Summary of the Previous Lecture

- Linear vector space
  - Linear (in)dependence, Dimension, Basis

- Inner product space
  - Generalized requirement for inner product
  - Ket ⇔ Bra: all the coefficient should be complex-conjugated → adjoint operation
  - Orthogonality, norm, orthonormal basis
  - Gram-Schmidt theorem
  - Schwarz inequality, triangular inequality
- Subspace
- Linear operator
  - Product of two operators
  - Commutator
  - Matrix representation

From Chap. 1 of "Principles of Quantum Mechanics", Ramamurti Shankar, 2nd ed. Plenum Press (1994)

Review: Matrix Representation of Linear Operators

- Assume that the original vector $|V\rangle = \sum_i v_i |i\rangle \Leftrightarrow \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$
- The transformed vector $|V'\rangle = \Omega|V\rangle$ is expanded as

$$|V'\rangle = \sum_j v'_j |j\rangle \Leftrightarrow \begin{bmatrix} v'_1 \\ v'_2 \\ \vdots \\ v'_n \end{bmatrix}$$

- $v'_j = \langle j|V'\rangle = \langle j|\Omega|V\rangle = \langle j|(\sum_i v_i \Omega|i\rangle) = \sum_i v_i \langle j|\Omega|i\rangle = \sum_i \Omega_{ji} v_i$
- $v'_j = \sum_i \Omega_{ji} v_i \Leftrightarrow \begin{bmatrix} v'_1 \\ v'_2 \\ \vdots \\ v'_n \end{bmatrix} = \begin{bmatrix} \langle 1|\Omega|1\rangle & \langle 1|\Omega|2\rangle & \cdots & \langle 1|\Omega|n\rangle \\ \langle 2|\Omega|1\rangle & & & \\ \vdots & & & \vdots \\ \langle n|\Omega|1\rangle & & \cdots & \langle n|\Omega|n\rangle \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$

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Matrix Representation of Linear Operators

- Identity operator I
  - $I_{ij} = \langle i|I|j\rangle = \langle i|j\rangle = \delta_{ij}$
- Projection operator $\mathcal{P}_i$
  - Consider the shape of expansion of vector

$$|V\rangle = \sum_{i=1}^{n} v_i|i\rangle = \sum_{i=1}^{n}\langle i|V\rangle|i\rangle = \sum_{i=1}^{n}|i\rangle\langle i|V\rangle = \left(\sum_{i=1}^{n}|i\rangle\langle i|\right)|V\rangle$$

  - $\sum_{i=1}^{n}|i\rangle\langle i|$ is an identity operator and also can be written as $\sum_{i=1}^{n}\mathcal{P}_i$.
  - $\mathcal{P}_i = |i\rangle\langle i|$ is called the projection operator for the ket $|i\rangle$
  - $I = \sum_{i=1}^{n}|i\rangle\langle i| = \sum_{i=1}^{n}\mathcal{P}_i$: **completeness relation** ⇔ The sum of the projections of a vector along all the n directions equals the vector itself. ➔ Used quite frequently in the calculation of quantum mechanics
  - $\mathcal{P}_i$ still works on bra as well: $\langle V|\mathcal{P}_i = \langle V|i\rangle\langle i| = v_i^*\langle i|$

Matrix Representation of Linear Operators

- Outer product
  - $\langle V|V'\rangle$ is a scalar
  - What about $|V\rangle\langle V'|$?
  - It is an operator
- Can we construct an operator that will map orthonormal basis $|1\rangle, |2\rangle, \dots, |n\rangle$ to $|1'\rangle, |2'\rangle, \dots, |n'\rangle$?

- Matrices corresponding to products of operators
  - $(\Omega\Lambda)_{ij} = \langle i|\Omega\Lambda|j\rangle = \langle i|\Omega(\sum_{k=1}^{n}|k\rangle\langle k|)\Lambda|j\rangle = \sum_{k=1}^{n}\langle i|\Omega|k\rangle\langle k|\Lambda|j\rangle = \sum_{k=1}^{n}\Omega_{ik}\Lambda_{kj}$

Linear Operators

- **Adjoint of an operator**
  - When a ket $\alpha|V\rangle$ is given, the corresponding bra is $\langle V|\alpha^*$.
  - Similarly when $\Omega|V\rangle = |\Omega V\rangle$ is given, there is a corresponding bra $\langle \Omega V|$ and we define the adjoint of operator Ω as $\Omega^\dagger$ that can transform $\langle V|$ to $\langle \Omega V|$ when applied from right. That is, $\langle V|\Omega^\dagger = \langle \Omega V|$.
  - Matrix component of adjoint operator
    - $(\Omega^\dagger)_{ij} = \langle i|\Omega^\dagger|j\rangle = \langle \Omega i|j\rangle = \langle j|\Omega i\rangle^* = (\langle j|\Omega|i\rangle)^* = \Omega_{ji}^*$
    - Transpose conjugate of matrix representing the original operator
    - If the field is real, adjoint corresponds to transpose of matrix
  - Adjoint of product of operator: $(\Omega\Lambda)^\dagger = \Lambda^\dagger\Omega^\dagger$

Hermitian Operators

- **Definition 13**: an operator Ω is **Hermitian** if $\Omega^\dagger = \Omega$
  - Equivalent to symmetric matrix for real field
- **Definition 14**: an operator Ω is **anti-Hermitian** if $\Omega^\dagger = -\Omega$
- Analogy between operator and number
  - Adjoint ⇔ Complex conjugation
- Any arbitrary operator Ω can be decomposed into its Hermitian part and anti-Hermitian part
  - $\Omega = \frac{\Omega+\Omega^\dagger}{2} + \frac{\Omega-\Omega^\dagger}{2}$

Unitary Operator

- **Definition 15**: an operator U is **unitary** if $UU^\dagger = U^\dagger U = I$
- Analogy between operator and number
  - Unitary operator ⇔ Complex number of unit modulus $u = e^{i\theta}$
- **Theorem 7**: unitary operators preserve the inner product between the vectors they act on. That is, if $|V'\rangle = U|V\rangle$, $\langle V'|V'\rangle = \langle V|V\rangle$
- Unitary operators are the generalization of rotation operator.
  - In typical 3-d vector space, unitary condition is equivalent to orthogonal matrix condition. ($O^{-1} = O^T$)
- Theorem 8: if one treats the columns of an n x n unitary matrix as components of n vectors, these vectors are orthonormal. The same for the rows.

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Trace

- Trace of a matrix
  - Definition: $\mathrm{Tr}(\Omega) = \sum_{i=1}^{n} \Omega_{ii}$
  - $\mathrm{Tr}(\Omega\Lambda) = \mathrm{Tr}(\Lambda\Omega)$
  - $\mathrm{Tr}(\Omega\Lambda\Theta) = \mathrm{Tr}(\Lambda\Theta\Omega) = \mathrm{Tr}(\Theta\Omega\Lambda)$ (cyclic permutation)
  - Trace of an operator is preserved even when the basis set is changed under unitary transformation

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Eigenvalue Problem

- Generally for $\Omega|V\rangle = |V'\rangle$, $|V'\rangle$ won't be parallel to $|V\rangle$.
- However, each operator has certain kets of its own, called as its **eigenkets**, on which the action of the operator is simply a rescaling of the ket: $\Omega|V\rangle = \omega|V\rangle$. In this case, $|V\rangle$ is called as an eigenket of operator Ω with eigenvalue ω.

- How to solve the eigenvalue problem?
  - We need to find eigenvalue ω and eigenvector $|V\rangle$ satisfying $(\Omega - \omega I)|V\rangle = |0\rangle$.
  - Re-write the above equation in terms of components by applying a basis bra $\langle i|$ to both sides: $\langle i|(\Omega - \omega I)|V\rangle = 0$
  - $\langle i|(\Omega - \omega I)\sum_{j=1}^{n}|j\rangle\langle j|\,|V\rangle = \sum_{j=1}^{n}\langle i|(\Omega - \omega I)|j\rangle v_j = \sum_{j=1}^{n}\left(\Omega_{\mathrm{ij}} - \omega\delta_{ij}\right)v_j = 0$
  - In matrix form, $\begin{bmatrix} \Omega_{11} - \omega & \Omega_{12} & \cdots \\ \Omega_{21} & \Omega_{22} - \omega & \\ \vdots & & \end{bmatrix}\begin{bmatrix} v_1 \\ v_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \end{bmatrix}$
  - For a non-trivial solution to exist, determinant of the above matrix should be zero.

Eigenvalue Problem

- (Continued) How to solve the eigenvalue problem?
  - In matrix form, $\begin{bmatrix} \Omega_{11}-\omega & \Omega_{12} & \cdots \\ \Omega_{21} & \Omega_{22}-\omega & \\ \vdots & & \end{bmatrix}\begin{bmatrix} v_1 \\ v_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \end{bmatrix}$
  - For a non-trivial solution to exist, determinant of the above matrix should be zero.

- Recall how to calculate **determinant of a matrix**
  - In the case of 2x2 matrix, $\det(\mathrm{A}) = |A| = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$
  - For the case of 3x3 matrix,

$$\det(\mathrm{A}) = \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a\begin{vmatrix} \square & \square & \square \\ \square & e & f \\ \square & h & i \end{vmatrix} - b\begin{vmatrix} \square & \square & \square \\ d & \square & f \\ g & \square & i \end{vmatrix} + c\begin{vmatrix} \square & \square & \square \\ d & e & \square \\ g & h & \square \end{vmatrix}$$

$$= a\begin{vmatrix} e & f \\ h & i \end{vmatrix} - b\begin{vmatrix} d & f \\ g & i \end{vmatrix} + c\begin{vmatrix} d & e \\ g & h \end{vmatrix} = a(ei - fh) - b(di - fg) + c(dh - eg)$$

  - It continues recursively for larger matrices

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The Characteristic Equation

- (Continued) How to solve the eigenvalue problem?

$$\det(\mathrm{A}) = \begin{vmatrix} \Omega_{11}-\omega & \Omega_{12} & \Omega_{13} \\ \Omega_{21} & \Omega_{22}-\omega & \Omega_{23} \\ \Omega_{31} & \Omega_{32} & \Omega_{33}-\omega \end{vmatrix}$$

$$= (\Omega_{11} - \boldsymbol{\omega})\{(\Omega_{22} - \boldsymbol{\omega})(\Omega_{22} - \boldsymbol{\omega}) - \Omega_{23}\Omega_{32}\}$$
$$-\Omega_{12}\{\Omega_{21}(\Omega_{33} - \boldsymbol{\omega}) - \Omega_{23}\Omega_{31}\}$$
$$+\Omega_{13}\{\Omega_{21}\Omega_{32} - (\Omega_{22} - \boldsymbol{\omega})\Omega_{31}\}$$

  - $\det\left(\Omega_{\mathrm{ij}} - \omega\delta_{ij}\right) = 0$ ➔ $\sum_{m=0}^{n} c_m \omega^m = 0$: characteristic equation
  - Every nth-order polynomial has n roots, not necessarily distinct and not necessarily real. ➔ **There exist n pairs of ($\boldsymbol{\omega}$, $|\boldsymbol{V}\rangle$)**
  - Note that even though the above equation is written in terms of specific basis, <u>the eigenvalue is independent of the basis choice</u>.

Eigenvalue Problem

- Example: find out the eigenvalues & eigenvectors for $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$
  - $\det(A - \omega I) = \begin{vmatrix} 1-\omega & 0 & 0 \\ 0 & -\omega & -1 \\ 0 & 1 & -\omega \end{vmatrix} = (1-\omega)(\omega^2+1) = 0$
  - For $\omega = 1$, find corresponding eigenvector
  - $\begin{bmatrix} 1-1 & 0 & 0 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \rightarrow \begin{matrix} 0 = 0 \\ -x_2 - x_3 = 0 \\ x_2 - x_3 = 0 \end{matrix} \rightarrow x_2 = x_3 = 0$
  - Notation: $|\omega = 1\rangle = |1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$
  - For other eigenvalues $\omega = \pm i$, verify that $|\omega = i\rangle = |i\rangle = \frac{1}{2^{1/2}} \begin{bmatrix} 0 \\ i \\ 1 \end{bmatrix}$ and $|\omega = -i\rangle = |-i\rangle = \frac{1}{2^{1/2}} \begin{bmatrix} 0 \\ -i \\ 1 \end{bmatrix}$
- When there are more than one eigenvector corresponding to a single eigenvalue, it is called **degeneracy**.
- The eigenvectors with the same eigenvalue form a subspace. $\rightarrow$ eigenspace of Ω with eigenvalue ω