Chapter 2

Introduction to Quantum Mechanics

2.1 Linear Algebra

2.1.1 Vector Spaces

For our purpose the most relevant vector space is a finite (or countable) dimensional space of vectors with complex components represented in the column matrix notation as

\[ |\psi\rangle \equiv \begin{pmatrix} \psi_1 \\ \cdot \\ \cdot \\ \cdot \\ \psi_n \end{pmatrix} \]  

(2.1)

where \( \psi_i \in \mathbb{C} \) and \( |\psi\rangle \in \mathbb{C}^n \) or \( \mathbb{C}^\infty \). These are the ket-vectors.

By definition the vector spaces comes with:

1. addition operation

\[ \begin{pmatrix} \psi_1 \\ \cdot \\ \cdot \\ \cdot \\ \psi_n \end{pmatrix} + \begin{pmatrix} \varphi_1 \\ \cdot \\ \cdot \\ \cdot \\ \varphi_n \end{pmatrix} = \begin{pmatrix} \psi_1 + \varphi_1 \\ \cdot \\ \cdot \\ \cdot \\ \psi_n + \varphi_n \end{pmatrix}, \]  

(2.2)
2. multiplication by a scalar, that is, a complex number (or c-number),

\[
\begin{pmatrix}
  \psi_1 \\
  \vdots \\
  \psi_n
\end{pmatrix}
\cdot z =
\begin{pmatrix}
  z \psi_1 \\
  \vdots \\
  z \psi_n
\end{pmatrix}
\tag{2.3}
\]

3. and a zero vector,

\[
\vec{0} =
\begin{pmatrix}
  0 \\
  \vdots \\
  0
\end{pmatrix}
\tag{2.4}
\]

not to be confused with a vacuum state \(|0\rangle\).

*Spanning set* in a vector space is a collection of vectors \(|\varphi_1\rangle, |\varphi_2\rangle...|\varphi_n\rangle\) such that an arbitrary vector can be written as their linear combination,

\[
|\psi\rangle = \sum_{i=1}^{n} a_i |\varphi_i\rangle.
\tag{2.5}
\]

### 2.1.2 Inner Product

An *inner product* \(\langle \cdot , \cdot \rangle\) is a function which takes two vectors \(|\psi\rangle\) and \(|\varphi\rangle\) to produce a single complex number denoted by \(\langle |\psi\rangle, |\varphi\rangle \rangle\) with following properties:

1. \(\langle \cdot , \cdot \rangle\) is linear in the second argument.

2. \(\langle |\psi\rangle, |\varphi\rangle \rangle = \langle |\varphi\rangle, |\psi\rangle \rangle^\ast\)

3. \(\langle |\psi\rangle, |\psi\rangle \rangle \geq 0\) with equality only iff \(|\psi\rangle = \vec{0}\).

For example the vector space \(\mathbb{C}^n\) has an inner product defined by

\[
\begin{pmatrix}
  \psi_1 \\
  \vdots \\
  \psi_n
\end{pmatrix}
\cdot
\begin{pmatrix}
  \varphi_1 \\
  \vdots \\
  \varphi_n
\end{pmatrix}
\equiv 
\sum_{i=1}^{n} \psi^*_i \varphi_i
\tag{2.6}
\]
The dual vector $\langle \psi |$ is a linear function from a vector space to complex numbers defined using the inner product,

$$\langle \psi | (| \varphi \rangle) \equiv \langle \psi | \varphi \rangle \equiv (| \psi \rangle, | \varphi \rangle).$$  \hfill (2.7)

In matrix representation it is a raw vector (also known as a dual vector, a co-vector or a bra-vectors),

$$\langle \psi | \equiv (\psi_1, \ldots, \psi_n).$$  \hfill (2.8)

when the column vector is known as a ket-vector. In a quantum mechanics a finite dimensional vector space with an inner product is called a Hilbert space. A number of definitions follow

- Two vectors $| \psi \rangle$ and $| \varphi \rangle$ are orthogonal if $\langle \psi | \varphi \rangle = 0$.
- Norm of a vector $| \psi \rangle$ is $\sqrt{\langle \psi | \psi \rangle}$.
- $| \psi \rangle$ is a unit vector if $\langle \psi | \psi \rangle = 1$.
- A set of vectors $| i \rangle$ is orthonormal if $\langle i | i \rangle = 1$ and $\langle i | j \rangle = 0$ for $i \neq j$.

With an orthonormal basis an inner product can be written in a matrix representation as

$$\langle \psi | \varphi \rangle = \left( \sum_{i=1}^{n} \psi_i | i \rangle, \sum_{j=1}^{n} \varphi_j | j \rangle \right) = \sum_{i=1}^{n} \sum_{j=1}^{n} \psi_i^* \varphi_j \langle i | j \rangle = \sum_{i=1}^{n} \psi_i^* \varphi_j = (\psi_1^*, \ldots, \psi_n^*) \begin{pmatrix} \varphi_1 \\ \vdots \\ \varphi_n \end{pmatrix}. \hfill (2.9)$$

2.1.3 Tensor product

Consider two vector spaces (e.g. Hilbert spaces) $V$ and $W$ with basis vectors $| v_i \rangle$’s and $| w_j \rangle$’s then we can form a tensor product space (denoted by $V \otimes W$) with basis vectors $| v_i \rangle \otimes | w_j \rangle$ (for brevity of notations often denoted by $| i \rangle | w_j \rangle$, $| v, w \rangle$ or even $| vw \rangle$).

$$| \psi \rangle = \sum_{i,j} \alpha_{ij} | v_i \rangle | w_j \rangle$$

For example if $V$ is the Hilbert space of the first q-bit and $W$ is the Hilbert space of the second q-bit then the tensor product space is a Hilbert space of two q-bits with basis vectors $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$. 

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The operators which act on vectors in \( V \otimes W \) are formed by a tensor product of operators in \( V \) and \( W \), e.g.,

\[
(A \otimes B) \sum_{i,j} \alpha_{ij} |v_i\rangle |w_j\rangle \equiv \sum_{i,j} \alpha_{ij} A |v_i\rangle B |w_j\rangle.
\]

A convenient matrix representation of the tensor products is given the so-called Kronecker product

\[
A \otimes B = \begin{pmatrix}
A_{11}B & A_{12}B & \cdots & A_{1n}B \\
A_{21}B & A_{22}B & \cdots & A_{2n}B \\
\vdots & \vdots & \ddots & \vdots \\
A_{n1}B & A_{n2}B & \cdots & A_{nn}B
\end{pmatrix}.
\]

For example

\[
\begin{pmatrix}1 & i \\
\end{pmatrix} \otimes \begin{pmatrix}1 \\
-i \\
\end{pmatrix} = \begin{pmatrix}-i \\
0 \\
1 \\
0
\end{pmatrix}
\]

or

\[
Y \otimes Z = \begin{pmatrix}0 & -i \\
i & 0 \\
\end{pmatrix} \otimes \begin{pmatrix}1 & 0 \\
0 & -1 \\
\end{pmatrix} = \begin{pmatrix}0 & 0 & -i & 0 \\
0 & 0 & 0 & i \\
i & 0 & 0 & 0 \\
0 & -i & 0 & 0
\end{pmatrix}
\]

### 2.1.4 Outer Product

Another convenient representation of linear operators is an outer product representation defined by,

\[
|\psi\rangle \langle \varphi| (|\varphi'\rangle) \equiv |\psi\rangle \langle \varphi| \varphi'\rangle = \langle \varphi| \varphi'\rangle |\psi\rangle.
\]  \hspace{1cm} (2.10)

For example an identity operator can be represented as a sum of outer product of an orthonormal basis, i.e.

\[
\hat{I} = \sum_{i=1}^{n} |i\rangle \langle i|
\]  \hspace{1cm} (2.11)

This is known as a completeness relation which can be used to obtain an outer product representations of operators,

\[
\hat{A} = \hat{I} \hat{A} \hat{I} = \sum_{i=1}^{n} \sum_{j=1}^{n} \langle i| \hat{A} | j\rangle | i\rangle \langle j|.
\]  \hspace{1cm} (2.12)
Eigenvectors $|i\rangle$ and their respective eigenvalues $\lambda_i$ of a linear operator $\hat{A}$ are defined by

$$\hat{A}|i\rangle = \lambda_i|i\rangle. \quad (2.13)$$

In a matrix representation the eigenvalues can be determined from a characteristic equation

$$\det(\hat{A} - \lambda \hat{I}) = 0. \quad (2.14)$$

Diagonal representation of an operator is given by

$$\hat{A} = \sum_{i=1}^{n} \lambda_i|i\rangle\langle i| \quad (2.15)$$

where $|i\rangle$ are the eigenvectors.

### 2.1.5 Linear Operators

_A linear operator_ on a vector space is a function which is linear in its inputs,

$$A \left( \sum_{i=1}^{n} a_i|\varphi_i\rangle \right) = \sum_{i=1}^{n} a_iA(|\varphi_i\rangle). \quad (2.16)$$

(To emphasize the difference from c-number or complex numbers the operators are sometimes called the q-numbers or quantum numbers.) The two simplest operators are the

- **identity operator** $\hat{I}$, defined by $\hat{I}|\psi\rangle = |\psi\rangle$ for all $|\psi\rangle$.
- **zero operator** $\hat{0}$, defined by $\hat{0}|\psi\rangle = \vec{0}$ for all $|\psi\rangle$.

Similarly to vectors, operators $A : \mathbb{C}^n \to \mathbb{C}^n$ can be represented in terms of matrices. In _matrix representation_ the linearity condition (2.16) can be rewritten as,

$$\hat{A} \sum_{i=1}^{n} a_i|\varphi_i\rangle = \sum_{i=1}^{n} a_i\hat{A}|\varphi_i\rangle, \quad (2.17)$$

where $\hat{A}$ is an $n \times n$ matrix and $|\varphi_i\rangle$'s are the $n \times 1$ column vectors. The entries $A_{ij}$ of the matrix $\hat{A}$ can be obtained for a given set of basis vectors $|\varphi_1\rangle, |\varphi_2\rangle ... |\varphi_n\rangle$ from

$$\hat{A}|\varphi_j\rangle = \sum_{i} A_{ij}|\varphi_i\rangle. \quad (2.18)$$

and then one can define trace of the matrix as the sum of diagonal elements

$$\text{tr}(\hat{A}) = \sum_{i} A_{ii}.$$
An important example of operators on $\mathbb{C}^2$ are the Pauli matrices,

$$
\begin{align*}
\sigma_0 & \equiv I \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
\sigma_1 & \equiv X \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
\sigma_2 & \equiv Y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\
\sigma_3 & \equiv Z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\end{align*}
$$

(2.19)

The Pauli matrices are related to each other through commutation relations

$$
\begin{align*}
[X,Y] & = 2iZ \\
[Y,Z] & = 2iX \\
[Z,X] & = 2iY
\end{align*}
$$

which can be compactly written

$$
[\sigma_j, \sigma_k] = 2i \sum_{l=1,2,3} \epsilon_{jkl} \sigma_l
$$

where

$$
\epsilon_{jkl} = \begin{cases} 
+1 & \text{if } jkl \text{ is an even permutation of } 123 \\
-1 & \text{if } jkl \text{ is an even permutation of } 123 \\
0 & \text{otherwise.}
\end{cases}
$$

is the Levi-Civita symbol.

### 2.1.6 Adjoint Operators

For every linear operator $\hat{A}$ on a Hilbert space there exist an adjoint (or Hermitian conjugate) operator defined as

$$
(|\psi\rangle, \hat{A}|\varphi\rangle) \equiv (\hat{A}^\dagger |\psi\rangle, |\varphi\rangle).
$$

(2.20)

It follows that

$$
(AB)^\dagger = B^\dagger A^\dagger
$$

(2.21)
and
\[
\left( \hat{A}|\psi\rangle \right)^\dagger = \langle \psi | \hat{A}^\dagger,
\]
where
\[
|\psi\rangle^\dagger \equiv \langle \psi |.
\]
In a matrix representation an adjoint operator is defined as
\[
\hat{A}^\dagger \equiv \left( \hat{A}^* \right)^T
\]
where \((\cdot)^*\) is a complex conjugation and \((\cdot)^T\) is a transpose operation.

Some useful definitions:

- \(\hat{A}\) is a \textit{positive definite} operator if \((|\psi\rangle, \hat{A}|\psi\rangle)\) is a positive real number for all \(|\psi\rangle \neq 0\).
- \(\hat{A}\) is a \textit{self-adjoint} (or Hermitian) operator if \(\hat{A}^\dagger = \hat{A}\). Any positive definite operator is Hermitian.
- \(\hat{A}\) is a \textit{normal} operator if \(\hat{A}\hat{A}^\dagger = \hat{A}^\dagger\hat{A}\). For example, any Hermitian operator is normal.
- \(\hat{P}\) is a \textit{projection} operator if \(\hat{P} = \hat{P}^2\). For example, \(\hat{P} = \sum_{i=1}^k |i\rangle\langle i|\), where \(|i\rangle\) is an orthonormal basis and \(k \leq n\).
- \(\hat{U}\) is a \textit{unitary} operator if \(\hat{U}^\dagger \hat{U} = \hat{I}\). Any pair of orthonormal basis \(|\psi_i\rangle\) and \(|\varphi_i\rangle\) can be used to define unitary operators, i.e. \(\hat{U} = \sum_{i=1}^n |\psi_i\rangle\langle \varphi_i|\).

Note that unitary operators preserve the inner product,
\[
(\hat{U}|\psi\rangle, \hat{U}|\varphi\rangle) = \langle \psi | \hat{U}^\dagger \hat{U} | \varphi \rangle = \langle \psi | \hat{I} | \varphi \rangle = \langle \psi | \varphi \rangle.
\]

2.1.7 Decompositions of operators

- Spectral decomposition. Any normal operator \(M\) on vector space \(V\) is diagonal with respect to some orthonormal basis \(|i\rangle\)'s for \(V\),
\[
M = \sum_i \lambda_i |i\rangle \langle i|
\]
Conversely, any diagonalizable operator is normal. For Hermitian operators the eigenvalues are real. Note that the spectral decomposition can be used to defined functions of operators,
\[
f(M) \equiv \sum_i f(\lambda_i) |i\rangle \langle i|
\]
• Polar decomposition. An arbitrary linear operator can be decomposed into product of unitary operator $U$ and positive operators $J$ and $K$ such that

$$A = UJ = KU$$

where

$$J \equiv \sqrt{A^\dagger A}$$

$$K \equiv \sqrt{AA^\dagger}.$$ 

• Singular value decomposition. For any square matrix $A$ there are exit unitary matrices $U$ and $V$, and a diagonal matrix $D$ such that

$$A = UDV.$$ 

The non-negative diagonal elements of $D$ are called the singular values of $A$.

2.2 Quantum Mechanics

2.2.1 Classical Physics

Classical physics is based on the two postulates:

1. **State space postulate**: Any closed system is associated with even dimensional space called the phase space. The state is described by a single point (or vector) in the phase space. The state is specified by $N$ position (usually denoted by $q_i$'s) and $N$ momentum (usually denoted by $p_i$'s) coordinates:

$$\left(q_1, q_2, ..., q_N, p_1, p_2, ..., p_N\right) \quad (2.26)$$

What is the dimensionality of the phase space of a simple harmonic oscillator? What is the dimensionality of the phase space of a single particle in a box? How many real numbers needed to specify a state of the harmonic oscillator and how many needed to specify a single particle?

2. **Evolution postulate**: Evolution of any closed system is described by function on the phase space. The function is called Hamiltonian and
denoted by \( H(q_1, q_2, \ldots, q_N, p_1, p_2, \ldots, p_N) \) and the evolution is described by the following equations

\[
\dot{p}_i = -\frac{\partial H}{\partial q_i}, \\
\dot{q}_i = \frac{\partial H}{\partial p_i}.
\]  

(2.27)

For a simple harmonic oscillator the Hamiltonian is

\[
H(q, p) = \frac{p^2}{2m} + \frac{kq^2}{2}.
\]  

(2.28)

and the corresponding equations of motion are

\[
\dot{p} = -kq, \\
\dot{q} = \frac{p}{m}
\]  

(2.29)

or equivalently

\[
\ddot{q} = \frac{\dot{p}}{m} = -\frac{kq}{m}.
\]  

(2.30)

2.2.2 Quantum Physics

In contrast the quantum physics is based on three postulates. We will first state the postulates and then introduce the necessary mathematical formalism that goes with it.

1. **State space postulate:** Any closed system is associated with a Hilbert space. The state of the system is described by a single point (or ket-vector) in the Hilbert space

\[
|\psi\rangle
\]  

(2.31)

with unit length

\[
\langle\psi|\cdot|\psi\rangle \equiv \langle\psi|\psi\rangle = 1
\]  

(2.32)

where \( \langle\psi| \) is a bra-vector.

2. **Evolution postulate:** Evolution of any closed system is described by a unitary operator, i.e.

\[
|\psi(t_2)\rangle = \hat{U}(t_2 - t_1)|\psi(t_1)\rangle
\]  

(2.33)

where

\[
\hat{U}(t_2 - t_1) \equiv e^{-\hat{H}(t_2-t_1)}.
\]  

(2.34)

and \( \hat{H} \) is a Hermitian operator known as Hamiltonian operator.
3. **Measurement postulate**: A measurement is described by a collection of measurement operators \( \{ \hat{M}_m \} \) with probability of an outcome \( m \) given by

\[
p(m) = \langle \psi | \hat{M}_m^\dagger \hat{M}_m | \psi \rangle
\]

(2.35)

where \( \hat{M}_m^\dagger \) is the Hermitian conjugate of \( \hat{M}_m \) and

\[
\sum_m \hat{M}_m^\dagger \hat{M}_m = I.
\]

Then the state after measurement

\[
\frac{\hat{M}_m | \psi \rangle}{\sqrt{p(m)}}
\]

(2.36)

Note that usually \( \hat{M}_m \) are assumed to be orthogonal projectors, i.e.

\[
\hat{M}_m = \hat{M}_m^\dagger = \hat{M}_m \hat{M}_m^\dagger \delta_{mm'}
\]

and then one can defined an observable operator

\[
\hat{M} = \sum_m m \hat{M}_m
\]

such that, of example,

\[
\langle \psi | \hat{M} | \psi \rangle = \sum_m m \langle \psi | \hat{M}_m | \psi \rangle = \sum_m m \langle \psi | \hat{M}_m^\dagger \hat{M}_m | \psi \rangle = \sum_m m p(m)
\]

or

\[
\langle \psi | \hat{M}^2 | \psi \rangle = \sum_{m,n} m n \langle \psi | \hat{M}_m \hat{M}_n | \psi \rangle = \sum_{m,n} m n \langle \psi | \hat{M}_m^\dagger \hat{M}_m | \psi \rangle \delta_{mn} = \sum_m m^2 p(m).
\]

### 2.2.3 Schrodinger Picture

Spectral decomposition implies that all normal operators have a diagonal representation,

\[
\hat{A} = \sum_{i=1}^{n} \lambda_i | i \rangle \langle i |.
\]

(2.37)

Therefore all positive definite operators as well as Hermitian operators have diagonal representations. Then one can define a function of Hermitian operators as
for an arbitrary function \( f \). This can be applied to Eq. (1.8) since the Hamiltonian operator \( \hat{H} \) must be Hermitian and thus has a spectral decomposition

\[
\hat{H} = \sum E_n |\psi_n\rangle \langle \psi_n | \tag{2.39}
\]

where \( E_n \) and \( |\psi_n\rangle \) are the eigenvalues and corresponding eigenstates of Hamiltonian operators, i.e.

\[
\hat{H} |\psi_n\rangle = E_n |\psi_n\rangle \tag{2.40}
\]

(The energy eigenstate \( |\psi_n\rangle \) with the lowest energy eigenvalue \( E_n \) is called the ground state.) Moreover, by expanding both sides of Eq. (1.8) we get

\[
|\psi(t_1)\rangle + (t_2 - t_1) \frac{d}{dt} |\psi(t_1)\rangle = \left(1 - (t_2 - t_1) \frac{i}{\hbar} \hat{H}\right) |\psi(t_1)\rangle \tag{2.41}
\]

which is the famous time-dependent Schrödinger equation

\[
i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \tag{2.42}
\]

in contrast to the time-independent Schrödinger equation (2.40). Using (1.8), (1.9), (2.38) and (2.39) we can find the most general solution of the time-dependent Schrödinger equation

\[
|\varphi(t)\rangle = \sum_n e^{-\frac{iE_n t}{\hbar}} [\langle \psi_n | \varphi(0) ] |\psi_n\rangle \tag{2.43}
\]

which is expressed as a linear sum over solutions of the time-independent Schrödinger equation. Note that each solution of the time-independent Schrödinger equation gives rise to a simple solution of the time-dependent Schrödinger equation

\[
|\varphi(t)\rangle = e^{-\frac{iE_n t}{\hbar}} |\psi_n\rangle. \tag{2.44}
\]

### 2.2.4 Heisenberg Picture

A framework where the state vectors evolves with time, but the operators remain constant is a Schrödinger picture. There is also a Heisenberg picture where the operators change with time, and the state vectors remain constant.
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Consider a time independent Hermitian operator \( \hat{A}_S \) in the Schrödinger picture then

\[
\langle \hat{A}_S \rangle(t) = \langle \psi_S(t)|\hat{A}_S|\psi_S(t) \rangle.
\] (2.45)

The time evolution is described by a Schrödinger equation whose solution is

\[
|\psi_S(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_t}|\psi_S(0)\rangle.
\] (2.46)

From (2.45) and (2.46) we obtain

\[
\langle \hat{A}_S \rangle(t) = \langle \psi_S(0)|e^{\frac{i}{\hbar}\hat{A}_H(t)}e^{-\frac{i}{\hbar}\hat{H}_t}|\psi_S(0)\rangle
= \langle \psi_H|\hat{A}_H(t)|\psi_H \rangle
= \langle \hat{A}_H(t) \rangle
\] (2.47)

where

\[
\hat{A}_H(t) \equiv e^{\frac{i}{\hbar}\hat{H}_t}\hat{A}_Se^{-\frac{i}{\hbar}\hat{H}_t}
|\psi_H\rangle \equiv |\psi_S(0)\rangle.
\] (2.48)

It is easy to calculate the time evolution of operators in Heisenberg picture,

\[
\frac{d\hat{A}_H(t)}{dt} = \frac{d}{dt}e^{\frac{i}{\hbar}\hat{H}_t}\hat{A}_Se^{-\frac{i}{\hbar}\hat{H}_t} + \frac{d}{dt}e^{\frac{i}{\hbar}\hat{H}_t}\hat{A}_Se^{-\frac{i}{\hbar}\hat{H}_t}
= \frac{i}{\hbar}\hat{H}e^{\frac{i}{\hbar}\hat{H}_t}\hat{A}_Se^{-\frac{i}{\hbar}\hat{H}_t} - e^{\frac{i}{\hbar}\hat{H}_t}\hat{A}_Se^{-\frac{i}{\hbar}\hat{H}_t}i\hbar \hat{H}e^{-\frac{i}{\hbar}\hat{H}_t}
= \frac{i}{\hbar} \left[ \hat{H}, \hat{A}_H(t) \right]
\] (2.50)

where the commutator is defined as

\[
[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}.
\] (2.51)

Expression (2.50) is known as the Heisenberg equations. It reduces to the Hamiltonian equations of motion in classical mechanics with commutators replaced by Poisson brackets,

\[
-\frac{i}{\hbar} \left[ \cdot, \cdot \right] \rightarrow \{ \cdot, \cdot \} \equiv \frac{\partial}{\partial q} \frac{\partial}{\partial p} - \frac{\partial}{\partial p} \frac{\partial}{\partial q}
\] (2.52)

i.e.

\[
\frac{dp}{dt} = \{ p, H \} = -\frac{\partial H}{\partial q}
\] (2.53)

\[
\frac{dq}{dt} = \{ q, H \} = \frac{\partial H}{\partial p}
\] (2.54)
Moreover, the Poisson bracket between conjugate variables
\[ \{ q, p \} = 1 \]  
(2.55)
is replaced by a commutation relation
\[ -\frac{i}{\hbar} [\hat{q}, \hat{p}] = 1. \]  
(2.56)

2.2.5 Density matrix

If the exact knowledge of the quantum microstate is not available, the system
is said to be in a not pure, but mixed state. Such states are not specified by
a unique vector in Hilbert space, but by a collection of vector \( \{ |\varphi_\alpha \rangle \} \) with
relative probabilities \( \{ p_\alpha \} \), such that
\[ \sum_\alpha p_\alpha = 1. \]  
(2.57)

And the entropy of a mixed state is defined as
\[ S = \sum_\alpha p_\alpha \log p_\alpha. \]  
(2.58)

Then, the ensemble average of a given operator \( \hat{O} \) is given by
\[ \langle \hat{O} \rangle = \sum_\alpha p_\alpha \langle \varphi_\alpha | \hat{O} | \varphi_\alpha \rangle. \]  
(2.59)

In a given set of orthonormal basis, \( |\psi_n \rangle \), the above expression takes the
following form
\[
\langle \hat{O} \rangle = \sum_{\alpha,n,m} p_\alpha \langle \varphi_\alpha | \psi_n \rangle \langle \psi_n | \hat{O} | \psi_m \rangle \langle \psi_m | \varphi_\alpha \rangle = \\
= \sum_{n,m} \left( \sum_\alpha p_\alpha \langle \psi_m | \varphi_\alpha \rangle \langle \varphi_\alpha | \psi_n \rangle \right) \langle \psi_n | \hat{O} | \psi_m \rangle = \\
= \sum_{n,m} \langle \psi_m | \hat{\rho} | \psi_n \rangle \langle \psi_n | \hat{O} | \psi_m \rangle = \\
= \sum_{n,m} \langle \psi_m | \hat{\rho} \hat{O} | \psi_m \rangle = \\
= \text{Tr}(\hat{\rho} \hat{O}) \]  
(2.60)
where the so-called density matrix is defined as

$$\hat{\rho} \equiv \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle \psi_\alpha|.$$  (2.61)

This is the Hermitian operator which replaces the probability distribution function in classical phase space.

Let $|\psi_n\rangle$ be the energy eigenstates, then

$$\langle \psi_n| i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) |\psi_m\rangle = i\hbar \frac{\partial}{\partial t} \sum_\alpha p_\alpha \langle \psi_n| \hat{H}|\psi_\alpha\rangle \langle \psi_\alpha|\psi_m\rangle$$

$$= \sum_\alpha p_\alpha \left( \langle \psi_n| i\hbar \frac{\partial}{\partial t} |\psi_\alpha\rangle |\psi_\alpha\rangle \langle \psi_\alpha|\psi_m\rangle + \langle \psi_n| |\psi_\alpha\rangle \langle \psi_\alpha| i\hbar \frac{\partial}{\partial t} |\psi_\alpha\rangle \right)$$

$$= \sum_\alpha p_\alpha \left( \langle \psi_n| \hat{H}|\psi_\alpha\rangle \langle \psi_\alpha|\psi_m\rangle + \langle \psi_n| |\psi_\alpha\rangle \left( i\hbar \frac{\partial}{\partial t} |\psi_\alpha\rangle \right) \right)$$

$$= \sum_\alpha p_\alpha \left( E_n \langle \psi_\alpha|\psi_\alpha\rangle \langle \psi_\alpha|\psi_m\rangle - E_m \langle \psi_\alpha|\psi_\alpha\rangle \langle \psi_\alpha|\psi_m\rangle \right)$$

$$= \langle \psi_n| \hat{\rho} (E_n - E_m) |\psi_m\rangle$$

$$= \langle \psi_n| \hat{H} \hat{\rho} - \hat{\rho} \hat{H} |\psi_m\rangle $$  (2.62)

Thus, independently of basis we get the Von Neumann equation:

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = [\hat{H}, \hat{\rho}],$$  (2.63)

which is a quantum version of Liouville's equation obtained (once again) by a formal substitution of Poisson brackets with commutator, i.e. $\{, \} \rightarrow -\frac{i}{\hbar} [ , ]$.

### 2.2.6 Schmidt decomposition

**Partial trace.** For a composite system $AB$ the reduced density operator of a subsystem $A$ is obtained by a partial trace

$$\rho^A \equiv tr_B(\rho^{AB})$$  (2.64)

which is defined by

$$tr_B(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) \equiv |a_1\rangle\langle a_2| tr(|b_1\rangle\langle b_2|).$$  (2.65)

**Schmidt decomposition.** What is perhaps surprising is that if the combined system is in a pure state,

$$\rho^{AB} = |\psi\rangle\langle \psi|$$  (2.66)
then there exist orthonormal basis $|a_i⟩'$s and $|b_i⟩'$s for subsystems such that the reduced density matrices are given by

$$\rho^A = \sum_i \lambda_i^2 |a_i⟩⟨a_i|$$  \hspace{1cm} (2.67)

$$\rho^B = \sum_i \lambda_i^2 |b_i⟩⟨b_i|.$$  \hspace{1cm} (2.68)

This is a consequence of the so-called Schmidt decomposition of a pure state of a combined system,

$$|ψ⟩ = \sum_i \lambda_i |a_i⟩ \otimes |b_i⟩$$  \hspace{1cm} (2.69)

where $\lambda_i$ are non-negative real numbers satisfying the normalization condition

$$\sum_i \lambda_i^2 = 1.$$  \hspace{1cm} (2.70)

The total number of non-zero $\lambda_i$'s is called the Schmidt number, and $|a_i⟩$ and $|b_i⟩$ are called the Schmidt bases.

In the case when the two subsystems have the same dimensionality the Schmidt decomposition can be obtained starting from a general expression

$$|ψ⟩ = \sum_{j,k} a_{jk} |j⟩ \otimes |k⟩$$  \hspace{1cm} (2.71)

where $a_{jk}$ is some square matrix of complex numbers. Using the singular value decomposition

$$a_{jk} = \sum_i u_{ji} d_{ii} v_{ik}$$  \hspace{1cm} (2.72)

where $u$ and $v$ are unitary matrices. Then

$$|ψ⟩ = \sum_{i,j,k} u_{ji} d_{ii} v_{ik} |j⟩ \otimes |k⟩$$  \hspace{1cm} (2.73)

which is equivalent to (2.69) with following identifications

$$d_{ii} = \lambda_i$$  \hspace{1cm} (2.74)

$$|a_i⟩ = \sum_j u_{ji} |j⟩$$  \hspace{1cm} (2.75)

$$|b_i⟩ = \sum_k v_{ik} |k⟩.$$  \hspace{1cm} (2.76)

**Purification.** An inverse operation to partial trace is purification. Suppose we start with a general mixed state $\rho^A$ with spectral decomposition

$$\rho^A = \sum_i p_i |a_i⟩⟨a_i|$$  \hspace{1cm} (2.77)
then one can construct an enlarged system in pure state

$$|\psi\rangle = \sum_i \sqrt{p_i} |a_i\rangle \otimes |r_i\rangle$$

(2.78)

described by density matrix

$$\rho_{AR} = |\psi\rangle \langle \psi|$$

$$= \sum_{ij} \sqrt{p_i p_j} |a_i\rangle \otimes |r_i\rangle \langle a_j| \otimes \langle r_j|$$

$$= \sum_i p_i |a_i\rangle \langle a_i| \otimes |r_i\rangle \langle r_i|$$

(2.79)

whose partial trace

$$tr_R(\rho_{AR}) = tr_R\left( \sum_i p_i |a_i\rangle \langle a_i| \otimes |r_i\rangle \langle r_i| \right) = \rho^A.$$  

(2.80)