Fundamentals of Quantum Mechanics in Liouville Space

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February 2020

Abstract. The purpose of this paper is to articulate a coherent and easy-to-understand way of doing quantum mechanics in any finite-dimensional Liouville space, based on the use of Kronecker product and what we have termed the 'bra-flipper' operator. Simple applications of the Liouville space formalism — for example, in solving master equations like the Lindblad equation — are also discussed, among other applications. The paper is addressed to students and researchers with some basic knowledge of quantum mechanics but who are new to the Liouville space formalism and seek a deeper understanding of it. The concepts are conveyed so as to make the application of the formalism to more complex problems in quantum physics straightforward and unencumbered.

Keywords: Liouville space, Hilbert space, Kronecker product, Bra-flipper operator

1. Introduction

For many complex problems in quantum mechanics, the Liouville space formalism turns out to be very effective in finding solutions or mathematically characterizing the problem. This is true, for example, in solving master equations in the theory of open quantum systems [1, 2]. To see why this is the case, we first have to recognize that the density matrix [3, 4] is a more pragmatic way of describing the quantum state of a system compared to vectors in the Hilbert space of pure states (HSPS) because it offers a general, compact and elegant way of describing quantum states. This makes it easier (with respect to the use of state vectors) to derive general formulas for probabilities and observable averages. Perhaps, nothing makes one appreciate the invention of density matrices than the quantum theory of relaxation [4]. The vast majority of quantum relaxation processes (from nuclear and electron spin magnetic resonance studies to relaxation processes in quantum optics) studied in physics, chemistry and biology become cumbersome and more likely to be fraught with unnecessary complications without the use of density matrices. However, though the equations of motion for the density matrix for such relaxation processes are often linear in the former, they are often not amenable to easy resolution. The Gorini-Sudarshan-Kossakowski-Lindblad master equation [5-7] is an excellent example. The Liouville space formalism offers a way around the problem. This is because, in this linear space, operators defined on HSPS become column vectors (called supervectors) and given that we are adept at solving equations of motion for vectors in HSPS (think of the Schrödinger equation, [7]), we can easily apply those same techniques also in Liouville space [1, 8].
The literature already provides a number of important introductions to the subject [1] [9] [10] [11] [12] [13] but for students and researchers new to it, grasping the basics is often challenging and confusing. A careful analysis of the literature points to one important source of this confusion. It has to do with the operational meaning an author assigns to the symbol ‘⊗’ (sometimes indicated as ‘×’ [9]). In some expositions (which we may call the ‘symbolic approach’), the common operational symbol ‘⊗’ is deprived of its common meaning and operations involving said symbol are assigned customized results which cannot be traced to any basic mathematical operations. This is the approach used, for example, in [14]. In fact, in referring to the symbol ‘⊗’ the authors clarify that it “is not a tensor product, but a related operation” [14, chap. 1, pg. 20].

Then there are those expositions (which we may call the ‘literal approach’) in which the symbol ‘⊗’ retains its normal operational meaning — namely, the tensor product. The literal approach is used, for example, in [11]. There are also those introductions where neither ‘⊗’ nor ‘×’ are explicitly used but either the symbolic approach or the literal one are implicitly implied in the operations (see for example [1, 15]).

The rationale behind this paper is threefold: 1) give a coherent account of quantum mechanics in Liouville space, 2) impact the readership with a simple and unified view of the subject so as to render the study of quantum systems of diverse nature in Liouville space conceptually and mathematically easy, and 3) strengthen further the literal approach. We emphasize that the present account is restricted to separable (see Appendix A.1 for definition) and finite Hilbert spaces (thus, separable and finite Liouville spaces as well). We shall rely solely on the basics of elementary quantum mechanics and only introduce here — as a matter of formality — a new operator, which we call the ‘bra-flipper’ operator (see §3.2). As we shall see later, this is all that we need (together with the tensor product operation and its properties) to make doing quantum mechanics in Liouville space easy and straightforward.

The paper is organized into three main sections. In the first section (§2) we give a quick overview of standard quantum mechanics in HSPS. We then gradually construct the notion of Liouville space and its related formalism in the second section (§3) — where, among other things, we introduce the bra-flipper operator (§3.2). This is followed by the third section (§4) where we apply the mathematical apparatus and concepts developed in the preceding section to formulate equations of motion in Liouville space according to Schrödinger, Heisenberg and interaction pictures. We also discuss in this section solutions to a specific class of master equations (for isolated or open quantum systems) to which the Lindblad equation belongs. Readers who may be less familiar with linear algebra and functional analysis may consult Appendix A.1 for some basic notions and definitions.

2. Overview of quantum mechanics in HSPS

The Reader will have noticed that in the preceding section, we always used the term Hilbert space of pure states (HSPS), instead of simply Hilbert space. This is because the notion of Hilbert space is a very broad one. Even the so-called Liouville space — the subject of this article — is in itself a Hilbert space (more on this later). In fact, any linear space which is complete and endowed with a norm is a Hilbert space (see Appendix A.1). In quantum mechanics, however, the term Hilbert space is often taken as synonymous with (or used as a shorthand for) what we refer to as ‘Hilbert space of
pure states. For the sake of clarity, we shall keep this distinction in our discussion. For a solid introduction to Hilbert spaces, we recommend [16, 17, 18, 19, 20, 21] — to name a few excellent references.

2.1. Pure states

What is then a pure state? The state of a quantum system is said to be pure when we have complete information on it [4, 22, 23]. ‘Complete information’ in the sense that there is no classical uncertainty as to what the quantum state is [22]. The set of all pure states of a quantum system form a complex linear space $\mathcal{H}$ — this is the gist of the superposition principle [23, 24] in quantum mechanics. $\mathcal{H}$ is complete and has a norm [16, 17]; thus, it is also a Hilbert space (Appendix A.1). This is the space we have been referring to as the Hilbert space of pure states (HSPS). And the pure states, being elements of the space, are said to be vectors of the latter (Appendix A.1).

Let $\mathcal{H}_d$ be a finite-dimensional HSPS of dimension $d$. Associated with $\mathcal{H}_d$ is an adjoint space (or dual space), indicated as $\mathcal{H}_d^*$. Using Dirac’s notation, let $|x\rangle$ be a vector in $\mathcal{H}_d$. $|x\rangle$ is a $(d \times 1)$ column vector. There is a one-to-one correspondence between the elements of $\mathcal{H}_d$ and $\mathcal{H}_d^*$: if $|x\rangle \in \mathcal{H}_d$, then there exists its corresponding element, denoted as $\langle x|$, in $\mathcal{H}_d^*$. The relation between the two is

$$\langle x| = |x\rangle^\dagger$$

(1)

where, for any vector, matrix or operator $A$, ‘$A^\dagger$’ indicates the conjugate transpose of $A$. We therefore see that $\langle x|$ must be a row vector of dimension $(1 \times d)$. $\langle x|$ is said to be the dual vector of $|x\rangle$.

For $|y\rangle \in \mathcal{H}_d^*$ and $|x\rangle \in \mathcal{H}_d$, $\langle y| |x\rangle$ maps $|x\rangle$ to a scalar through the matrix product

$$\left(\langle y|\right)\left(|x\rangle\right) \equiv \langle y| x \rangle .$$

(2)

Equation (2) also defines an inner product (or scalar product) for $\mathcal{H}_d$ [16, 18, 19] (Appendix A.1). That is, given two vectors $|y\rangle, |x\rangle \in \mathcal{H}_d$, we can choose their inner product to be defined as

$$\langle |y\rangle, |x\rangle \rangle := \langle y| x \rangle .$$

(3)

For separable Hilbert spaces, (3) is the commonly used inner product, and so shall we in this paper.

Let $|\psi(t)\rangle$ be a generic pure state in $\mathcal{H}_d$. The vector $|\psi(t)\rangle$ can be expanded in any orthonormal basis $\{|\phi_n\rangle\}$ ($n = 1, \ldots, d$) of the Hilbert space $\mathcal{H}_d$. That is,

$$|\psi(t)\rangle = \sum_{n=1}^{d} \phi_n(t) |\phi_n\rangle , \quad \langle \phi_n|\phi_{n'} \rangle = \delta_{n,n'} .$$

(4)

Since there is an infinite number of possible orthonormal bases, we deduce that there is an infinite number of ways of expressing the same vector $|\psi(t)\rangle$ of the system. Because the elements of the set $\{|\phi_n\rangle\}$ form an orthonormal basis, it follows from (4) that the complex coefficient $\phi_n(t)$ is given by the expression

$$\phi_n(t) = \langle \phi_n|\psi(t)\rangle$$

(5)
which, when introduced into (4), yields the identity

\[ \mathbb{I}_d = \sum_{n=1}^{d} |\phi_n\rangle \langle \phi_n| \]  

(6)

where \( \mathbb{I}_d \) is the identity operator on \( \mathcal{H}_d \). Equation (6) is valid for any arbitrary orthonormal basis of \( \mathcal{H}_d \). If \( |\psi(t)\rangle \) is normalized, such that \( \langle \psi(t)|\psi(t)\rangle = 1, \forall t \geq 0 \), then the normalization condition \( \sum_{n=1}^{d} |\phi_n(t)|^2 = 1 \) readily follows. It must be emphasized that in (4), the state of the system is simultaneously \( |\phi_1\rangle, \ldots, |\phi_d\rangle \), each to some degree; for each \( |\phi_n\rangle \), this degree is quantified by the respective coefficient \( \phi_n(t) \) and we say there is quantum coherence [23, 24].

If the system also happens to be isolated, for example, then Schrödinger’s equation applies and its equation of motion reads

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

(7)

where \( H \) is the system’s Hamiltonian operator.

2.2. Mixed states

When there is classical uncertainty on the system’s quantum state, we resort to an ensemble of vectors in HSPS to describe it. The result is what we call a mixed state [4, 22, 23]. This is a collection of positive real numbers \( 0 \leq p_k \leq 1 \) and their corresponding vectors \( |\psi_k\rangle \in \mathcal{H}_d \), where \( p_k \) is the probability that the quantum system is in the pure state \( |\psi_k\rangle \). Mixed states are therefore typically expressed in the form of the collection \( \{p_k, |\psi_k\rangle\} \) and they are symptom of the observer’s lack of complete information on the quantum state of the system under study. Either \( p_k \) or \( |\psi_k\rangle \) (or both) may depend on time. Nonetheless, the condition \( \sum_k p_k = 1 \) always holds.

Given the mixed state \( \{p_k, |\psi_k\rangle\} \), where the pure states \( |\psi_k\rangle \) form an orthonormal basis of \( \mathcal{H}_d \), we may introduce an operator \( \rho \), the density matrix (or density operator), defined on \( \mathcal{H}_d \) such that

\[ \langle \psi_k|\rho|\psi_k\rangle = p_k, \forall k. \]  

(8)

Then, the operator \( \rho \) must be of the form

\[ \rho = \sum_{k=1}^{d} p_k |\psi_k\rangle \langle \psi_k|. \]  

(9)

Equation (9) is the diagonal representation of \( \rho \). If we choose to represent \( \rho \) in a different orthonormal basis — say \( \{\phi_n\} \) — , then, from (9) and (6), we have

\[
\rho = \sum_{k=1}^{d} p_k \mathbb{I}_d |\psi_k\rangle \langle \psi_k| \mathbb{I}_d = \sum_{k=1}^{d} p_k \sum_{n=1}^{d} \sum_{n'=1}^{d} |\phi_n\rangle \langle \phi_n| |\psi_k\rangle \langle \psi_k| |\phi_n'\rangle \langle \phi_n'| |\phi_n\rangle \langle \phi_n'| \\
= \sum_{n=1}^{d} \sum_{n'=1}^{d} \left( \sum_{k=1}^{d} p_k |\phi_n| \langle \psi_k| |\phi_n'\rangle \langle \psi_k| |\phi_n'\rangle \right) |\phi_n\rangle \langle \phi_n'| \\
= \sum_{n=1}^{d} \sum_{n'=1}^{d} \lambda_{nn'} |\phi_n\rangle \langle \phi_n'| .
\]  

(10)
Thus, in a different orthonormal basis, $\rho$ ceases to be diagonal even though the statistics of measurement outcomes remain the same. Such different representations of the same density matrix $\rho$ are related to each other through a unitary transformation. If the system is isolated, with Hamiltonian $H$, and we take the time derivative of $\rho(t)$, then, from (7) and (9), we obtain

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar} [H, \rho(t)]$$

(11)

which is the Liouville-von Neumann equation.

Note that a pure state may also be expressed in the form of a density matrix. If we take $|\psi(t)\rangle$ in (4) for example, its associated density matrix is

$$\rho(t) = \sum_{n=1}^{d} \sum_{n'=1}^{d} a_{nn'}(t) \langle \phi_n | \phi_{n'} \rangle$$

(12)

where we notice the similarity between the final forms of $\rho$ in (10) and (12). This tells us that the fact that a density matrix $\rho$ has nonzero off-diagonal elements (i.e. coherence) in a basis, does not necessarily mean it represents a mixed state. To check whether a density matrix represents a mixed or pure state, one has to put it in its diagonal form, (9): if there are more than one nonzero $p_k$, then the state is mixed, otherwise it is pure. Put more elegantly, $\rho$ represents a pure state if its rank (i.e. the number of nonzero eigenvalues) is 1; if the rank is greater than 1 then the state is mixed. For example, all the following qubit density matrices represent pure states:

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & -e^{i\theta} \\ -e^{-i\theta} & 1 \end{pmatrix}$$

$$\rho = \frac{3}{4} \begin{pmatrix} 1 & \frac{\sqrt{3}}{3} e^{i2\theta} \\ \frac{\sqrt{3}}{3} e^{-i2\theta} & \frac{1}{3} \end{pmatrix}$$

(13)

The fact that the rank of a pure state’s density matrix is 1 also leads to the assertion that $\text{Tr}[\rho^2] = 1$ if $\rho$ represents a pure state; while for a mixed state, $\text{Tr}[\rho^2] < 1$.

2.3. The Hilbert space of operators $O_d$ and the extended Hilbert-Schmidt inner product

Thus far, we have only met three linear operators defined on $H_d$: the Hamiltonian $H$, the density matrix $\rho$ and the identity operator $I_d$. Certainly, for a given $H_d$ there is an infinite number of linear operators one can define on it. These operators also form a finite-dimensional linear space. Let it be denoted as $O_d$. In reality, there is a one-to-one correspondence between elements of $O_d$ and $(d \times d)$ square matrices, so we shall speak of the elements of $O_d$ as operators or matrices, interchangeably. The corresponding adjoint space is $O_d^*$. As usual, there is a one-to-one correspondence between the elements of $O_d$ and $O_d^*$; if $A \in O_d$, then its dual is $A^\dagger (\in O_d^*)$. Also, since it is a linear space, we would expect to be able to define an inner product on $O_d$. The commonly used one here is the Hilbert-Schmidt inner product. If $A$ and $B$ are two elements of $O_d$, then their Hilbert-Schmidt inner product is

$$\langle A, B \rangle = \text{Tr} [BA^\dagger]$$

(14)

$A$ and $B$ are square matrices so $\langle A, B \rangle = \text{Tr} [A^\dagger B]$, due to trace property. But on close examination, one observes that if we define an ordered inner product as given
in (14) (which may be called ‘extended Hilbert-Schmidt’ to differentiate it from the conventional one), then the inner product we defined for $H_d$, (3), is also of the same kind. Indeed, from (3) and (6),

$$\langle |y\rangle, |x\rangle \rangle = \langle y|I_d|x\rangle = \sum_{n=1}^{d} \langle \phi_n|\phi_n\rangle = \sum_{n=1}^{d} \langle \phi_n|x\rangle \langle y|\phi_n\rangle = \text{Tr}[|x\rangle \langle y|].$$

(15)

Thus, for both $H_d$ and $O_d$, we have the extended Hilbert-Schmidt inner product, (14), as the scalar product. Moreover, if $\{|\phi_n\rangle\}$ is an orthonormal basis for $H_d$, then the set of operators $\{|\phi_n\rangle \langle \phi_{n'}|\}$ — where $n,n' = 1,2,\ldots,d$ — constitute an orthonormal basis for $O_d$. The orthonormality of the elements of $\{|\phi_n\rangle \langle \phi_{n'}|\}$ can be verified with the extended Hilbert-Schmidt inner product, (14). The linear space $O_d$ is therefore complete and normed, which makes it a (complex) Hilbert space. The dimension of the set $\{|\phi_n\rangle \langle \phi_{n'}|\}$ — and, therefore, of $O_d$ — is easily seen to be $d^2$.

3. Mathematical foundations of Quantum Mechanics in Liouville space

3.1. Some initial considerations

For separable Hilbert spaces (Appendix A.1) like $H_d$ and $O_d$, it is always possible to represent their elements as column vectors and operators as matrices. Thus, quantum mechanics in separable Hilbert spaces turns out to be essentially matrix analysis [25, 26]. If we consider again Schrödinger’s equation, (7), we may conveniently view it as the classic matrix calculus problem

$$\frac{d}{dt} x(t) = A x(t), \quad x(0) = c$$

(16)

where $x(t)$ and $c$ are $(d \times 1)$ complex column matrices and $A$ is a $(d \times d)$ complex square matrix. We know from matrix analysis (via the theory of matrix functions) that the differential equation in (16) has as solution [26, 29, 30]

$$x(t) = e^{tA} c$$

(17)

where $e^{tA}$ (sometimes also indicated as exp$[tA]$) is a $(d \times d)$ complex square matrix defined as

$$e^{tA} := I_d + tA + \frac{t^2}{2!} A^2 + \frac{t^3}{3!} A^3 + \ldots = \sum_{n=0}^{\infty} \frac{t^n}{n!} A^n$$

(18)

where we define $A^n := I_d$ (here $I_d$ is the $d \times d$ identity matrix) for $n = 0$. For a review on how $e^{tA}$ may be effectively computed, we recommend the updated version of Moler and Van Loan’s celebrated “Nineteen dubious ways” paper [31]. If we set $x(t) = |\psi(t)\rangle$ and $A = -\frac{i}{\hbar} H$, (17) solves the Schrödinger equation, (7).

Had $x(t)$ and $A$ been scalars, the solution to the differential equation in (16) would still be of the form given in (17). This equivalence does not hold true in general. If we consider the Liouville-von Neumann equation — (11) —

$$\frac{d}{dt} \rho(t) = -\frac{i}{\hbar} (H \rho(t) - \rho(t) H)$$

(19)
for example, we cannot solve it assuming $\rho(t)$ and $H$ were scalars. What makes matrix differential equations of this sort challenging to solve is the fact that given two matrices $A$ and $B$, in general, $AB \neq BA$. Solving the linear equation

$$AX + XB = C$$  \hspace{1cm} (20)

for $X$ (where $X, A, B$ and $C$ are square matrices of the same dimension $n$) also poses similar problems. The conundrum can be put to rest by resorting to Kronecker product. The point is that solving a problem like (20) for $X$ is, in ultimate analysis, solving for a countable set of functions (i.e. the elements of $X$): however these functions may be organized — in the form of a square matrix or otherwise — is of secondary importance. With the help of the Kronecker product, a problem like (20) may be solved by factoring out $X$ in the form of a column vector from the l.h.s. turning the equation into (see for example [32, 33])

$$\tilde{D} \text{vec}[X] = \text{vec}[C]$$  \hspace{1cm} (21)

where $\tilde{D}$ is a square matrix that depends on $A$ and $B$, while $\text{vec}[X]$ and $\text{vec}[C]$ are the column vector representation of $X$ and $C$, respectively. Note that while $\text{vec}[X]$ and $\text{vec}[C]$ are column vectors of dimension $(n^2 \times 1)$, $\tilde{D}$ is a square matrix of dimension $(n^2 \times n^2)$. Moreover, while the form in (21) can always be achieved from (20), care must be taken when solving the former for $\text{vec}[X]$. The solution set for $\text{vec}[X]$ may consist of a unique element, infinite elements or be empty (i.e. no solution), depending on the nature of $\tilde{D}$ and $\text{vec}[C]$. For example, if $\tilde{D}$ is invertible and $\text{vec}[C]$ is not a null column vector, then

$$\text{vec}[X] = \tilde{D}^{-1} \text{vec}[C].$$  \hspace{1cm} (22)

If the transformation $AX + XB = C \mapsto \tilde{D} \text{vec}[X] = \text{vec}[C]$ is always possible, then it is easy to imagine also the following transformation of the Liouville-von Neumann equation

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}(H\rho(t) - \rho(t)H) \mapsto \frac{d}{dt}\text{vec}[\rho(t)] = \mathcal{L} \text{vec}[\rho(t)]$$  \hspace{1cm} (23)

from which follows the general solution

$$\text{vec}[\rho(t)] = e^{t\mathcal{L}} \text{vec}[\rho(0)]$$  \hspace{1cm} (24)

where $\mathcal{L}$ and $e^{t\mathcal{L}}$ are $(d^2 \times d^2)$ matrices which depend on the Hamiltonian $H$, while $\text{vec}[\rho(t)]$ and $\text{vec}[\rho(0)]$ are $(d^2 \times 1)$ column vectors. The square matrix $e^{t\mathcal{L}}$ still has a series expression similar to (18), namely,

$$e^{t\mathcal{L}} = I_{d^2} + t\mathcal{L} + \frac{t^2}{2!}\mathcal{L}^2 + \frac{t^3}{3!}\mathcal{L}^3 + \ldots = \sum_{n=0}^{\infty} \frac{t^n}{n!}\mathcal{L}^n.$$  \hspace{1cm} (25)

The transformation in (23) is the quintessence of the Liouville space formalism: viz. the linear space where HSPS linear operators become column vectors.

Before going any further, it is important we introduce the Kronecker product and its properties in the next subsection. In the subsequent subsections, we employ these properties to develop the Liouville space formalism.
3.1.1. Kronecker product and properties. Let \( X = [x_{ij}] \) be a matrix of dimension \((m \times n)\) and \( Y = [y_{ij}] \) a matrix of dimension \((m' \times n')\),

\[
X = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{pmatrix}, \quad Y = \begin{pmatrix} y_{11} & y_{12} & \cdots & y_{1n'} \\ y_{21} & y_{22} & \cdots & y_{2n'} \\ \vdots & \vdots & \ddots & \vdots \\ y_{m'1} & y_{m'2} & \cdots & y_{m'n'} \end{pmatrix}. \tag{26}
\]

Then, the Kronecker product (also called ‘tensor product’ or ‘direct product’) \( X \otimes Y \) is a \((mm' \times nn')\) matrix defined as

\[
X \otimes Y := \begin{pmatrix} x_{11}Y & x_{12}Y & \cdots & x_{1n}Y \\ x_{21}Y & x_{22}Y & \cdots & x_{2n}Y \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1}Y & x_{m2}Y & \cdots & x_{mn}Y \end{pmatrix}. \tag{27}
\]

For example, if

\[
X = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix}, \quad Y = \begin{pmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{pmatrix}, \tag{28}
\]

then

\[
X \otimes Y = \begin{pmatrix} x_{11}y_{11} & x_{11}y_{12} & x_{12}y_{11} & x_{12}y_{12} \\ x_{11}y_{21} & x_{11}y_{22} & x_{12}y_{21} & x_{12}y_{22} \\ x_{21}y_{11} & x_{21}y_{12} & x_{22}y_{11} & x_{22}y_{12} \\ x_{21}y_{21} & x_{21}y_{22} & x_{22}y_{21} & x_{22}y_{22} \end{pmatrix}. \tag{29}
\]

We note that, in general, \( X \otimes Y \neq Y \otimes X \). Here are some useful properties and identities involving the Kronecker product (\( V, X, Y, Z \) are matrices) (proofs can be found in [32]):

(i) **Multiplication by scalar**: If \( c \) is complex scalar, then

\[
X \otimes (cY) = c(X \otimes Y) \tag{30}
\]

(ii) **Distributive property with respect to addition**:

\[
(X + Y) \otimes Z = X \otimes Z + Y \otimes Z \tag{31a}
\]

\[
X \otimes (Y + Z) = X \otimes Y + X \otimes Z \tag{31b}
\]

(iii) **Associative property**:

\[
X \otimes (Y \otimes Z) = (X \otimes Y) \otimes Z \tag{32}
\]

(iv) **Mixed product rule**: If \( X, Y, Z, V \) are matrices of dimension \((m \times n), (n \times m), (m' \times n')\) and \((n' \times m')\), respectively, then

\[
(X \otimes Z)(Y \otimes V) = (XY) \otimes (ZV) \tag{33}
\]

(v) **The inverse of a Kronecker product**: If \( X \) and \( Y \) are invertible matrices, then

\[
(X \otimes Y)^{-1} = X^{-1} \otimes Y^{-1} \tag{34}
\]
(vi) The conjugate transpose of a Kronecker product:

\[(X \otimes Y)^\dagger = X^\dagger \otimes Y^\dagger\]  

(vii) Eigenvalues and eigenvectors: Let \(X\) and \(Y\) be diagonalizable matrices of dimension \((n \times n)\) and \((m \times m)\), respectively. Let \(\{\lambda_j\}\) and \(\{x_j\}\) \((j = 1, 2, \ldots, n)\) be the eigenvalues and eigenvectors of \(X\), respectively. Similarly, let \(\{\mu_k\}\) and \(\{y_k\}\) \((k = 1, 2, \ldots, m)\) be the eigenvalues and eigenvectors of \(Y\), respectively. Then, \(\{\lambda_j\mu_k\}\) and \(\{x_j \otimes y_k\}\) are eigenvalues and eigenvectors of \(X \otimes Y\), respectively.

That is

\[(X \otimes Y)(x_j \otimes y_k) = \lambda_j \mu_k (x_j \otimes y_k)\]  

(viii) Trace function of a Kronecker product:

\[\text{Tr}[X \otimes Y] = \text{Tr}[X] \cdot \text{Tr}[Y]\]  

(ix) Determinant of a Kronecker product: If \(X\) is a \((n \times n)\) matrix, and \(Y\) is a \((m \times m)\) matrix then

\[\det[(X \otimes Y)] = (\det[X])^m \cdot (\det[Y])^n\]  

(x) Analytic function of a Kronecker product involving an identity matrix: Let \(X\) be a \((n \times n)\) square matrix, and \(I_m\) the \((m \times m)\) identity matrix. If \(f\) is an analytic function defined for both the Kronecker product (between \(X\) and \(I_m\)) and for \(X\), then

\[f(X \otimes I_m) = f(X) \otimes I_m\]  

\[f(I_m \otimes X) = I_m \otimes f(X)\]  

Examples of matrix analytic functions include \(\exp[\bullet]\) and the trigonometric functions \(\sin(\bullet)\) and \(\cos(\bullet)\). So, we have, for example, that

\[e^{X \otimes I_m} = e^X \otimes I_m\]  

\[\sin(I_m \otimes X) = I_m \otimes \sin(X)\]  

\[\cos(X \otimes I_m) = \cos(X) \otimes I_m\]  

where

\[\cos(X) := I_n - \frac{X^2}{2!} + \frac{X^4}{4!} - \frac{X^6}{6!} + \ldots = \sum_{k=0}^{\infty} (-1)^k \frac{X^{2k}}{(2k)!}\]  

\[\sin(X) := X - \frac{X^3}{3!} + \frac{X^5}{5!} - \frac{X^7}{7!} + \ldots = \sum_{k=0}^{\infty} (-1)^k \frac{X^{2k+1}}{(2k+1)!}\]  

3.2. The bra-flipper operator, \(\mathcal{U}\)

We saw in the last subsection that in the Liouville space formalism, operators like the density matrix become column vectors. These ‘vectorized’ operators are commonly referred to as ‘supervectors’ or ‘superkets’. Consider the qubit pure state

\[|\psi(t)\rangle = a(t) |0\rangle + b(t) |1\rangle\]
where \( a(t) \) and \( b(t) \) are complex scalars which satisfy the normalization condition \( |a(t)|^2 + |b(t)|^2 = 1 \). The matrix representation of the elements of the basis \( \{ 0, 1 \} \) is

\[
|0 \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1 \rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
\]

Consequently,

\[
\langle 0 | = |0 \rangle^\dagger = \begin{pmatrix} 1 & 0 \end{pmatrix} \quad \langle 1 | = |1 \rangle^\dagger = \begin{pmatrix} 0 & 1 \end{pmatrix}
\]

and the matrix representation of the generic qubit pure state \( |\psi(t)\rangle \) is

\[
|\psi(t)\rangle = a(t) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b(t) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}.
\]

The density matrix \( \rho(t) \) corresponding to this pure state is of the form

\[
\rho(t) = |\psi(t)\rangle \langle \psi(t)| = |a(t)|^2 |0\rangle \langle 0| + a(t)b^*(t) |0\rangle \langle 1| + a^*(t)b(t) |1\rangle \langle 0| + |b(t)|^2 |1\rangle \langle 1|.
\]

The matrix representation of \( \rho(t) \) can be obtained either from (48a) or (48b). If we use (48a), then

\[
\rho(t) = |\psi(t)\rangle \langle \psi(t)| = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} \begin{pmatrix} a^*(t) & b^*(t) \end{pmatrix} = \begin{pmatrix} |a(t)|^2 & a(t)b^*(t) \\ a^*(t)b(t) & |b(t)|^2 \end{pmatrix}.
\]

Now, if we want to represent \( \rho(t) \) in the form of a column vector, we have different choices as to how to rearrange the elements of \( \rho(t) \) in the vector. The following, for example, are some of the possible choices

\[
\begin{pmatrix} |a(t)|^2 \\ a^*(t)b(t) \\ a(t)b^*(t) \\ |b(t)|^2 \end{pmatrix} \quad \begin{pmatrix} |a(t)|^2 \\ a(t)b^*(t) \\ a^*(t)b(t) \\ |b(t)|^2 \end{pmatrix} \quad \begin{pmatrix} |a(t)|^2 \\ a^*(t)b(t) \\ a(t)b^*(t) \\ |b(t)|^2 \end{pmatrix} \quad \begin{pmatrix} |a(t)|^2 \\ a^*(t)b(t) \\ a(t)b^*(t) \\ |b(t)|^2 \end{pmatrix}.
\]

In matrix analysis, given a \((m \times n)\) matrix \( X \), the column vector vec\([X]\) is meant to correspond to the following arrangement

\[
\text{vec}[X] \equiv \begin{pmatrix} X_{\bullet 1} \\ X_{\bullet 2} \\ \vdots \\ X_{\bullet n-1} \\ X_{\bullet n} \end{pmatrix}, \quad \text{where } X_{\bullet i} = \begin{pmatrix} x_{1i} \\ x_{2i} \\ \vdots \\ x_{mi} \end{pmatrix}.
\]

\( X_{\bullet i} \) is the \( i \)-th column of the matrix (counting from the left). So if we take \( \rho(t) \) in (49), for example,

\[
\text{vec}[\rho(t)] = \begin{pmatrix} |a(t)|^2 \\ a^*(t)b(t) \\ a(t)b^*(t) \\ |b(t)|^2 \end{pmatrix}
\]

which is the first vector we wrote in (50). In quantum mechanics, different choices may be made. Some authors, for example, prefer the arrangement whereby the diagonal
which in matrix representation reads

$$\vec{vec}[X] \equiv \begin{pmatrix} X_1 \vdots X_m \end{pmatrix}, \quad \text{where } X_{k\bullet} = \begin{pmatrix} x_{k1} \\ \vdots \\ x_{kn} \end{pmatrix}. \tag{53}$$

$X_{k\bullet}$ is the $k$-th row of the matrix $X$. One major advantage of this choice is that, unlike (51) used in matrix analysis, it can be easily created using the Kronecker product (without any further rearrangements). As a result, the mathematics become greatly simplified. There is, indeed, a direct correlation between the arrangement chosen and the straightforwardness of the mathematics which come into play as a consequence.

We choose the arrangement in (53) in our discussion. To see how it can be easily implemented, we introduce the ‘bra-flipper’ operator $\bar{\mathcal{O}}$:

Let $|a\rangle \langle b|$ be an operator defined on the Hilbert space $\mathcal{H}_d$ of dimension $d$. The bra-flipper operator $\bar{\mathcal{O}}$, defined on the same $\mathcal{H}_d$, is a superoperator which acts on $|a\rangle \langle b|$ and transforms it into a superket according to the transformation

$$\bar{\mathcal{O}}[|a\rangle \langle b|] = |a\rangle \otimes |b|^\ast \equiv |a, b\rangle \tag{54}$$

where $|b|^\ast$ is the complex conjugate of $|b\rangle$.

The appearance of the Kronecker product in (54) must be noted. Moreover, $\bar{\mathcal{O}}$ is a linear superoperator. That is,

(i) If $\lambda$ is a complex scalar, then

$$\bar{\mathcal{O}}[\lambda |a\rangle \langle b|] = \lambda \bar{\mathcal{O}}[|a\rangle \langle b|] \tag{55}$$

(ii) Let $|a'\rangle \langle b'|$ also be an operator defined on $\mathcal{H}_d$ and $\lambda'$ a complex scalar. Then

$$\bar{\mathcal{O}}[\lambda |a\rangle \langle b| + \lambda' |a'\rangle \langle b'|] = \lambda \bar{\mathcal{O}}[|a\rangle \langle b|] + \lambda' \bar{\mathcal{O}}[|a'\rangle \langle b'|]. \tag{56}$$

Since the set of operators defined on $\mathcal{H}_d$ form a linear space, it follows from the above properties of $\bar{\mathcal{O}}$ that the superkets $\{|a, b\rangle\}$ also form a linear space. (We leave it to the Reader to prove.) This linear space is none other but the finite-dimensional Liouville space associated with $\mathcal{H}_d$, which we denote as $\mathcal{L}_d$.

Observe that if we apply $\bar{\mathcal{O}}$ to $\rho(t)$ in (49), we get

$$|\rho(t)\rangle \equiv \bar{\mathcal{O}}[\rho(t)] = \bar{\mathcal{O}}[|\psi(t)\rangle \langle \psi(t)|] = |\psi(t)\rangle \otimes |\psi(t)|^\ast \tag{57}$$

which in matrix representation reads

$$|\rho(t)\rangle = |\psi(t)\rangle \otimes |\psi(t)|^\ast = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} \otimes \begin{pmatrix} a^\ast(t) \\ b^\ast(t) \end{pmatrix} = \begin{pmatrix} |a(t)|^2 \\ a(t)b^\ast(t) \\ a^\ast(t)b(t) \\ |b(t)|^2 \end{pmatrix}. \tag{58}$$
and coincides with the second vector in (50).

With the help of the bra-flipper operator, we can also transform any mixed state density operator into a superket. If we take \( \rho \) in (10), for example, we have

\[
|\rho\rangle\rangle = \mathcal{U}[\rho] = \sum_{n=1}^{d} \sum_{n'=1}^{d} \lambda_{n'n} |\phi_n\rangle \otimes |\phi_{n'}\rangle^* = \sum_{n=1}^{d} \sum_{n'=1}^{d} \lambda_{n'n} |\phi_n, \phi_{n'}\rangle .
\]

This also applies to any operator \( A \) defined on \( \mathcal{H}_d \). Indeed, since

\[
A = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} A_{\nu\nu'} |\nu\rangle \langle \nu' |, \quad A_{\nu\nu'} \equiv \langle \nu | A |\nu' \rangle
\]

for an arbitrary orthonormal basis \( \{|\nu\rangle\} \) of \( \mathcal{H}_d \), it readily follows that

\[
|A\rangle\rangle = \mathcal{U}[A] = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} A_{\nu\nu'} |\nu\rangle \otimes |\nu'\rangle^* = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} A_{\nu\nu'} |\nu, \nu'\rangle .
\]

If we indicate each superket \( |\nu, \nu'\rangle \) with a distinct single character so that \( |\nu, \nu'\rangle \rightarrow |\alpha\rangle \), then

\[
|A\rangle\rangle = \sum_{\alpha=1}^{d^2} A_{\alpha} |\alpha\rangle .
\]

We recognize (62) as the expansion of the supervector \( |A\rangle\rangle \) in the basis (or ‘superbasis’) \( \{|\alpha\rangle\} \) (more on this in the next subsection). This is formally similar to the expansion in (4). In fact, the set \( \{|\alpha\rangle\} \) form an orthonormal superbasis for \( \mathcal{L}_d \). And since the cardinality of \( \{|\alpha\rangle\} \) is \( d^2 \), it follows that \( \mathcal{L}_d \) is a \( d^2 \)-dimensional linear space (Appendix A.1). We prove the orthonormality of the set \( \{|\alpha\rangle\} \) in the next subsection when we define the adjoint space for \( \mathcal{L}_d \).

3.3. The Liouville adjoint space \( \mathcal{L}_d^* \) and inner product

To every superket \( |a, b\rangle \) of \( \mathcal{L}_d \) is associated a unique dual vector \( \langle \langle a, b | \) called ‘superbra’. The superbases form the adjoint space \( \mathcal{L}_d^* \). Just as the vector \( |x\rangle \) and its dual \( \langle x | \) are related through the operation of conjugate transpose, (1), so is the superket \( |a, b\rangle \) and its dual \( \langle \langle a, b | \). That is,

\[
\langle \langle a, b | = |a, b\rangle \rangle = (|a\rangle \otimes |b\rangle)^* = |a| \otimes |b|^* .
\]

Here too, the matrix product between a superbra and superket constitute an inner product on \( \mathcal{L}_d \). Specifically, if \( |a', b'\rangle, |a, b\rangle \in \mathcal{L}_d \), then their inner product is defined as

\[
\langle \langle a', b' | , |a, b\rangle \rangle := \langle \langle a', b' | a, b \rangle \rangle .
\]

Thus, \( \mathcal{L}_d \) is a normed linear space. Given that every finite-dimensional complex linear space is complete (Appendix A.1), \( \mathcal{L}_d \) must also be complete [16, 18, 19]. Furthermore, since every normed and complete linear space is a Hilbert space, we also conclude that

- \( \mathcal{L}_d \) is a Hilbert space.
- The inner product of \( \mathcal{L}_d \) is complete.

Therefore, every superket in \( \mathcal{L}_d \) has a unique dual, and every inner product in \( \mathcal{L}_d \) is complete.
\( \mathcal{L}_d \) is also a Hilbert space (Appendix A.1). Specifically, it is a complex and separable Hilbert space.

Note that, according to (54) and (63),
\[
\langle \langle a', b' | a, b \rangle \rangle = \langle \langle a' | \otimes \langle \langle b' | b \rangle \rangle^* \rangle \langle a \rangle \otimes \langle b \rangle^* \tag{65a}
\]
\[
= \langle a' | a \rangle \otimes \langle b' | b \rangle^* \tag{65b}
\]
\[
= \langle a' | a \rangle \cdot \langle b' | b \rangle^* \tag{65c}
\]
where we have made use of the mixed product rule of the Kronecker product, (33).

If the vectors \( \langle \langle a \rangle \rangle, \langle \langle a' \rangle \rangle, \langle \langle b \rangle \rangle, \langle \langle b' \rangle \rangle \) belong to the same orthonormal basis of \( \mathcal{H}_d \), then it follows from (65c) that
\[
\langle \langle a' , b' | a, b \rangle \rangle = \delta_{a', a} \delta_{b', b} \tag{66}
\]
which means the set of superkets \( \{ |a, b\rangle \rangle \} \) form an orthonormal (super)basis for the Liouville space \( \mathcal{L}_d \).

Consequently, the superket \( |A\rangle \rangle \) we saw in (62) and its dual \( \langle \langle A | \) are also related through the conjugate transpose operation,
\[
\langle \langle A | = |A\rangle \rangle^\dagger = \sum_{\alpha=1}^{d^2} A_{\alpha}^* |\alpha\rangle \rangle = \sum_{\alpha=1}^{d^2} A_{\alpha}^* \langle \langle \alpha | . \tag{67}
\]

3.4. The superoperator \( I_{d^2} \) and change of superbasis
If we take the inner product between \( |\nu''\rangle \rangle, |\nu'''\rangle \rangle \in \mathcal{L}_d \) and \( |A\rangle \rangle \) (defined in (61)), it yields the expression
\[
\langle \langle \nu'', \nu''' | A \rangle \rangle = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} A_{\nu \nu'} \langle \langle \nu'', \nu''' | \nu, \nu' \rangle \rangle. \tag{68}
\]

If \( |\nu\rangle \rangle, |\nu'\rangle \rangle, |\nu''\rangle \rangle, |\nu'''\rangle \rangle \) are elements of the same set of orthonormal basis of \( \mathcal{H}_d \), then it follows from (66) that
\[
\langle \langle \nu'', \nu''' | A \rangle \rangle = A_{\nu'' \nu'''} = \langle \nu''' | A | \nu''' \rangle. \tag{69}
\]
This is an important identity because it allows us to rewrite (61) as
\[
|A\rangle \rangle = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} |\nu, \nu'\rangle \rangle A_{\nu \nu'} \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} \langle \nu, \nu' | \langle \langle \nu, \nu' | A \rangle \rangle \tag{70}
\]
from which we deduce that
\[
\sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} |\nu, \nu'\rangle \rangle \langle \langle \nu, \nu' | = I_{d^2} \tag{71}
\]
where \( I_{d^2} \) is the identity superoperator defined on \( \mathcal{L}_d \). In a single index notation, we may write
\[
\sum_{\alpha=1}^{d^2} |\alpha\rangle \rangle \langle \langle \alpha | = I_{d^2}. \tag{72}
\]
Now, suppose the expansion of $|A\rangle$ in the orthonormal superbasis $\{ |\alpha\rangle \}$ holds. Suppose $\{ |\eta\rangle \}$ is another orthonormal superbasis of $\mathcal{L}_d$. We want to change (61) from the superbasis $\{ |\alpha\rangle \}$ to $\{ |\eta\rangle \}$. This can be easily achieved in light of (72). Indeed, we may write

$$
|A\rangle = \sum_{\alpha=1}^{d^2} A_\alpha \; |\alpha\rangle = \sum_{\alpha=1}^{d^2} A_\alpha \sum_{\eta=1}^{d^2} |\eta\rangle \langle \eta | \alpha\rangle = \sum_{\eta=1}^{d^2} A_\eta \; |\eta\rangle
$$

with

$$
A_\eta = \sum_{\alpha=1}^{d^2} A_\alpha \langle \eta | \alpha\rangle .
$$

3.5. $\Phi$ is an isomorphism

We have seen that $\mathcal{H}_d$ (the linear space of pure states), $\mathcal{O}_d$ (the linear space of operators on $\mathcal{H}_d$) and $\mathcal{L}_d$ are all complex separable Hilbert spaces; but while $\mathcal{H}_d$ is $d-$dimensional, $\mathcal{O}_d$ and $\mathcal{L}_d$ are $d^2-$dimensional. We prove here that $\Phi$ is an isomorphism between $\mathcal{O}_d$ and $\mathcal{L}_d$. That is, $\Phi$ preserves the inner product between these two spaces.

In general, a linear surjective map $M : \mathcal{X} \to \mathcal{Y}$ (where $\mathcal{X}$ and $\mathcal{Y}$ are Hilbert spaces) is said to be an isomorphism between the two spaces if for $x_1, x_2 \in \mathcal{X}$

$$
\langle M(x_1), M(x_2) \rangle = \langle x_1, x_2 \rangle .
$$

Therefore, to prove $\Phi$ is an isomorphism, we need to prove first of all that it is surjective, and then prove that it preserves the inner product. To prove $\Phi$ is surjective, it suffices to notice that it is a bijection (that is, a one-to-one correspondence). We give the proof in Appendix A.2.

To prove $\Phi$ preserves the extended Hilbert-Schmidt inner product defined in (63), let $A$ and $B$ be any two operators which belong to $\mathcal{O}_d$. Then, according to (61) and (64),

$$
\langle \Phi[A], \Phi[B] \rangle = \langle |A\rangle , |B\rangle \rangle = \langle |A| B \rangle
$$

We know in general, $|A\rangle = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} A_{\nu \nu'} |\nu, \nu'\rangle$ and $|B\rangle = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} B_{\nu \nu'} |\nu, \nu'\rangle$, where $\{ |\nu, \nu'\rangle \}$ constitute an orthonormal superbasis of $\mathcal{L}_d$, so

$$
\langle |A| B \rangle = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} A_{\nu \nu'}^* B_{\nu \nu'} = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} B_{\nu \nu'} A_{\nu \nu'}^* .
$$

But since $A_{\nu \nu'}^*$ is scalar, it is invariant under transpose. Hence,

$$
A_{\nu \nu'}^* = (A_{\nu \nu'}^*)^T = \langle \nu' | A | \nu \rangle .
$$

Thus,

$$
\langle |A| B \rangle = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} \langle \nu | B | \nu' \rangle \; \langle \nu' | A | \nu \rangle = \sum_{\nu=1}^{d} \langle \nu | B A^\dagger | \nu \rangle = \text{Tr} [ B A^\dagger ]
$$

which is the extended Hilbert-Schmidt inner product, (14). This proves that $\mathcal{O}_d$ and $\mathcal{L}_d$ are truly isomorphic.
we indicate as $S$ matrices of dimension $(d \times d)$. Similar to the trace function on $O_d$, $\text{Tr}(\rho(t)) = \langle \rho(t) | A \rangle = \langle A | \rho(t) \rangle$.

At this point, we must observe that the expectation value $\langle A(t) \rangle$ of a Hermitian observable $A = A^\dagger \in O_d$ is simply a scalar product in Liouville space,

$$\langle A(t) \rangle = \text{Tr} \left[ \rho(t) A \right] = \langle \rho(t) | A \rangle = \langle A | \rho(t) \rangle .$$

And for an arbitrary operator $B \in O_d$, $\text{Tr}[B] = \langle I_d | B \rangle = \langle B^\dagger | I_d \rangle$.

### 3.6. Superoperators and the trace functional on $L_d$

Like operators on $H_d$, we can think of operators acting on $L_d$. These operators are called superoperators. For a given $L_d$, it is easy to see that its superoperators are matrices of dimension $(d^2 \times d^2)$ and they form a linear space of dimension $d^4$ — which we indicate as $S_d$. If $\{\nu, \nu'\}$ is a basis of $L_d$, then the set $\{|\alpha\rangle \langle \alpha'|\}$ spans $S_d$ and is called a superoperator basis of $S_d$. $I_{d^2}$, (72), is the identity superoperator on $L_d$.

Before we define the inner product on $S_d$, we need to define the trace function on $L_d$. Similar to the trace function on $O_d$, if $\mathcal{B}$ is a superoperator, element of $S_d$, then its trace $\text{Tr}(\mathcal{B})$ is defined as

$$\text{Tr}(\mathcal{B}) = \sum_{\alpha=1}^{d^2} \langle \alpha | \mathcal{B} | \alpha \rangle .$$

Not surprisingly, we choose the extended Hilbert-Schmidt inner product as the scalar product on $S_d$. In particular, given the two superoperators $\mathcal{A}, \mathcal{B} \in S_d$, we define their inner product as

$$\langle \mathcal{A}, \mathcal{B} \rangle := \text{Tr}(\mathcal{B} \mathcal{A}^\dagger) .$$

Note that in analogy to (15), we observe that $\langle A | B \rangle$, (79), may also be written as

$$\langle A | B \rangle = \sum_{\alpha=1}^{d^2} \langle A | \alpha \rangle \langle \alpha | B \rangle = \sum_{\alpha=1}^{d^2} \langle \alpha | B \rangle \langle A | \alpha \rangle = \text{Tr}(\langle B | \langle A \rangle) .$$

Thus, the linear spaces $H_d, O_d, L_d$ and $S_d$ share the same type of inner product. Also, since $S_d$ is normed and finite-dimensional (thus, complete), it is also a Hilbert space like the other three. These concepts are summarized in table 1.

We can also expand any given superoperator $\mathcal{B} \in S_d$ in any given orthonormal superbasis $\{|\alpha\rangle \langle \alpha|\}$ of $S_d$:

$$\mathcal{B} = \sum_{\alpha=1}^{d^2} \sum_{\alpha' = 1}^{d^2} |\alpha\rangle \langle \alpha | \mathcal{B} | \alpha' \rangle \langle \alpha' | = \sum_{\alpha=1}^{d^2} \sum_{\alpha' = 1}^{d^2} \mathcal{B}_{\alpha, \alpha'} \ |\alpha\rangle \langle \alpha' |$$

### Table 1. Some characteristics of the linear spaces $H_d, O_d, L_d, S_d$. (HS=Hilbert space; LO=Linear operators)

| Symbol | Name | Dimension | Elements |
|--------|------|-----------|----------|
| $H_d$  | HS of pure states | $d$ | $(d \times 1)$ column vectors |
| $O_d$  | HS of LO on $H_d$ | $d^2$ | $(d \times d)$ matrices |
| $L_d$  | HS of ‘vectorized’ LO on $H_d$ | $d^2$ | $(d^2 \times 1)$ column vectors |
| $S_d$  | HS of LO on $L_d$ | $d^4$ | $(d^2 \times d^2)$ matrices |

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where
\[ \mathcal{B}_{\alpha,\alpha'} = \langle \alpha | \mathcal{B} | \alpha' \rangle \]  \hspace{1cm} (85)

If instead of the single index \( \alpha \) we use the two index representation (see (71) and (72)), the expansion becomes
\[ \mathcal{B} = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} \sum_{\nu''=1}^{d} \sum_{\nu'''=1}^{d} \mathcal{B}_{\nu\nu',\nu''\nu'''} |\nu,\nu'\rangle \langle \nu''| \langle \nu'''| \]  \hspace{1cm} (86)
with
\[ \mathcal{B}_{\nu\nu',\nu''\nu'''} = \langle \nu,\nu' | \mathcal{B} | \nu'',\nu''' \rangle \]  \hspace{1cm} (87)
where the set \( \{ |\nu\rangle \} \) is an orthonormal basis of \( \mathcal{H}_d \).

3.7. The superket triple product identity

The results of this subsection bring to light the full glory of the Liouville space formalism. Say \( A, B, C \) are linear operators acting on \( \mathcal{H}_d \); thus, they are also elements of \( \mathcal{O}_d \). The product \( ABC \) is still an operator on \( \mathcal{H}_d \). The superket triple product identity states that
\[ |\text{ABC}\rangle = (A \otimes C^T) |\text{B}\rangle \]  \hspace{1cm} (88)
where \( C^T \) is the transpose of \( C \). In other words, the superket corresponding to the product \( ABC \in \mathcal{O}_d \), i.e. \( |\text{ABC}\rangle \in \mathcal{L}_d \), can be written as the result of the superoperator \( (A \otimes C^T) \) acting on the superket \( |\text{B}\rangle \in \mathcal{L}_d \). As a corollary, the following identities also follow from (88):
\[ |\text{ABC}\rangle = (AB \otimes \mathcal{I}_d) |\text{C}\rangle \]  \hspace{1cm} (89a)
\[ |\text{ABC}\rangle = (\mathcal{I}_d \otimes C^T B^T) |\text{A}\rangle \]  \hspace{1cm} (89b)

Let \( \{ |\nu\rangle \} \) be an orthonormal basis for \( \mathcal{H}_d \). To prove (88), we need to observe that the product of matrix elements
\[ A_{\nu\nu'} B_{\nu''\nu'''} = \langle \nu | A | \nu' \rangle \langle \nu'' | B | \nu''' \rangle \]  \hspace{1cm} (90)
may be written as an element of the superoperator \( A \otimes B^T \). Namely,
\[ A_{\nu\nu'} B_{\nu''\nu'''} = \langle \nu,\nu''| A \otimes B^T |\nu',\nu'''\rangle \]  \hspace{1cm} (90)
Equation (90) can be easily verified using the mixed product rule, (33). Since the expansion of \( ABC \) in the basis \( \{ |\nu\rangle \} \) is
\[ ABC = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} (ABC)_{\nu\nu'} |\nu\rangle \langle \nu'| \]  \hspace{1cm} (91)
after applying the bra-flipper superoperator to this expansion, we get
\[ |\text{ABC}\rangle = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} (ABC)_{\nu\nu'} |\nu',\nu\rangle \]  \hspace{1cm} (92)
But,
\[ (ABC)_{\nu\nu'} = \sum_{\nu''=1}^{d} \sum_{\nu'''=1}^{d} \langle \nu | A | \nu'' \rangle \langle \nu'' | B | \nu''' \rangle \langle \nu''' | C | \nu' \rangle \]  \hspace{1cm} (93)
Substituting this into (92), we finally obtain

\[
(ABC)_{\nu\nu'} = \sum_{\nu''=1}^{d} \sum_{\nu'''=1}^{d} \langle [\nu',\nu'] | A \otimes C^T | \nu'',\nu''' \rangle \langle \nu'',\nu''' | B \rangle
\]

\(= \langle [\nu',\nu'] | A \otimes C^T | B \rangle \). \hspace{2cm} (94)

Substituting this into (92), we finally obtain

\[
|ABC\rangle = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} |[\nu',\nu]| \langle [\nu',\nu'] | A \otimes C^T | \nu \rangle \langle \nu | B \rangle
\]

\(= (A \otimes C^T) | B \rangle \). \hspace{2cm} (95)

The superket triple product identity is very important in Liouville space formalism and comes in handy, for example, when solving master equations. We shall see this application in the next section \(\text{[8]}\). Nonetheless, the following relations for the superket of the commutation \([A,B]\) can be easily proved using (88):

\[
| [A,B] \rangle = [A,1_B] | B \rangle = [1_d,B] | A \rangle = [A,B] | 1_d \rangle ,
\]

where the “super-commutator” \([X,Y]\) is defined as

\[
[X,Y] \equiv X \otimes Y^T - Y \otimes X^T .
\]

(97)

We also note that \([X,Y] = -[Y,X]\). Analogously, we define the “super-anticommutator” \([X,Y]_+\) as

\[
[X,Y]_+ \equiv X \otimes Y^T + Y \otimes X^T .
\]

(98)

As a result, \([X,Y]_+ = [Y,X]_+\).

\[3.8. \text{Liouville space formalism and composite quantum systems}\]

The mathematical foundations for the Liouville space formalism laid above can be easily extend to any aggregate of quantum systems, each with a finite-dimensional HSPS. For simplicity, let us consider a bipartite quantum system \(S_1 + S_2\). Let \(H_d\) be the HSPS of system \(S_i\), and of dimension \(d_i\) \((i = 1, 2)\). Also, let \(\{|\nu\rangle\}\) and \(\{[\mu]\}\) be an orthonormal basis of \(H_{d_1}\) and \(H_{d_2}\), respectively. Then, the HSPS \(H_d\) of the composite system \(S_1 + S_2\) is given by the tensor product \(H_d = H_{d_1} \otimes H_{d_2}\), with \(d = d_1 \cdot d_2\). The set \(\{|\nu\rangle \otimes [\mu]\}\) then constitutes an orthonormal basis for \(H_d\).

Consider now the operator \(\mathcal{Z} = A \otimes B\) acting on \(H_d\), where \(A \in \mathcal{O}_{d_1}\) and \(B \in \mathcal{O}_{d_2}\). We know \(A = \sum_{\nu=1}^{d_1} \sum_{\nu'=1}^{d_1} A_{\nu\nu'} |\nu\rangle \langle \nu'|\) and \(B = \sum_{\mu=1}^{d_2} \sum_{\mu'=1}^{d_2} B_{\mu\mu'} |\mu\rangle \langle \mu'|\), so

\[
\mathcal{Z} = \sum_{\nu=1}^{d_1} \sum_{\nu'=1}^{d_1} \sum_{\mu=1}^{d_2} \sum_{\mu'=1}^{d_2} A_{\nu\nu'} B_{\mu\mu'} |\nu\rangle \langle \nu'| \otimes |\mu\rangle \langle \mu'|\)
\]

\(= \sum_{\nu=1}^{d_1} \sum_{\nu'=1}^{d_1} \sum_{\mu=1}^{d_2} \sum_{\mu'=1}^{d_2} A_{\nu\nu'} B_{\mu\mu'} (|\nu\rangle \otimes |\mu\rangle ) (\langle \nu'| \otimes \langle \mu'|\)). \hspace{2cm} (99)\]
where we have applied the mixed product rule of the Kronecker product, (33). To transform \( Z \) into a superket, we simply apply to it the bra-flipper superoperator \( \mathcal{U} \), obtaining

\[
|Z\rangle \rangle = \mathcal{U} \left( \langle \nu | \otimes \langle \mu | \right) \left( |\nu\rangle \otimes |\mu\rangle \right) = \sum_{\nu=1}^{d_1} \sum_{\nu' = 1}^{d_1} \sum_{\mu = 1}^{d_2} \sum_{\mu' = 1}^{d_2} A_{\nu
u'} B_{\mu\mu'} |\nu\mu, \nu'\mu'\rangle \rangle \tag{100}
\]

where \(|\nu\mu, \nu'\mu'\rangle \rangle = |\nu\rangle \otimes |\mu\rangle \otimes |\nu'\rangle^* \otimes |\mu'\rangle^*\). Because the set \(|\nu\mu, \nu'\mu'\rangle \rangle\) is certainly an orthonormal superbasis of the Liouville space \( L_d \), we may also write

\[
|Z\rangle \rangle = \sum_{\nu=1}^{d_1} \sum_{\nu' = 1}^{d_1} \sum_{\mu = 1}^{d_2} \sum_{\mu' = 1}^{d_2} \mathcal{L}_{\nu\mu, \nu'\mu'} |\nu\mu, \nu'\mu'\rangle \rangle \tag{101}
\]

Comparing (100) and (101) with each other, we conclude the following equations — which are equivalent to each other — must hold

\[
\mathcal{L}_{\nu\mu, \nu'\mu'} = A_{\nu
u'} B_{\mu\mu'} \tag{103a}
\]

\[
\langle \nu\mu, \nu'\mu'| A \otimes B \rangle = A_{\nu\nu'} B_{\mu\mu'} \tag{103b}
\]

\[
\langle \nu\mu, \nu'\mu'| A \otimes B \rangle = \langle \nu\mu | A \rangle \langle \nu'\mu' | B \rangle \tag{103c}
\]

where, in arriving at (103c), we have made use of (69). These results can be easily extended to multipartite quantum systems.

### 4. Applications

In this section, we apply — for the purpose of illustration — the concepts and mathematical tools developed in the preceding section to some problems in quantum mechanics. In §4.1 we explore the derivation of equations of motion in the Schrödinger, Heisenberg and interaction pictures — according to the Liouville space formalism. We then discuss in §4.2 the Liouville space solution to a certain class of equations of motion.

#### 4.1. Equations of motion in Liouville space

##### 4.1.1. Schrödinger picture in Liouville space

If we apply the bra-flipper superoperator on the Liouville-von Neumann equation, (11), and employ the relation in (96), we obtain

\[
\frac{d}{dt} |\rho(t)\rangle \rangle = -\frac{i}{\hbar} \left[ H, |\rho(t)\rangle \rangle \right] \tag{104a}
\]

\[
\frac{d}{dt} |\rho(t)\rangle \rangle = -\frac{i}{\hbar} [H, |\rho(t)\rangle \rangle] \equiv -\frac{i}{\hbar} \Sigma |\rho(t)\rangle \rangle \tag{104b}
\]


Taking the time derivative, we get

\[ \mathcal{L} = [H, \mathbb{I}_d] = H \otimes \mathbb{I}_d - \mathbb{I}_d \otimes H^T. \quad (105) \]

It is instructive to rederive (104b) following a more laborious route which begins with the general definition for the density matrix \( \rho(t) \) of an isolated system [3, 4]

\[ \rho(t) = \sum_{n=1}^{d} p_n |\psi_n(t)\rangle \langle \psi_n(t)| \quad (106) \]

where \( p_n \) is the probability of finding the system in the \( n \)-th state. Moreover, we know — according to Schrödinger’s equation — that [3, 4]

\[ \frac{d}{dt} |\psi_n(t)\rangle = -\frac{i}{\hbar} H |\psi_n(t)\rangle. \quad (107) \]

Now, upon the application of the bra-flipper superoperator, (106) becomes

\[ |\rho(t)\rangle = \sum_{n=1}^{d} p_n |\psi_n(t)\rangle \otimes |\psi_n(t)^*\rangle. \quad (108) \]

Taking the time derivative, we get

\[
\frac{d}{dt} |\rho(t)\rangle = \sum_{n=1}^{d} p_n \left[ \left( \frac{d}{dt} |\psi_n(t)\rangle \right) \otimes |\psi_n(t)^*\rangle + |\psi_n(t)\rangle \otimes \left( \frac{d}{dt} |\psi_n(t)^*\rangle \right) \right]
\]

\[ = -\frac{i}{\hbar} \sum_{n=1}^{d} p_n \left[ H |\psi_n(t)\rangle \otimes |\psi_n(t)^*\rangle - |\psi_n(t)\rangle \otimes H^* |\psi_n(t)^*\rangle \right] \quad (109a) \]

\[ = -\frac{i}{\hbar} \sum_{n=1}^{d} p_n \left[ (H \otimes \mathbb{I}_d) (|\psi_n(t)\rangle \otimes |\psi_n(t)^*\rangle) - (\mathbb{I}_d \otimes H^*) (|\psi_n(t)\rangle \otimes |\psi_n(t)^*\rangle) \right] \quad (109b) \]

\[ = -\frac{i}{\hbar} \left[ (H \otimes \mathbb{I}_d) - (\mathbb{I}_d \otimes H^*) \right] \sum_{n=1}^{d} p_n (|\psi_n(t)\rangle \otimes |\psi_n(t)^*\rangle) \quad (109c) \]

\[ = -\frac{i}{\hbar} \mathcal{L} |\rho(t)\rangle \quad (109d) \]

\[ = -\frac{i}{\hbar} \left[ H \otimes \mathbb{I}_d - \mathbb{I}_d \otimes H^T \right] |\rho(t)\rangle \quad (109e) \]

where in the last line we have exploited the fact that \( H \) is Hermitian. We note that (109c) agrees with (104b) — which confirms how logically consistent this approach is.

As a common practice in the literature [3, 9, 10, 11], we may want to express (104b) in some orthonormal basis \( \{|\nu\rangle\} \) of \( \mathcal{H}_d \). This can easily be achieved as follows: surely, the set \( \{|\nu\rangle\} \) generates the orthonormal basis \( \{|\nu, \nu'\rangle\} \) for \( \mathcal{L}_d \), and we may multiply (104b) from the left by a generic superbra \( \langle \nu, \nu'| \), obtaining

\[
\frac{d}{dt} \langle \nu, \nu' | \rho(t) \rangle = -\frac{i}{\hbar} \langle \nu, \nu' | \mathcal{L} |\rho(t)\rangle \quad (110a) \]

\[ \frac{d}{dt} \rho_{\nu \nu'}(t) = -\frac{i}{\hbar} \sum_{\nu'', \nu'''} \langle \nu, \nu' | \mathcal{L} |\nu'', \nu'''\rangle \langle \nu'', \nu''' | \rho(t) \rangle \quad (110b) \]

\[ \frac{d}{dt} \rho_{\nu \nu'}(t) = -\frac{i}{\hbar} \sum_{\nu'', \nu'''} \mathcal{L}_{\nu \nu'; \nu'' \nu'''} \rho_{\nu'' \nu'''}(t) \quad (110c) \]
where, naturally, $\mathcal{L}_{\nu', \nu''} = \langle \nu | H(\otimes \mathbb{I}_d - I_d \otimes H^T) | \nu'' \rangle$. We can easily find an explicit expression for the matrix elements $\mathcal{L}_{\nu', \nu''}$ using the definition in (105) for $\mathcal{L}$ and the mixed product rule, (33). As a matter of fact,

\begin{align}
\mathcal{L}_{\nu', \nu''} &= \langle \nu | H(\otimes \mathbb{I}_d - I_d \otimes H^T) | \nu'' \rangle \\
&= \langle \nu | (H \otimes \mathbb{I}_d - I_d \otimes H^T) | \nu'' \rangle \\
&= \langle \nu | (H | \nu'' \rangle) \otimes (H^* | \nu'' \rangle) \\
&= \langle \nu | H | \nu'' \rangle \otimes (H^* | \nu'' \rangle) \\
&= H_{\nu', \nu''} \delta_{\nu', \nu''}. 
\end{align}

Obviously, for the first term in (111b), we have

\begin{align}
\langle \nu, \nu' | H \otimes \mathbb{I}_d | \nu'' \rangle &= \langle \nu, \nu' | (H \otimes \mathbb{I}_d - I_d \otimes H^T) | \nu'' \rangle \\
&= \langle \nu, \nu' | H | \nu'' \rangle \\
&= H_{\nu', \nu''} \delta_{\nu', \nu''}. 
\end{align}

On a similar note, the second term in (111b) gives

\begin{align}
\langle \nu, \nu' | I_d \otimes H^T | \nu'' \rangle &= \langle \nu | I_d \otimes H^T | \nu'' \rangle \\
&= \delta_{\nu, \nu'} \delta_{\nu', \nu''}
\end{align}

Thus, $\mathcal{L}_{\nu', \nu''} = H_{\nu', \nu''} \delta_{\nu', \nu''} - \delta_{\nu, \nu'} H^*_{\nu', \nu''}$, and (110c) becomes

\begin{equation}
\frac{d}{dt} \rho_{\nu
u'}(t) = -\frac{i}{\hbar} \sum_{\nu, \nu'} (H_{\nu, \nu'} \delta_{\nu', \nu''} - \delta_{\nu, \nu'} H^*_{\nu', \nu''}) \rho_{\nu, \nu'}(t)
\end{equation}

— which is the expression one usually finds in the literature [10].

Let us now solve (104b) for $|\rho(t)\rangle$. Certainly, (104b) is formally equivalent to the classic matrix differential equation in (10) (or even the Schrödinger equation, (7)). Its solution is therefore

\begin{equation}
|\rho(t)\rangle = e^{-\frac{i}{\hbar} t H} |\rho(0)\rangle = e^{-\frac{i}{\hbar} t [H \otimes \mathbb{I}_d - I_d \otimes H^T]} |\rho(0)\rangle.
\end{equation}

Because $H \otimes \mathbb{I}_d$ commutes with $\mathbb{I}_d \otimes H^T$, it follows that

\begin{equation}
|\rho(t)\rangle = e^{-\frac{i}{\hbar} t [H \otimes \mathbb{I}_d]} e^{\frac{i}{\hbar} t [I_d \otimes H^T]} |\rho(0)\rangle.
\end{equation}

Applying the properties stated in (59) of the Kronecker product, we obtain

\begin{equation}
|\rho(t)\rangle = \left( e^{-\frac{i}{\hbar} t H} \otimes \mathbb{I}_d \right) \left( I_d \otimes e^{\frac{i}{\hbar} t H^T} \right) |\rho(0)\rangle
\end{equation}

This solution can be reversed to the square matrix form of $\rho(t)$ by resorting to the triple product identity in (SS). Indeed, from the latter equation, we have

\begin{equation}
|\rho(t)\rangle = \left( e^{-\frac{i}{\hbar} t H} \rho(0) \right) \rho(0) e^{\frac{i}{\hbar} t H}
\end{equation}

from which follows that

\begin{equation}
\rho(t) = e^{-\frac{i}{\hbar} t H} \rho(0) e^{\frac{i}{\hbar} t H}
\end{equation}

since $\mathcal{D}$ is a bijection [Appendix A.1]. The solution in (119) is widely known and derived in every undergraduate textbook on quantum mechanics, but the purpose of
deriving it here starting from (104b) is to show how consistent the Liouville space formalism we developed earlier is with standard quantum mechanics in $H_d$.

To further appreciate the formal similarities between quantum mechanics in $H_d$ and $L_d$, we note that
$$e^{-\frac{i}{\hbar}tH} \otimes e^{\frac{i}{\hbar}tH^T}$$
is the equivalent of evolution operator in $L_d$.

Hence, (117) may be written as
$$\rho(t) = U(t) \rho(0)$$

(120)

From its definition, we see that $U(0) = I_d \otimes I_d = I_{d^2}$. Also, $U(t)$ is clearly unitary.

Indeed, the Liouvillian $L$, (105), is Hermitian, so
$$U(t)U(t)^\dagger = U(t)^\dagger U(t) = I_{d^2}.$$ (121)

Furthermore, after introducing (120) into (104b), we observe that the evolution superoperator $U(t)$ satisfies the differential equation
$$\frac{d}{dt}U(t) = -\frac{i}{\hbar}L U(t)$$ (122)

— as one would expect from the second equation in (120).

4.1.2. Heisenberg picture in Liouville space. As it is well-known, in the Heisenberg picture, we let operators other than the density matrix evolve in time [34, 35]. If $A$ is a generic operator and element of $O_d$, then it follows from (120) that the relations
$$\langle A(t) \rangle = \langle A(0) \rangle$$

(123)

hold, where $|A_H(t)\rangle$ — the Heisenberg representation of the superket $|A\rangle$ — is defined as
$$|A_H(t)\rangle := U(t)^\dagger |A\rangle.$$ (124)

Taking the time derivative, we obtain
$$\frac{d}{dt} |A_H(t)\rangle = \frac{i}{\hbar}L |A_H(t)\rangle + U(t)^\dagger \frac{\partial}{\partial t} |A\rangle$$ (125)

where the last term becomes zero for time-independent $A$. Equation (125) is the operator $A$'s equation of motion in the Heisenberg picture in Liouville space.

4.1.3. Interaction picture in Liouville space. In the interaction picture, the time evolution of the system is shared between the density matrix and other operators [34, 35]. To see how that can be achieved in Liouville space, consider now the equation of motion
$$\frac{d}{dt} |\rho(t)\rangle = -\frac{i}{\hbar}L(t) |\rho(t)\rangle$$ (126)

where the Liouvillian $L(t)$ is now time-dependent and given by the sum
$$L(t) = L_o + L'(t)$$ (127)

where $L_o$ originates from a known time-independent Hamiltonian $H_o$, i.e. $L_o = [H_o, I_d]$, and $L'(t)$ is a perturbation respect to $L_o$. For Hermitian $H_o$, $L_o$ remains
leads to the equation of motion in accordance with (131).

where we set \( U \) where we have employed (134), and \( O \) belonging to \( U \).

Integrating the differential equation in (131) for \( U \) where

\[
\frac{d}{dt} U(t) = -\frac{i}{\hbar} [\mathcal{L}_0 + \mathcal{L}'(t)] U(t).
\]

The superpropagator \( \Phi(t) \) here is different from that in (129). We may decompose \( \Phi(t) \) according to the product

\[
\Phi(t) = \Phi_{\text{int}}(t) \Phi(t)
\]

where we set \( \Phi_{\text{int}}(t) = e^{-\frac{\hbar}{2} \mathcal{L}_0} \). Given that \( \Phi(0) = \mathbb{I}_{d^2} \) and \( \Phi_{\text{int}}(0) = \mathbb{I}_{d^2} \), we find that \( \Phi_{\text{int}}(0) = \mathbb{I}_{d^2} \).

Substituting (129) into (128), we get

\[
\Phi_{\text{int}}(t) \frac{d}{dt} \Phi_{\text{int}}(t) = -\frac{i}{\hbar} \mathcal{L}'(t) \Phi_{\text{int}}(t) \Phi(t)
\]

from which we obtain the final result

\[
\frac{d}{dt} \Phi_{\text{int}}(t) = -\frac{i}{\hbar} \mathcal{L}'(t) \Phi_{\text{int}}(t), \quad \text{where} \quad \mathcal{L}'(t) = \Phi_{\text{int}}(t) \mathcal{L}'(t) \Phi_{\text{int}}(t).
\]

Integrating the differential equation in (131) for \( \Phi_{\text{int}}(t) \) results in

\[
\Phi_{\text{int}}(t) = \mathbb{I}_{d^2} - \frac{i}{\hbar} \int_0^t dt_1 \mathcal{L}'(t_1) + \left( -\frac{i}{\hbar} \right)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \mathcal{L}'(t_1) \mathcal{L}'(t_2) \\
+ \left( -\frac{i}{\hbar} \right)^3 \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \mathcal{L}'(t_1) \mathcal{L}'(t_2) \mathcal{L}'(t_3) + \ldots
\]

\[
\equiv \mathcal{T} \exp \left[ -\frac{i}{\hbar} \int_0^t dt' \mathcal{L}'(t') \right]
\]

where \( \mathcal{T} \) denotes the time-ordering operator.

With \( \Phi(t) \) as defined in (129), it turns out that

\[
|\rho(t)\rangle = \Phi(t) |\rho(0)\rangle = \Phi_{\text{int}}(t) |\rho_{\text{int}}(t)\rangle
\]

where

\[
|\rho_{\text{int}}(t)\rangle \equiv \Phi_{\text{int}}(t) |\rho(0)\rangle = \Phi_{\text{int}}(t) |\rho(t)\rangle.
\]

\(|\rho(t)\rangle\rangle\) is the superket of the density matrix in the interaction picture, and its equation of motion is easily found to be

\[
\frac{d}{dt} |\rho(t)\rangle = -\frac{i}{\hbar} \mathcal{L}'(t) |\rho(t)\rangle
\]

in accordance with (131).

In regards to the time evolution of other operators, let \( A \) be a generic operator belonging to \( \mathcal{O}_d \). Then, the inner product \( \langle \rho(t) | A \rangle \) yields

\[
\langle \rho(t) | A \rangle = \langle \rho_{\text{int}}(t) | A \rangle = \langle \rho_{\text{int}}(t) | A_{\text{int}}(t) \rangle
\]

where we have employed (134), and

\[
|A_{\text{int}}(t)\rangle \rangle = \Phi_{\text{int}}(t) |A\rangle \rangle.
\]
\( |A_I(t)\rangle \) is said to be the interaction picture representation of the superket \(|A\rangle\). Its corresponding equation of motion is easily derived from (137) to be
\[
\frac{d}{dt} |A_I(t)\rangle = \frac{i}{\hbar} \mathcal{L}_o(t) |A_I(t)\rangle + \mathsf{U}_o(t) \frac{\partial}{\partial t} |A\rangle .
\] (138)
for Hermitian \( \mathcal{L}_o \). Equation (138) is the Liouville space equation of motion of \( A \) in the interaction picture. All these results bear very close similarities, formally speaking, to their equivalent counterparts in standard quantum mechanics \[34, 35\].

4.2. Solving master equations in Liouville space and the connection to non-Hermitian quantum mechanics.

We have so far dealt only with isolated quantum systems — where the Liouvillian \( \mathcal{L} \), (105), is Hermitian. This makes it possible to apply the quantum mechanical spectral decomposition theorem \[16, 17, 21\] which is an important result frequently applied in what is commonly referred to as Hermitian quantum mechanics \[36, 37, 38\] — i.e. the kind of quantum mechanics where observables are postulated to be represented by Hermitian operators. For finite-dimensional Hilbert spaces, the spectral decomposition theorem states that given a Hermitian operator \( A \in \mathcal{O}_d \), there exists an orthonormal basis \( \{ |\nu\rangle \} \) of \( \mathcal{H}_d \) such that
\[
A = \sum_\nu A_{\nu\nu} |\nu\rangle \langle \nu|
\] (139)
and the coefficients \( A_{\nu\nu} \) are real. The expansion of \( A \) in (139) is its so-called spectral decomposition. Similarly, in a finite-dimensional Liouville space, the Hermitian superoperator \( \mathcal{B} \in \mathcal{S}_d \), i.e. \( \mathcal{B} = \mathcal{B}^\dagger \), has its spectral decomposition
\[
\mathcal{B} = \sum_{\alpha=1}^{d^2} \mathfrak{B}_{\alpha,\alpha} |\alpha\rangle \langle \alpha|
\] (140)
or, in the two-indexed representation,
\[
\mathcal{B} = \sum_{\nu=1}^{d} \sum_{\nu'=1}^{d} \mathfrak{B}_{\nu\nu',\nu\nu'} |\nu,\nu'\rangle \langle \nu,\nu' | .
\] (141)
Here too, the expansion coefficients \( \{ \mathfrak{B}_{\alpha,\alpha} \} \equiv \{ \mathfrak{B}_{\nu\nu',\nu\nu'} \} \) are real and the eigen-superkets \( \{ |\nu,\nu'\rangle \} \) constitute a complete orthonormal basis for \( \mathcal{L}_d \). However, not all elements of \( \mathcal{S}_d \) are Hermitian (or skew-Hermitian, \[112,24\]). For these superoperators, the spectral decomposition theorem cannot be applied.

To explore these problems, we consider in this subsection the solution to equations of motion of the type
\[
\frac{d}{dt} |\rho(t)\rangle = \mathcal{L} |\rho(t)\rangle
\] (142)
where the generator of the dynamics \( \mathcal{L} \) is time-independent. It is important to note that, in general, all equations of motions for \( \rho(t) \) which are linear in the latter can be reduced to the form in (142) by means of the superket triple product identity in (88). However, in the general case, \( \mathcal{L} \) may be time-dependent. The solution to (142) is evidently,
\[
|\rho(t)\rangle = e^{t\mathcal{L}} |\rho(0)\rangle .
\] (143)
We may want to proceed further by expanding $e^{t\mathcal{L}} \rho(0)$ in the `eigenvectors' of $\mathcal{L}$. Caution is needed here because, as a matrix, $\mathcal{L} \in \mathcal{S}_d$ may be diagonalizable (i.e. has $d^2$ independent genuine eigenvectors [20] (more on this latter in §4.2.3) or non-diagonalizable. As we shall shortly see, for isolated quantum systems, $\mathcal{L}$ in (142) is skew-Hermitian (i.e. $\mathcal{L}^\dagger = -\mathcal{L}$) and therefore diagonalizable. On the other hand, for open quantum systems $\mathcal{L}$ is neither Hermitian nor skew-Hermitian, so could be diagonalizable or not. For isolated systems, $e^{t\mathcal{L}}$ can be expanded in an orthonormal basis of $\mathcal{S}_d$ which diagonalizes the former. But for open quantum systems, the analogous expansion of $e^{t\mathcal{L}}$ will require either a biorthonormal basis (112.2) or a generalized basis (112.3) of $\mathcal{S}_d$, depending on the nature of $\mathcal{L}$. It goes without saying that orthonormal and biorthonormal bases are special instances of generalized bases.

4.2.1. Isolated quantum systems. Orthonormal basis expansion of $e^{t\mathcal{L}}$. If we go back to (104b) and set

$$\mathcal{L} \equiv -\frac{i}{\hbar} [H, \mathbb{I}_d] = -\frac{i}{\hbar} (H \otimes \mathbb{I}_d - \mathbb{I}_d \otimes H^T) ,$$

equation (114) then becomes $\rho(t) = e^{t\mathcal{L}} \rho(0)$, which is equivalent to the expression in (113). As remarked earlier, $[H, \mathbb{I}_d]$ is Hermitian (for Hermitian Hamiltonian $H$), so $\mathcal{L}$ is skew-Hermitian. Thus, according to the spectral decomposition theorem, we can find an orthonormal basis of $\mathcal{S}_d$ which diagonalizes $[H, \mathbb{I}_d]$, and by extension $\mathcal{L}$, (144). The first thing we need to observe is that $\mathcal{L}$ is proportional to the sum of two Hermitian superoperators $H \otimes \mathbb{I}_d$ and $\mathbb{I}_d \otimes H^T$. Second, since they commute, i.e. $[H \otimes \mathbb{I}_d, \mathbb{I}_d \otimes H^T] = 0$, the two superoperators must share the same eigen-supervectors.

Now, since $H$ is Hermitian, let $H = \sum_\nu \epsilon_\nu |\nu\rangle \langle \nu|$ be its spectral decomposition, where $\epsilon_\nu \equiv \langle \nu|H|\nu\rangle$ and $\{\epsilon_\nu\}$ are the eigenvalues of $H$. If we take $H \otimes \mathbb{I}_d$, we see that

$$H \otimes \mathbb{I}_d = \sum_\nu \epsilon_\nu |\nu\rangle \otimes \mathbb{I}_d = \sum_\nu \epsilon_\nu |\nu\rangle \otimes \sum_\nu' \langle \nu'| \langle \nu'|T\rangle$$

where we have made use of the completeness of the orthonormal basis $\{|\nu\rangle\}$, (10), and the fact that $\mathbb{I}_d$ is invariant under transpose. After applying the mixed product rule of the Kronecker product — (33) — on (144), we get

$$H \otimes \mathbb{I}_d = \sum_\nu \sum_\nu' \epsilon_\nu \langle \nu| \otimes |\nu'|^*\rangle (\langle \nu| \otimes \langle \nu'|^*) = \sum_\nu \sum_\nu' \epsilon_\nu \langle \nu, \nu'\rangle \langle \nu, \nu'|$$

Comparing (146b) with (141), we clearly see that (146b) is the spectral decomposition of the superoperator $(H \otimes \mathbb{I}_d)$, and $\epsilon_\nu = \langle \nu|H|\nu\rangle$. Likewise, for the superoperator $(\mathbb{I}_d \otimes H^T)$, it is easy to prove that

$$\mathbb{I}_d \otimes H^T = \sum_\nu \sum_\nu' \epsilon_\nu' |\nu, \nu'| \langle \nu, \nu'|$$

Thus, putting these last two equations together, it follows from (144) that

$$\mathcal{L} = -\frac{i}{\hbar} \sum_\nu \sum_\nu' (\epsilon_\nu - \epsilon_\nu') |\nu, \nu'| \langle \nu, \nu'|$$
which is the spectral decomposition of $\mathcal{L}$. So, the eigenvalues of $\mathcal{L}$ are simply proportional to the energy gap $(\epsilon_\nu - \epsilon_{\nu'})$ between the eigenstates of $H$. We also observe that

(i) for those eigen-superkets $|\nu, \nu'\rangle$ where $\nu = \nu'$, their corresponding eigenvalue is identically zero. Hence, $\mathcal{L}$ is a singular matrix (that is, not invertible).

(ii) for fixed $\nu$ and $\nu'$, $\mathcal{L}_{\nu \nu', \nu \nu'} = -\mathcal{L}_{\nu' \nu, \nu' \nu}$. This implies that $\mathcal{L}$ is a zero-trace superoperator (an observation which can alternatively be proved from the definition of $\mathcal{L}$ in (144) by taking the trace).

The fact that the eigen-superkets $\{ |\nu, \nu'\rangle \}$ of $\mathcal{L}$ form a complete orthonormal basis for the Liouville space $\mathcal{L}_d$ — leading therefore to the completeness relation in (71) — can be used to greatly simplify derivations and calculations. Back to $|\rho(t)\rangle$, (149), for example, we can expand $e^{\mathcal{L}t}$ in the basis $\{ |\nu, \nu'\rangle \}$, yielding

$$
|\rho(t)\rangle = e^{\mathcal{L}t} |\rho(0)\rangle = \sum_{\nu, \nu'} e^{\mathcal{L}t} |\nu, \nu'\rangle \langle \nu, \nu' | \rho(0)\rangle = \sum_{\nu, \nu'} e^{-i\frac{\hbar}{\mathcal{L}}(\epsilon_{\nu} - \epsilon_{\nu'})} |\nu, \nu'\rangle \langle \nu, \nu' | \rho(0)\rangle
$$

(149)
or, alternatively,

$$
|\rho(t)\rangle = \sum_{\nu} \rho_{\nu \nu} |\nu, \nu\rangle + \sum_{\nu \neq \nu'} e^{-i\frac{\hbar}{\mathcal{L}}(\epsilon_{\nu} - \epsilon_{\nu'})} \rho_{\nu \nu'} |\nu, \nu'\rangle
$$

(150)

where $\rho_{\nu \nu'} = \langle \nu, \nu' | \rho(0)\rangle$. It is quite clear from (150) that the populations $\langle \nu, \nu | \rho(t)\rangle$ remain invariant during the evolution. Namely, $\langle \nu, \nu | \rho(t)\rangle = \langle \nu, \nu | \rho(0)\rangle = \rho_{\nu \nu}$. Meanwhile, each initial coherence simply gains a phase factor for $t > 0$; i.e. $\langle \nu, \nu' | \rho(t)\rangle = e^{-i\frac{\hbar}{\mathcal{L}}(\epsilon_{\nu} - \epsilon_{\nu'})} \langle \nu, \nu' | \rho(0)\rangle$, $\nu \neq \nu'$. These observations are all in agreement with standard quantum mechanics of isolated systems and deducible from (119). But more importantly, since an isolated system is always in a steady state, these observations also set general criteria for steady states. Put succinctly,

**P1:** for an open or isolated quantum system with $|\rho(t)\rangle = e^{\mathcal{L}t} |\rho(0)\rangle$, if the generalized eigen-superket $|\alpha\rangle$ of $\mathcal{L}$ has eigenvalue $\lambda_\alpha$ and $\text{Re}[\lambda_\alpha] = 0$, then $|\alpha\rangle$ is a steady-state.

The keyword to note here is generalized eigen-superket — which we discuss in subsection 4.2.3. By the end of 4.2.3 it will be clear why the proposition P1 holds.

4.2.2. Open quantum systems. Biorthonormal basis expansion of $e^{\mathcal{L}t}$. In standard formulation of quantum mechanics (commonly referred to as Hermitian quantum mechanics), it is postulated that all physical observables are represented by Hermitian operators. In non-Hermitian quantum mechanics [36, 37, 38, 39], the formal definition of an operator representing a physical observable poses on entirely different criteria and are more relaxed with respect to the Hermiticity requirement in Hermitian quantum mechanics. In the so-called $PT$-symmetric formulation [36, 37, 38, 39], for example, an operator qualifies as an observable if it is simultaneously invariant with respect to both parity ($P$) and time-reversal ($T$) operations. The concept of biorthonormal basis [40, 41] plays an important role in non-Hermitian quantum
mechanics. And it should come as no surprise if we encounter it here in Liouville space formalism dealing with open quantum systems because non-Hermitian quantum mechanics handles exceptionally well resonance phenomena \[38\], which — conceptually speaking — are a consequence of a quantum system being open.

In the study of open quantum systems, for example, the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL, or simply Lindblad) equation plays a crucial role and has found diverse applications: from tackling fundamental problems like the quantum-to-classical transition to the development of quantum technologies \[5, 7, 20, 23, 24, 42\]. For $\rho(t)$ defined on a finite-dimensional HSPS of dimension $d$, the GKSL equation reads \[7\]

$$
\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H, \rho(t)] + \sum_{k=1}^{d^2-1} \gamma_k \left( A_k \rho(t) A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho(t) - \frac{1}{2} \rho(t) A_k^\dagger A_k \right)
$$

(151)

where the first and second terms represent the unitary and the dissipative parts of the system’s evolution, respectively. The constants $\{\gamma_k\}$ are positive and represent relaxation rate constants (if the $A_k$ are dimensionless). Naturally, $H$ and $\{A_k\}$ are operators; so even though the GSKL equation is linear in $\rho(t)$, it does not easily lend itself to a solution. However, we can circumvent the problem by transitioning to the Liouville space. Namely, we first apply the bra-flipper superoperator on both sides of (151) and then make use of the superket triple product identity in (88) to factorize out $\rho(t)$ as $|\rho(t)\rangle \rangle$ on the l.h.s. of (151). This leads to a differential equation of the same form as that in (142), and the solution in (143) still holds, with

$$
\mathfrak{L} = -\frac{i}{\hbar}[H, \mathbb{I}_d] + \sum_{k=1}^{d^2-1} \gamma_k \left( A_k \otimes A_k^\dagger - \frac{1}{2} [A_k^\dagger A_k, \mathbb{I}_d] \right)
$$

(152)

where we have made use of the definitions in (97) and (98) (see also Appendix A of [2]). Unlike the generator $\mathfrak{L}$ for an isolated system, the generator $\mathfrak{L}$ in (152) is not skew-Hermitian (nor is it Hermitian). This means $\mathfrak{L}$ and $\mathfrak{L}^\dagger$, in general, do not share the same eigen-supervectors as one would expect for a Hermitian (or skew-Hermitian) superoperator.

Suppose the generator $\mathfrak{L} \in \mathcal{S}_d$ in (152) is diagonalizable. This will mean that there exists an invertible matrix $\mathfrak{A} \in \mathcal{S}_d$ \[20, 27, 28\] such that

$$
\mathfrak{A}^{-1} \mathfrak{L} \mathfrak{A} = \mathfrak{D}
$$

(153)

where $\mathfrak{D}$ is a $(d^2 \times d^2)$ diagonal matrix. In matrix theory, $\mathfrak{A}$ and $\mathfrak{D}$ are the eigenvector and eigenvalue matrices, respectively, of $\mathfrak{L}$. Let $\{\lambda_1, \lambda_2, \ldots, \lambda_{d^2}\}$ be the eigenvalues of $\mathfrak{L}$. There could be repeated eigenvalues. Then,

$$
\mathfrak{D} = \sum_{k=1}^{d^2} \lambda_k \langle k | \langle k |
$$

(154)

where $|k\rangle$ is the $k$–th element of $\mathfrak{L}$’s canonical basis. That is, $|k\rangle$ is the $(d^2 \times 1)$ column vector whose entries are all equal to zero except for that at the $k$–th row, where the entry has value 1, i.e.

$$
|k\rangle = \begin{pmatrix} 0 & \ldots & 0 & 1 & 0 & \ldots & 0 \end{pmatrix}^T.
$$

(155)
Surely,
\[ \langle \langle k | k' \rangle \rangle = \delta_{k,k'} \quad \text{and} \quad \sum_{k=1}^{d^2} |k\rangle \langle \langle k | = I_{d^2} . \quad (156) \]

Substituting (154) into (153), we derive that
\[ \mathcal{L} = \sum_{k=1}^{d^2} \lambda_k \mathfrak{A} |k\rangle \langle \langle k | \mathfrak{A}^{-1} \]
\[ = \sum_{k=1}^{d^2} \lambda_k \langle \langle \xi_k | \langle \langle \xi_k | \quad (157) \]
where
\[ |\xi_k\rangle \equiv \mathfrak{A} |k\rangle \quad \langle \langle \xi_k | \equiv \langle \langle k | \mathfrak{A}^{-1} . \quad (158) \]

In general, \( |\xi_k\rangle \neq \langle \langle k | \mathfrak{A}^\dagger \). The equality only holds when \( \mathfrak{A}^\dagger = \mathfrak{A}^{-1} \) — that is, when \( \mathfrak{A} \) is unitary; but this can be true only when \( \mathcal{L} \) is Hermitian or skew-Hermitian, which we know is not the case for open quantum systems.

Proceeding, we also observe that
\[ \langle \langle \xi_k | \langle \langle k | \rangle \rangle = \delta_{k,k'} \quad . \quad (159) \]

Moreover, multiplying from the left the completeness relation \( I_{d^2} = \sum_{k=1}^{d^2} |k\rangle \langle \langle k | \) by \( \mathfrak{A} \), and then from the right by \( \mathfrak{A}^{-1} \), we end up with the following completeness relation
\[ \mathbb{I}_{d^2} = \sum_{k=1}^{d^2} |\xi_k\rangle \langle \langle \xi_k | . \quad (160) \]

We hence conclude from (160) that the superoperators \( \{ |\xi_k\rangle \langle \langle k | \} \) also form a complete basis for \( \mathcal{S}_d \). In addition, the fact that \( \langle \langle \xi_k | \) is orthogonal to \( |\xi_k| \) \( , \) (159), even though the two sets \( \{ \langle \langle \xi_k | \} \) and \( \{ |\xi_k| \} \) are not conjugate transpose of each other, implies that the superoperators \( \{ |\xi_k\rangle \langle \langle k | \} \) constitute what we call a biorthonormal basis \( [40, 41] \) for \( \mathcal{S}_d \). In particular, \( \{ |\xi_k| \} \) are the right eigenvectors (or right eigen-supervectors) of \( \mathcal{L} \), while \( \{ \langle \langle \xi_k | \} \) are the corresponding left eigen-supervectors. To see why this is so, let us go back to (157) where we saw that \( \mathcal{L} = \sum_{k=1}^{d^2} \lambda_k \langle \langle \xi_k | \langle \langle \xi_k | \). If we multiply this relation from the left by \( \langle \langle \xi_k |' \), we get
\[ \langle \langle \xi_k |' \mathcal{L} = \sum_{k=1}^{d^2} \lambda_k \langle \langle \xi_k |' \langle \langle \xi_k | = \sum_{k=1}^{d^2} \lambda_k \delta_{k,k'} \langle \langle \xi_k | \]
\[ = \lambda_{k'} \langle \langle \xi_k |' . \quad (161) \]

Similarly, multiplying (157) from the right by \( |\xi_k|' \) yields
\[ \mathcal{L} |\xi_k|' = \lambda_{k'} |\xi_k|' . \quad (162) \]

Finally, if we now go back to (143), and introduce the biorthonormal completeness relation in (160), the result is
\[ |\rho(t)\rangle = \sum_{k=1}^{d^2} e^{i \lambda_k} |\xi_k\rangle \langle \langle \xi_k | \rho(0) \langle \langle \xi_k |) . \quad (163) \]
The eigenvalues $\lambda_k$ are, generally speaking, complex. For dissipative systems, the stability conditions require that $\text{Re}[\lambda_k] \leq 0$. And the steady states are those (right) eigen-supervectors with $\text{Re}[\lambda_k] = 0$ [2] [5] [23].

4.2.3. Open quantum systems. Generalized basis expansion of $e^{tL}$. For non-diagonalizable $L$, the spectral theorem [26] of linear algebra asserts that it is possible to expand $L$ in its generalized super-eigenvectors. Let us see briefly what we mean by generalized eigenvectors.

For ordinary or genuine (right) eigenvectors of the superoperator $L$ we mean the non-null superkets satisfying the relation [21] [26] [27] [28]

$$L \, |\zeta_\alpha\rangle = \lambda_\alpha \, |\zeta_\alpha\rangle$$  (164)

which may also be written as

$$(L - \lambda_\alpha I_d^2) \, |\zeta_\alpha\rangle = 0$$  (165)

where $\lambda_\alpha$, a complex scalar, is the eigenvalue of $L$ associated with the eigenvector $|\zeta_\alpha\rangle$. Say $L$ has $L$ distinct eigenvalues, which we indicate as $\{\lambda_\alpha\}$, $\alpha = 1, 2, \ldots, L$. Let $p_\alpha$ be the multiplicity of the eigenvalue $\lambda_\alpha$. Naturally, $\sum_\alpha p_\alpha = d^2$. The positive integer $p_\alpha$ is also commonly referred to as the algebraic multiplicity of $\lambda_\alpha$ [27]. Let $g_\alpha$ denote the number of independent genuine eigenvectors associated with the eigenvalue $\lambda_\alpha$. The positive integer $g_\alpha$ is called the geometric multiplicity of $\lambda_\alpha$ [27]. In general, $g_\alpha \leq p_\alpha$. This also means, $\sum_\alpha g_\alpha \leq d^2$. We thus have that $L$ is diagonalizable when $g_\alpha = p_\alpha$ for all $\alpha$ — or, in other terms, when $\sum_\alpha g_\alpha = d^2$. On the other hand, it only takes one eigenvalue $\lambda_{\alpha'}$ with $g_{\alpha'} < p_{\alpha'}$ to make $L$ non-diagonalizable.

If a given eigenvalue $\lambda_\alpha$ has $g_\alpha < p_\alpha$, with $p_\alpha \geq 2$, the spectral theorem [21] [26] [27] [28] of linear algebra asserts that it is possible to find $p_\alpha$ independent eigenvectors, $\{ |\zeta_\alpha(m)\rangle \}$, $m = 1, 2, \ldots, p_\alpha$, all with eigenvalue $\lambda_\alpha$. The vectors $\{ |\zeta_\alpha(m)\rangle \}$ are called generalized eigenvectors and are defined as follows

$$(L - \lambda_\alpha I_d^2) \, |\zeta_\alpha(1)\rangle = 0$$  (166a)

$$(L - \lambda_\alpha I_d^2) \, |\zeta_\alpha(m)\rangle = |\zeta_\alpha(m-1)\rangle$$  \hspace{1cm} m = 2, \ldots, p_\alpha  \hspace{1cm} (166b)

from which follows that

$$(L - \lambda_\alpha I_d^2)^m \, |\zeta_\alpha(m)\rangle = 0$$  \hspace{1cm} k = 1, 2, \ldots, p_\alpha .  \hspace{1cm} (167)

The vector $|\zeta_\alpha(m)\rangle$ satisfying (167) is said to be a generalized eigenvector of rank $m$ [21] [26] [44]. An important implication of (167) is that

$$(L - \lambda_\alpha I_d^2)^n \, |\zeta_\alpha(m)\rangle = 0$$  \hspace{1cm} \text{for} \hspace{1cm} n \geq m . \hspace{1cm} (168)

We may collect the vectors $\{ |\zeta_\alpha(k)\rangle \}$ into a single matrix $\mathfrak{B}$ according to the arrangement

$$\mathfrak{B} = \begin{pmatrix} |\zeta_1(1)\rangle & \ldots & |\zeta_1(p_1)\rangle & \ldots & |\zeta_L(1)\rangle & \ldots & |\zeta_L(p_L)\rangle \end{pmatrix} . \hspace{2cm} (169)$$
That is, the vector $|\zeta(\alpha,m)\rangle$ occupies the $n(\alpha,m)$--th column of $\mathcal{B}$, where

$$n(\alpha,m) = F(\alpha - 1) + m , \quad F(\alpha') = \begin{cases} 0 , & \text{if } \alpha' = 0 \\ \sum_{\alpha=1}^{\alpha'} p_\alpha , & \text{otherwise} \end{cases} .$$  \hfill (170)

The superoperator $\mathcal{B}$ is invertible and the similarity transformation

$$\mathcal{B}^{-1} \mathcal{L} \mathcal{B} = \mathcal{J}$$  \hfill (171)

is called the *Jordan canonical form* \cite{21, 26, 27, 28, 44} of $\mathcal{L}$. For non-diagonalizable $\mathcal{L}$, the Jordan form $\mathcal{J}$ is *almost* diagonal. In particular, $\mathcal{J}$ is composed of $L$ blocks of matrices

$$\mathcal{J} = \begin{pmatrix} \mathcal{J}_1 & & \\ & \ddots & \\ & & \mathcal{J}_L \end{pmatrix}$$  \hfill (172)

where the block matrix $\mathcal{J}_\alpha$ is a triangular square matrix of dimension $p_\alpha$, whose diagonal has the fixed value $\lambda_\alpha$ and its immediate upper diagonal has the fixed value of 1, while all other entries are zero. That is,

$$\mathcal{J}_\alpha = \begin{pmatrix} \lambda_\alpha & 1 & & \\ & \lambda_\alpha & 1 & & \\ & & \ddots & \ddots & \\ & & & \lambda_\alpha & 1 \\ & & & & \lambda_\alpha \end{pmatrix}.$$  \hfill (173)

With the concept of generalized eigenvectors in our possession, we can now proceed to show how we can conveniently expand $e^{t \mathcal{L}} |\rho(0)\rangle$ in terms of the generalized eigen-superkets $\{ |\zeta(\alpha,m)\rangle\}$ of $\mathcal{L}$. To begin with, let $\{ |k\rangle\}$ ($k = 1, \ldots, d^2$) be once again the canonical basis for $\mathcal{L}_d$ \cite{155}. It is easy to see that the column vector $\mathcal{B} |k\rangle$ is non other but the $k$--th column of $\mathcal{B}$. Since there is a one-to-one correspondence between the set of integers $\{n(\alpha,m)\}$, \cite{171}, and $\{k\}$, it follows that for fixed $\alpha$ and $m$, if

$$\mathcal{B} |k\rangle = |\zeta(\alpha,m)\rangle \quad \text{then} \quad k = n(\alpha,m) \quad \text{(174)}$$

— in virtue of \cite{169} — , and we may therefore write

$$\mathcal{B} |n(\alpha,m)\rangle = |\zeta(\alpha,m)\rangle.$$  \hfill (175)

In other words, the integers $\{n(\alpha,m)\}$ are simply a two-indexed representation of the integers $\{k\}$. Thus, from \cite{150}, we see that the following chain of completeness relations hold

$$I_{d^2} = \sum_{k=1}^{d^2} |k\rangle \langle k| = \sum_{\alpha=1}^{L} \sum_{m=1}^{p_\alpha} |n(\alpha,m)\rangle \langle n(\alpha,m)|$$  \hfill (176)

and

$$\langle n(\alpha',m')| n(\alpha,m)\rangle = \delta_{\alpha',\alpha} \delta_{m',m}.$$  \hfill (177)
If we multiply (176) from the left by $\mathcal{B}$ and from the right by $\mathcal{B}^{-1}$, we get

$$
\mathcal{I}_{\xi} = \sum_{\alpha=1}^{L} \sum_{m=1}^{p_{\alpha}} |\zeta_{\alpha}(m)\rangle \langle \xi_{\alpha}(m)|
$$

(178)

where

$$
\langle \xi_{\alpha}(m)| = \langle n(\alpha, m)| \mathcal{B}^{-1}.
$$

(179)

Note that $\langle n(\alpha, m)| \mathcal{B}^{-1}$ is the $n(\alpha, m)-th$ row vector of $\mathcal{B}^{-1}$. $\langle \xi_{\alpha}(m)|$ is the left generalized eigenvector of $\mathcal{L}$ of rank $n$ and with eigenvalue $\lambda_{\alpha}$. From (175), (179) and (177), we readily conclude that

$$
\langle \xi_{\alpha}(m)| \zeta_{\alpha'}(m')\rangle = \delta_{\alpha',\alpha} \delta_{m',m}
$$

(180)

which is the orthogonality relation between these generalized left and right eigenvectors.

With the aid of the completeness relation in (178), we have

$$
|\rho(t)\rangle = e^{\mathcal{L}t} |\rho(0)\rangle = \sum_{\alpha=1}^{L} \sum_{m=1}^{p_{\alpha}} e^{\mathcal{L}t} |\zeta_{\alpha}(m)\rangle \langle \xi_{\alpha}(m)| \langle \rho(0)|
$$

(181)

$$
= \sum_{\alpha=1}^{L} e^{\lambda_{\alpha}t} \sum_{m=1}^{p_{\alpha}} e^{t(\mathcal{L}-\lambda_{\alpha}1_{d}2)} |\zeta_{\alpha}(m)\rangle \langle \xi_{\alpha}(m)| \langle \rho(0)|
$$

which leads to the final result (see also [4] for a similar result in $\mathcal{H}_{d}$)

$$
|\rho(t)\rangle = \sum_{\alpha=1}^{L} e^{\lambda_{\alpha}t} \sum_{m=1}^{p_{\alpha}} \sum_{n=0}^{m-1} \frac{t^{n}}{n!} |\zeta_{\alpha}(m-n)\rangle \langle \xi_{\alpha}(m)| \langle \rho(0)|
$$

(182)

where we have made use of (166b) and (168). Here too, the stability of $|\rho(t)\rangle$ demands that $\text{Re}[\lambda_{\alpha}] \leq 0$. Naturally, the generalized eigen-superkets with $\text{Re}[\lambda_{\alpha}] = 0$ define the steady states of the dynamics. More importantly, the stability of the steady states requires that each eigenvalue $\lambda_{\alpha}$ with $\text{Re}[\lambda_{\alpha}] = 0$ must necessarily have a geometric multiplicity of 1, so that $|\rho(\infty)\rangle \equiv \lim_{t \to +\infty} |\rho(t)\rangle$ is a well-defined state. Note also that if $\mathcal{L}$ is diagonalizable but not skew-Hermitian (nor Hermitian), (182) reduces to (169); while for skew-Hermitian $\mathcal{L}$, (182) simply reduces to (149). This, together with the observations made in §4.2.2 and §4.2.4 explains why the proposition P1 holds.

5. Concluding Remarks

We have illustrated how a finite-dimensional Liouville space $\mathcal{L}_{d}$ can be built from a finite-dimensional HSIS $\mathcal{H}_{d}$, using essentially the same mathematical tools and concepts students learn in their first course in non-relativistic quantum mechanics. These mathematical tools are only augmented by the use of the Kronecker product (3.1.14) and the introduction of the bra-flipper operator $\mathcal{B}$ (3.2). We have also stressed that, like $\mathcal{H}_{d}$, the Liouville space $\mathcal{L}_{d}$ is also a Hilbert space. Whereas the vectors in $\mathcal{H}_{d}$ are only pure states, the quantum state vectors in $\mathcal{L}_{d}$ are either pure or mixed.
In this view, $\mathcal{L}_d$ is an enriched extension of $\mathcal{H}_d$. Both Hilbert spaces also share the same form of scalar product, namely, the extended Hilbert-Schmidt inner product. The same type of inner product also applies to the Hilbert spaces $\mathcal{O}_d$ and $\mathcal{S}_d$ (table 1).

From a conceptually practical perspective, an important argument can be further made for the Liouville space formalism — and it relates to spectroscopy. In ordinary quantum mechanics in $\mathcal{H}_d$, the eigenvalues of observables — like the Hamiltonian or magnetization vector — , which are absolute quantities (at least, up to a constant), are the natural occurrences. Meanwhile, what we experimentally measure in spectroscopic experiments like nuclear magnetic resonance (NMR) are quantities related to the differences between these eigenvalues [45]. We need not look further than the resonance conditions of such experiments to see this is the case. A formalism in quantum mechanics where these differences naturally appear as proportional to the eigenvalues of a corresponding operator would be much more practical. And the Liouville space formalism satisfies this need. (If we look at the Liouvillian $\mathcal{L}$ in (144) for an isolated quantum system, for example, it is clear from its diagonal form in (148) that its eigenvalues are proportional to the energy differences ($\epsilon_\nu - \epsilon_{\nu'}$).) This makes the Liouville space formalism particularly suited for theoretical studies in diverse spectroscopies [1, 10, 11]. The usefulness of the formalism is further accentuated by the superket triple product identity (88) — which enables one to, at least, formally solve any kind of master equation linear in the density matrix $\rho(t)$ (or any other operator which is the subject of the differential equation).

One important question we may want to discuss is whether there is a higher Hilbert space than the Liouville space $\mathcal{L}_d$ where one can still do quantum mechanics as in $\mathcal{H}_d$. The answer is NO. To see why, recall that $\mathcal{L}_d$ is nothing but the Hilbert space of the column ‘vectorized’ operators on $\mathcal{H}_d$ (table 1). Technically speaking, one can column ‘vectorize’ the superoperators on $\mathcal{L}_d$ (that is, the elements of $\mathcal{S}_d$) and create another Hilbert space $\mathcal{T}_d$ whose dimension will be $d^4$. The $(d^2 \times d^2)$ matrices of $\mathcal{S}_d$ will now be $(d^4 \times 1)$ column vectors in $\mathcal{T}_d$. The operators on $\mathcal{T}_d$, which will be $(d^4 \times d^4)$ matrices will also constitute a Hilbert space whose elements can be column ‘vectorized’ to get another Hilbert space $\mathcal{U}_d$ of dimension $d^{16}$, and so on. The point is, mathematically speaking, we can build an infinite sequence of finite-dimensional Hilbert spaces from $\mathcal{H}_d$. Despite this fact, we cannot do quantum mechanics beyond $\mathcal{L}_d$ because the density matrix $\rho(t)$, as far as current quantum physics goes, is the most general way of describing a quantum state, and in $\mathcal{L}_d$ it becomes a column vector — which is the most rudimentary element a finite-dimensional linear space can have. A square matrix can be reduced to a column vector, but what can a column vector be reduced to without losing any information? We do not have anything like that. The transition from $\mathcal{H}_d$ to $\mathcal{L}_d$, in regards to quantum mechanics, was made possible simply because we can reduce the matrix $\rho(t)$ to the column vector $|\rho(t)\rangle$ without losing information on the quantum state. This means, there won’t be any equivalent representation of $|\rho(t)\rangle$ (as far as information content is concerned) in $\mathcal{T}_d$, so quantum mechanics will be incomplete in this space and any other subsequent higher space.

Finally, we remark that the formalism discussed above can be extended to any kind of Liouville space $\mathcal{L}$ (separable or continuous) [10, 13], following the general theory of Hilbert spaces expounded, for example, in [16, 17, 18, 19].
Acknowledgments

The author is grateful to Mr. Matteo Bruschi and Dr. Andrea Piserchia for proofreading the manuscript and sharing their thoughts.

Appendix

Appendix A.1. Vector spaces, Hilbert spaces — a brief overview.

The definitions and propositions listed below can be found in books like \[16, 18, 19, 20, 21, 26, 27, 28\].

- A vector space or linear space $\mathcal{X}$ over a field $\mathbb{F}$ is a set of elements (called vectors) endowed with two operations:
  - (i) addition: if $x$ and $y$ are both elements of $\mathcal{X}$ then $x + y$ is also an element of $\mathcal{X}$
  - (ii) scalar multiplication: if $c \in \mathbb{F}$ and $x \in \mathcal{X}$, then $cx \in \mathcal{X}$ such that for any vectors $x, y, z \in \mathcal{X}$ and scalars $c, c' \in \mathbb{F}$
    - (i) $x + y = y + x$
    - (ii) $x + (y + z) = (x + y) + z$
    - (iii) there exists a unique vector 0 such that $x + 0 = x$
    - (iv) $c(x + y) = cx + cy$
    - (v) $(c + c')x = cx + c'x$
    - (vi) $c(c'x) = (cc')x$

$\mathcal{X}$ is said to be a complex vector space if $\mathbb{F} = \mathbb{C}$ (the set of complex numbers).
If $\mathbb{F} = \mathbb{R}$ (the set of real numbers), then $\mathcal{X}$ is said to be real.

- Let $S$ be a subset of $\mathcal{X}$. $S$ is said to be a linear manifold if it is a linear space itself.

- A set of vectors $\{x_1, x_2, \ldots, x_l\}$ is said to be linearly independent if the only solution to the equation $\sum_{i=1}^{l} c_i x_i = 0$ in the variables $c_1, c_2, \ldots, c_l$ is that $c_1 = c_2 = \cdots = c_l = 0$. Otherwise, the set is said to be linearly dependent.

- A set of vectors $\{x_1, x_2, \ldots, x_l\}$ is said to span a linear space $\mathcal{X}$ defined over the field $\mathbb{F}$ if every element $x$ of $\mathcal{X}$ can be expressed as a linear combination of $\{x_1, x_2, \ldots, x_l\}$: i.e. $x = c_1 x_1 + c_2 x_2 + \cdots + c_l x_l$, where $c_1, c_2, \ldots, c_l \in \mathbb{F}$.

- A set of vectors $\{x_1, x_2, \ldots, x_l\}$ is said to be the basis of a linear space $\mathcal{X}$ if: a) it is linearly independent, and b) spans $\mathcal{X}$.

- A linear space $\mathcal{X}$ is $n$-dimensional if and only if its basis consists of $n$ vectors.

- An inner product or scalar product for a linear space $\mathcal{X}$ is a map $F$ which assigns to each pair of vectors $x, y \in \mathcal{X}$ a scalar, denoted symbolically $\langle x, y \rangle$. An inner product for $\mathcal{X}$ must satisfy the following properties for vectors $x, y, z \in \mathcal{X}$ and scalar $c$:
  - (i) $\langle x, y + z \rangle = \langle x, y \rangle + \langle x, z \rangle$
  - (ii) $\langle cx, y \rangle = c \langle x, y \rangle$
  - (iii) $\langle x, y \rangle = \langle y, x \rangle^*$
  - (iv) $\langle x, x \rangle \geq 0$, the equality holding only if $x = 0$

- For a given inner product $F$ on linear space $\mathcal{X}$, the norm or length (according to $F$) of the vector $x \in \mathcal{X}$ is the non-negative real number $\|x\| := \sqrt{\langle x, x \rangle}$. 

A normed space is a linear space with a norm.

Two vectors \( x, y \in \mathcal{X} \) are said to be orthogonal to each other if \( \langle x, y \rangle = 0 \).

Two vectors \( x, y \in \mathcal{X} \) are said to be orthonormal if: a) they are orthogonal, and b) \( \|x\| = \|y\| = 1 \).

We say a sequence of vectors \( \{w_n\} \) \( (w_n = \sum_{k=1}^{n} c_k x_k) \) converges to a limit vector \( w \) if \( \|w_n - w\| \to 0 \) as \( n \to \infty \).

A Cauchy sequence of vectors is a sequence of vectors \( \{w_n\} \) such that \( \|w_m - w_n\| \to 0 \) as \( m, n \to \infty \).

A linear space \( \mathcal{X} \) is said to be complete if every Cauchy sequence of vectors converges to a limit vector which also belongs to \( \mathcal{X} \).

Every finite-dimensional complex linear space is complete. (See [16] for proof.)

A linear space \( \mathcal{X} \) is called a Hilbert space if \( \mathcal{X} \) is: a) normed and b) complete.

A separable Hilbert space is one whose orthonormal basis consists of a countable (finite or infinite) number of vectors.

Appendix A.2. \( \mathcal{U} \) is a bijection

We prove the proposition by reductio ad absurdum. We assume the proposition

\[ \mathbf{P2: \mathcal{U} \text{ is not a bijection}} \]

is true. Suppose then that we take two non-null operators \( A, B \in \mathcal{O}_d \), where \( A \neq B \) but \( \mathcal{U}[A] = \mathcal{U}[B] \). Let \( \{|\nu\rangle \langle \nu'|\} \) \( (\nu, \nu' = 1, \ldots, d) \) be an orthonormal basis of \( \mathcal{O}_d \). Thus, we have the expansions

\[ A = \sum_{\nu} \sum_{\nu'} A_{\nu \nu'} |\nu\rangle \langle \nu'| \text{ and } B = \sum_{\nu} \sum_{\nu'} B_{\nu \nu'} |\nu\rangle \langle \nu'| \],

from which — upon applying \( \mathcal{U} \) — we obtain

\[ \mathcal{U}[A] = |A\rangle\rangle = \sum_{\nu, \nu'} A_{\nu \nu'} |\nu, \nu'\rangle \rangle, \quad \mathcal{U}[B] = |B\rangle\rangle = \sum_{\nu, \nu'} B_{\nu \nu'} |\nu, \nu'\rangle \rangle. \quad (A.1) \]

Since \( \mathcal{U}[A] = \mathcal{U}[B] \), it follows that

\[ 0 = \mathcal{U}[A] - \mathcal{U}[B] = \sum_{\nu, \nu'} (A_{\nu \nu'} - B_{\nu \nu'}) |\nu, \nu'\rangle \rangle \]

(A.2)

which can only be true if \( (A_{\nu \nu'} - B_{\nu \nu'}) = 0 \) for any arbitrary \( \nu, \nu' \) — given that the superkets \( \{|\nu, \nu'\rangle \rangle\} \) are linearly independent (Appendix A.1). But for non-null operators \( A \) and \( B \), \( (A_{\nu \nu'} - B_{\nu \nu'}) = \langle \nu|(A - B)|\nu'\rangle = 0, \forall \nu, \nu' \) can be true iff \( A = B \). This contradicts our initial assertion that \( A \neq B \). Thus, the proposition \( \mathbf{P2} \) is false.

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