle \left\langle\boldsymbol{\phi}_k|\boldsymbol{\phi}_i\right\rangle \left\langle\boldsymbol{\psi}_j|\boldsymbol{\phi}_j\right\rangle \left|\boldsymbol{\phi}_k\right\rangle \\ &= \rho_1.\end{aligned}$$
- Note that the original mixed state ρ_1 is *purified* to become a pure state $\left|\boldsymbol{\Psi}\right\rangle$.
  - ◇ There are infinitely many ways to purify a mixed state.