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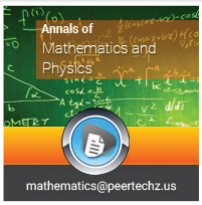

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Research Article

From linear algebra to quantum information

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Abstract

Anticipating the realization of quantum computers, we propose the most reader-friendly exposition of quantum information and qubits theory. Although the latter lies within framework of linear algebra, it has some flavor of quantum mechanics and it would be easier to get used to special symbols and terminologies. Quantum mechanics is described in the language of functional analysis: the state space (the totality of all states) of a quantum system is a Hilbert space over the complex numbers and all mechanical quantities are taken as Hermite operators. Hence some basics of functional analysis is necessary. We make a smooth transition from linear algebra to functional analysis by comparing the elements in these theories: Hilbert space vs. finite dimensional vector space, Hermite operator vs. linear map given by a Hermite matrix. Then from Newtonian mechanics to quantum mechanics and then to the theory of qubits. We elucidate qubits theory a bit by accommodating it into linear algebra framework under these precursors.

Introduction

Our purpose is to provide basics of quantum information by accommodating it within framework of linear algebra via quantum mechanics and functional analysis in plausibly the most reader-friendly way. This attempt was made in [1, pp. 16-46] and our presentation here is its development with more elucidation. It is usually the case that one takes some basic knowledge for granted without recourse to its source. E.g. the Kronecker product of two matrices is taken as heaven-sent axiom. It is, however, the matrix associated to the tensor product of two linear maps. Or one uses C^n as an n-dimensional C-vector space and the underlying result is neglected that an n-dimensional K vector space is isomorphic to K^n, i.e. vector space structure, linear maps, etc. are all ignored. In this paper we make pavement of some of such cracks on the road. We also restore the lost legay by rferring to standard classics on the subject, Chebyshev, Hermite, Dirac, Pauling, et al.

Quantum mechanics is described by the language of functional analysis, Hilbert spaces and linear operators. In the beginning of development, however, infinite matrices used to be used. Cf. e.g. [2]. Also in [3] and [4] infinite matrices are extensively used. Cf. § 4.

In [5] we remarked the following. True that Chen [6] has rather diligently searched for lost references after 1983, especially [7] which is not mentioned in [8] but is the very genesis of Chebyshev-Markov Expansion (CME) and arithmetical Fourier transforms in [9]. It is taken up in [10] as a paper containing infinite matrices in connection with Möbius inversion formula.

More recently [11] treats infinite matrices in another context: "An infinite dimensional vector whose components are Fourier coefficients of an automorphic form is characterized as one which is annihilated by an infinite matrix whose entries are the values of a Bessel function."

Along with development of functional analysis, the use of infinite matrices has been abandoned and replaced totally by linear operators. Since functional analysis may be thought of as an advanced deviation of linear algebra, it may be the most accessible way to grasping quantum mechanics passing from linear algebra to functional analysis and thence to quantum theory. This will be given in § 2.

One of the main possible menace on any Grid system connected to many users will come from using conventional crypto-system. There is a possibility of realization of quantum

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computers which will break many crypto-systems. § 4 is a prelude to quantum information which hopefully will help the readers to recognize the underlying structures.

However, in order to recognize the idea of quantum computers, it is necessary to have some basics in quantum mechanics and for this one needs some basics of mechanics since the former is a modification of Newtonian one. In § 3 we give basics on transition from Newtonian mechanics to quantum mechanics,

Then there are two extremal cases. One is qubits theory and the other extreme is continuous variable quantum mechanics which is the theory of infinite objects and is directly connected to quantum mechanics.

We specify to the theory of **qubits (quantum bits)** in § 4. For implementation purpose it is more favorable to have simple structures and qubits are simpler and suitable for implementation as quantum circuits, cf. e.g. [12].

Functional analysis as an advanced deviation of linear algebra

In this section we make a brief transition from linear algebra to functional analysis, stating different notation and terminologies. There are enormous amount of literature on linear algebra and functional analysis. We refer to [13] or [14] for the former and [15] etc. for the latter.

A **vector space** V over a field K is an algebraic system in which V is an additive Abelian group with scalar multiplication λx by elements λ of K, where $x \in V$. The scalar multiplication satisfies standard laws in algebra. It follows that V is the set of all linear combinations with coefficients in K. As is always the case with mathematics, given two systems V, V' with the same structure, the map is of the most importance that keeps algebraic structure, i.e. $f(x-y)= f(x)-f(y)$ and $\lambda f(x)=f(\lambda x)$. These two conditions are equivalent ot linearity $f(\lambda x+\mu y) = \lambda f(x)+\mu f(y)$ and we call such a map a linear map $f : V \to V'$. Every vector space V has a basis $\{u_i \mid i \in I\}$, which is the smallest set of generators. I.e. every element $x \in V$ may be expressed uniquely as a linear combination $x = \sum_{i\in I}\lambda_i u_i$ with only finitely many λ_i's are non-zero, denoted $V = \oplus_{i\in I} Ku_i$. If the basis consists of finitely many elements, V is called finite-dimensional and otherwise infinite-dimensional. In the former case, *an n-dimensional K-vector space is isomorphic to K^n.*

Theorem 2.1 *Let*

$$V = \bigoplus_{i=1}^{n} Ku_i, \quad V' = \bigoplus_{j=1}^{m} Kv_j, \quad V'' = \bigoplus_{k=1}^{\ell} Kw_k \tag{1}$$

be vector spaces and let $f : V \to V'$ be a linear map. Then we have the **basis correspondence formula**

$$f(u_j) = \sum_{i=1}^{m} a_{ij} v_i, \quad a_{ij} \in K, \quad 1 \le j \le n. \tag{2}$$

or in row form

$$(f(u_1), \cdots, f(u_n)) = (v_1, \cdots, v_m)A, \quad A = (a_{ij}) \in M_{m,n}(K), \tag{3}$$

Under (3), the linear map y=f(x) is in column form

$$\begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix} = \mathrm{y} = f_A(\mathrm{x}) = A\mathrm{x} = A\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}, \tag{4}$$

which means

$$\sum_{i=1}^{m} y_i v_i = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} a_{ij} x_j \right) v_i \tag{5}$$

and is referred to as the **coordinate correspondence formula**. The representation matrix of $g \circ f$ is BA, where $g : V' \to V''$ is a linear map satisfying the same conditions as f with the representation matrix B.

The correspondence between a linear map f and a matrix A is one-to-one and a linear map may be treated as f_A in (4).

Here matrix product is carried out according to the rule: row × column. It has chirality and if we express (2) in column vector form, we have ${}^tA$ in (4).

The field K of scalars may be any field, e.g. in coding theory, finite fields are taken. We choose K to be the complex number field C.

The inner product (scalar product) of two vectors a,b is defined by

$$(a, b) = {}^t\mathrm{a}\overline{\mathrm{b}} = {}^t\overline{\mathrm{b}}\mathrm{a} = ba^* \tag{6}$$

This entails non-negativity

$$(\mathrm{a}, \mathrm{a}) = \sum_{i=1}^{n} |\, a_i \,|^2 = |\, \mathrm{a} \,|^2 \ge 0. \tag{7}$$

The inner product satisfies linearity in the first entry

$$(\mathrm{a} + \mathrm{b}, \mathrm{c}) = (\mathrm{a}, \mathrm{c}) + (\mathrm{b}, \mathrm{c}), \quad (c\mathrm{a}, \mathrm{b}) = c(\mathrm{a}, \mathrm{b}) \tag{8}$$

and because of the complex conjugation property

$$(\mathrm{b}, \mathrm{a}) = \overline{(\mathrm{a}, \mathrm{b})} \tag{9}$$

it satisfies modified linearity

$$(\mathrm{a}, c\mathrm{b}) = \overline{c}(\mathrm{a}, \mathrm{b}), \quad (\mathrm{a} + \mathrm{b}, \mathrm{c}) = (\mathrm{a}, \mathrm{c}) + (\mathrm{b}, \mathrm{c}). \tag{10}$$

Definition 1: *The inner product on a C -vector space V is defined as a map V×V→C satisfying the non-negativity (7), linearity in the first entry (8), complex conjugation property (9) and linearity in the second entry (10). A C-vector space is called an inner product space if there is defined an inner product. In this case, the norm is defined by (7), i.e.*

$$\| \mathrm{a} \| = \sqrt{(\mathrm{a}, \mathrm{a})}. \tag{11}$$

We may speak of orthogonality of vectors. Two vectors $\mathrm{a} \neq \mathrm{o}, \mathrm{b} \neq \mathrm{o}$ are said to be orthogonal if (a,b) =0 as suggested by the cosine theorem. Given an orthogonal system (OS) we may normalize it to be an orthonormal system (ONS) by the Gram-Schmidt process. If a basis of a vector space is an ONS, it

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is called an Orthonormal Basis (ONB). C^n

Lemma 2.1: (i) *For a degree K matrix A with complex numbers entries, the following conditions are equivalent.*

(a) A is a normal matrix ($A A^* = A^* A$) and all eigenvalues of A are real numbers.

(b) A can be diagonalized by a unitary matrix $U \in U_k(\mathbb{C})$ as

$$U^{-1} A U = \begin{pmatrix} \lambda_1 & & O \\ & \ddots & \\ O & & \lambda_k \end{pmatrix} = D, \tag{12}$$

where λ_i are real.

(c) A is a Hermite matrix.

(ii) Suppose a Hermite matrix A of degree k is diagonalized by a unitary matrix U as (12). Then

$$e^A = \sum_{n=0}^{\infty} \frac{1}{n!} A^n = U \begin{pmatrix} e^{\lambda_1} & & O \\ & \ddots & \\ O & & e^{\lambda_k} \end{pmatrix} U^{-1}. \tag{13}$$

In what follows we assume the coefficient matrix $A = (a_{ij})_{1 \le i,j \le k}$ has constant entries. We consider the homogeneous system of DEs ($x_j = x_j(t)$

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} x_1 \\ \vdots \\ x_k \end{pmatrix} = A \begin{pmatrix} x_1 \\ \vdots \\ x_k \end{pmatrix}$$

in the form

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{x}(t) = A\mathrm{x}(t), \tag{14}$$

by writing

$$\mathrm{x} = \mathrm{x}(t) = {}^t(x_1(t), \cdots, x_k(t))$$

as a generalization of the DE for the first-order reaction (a is a constant)

$$\frac{\mathrm{d}}{\mathrm{d}t} x(t) = a x(t). \tag{15}$$

It is weell-known that the solution to (15) is

$$x(y) = e^{at} x(0), \tag{16}$$

so that the system obeying (15) is an *exponential phenomenon*. This will be applied very often in what follows.

We may also treat the linear DE of degree k

$$\frac{\mathrm{d}^k x}{\mathrm{d}t^k} + a_1 \frac{\mathrm{d}^{k-1} x}{\mathrm{d}t^{k-1}} + \cdots + a_{k-1} x = 0 \tag{17}$$

as a special case of (14) with

$$\mathrm{x} = \begin{pmatrix} x(t) \\ \vdots \\ x^{(k-1)}(t) \end{pmatrix} \tag{18}$$

and

$$A = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ & & \cdots & & \\ -a_{k-1} & & \cdots & & -a_1 \end{pmatrix}. \tag{19}$$

For differentiation of (18) gives $\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{x}(t) = {}^t(x', \cdots, x^{(k)})$ and the last entry is $-a_{k-1} x - \cdots - a_1 \frac{\mathrm{d}^{k-1} x}{\mathrm{d}t^{k-1}}$ by (17) and so (17) amounts to (14).

Theorem 2.2: *Suppose A is a square matrix of degree k which is diagonalizable as in (12). Then the solution of the system of differential equations (14) under the initial condition* $\mathrm{x}(0) = {}^t(x_1(0), \cdots, x_n(0))$ *is given by*

$$\mathrm{x}(t) = e^{At} \mathrm{x}(0). \tag{20}$$

A Hilbert space H is an inner product vector spaces over C which is complete with respect to the norm $\|.\|$, induced by the scalar product (,) (as in (11)). Here completeness means that every Cauchy sequence is convergent which enables analysis to be conducted on H. The elements of H are usually complex-valued functions defined on a certain domain. A typical example is $L^2(a,b)$ the Hilbert space of square integrable function on the interval (a,b). Thus we call a linear map a linear operator (or an additive operator) which sends a function to another object. Hilbert spaces come in quantum mechanics as the state space (totality of all states) of a quantum system and all (quantum) mechanical quantities are expressed as Hermitian operators (or self-adjoint operators), i.e. linear operators T: $H \to H$ satisfying $T^* = T$, where T^* means the conjugate operator, i.e.

$$(T\Psi_1, \Psi_2) = (\Psi_1, T^* \Psi_2). \tag{21}$$

Let $\{E(\lambda)\}$ be a resolution of the identity, i.e. each $E(\lambda)$ is a projector having the properties in Proposition 4.1 and they satisfy certain other conditions.

Theorem 2.3: *Let $\{E(\lambda)\}$ be a resolution of the identity. Then for a real-valued continuous function $\emptyset(x)$, we have*

$$(Tx, y) = \int_{-\infty}^{\infty} \phi(\lambda) \mathrm{d}(E(\lambda)x, y) \tag{22}$$

defines the self-adjoint operator T with domain of definition H satisfying $TE(\lambda) \supset E(\lambda)T$. In particular for $\emptyset(\lambda)=\lambda$

$$(Tx, y) = \int_{-\infty}^{\infty} \lambda \, \mathrm{d}(E(\lambda)x, y) \tag{23}$$

defines the self-adjoint operator T with domain of definition H. abbreviated as

$$T = \int_{-\infty}^{\infty} \lambda \, \mathrm{d}E(\lambda) \tag{24}$$

called the spectral decomposition of T. Here integrals are Stieltjes integrals and reduce to sums for discrete $\{\lambda\}$.

Definition 2: *Let T be a Hermitian operator with dense domain of definition. For a complex number λ let*

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$$T_\lambda = T - \lambda I \tag{25}$$

and consider its inverse. λ belongs to the spectra $S(T)$ of T if there is no continuous inverse operator T_λ^{-1} such that $\overline{D(T_\lambda^{-1})} = \mathcal{H}$. $S(T)$ is divided into two subsets:

$$S(T) = P(T) \cup C(T), \tag{26}$$

where $P(T)$ is the point spectra and $C(T)$ is the continuous spectra. (In general there is residual spectra), defined respectively as follows.

- $\lambda \in P(T)$ means $D(T_\lambda^{-1}) = \varnothing$, i.e. the inverse operator T_λ^{-1} does not exist.
- $\lambda \in C(T)$ means $\overline{D(T_\lambda^{-1})} = H$ but T_λ^{-1} is not continuous.

Theorem 2.4: *That $\lambda \in P(T)$ is equivalent to the fact that the equation $Tx = \lambda x$ has a non-trivial solution. If this is the case, λ is called the* eigenvalue *of T and $x \neq 0$ the* eigenvetor *of T.*

The set of all eigenvectors and the zero vector forms a subspace $E_T(\lambda)$ of H called the eigenspace of T.

For a Hermitian operator $T = \int \lambda \mathrm{d}E(\lambda)$ we have

- $S(T) \subset \mathbb{R}$.
- $\lambda \notin S(T)$ is equivalent to $E(\lambda_1) \neq E(\lambda_2)$ for some open interval (λ_1, λ_2) containing λ.
- $\lambda \in P(T)$ is equivalent to $E(\lambda) \neq E(\lambda - 0)$ and $E_T(\lambda) = \mathrm{Im}(E(\lambda) - E(\lambda - 0))$.
- $\lambda \in C(T)$ is equivalent to $E(\lambda) = E(\lambda - 0)$ and for any open interval (λ_1, λ_2) contaning λ we have $E(\lambda_1) \neq E(\lambda_2)$.

For a compact operator (or a completely continuous operator), Theorem 2.3 reduces to the spectral decomposition in the form of a series [16, p. 189](1990),p. 189], whose special case is Theorem 4.2 below.

From classical to quantum mechanics

In this section we provide a transition from classical to quantum mechanics. We shall use notation in [17, 5.1] rather than the commonly used one in quantum mechanics.

We shall first see that taking for granted that every physical quantity T can be represented by a linear operator, which by abuse of language is denoted by the same letter T, Hermitian operators are the ones that are needed. For the expectation value of T is given as the inner product

$$(\psi, T\psi) = \langle \psi \mid T\psi \rangle = \int \psi^* T\psi \, \mathrm{d}\mathrm{r}, \tag{27}$$

where $(T\psi, \psi)$ indicates the inner product in the vector space H and r = (x,y,z) is the position vector. Since expectation value is the average of the measured real values of a physical quantity, it must be real. For this it suffices that the conjugate operator T^* exists such that $T^* \supset T$, which means that T^* is an extension of T. T is then called **symmetric**. Symmetric operators are not always self-adjoint but physical interpretation requires that operators which represent measurable physical quantities must be self-adjoint, and we *use symmetric and Hermitian synonymously* so is customary.

For a Hermitian operator T, the eigenvectors $|\psi\rangle$ belonging to its eigenvalue $\lambda (\in \mathbb{R})$ are viewed as the quantum state whose mechanical quantity is equal to λ.

The Hermitian operator H expressing the total energy of a system is called the Hamiltonian. In most of quantum physics books, the Hamiltonian is denoted $\hat{H}$ but we use the same letter H as with the Hamiltonian function.

The wave function (denoted as a ket vector $|\Psi\rangle = |\Psi(\mathrm{r}, t)\rangle$, cf. § 4) is a (vector-valued) function in the position vector r and time t and is to satisfy the (time dependent) Schrödinger equation.

$$i\hbar \frac{\partial}{\partial t} |\Psi(\mathrm{r}, t)\rangle = H |\Psi(\mathrm{r}, t)\rangle, \tag{28}$$

where

$$\hbar = \frac{h}{2\pi} \tag{29}$$

is called the reduced Planck constant, referred to as the Planck constant and where

$$h = 2\pi\hbar = 6.624 \times 10^{-27} \, erg \times sec$$

is the Planck constant.

More concretely, consider a system of N point particles $\mathrm{r}_j = (x_j, y_j, z_j)$ with mass m_i, $1 \leq j \leq N$ moving around a three dimensional space under the influence of forces given as a potential energy $V = V(\mathrm{R}, t)$, where

$$\mathrm{R} = (\mathrm{r}_1, \cdots, \mathrm{r}_N) = (x_1, \cdots, z_N) \in \mathbb{R}^{3N} \tag{30}$$

is a $3N$-dimensional vector. For this the Hamiltonian H in (28) reads

$$H = -\frac{\hbar^2}{2} \sum_{j=1}^{N} \frac{1}{m_j} \Delta_j + V, \tag{31}$$

where Δ_j is the Laplacian operating on each r_j defined by

$$\Delta_j = \frac{\partial^2}{\partial x_j^2} + \frac{\partial^2}{\partial y_j^2} + \frac{\partial^2}{\partial z_j^2}. \tag{32}$$

Hence the Schrödinger equation (28) amounts to the non-relativistic Schrödinger equation in position basis

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathrm{R}, t) = H\Psi(\mathrm{R}, t), \tag{33}$$

where $\Psi(\mathrm{R}, t)$, called the (position-space) wave function, describes the state of the system at time t. In this case, there is a postulate (M. Born) that the probability of the positions

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of N particles lying in a certain region $D \subset \mathbb{R}^{3N}$ is to be proportional to

$$\int \cdots \int_D |\Psi(\mathrm{R},t)|^2 \mathrm{d}\mathrm{R}. \tag{34}$$

For this we must have the probability of the total event is to be **1**, and *a fortiori*

$$\int \cdots \int_{\mathbb{R}^{3N}} |\Psi(\mathrm{R},t)|^2 \mathrm{d}\mathrm{R} < \infty, \tag{35}$$

i.e. the L^2-space $L^2(\mathbb{R}^{3N})$ is the place where the wave functions are to lie.

In the form (31), we may easily check the condition for H to be symmetric. Let $D \subset \mathbb{R}^{3N}$ be either bounded or equal to the whole set. In the former case, we consider only those wave functions which are 0-extensions, i.e. $\Psi(\mathrm{R},t) - 0$ if $\mathrm{R} \notin D$ and in the case $D = \mathbb{R}^{3N}$, we take account that $\Psi(\mathrm{R},t) \to 0$ quickly enough as one of the position variables tends to ∞ in view of (35). We refer to this as a boundary condition. It suffices to consider the case $\mathrm{R}\,x$, say. By integration by parts, we have (R' denoting the $(3N-1)$-dimensional vector)

$$\int \cdots \int_D \overline{\Psi_1(\mathrm{R},t)} \frac{\partial^2}{\partial^2 x} \Psi_2(\cdots, x, \cdots, t) \mathrm{d}\mathrm{R}$$

$$= -\int \cdots \int_{\partial D} \frac{\partial}{\partial x} \overline{\Psi_1(\mathrm{R},t)} \frac{\partial}{\partial x} \Psi_2(\cdots, x, \cdots, t) \mathrm{d}\mathrm{R}'$$

$$= \int \cdots \int_D \frac{\partial^2}{\partial^2 x} \overline{\Psi_1(\mathrm{R},t)} \Psi_2(\cdots, x, \cdots, t) \mathrm{d}\mathrm{R},$$

or (21) with $T^* = T = H$.

We shall explain how the Hamiltonian (31) is deduced from the Hamiltonian function. For a conservative system (in which the potential energy does not depend on time) the Hamiltonian function $H = H(R)$ is the total energy (kinetic and potential) of the system:

$$H = H(\mathrm{R}) = T(\mathrm{p}) + V(\mathrm{R}) = W. \tag{36}$$

Here the momentum p_k related to the direction x_k is $m_k \dot{x}_k$, so that

$$\mathrm{p} = (p_1, \cdots, p_N) = (m_1 \dot{x}_1, \cdots, m_N \dot{x}_N) \tag{37}$$

and the kinetic energy $T = T(\mathrm{p})$ is

$$T = \frac{1}{2} \sum_{k=1}^{n} m_k (\dot{x}_k^2 + \dot{y}_k^2 + \dot{z}_k^2) = \frac{1}{2} \sum_{k=1}^{n} \frac{1}{m_k} p_k^2. \tag{38}$$

Substituting (38) into (36), we deduce that

$$H(\mathrm{R}) = \frac{1}{2} \sum_{k=1}^{n} \frac{1}{m_k} p_k^2 + V(\mathrm{R}) = W. \tag{39}$$

Making the *replacement*

$$p_k \leftrightarrow \frac{h}{2\pi i} \frac{\partial}{\partial x_k} = -i\hbar \frac{\partial}{\partial x_k}, \quad W \leftrightarrow -\frac{h}{2\pi i} \frac{\partial}{\partial t} = i\hbar \frac{\partial}{\partial t}, \tag{40}$$

we obtain the Hamiltonian (31).

The Hamiltonian (31) operates on the wave function $\Psi(\mathrm{R},t)$ as

$$H\Psi(\mathrm{R},t) = -\frac{\hbar^2}{2} \sum_{j=1}^{N} \frac{1}{m_j} \Delta_j \Psi(\mathrm{R},t) + V\Psi(\mathrm{R},t) = i\hbar \frac{\partial \Psi}{\partial t}. \tag{41}$$

Hence the wave equation (33) amounts to (41).

In case the boundary conditions can be so chosen that the Hamiltonian is Hermitian, then (41) can be solved using the spectral decomposition. [18, pp. 172-185]:

$$\Psi(\mathrm{R},t) = U_t \Psi(\mathrm{R},0), \quad U_t = e^{-\frac{i}{\hbar} Ht} \tag{42}$$

where e^B is the exponential function in the bounded operator. Hence this may be thought of as a manifestation of exponential phenomenon. We note that U_t is a unitary operator [17, p. 175]. We add a standard characterization [18, p. 41].

Theorem 3.1: *For a bounded operator U to be unitary it is necessary and sufficient that*

$$U^* = U^{-1}. \tag{43}$$

Our aim from here is to solve (41) under the assumption that Ψ is of variables separable type

$$\Psi(\mathrm{R},t) = \varphi(t)\psi(\mathrm{R}) \tag{44}$$

and prove Theorem 3.3 generalizing the standard Theorem 3.2. Both of them hold on the assumption that $\psi(\mathrm{R})$ is also of variables separable type. Substituting (44) in (41), we have

$$\left(-\frac{\hbar^2}{2} \sum_{j=1}^{N} \frac{1}{m_j} \Delta_j \psi(\mathrm{R}) + V(\mathrm{R})\psi(x) \right) \varphi(t) = i\hbar \psi(\mathrm{R}) \frac{\mathrm{d}\varphi(t)}{\mathrm{d}t}, \tag{45}$$

whence dividing both sides by $\varphi(t)\psi(\mathrm{R})$ we have

$$\frac{1}{\psi(\mathrm{R})} \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(\mathrm{R})\psi(\mathrm{R}) \right) = \frac{1}{\varphi(t)} \left(i\hbar \frac{\mathrm{d}\varphi(t)}{\mathrm{d}t} \right). \tag{46}$$

Since the left-hand side of (46) is a function in R only and the right-hand side in t only, it follows that (46) must be a constant, say W. Hence (46) is equivalent to the system

$$\left\{ \begin{array}{ll} \dfrac{\mathrm{d}\varphi(t)}{\mathrm{d}t} & = -\dfrac{i}{\hbar} W\varphi(t) \\ -\dfrac{\hbar^2}{2} \sum\limits_{j=1}^{N} \dfrac{1}{m_j} \Delta_j \psi(\mathrm{R}) + V(\mathrm{R})\psi(\mathrm{R}) & = W\psi(\mathrm{R}). \end{array} \right\} \tag{47}$$

The second equation in (47) is often written as

$$\sum_{j=1}^{N} \frac{1}{m_j} \Delta_j \psi(\mathrm{R}) + \frac{2}{\hbar^2} (W - V)\psi(\mathrm{R}) = 0 \tag{48}$$

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and called the Schrödinger amplitude equation for a conservative system of point particles. $W = W_n$ represents the energy of the system at its various stationary states and is called the characteristic energy values or eigenvalues of the wave equation.

Since the first equation in (47) is one for the first-order reaction (15), the solution is given by $e^{-\frac{i}{\hbar}W_n t}$. Hence by the principle of superposition, the general solution $\Psi(\mathrm{R},t)$ of (41) is given by

$$\Psi(\mathrm{R},t) = \sum_n a_n \Psi_n(\mathrm{R},t) = \sum_n a_n \psi_n(\mathrm{R}) e^{-i\frac{W_n}{\hbar}t}. \tag{49}$$

Up here the variable separation condition on $\psi_n(\mathrm{R})$ was not assumed. From here we assume that $\psi(\mathrm{R})$ is also of variables separable type, in which case we may separate the components as in [19, p. 101] and treat the case (48) for R = x.

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(W - V)\psi(x) = 0. \tag{50}$$

Since this is a linear DE of degree 2 with variable coefficients, we apply the Lagrange constant variation method) to find its (approximate) solutions (66). Let

$$\psi = \psi(x) = e^{q(x)}, \tag{51}$$

say, where

$$q(x) = \frac{i}{\hbar}\int y\,\mathrm{d}x \tag{52}$$

and $y = y(x)$. Then

$$\frac{\mathrm{d}\psi}{\mathrm{d}x} = \frac{i}{\hbar} y e^{q(x)}. \tag{53}$$

Hence differentiating again, we obtain

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \frac{i}{\hbar}\left(\frac{\mathrm{d}y}{\mathrm{d}x} + \frac{i}{\hbar}y^2\right)e^{q(x)}. \tag{54}$$

Substituting (54) and (51) into (50) and dividing both sides by $\frac{1}{\hbar^2}e^{q(x)}$, we transform (50) into

$$-\frac{\hbar}{i}\frac{\mathrm{d}y}{\mathrm{d}x} + y^2 + 2m(W - V) = 0$$

or

$$\frac{\hbar}{i}\frac{\mathrm{d}y}{\mathrm{d}x} = 2m(W - V) - y^2 = p^2 - y^2, \tag{55}$$

say, where

$$p = \sqrt{2m(W - V)} \tag{56}$$

is the classical expression for the momentum.

The Wentzel-Kramers-Billouin Method (WKB method) consists in giving an approximation to the solution of the wave equation. The first term leads to the result obtained by classical mechanics (Newtonian mechanics), the second term to the old-quantum theory result, and higher terms to corrections which brings in the effects characteristic of the new (quantum) mechanics.

In [19], they apply WKB method by viewing y *a priori* as a function in h and expand it into the Maclaurin series in $t := \frac{\hbar}{i}$:

$$y = y(x,h) = \sum_{n=0}^{\infty} y_n t^n, \tag{57}$$

where y_j are functions in x. We compare the coefficients of (57) and (55) in the form

$$t\frac{\mathrm{d}y}{\mathrm{d}x} = t\left(\sum_{n0}^{\infty} y_n' t^n\right) = p^2 - y^2 = p^2 - (y_0^2 + 2y_0y_1t + (y_1^2 + 2y_0y_2)t^2 + \cdots). \tag{58}$$

Hence

$$p^2 - y_0^2 = 0, \quad 2y_0y_1 = -y_0', \quad y_1^2 + 2y_0y_2 = -y_1', \cdots \tag{59}$$

so that

$$y_0 = p, \quad y_1 = \frac{-y_0'}{2y_0} = \frac{-p'}{2p}, \quad y_2 = -\frac{1}{2y_0}\left(y_1' + y_1^2\right)\cdots. \tag{60}$$

Since

$$p' = \frac{-2mV'}{2p}, \tag{61}$$

it follows that

$$y_1 = \frac{2mV'}{(2p)^2} = \frac{V'}{4(W - V)}. \tag{62}$$

Substituting the expressions for y_1' and y_1^2 in the third equality in (60), we find that

$$y_2 = -\frac{1}{2p}\frac{1}{16(W - V)^2}(4V''(W - V) + 5V'^2) \tag{63}$$

$$= -\frac{1}{32}\frac{1}{\sqrt{2m}(W - V)^{5/2}}(4V''(W - V) + 5V'^2)$$

Incorporating the coefficients y_0, y_1, y_2 from (57), (62) and (63), we have an approximation to (52)

$$y = y_0 + \frac{\hbar}{i}y_1 + \left(\frac{\hbar}{i}\right)^2 y_2 + \cdots = p + \frac{\hbar}{i}\frac{V'}{4(W - V)} \tag{64}$$

$$-\left(\frac{\hbar}{i}\right)^2 \frac{1}{32}\frac{1}{\sqrt{2m}(W - V)^{5/2}}(4V''(W - V) + 5V'^2) + \cdots.$$

Substituting (64) up to the second term and noting that by (62)

$$\int y_1\,\mathrm{d}x = -\frac{1}{4}\log(W - V) + C, \tag{65}$$

we find an approximation

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$$\psi = M(W-V)^{-\frac{1}{4}} e^{\int\sqrt{2m(W-V)}\,dx} \tag{66}$$

with M a constant. The probability distribution function is

$$\bar{\psi}\psi \approx C(W-V)^{-\frac{1}{2}} \approx \frac{1}{p} \tag{67}$$

in conformity with the classical result that the probability of finding a particle in a range *dx* is inversely proportional to the velocity in that range and the velocity is proportional to *p*.

Quantization occurs when one attempts to extend the region for *W* by an associated condition

$$\int_C y\,dx = 2\pi\hbar n, \quad n = 0,1,2,\cdots, \tag{68}$$

where the integral is a certain contour integral. The first approximation in (64) amounts to the classical quantum theory condition (68) with *p* in place of *y*. The second approximation in (64) gives

$$\int_C p\,dx = 2\pi\hbar\left(n+\frac{1}{2}\right), \quad n = 0,1,2,\cdots. \tag{69}$$

Lemma 3.1: *Writing in (50)*

$$\alpha = \alpha(x) = \frac{1}{\hbar^2}p^2, \tag{70}$$

where *p* is defined by (56), we find that (50) amounts to the homogeneous equation for a one-dimensional wave $y(x)$

$$y'' + \alpha y = 0, \tag{71}$$

which entails (78).

Corollary 3.1 *In the case where* α *is a constant (we may suppose* α>0*), this can be solved e.g. by the method of diagonalization, cf. Theorem 2.2 or by the Laplace transform method and the solution to (71) is*

$$y(x) = y(0)\cos\sqrt{\alpha}x + \frac{y'(0)}{\sqrt{\alpha}}\sin\sqrt{\alpha}x = A\sin(\sqrt{\alpha}x+\theta), \tag{72}$$

say. Further if $y(x)$ has the initial value $y(0)=0$ and satisfies the boundary condition that $y(x)=0$ for $x>a>0$, *a* being big enough. Then (71) amounts to the one-dimensional Schrödinger equation

$$-\frac{\hbar}{2m^2}y'' = Ey, \tag{73}$$

where $E = \frac{\hbar}{2m^2}\alpha$. By continuity, $y(a)=0$. The solution (72) reads

$$y(x) = \frac{y'(0)}{\sqrt{\alpha}}\sin\sqrt{\alpha}x. \tag{74}$$

For this to vanish at $x=a$, we must have $\sqrt{\alpha}a = \pi n$, $n\in\mathbb{N}$ or

$$\alpha = \left(\frac{\pi n}{a}\right)^2. \tag{75}$$

Hence

$$E = E_n = \frac{\hbar}{2m^2}\left(\frac{\pi n}{a}\right)^2 \tag{76}$$

are energy levels and

$$y_n(x) = c\sin\frac{\pi n}{a}x \tag{77}$$

are eigenfunctions belonging to E_n.

We are in a position to prove Theorem 3.2.

(71) contains the case of simple harmonic motion of a point particle under the restoring force directly proportional to the displacement x acting on it in the direction opposite to x, i.e.

$$mx'' = -kx \tag{78}$$

which is the case (71) with $\alpha = \frac{k}{m}$. It is customary to write ω for the frequency, i.e. $\alpha = \frac{k}{m}$ or $k = m\omega^2$. Since the potential inducing the restoring force on the left-hand side of the above equation is $V(x) = \frac{1}{2}x^2$, the Hamiltonian function (39) is

$$H = H(x) = \frac{1}{2}mp_x^2 + \frac{1}{2}m\omega^2x^2. \tag{79}$$

Making the replacement (40), we find the Hamiltonian—harmonic oscillator

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2 \tag{80}$$

and the Schrödinger equation corresponding to (48) with *W*=*E* reads

$$H\Psi(x) = E\Psi(x). \tag{81}$$

Introducing the notation

$$x \leftrightarrow \sqrt{\frac{m\omega}{\hbar}}x, \quad \lambda = \frac{2}{\hbar\omega}E,$$

(81) amounts to

$$\left(\frac{d^2}{dx^2} + x^2\right)\Psi(x) = \lambda\Psi(x) \tag{82}$$

which is (86) below satisfied by Hermite polynomials. The solutions satisfying the boundary condition that $\Psi(x)\to 0$ as $x\to\infty$ are possible only for $\lambda = \lambda_n$ with $2n+1$, $n = 0,1,\cdots$ and are proportional to (85).

Invoking the normalization of Ψ we have proved

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Theorem 3.2: *Under the assumption of (??), eigenfunctions corresponding to eigenvalues* $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$ *are*

$$\Psi_n(x) = \sqrt{\frac{1}{2^n n!}\sqrt{\frac{m\omega}{\pi\hbar}}}H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-\frac{m\omega}{2\hbar}x^2}. \tag{83}$$

Cf. e.g. [20].

Here the **Hermite polynomial** $y = H_n(x)$ is a solution of the DE

$$\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + 2ny = 0 \tag{84}$$

and

$$w = e^{-\frac{1}{2}x^2}H_n(x) \tag{85}$$

is a solution of

$$\frac{d^2w}{dx^2} + (2n + 1 - x^2)w = 0. \tag{86}$$

Hermite polynomials are one of well-known class of orthogonal polynomials (cf. e.g. [21, II, pp.153-231]) and the class of functions given by (83) forms an ONB (orthonormal basis).

There is an explicit formula ([21, II, p. 193 (9)])

$$H_n(x) = \sum_{m=0}^{[n/2]}\frac{(-1)^m(2x)^{n-2m}}{m!(n-2m)!} \tag{87}$$

which may be proved by the formula

$$H_n(x) = (-1)^n e^{x^2}D^n e^{-x^2} \tag{88}$$

with $D = \frac{d}{dx}$. First a few terms are

$$H_0(x) = 1, H_1(x) = 2x.H_2(x)4x^2 - 2, H_3(x) = 8x^3 - 12x, \cdots.$$

Below we give proofs of some of the properties of Hermite polynomials.

(84) reduces to (86).

Proof. We determine the constants α so that by the change of variable

$$y = e^{\alpha x^2}w \tag{89}$$

(84) reduces to the one without $\frac{dw}{dx}$. We have

$$\frac{dy}{dx} = e^{\alpha x^2}\left(2\alpha xw + \frac{dw}{dx}\right)$$

and

$$\frac{d^2y}{dx^2} = e^{\alpha x^2}\left(\frac{d^2w}{dx^2} + 4\alpha x\frac{dw}{dx} + 2\alpha\left(2\alpha x^2 + 1\right)w\right)$$

Substituting these and dividing by $e^{\alpha x^2}$, we see that (84) reads

$$\frac{d^2w}{dx^2} + \left(4\alpha - 2\right)\frac{dw}{dx} + \left(4\alpha(\alpha-1)x^2 + 2\alpha + 2n\right)w = 0. \tag{90}$$

We choose $\alpha = \frac{1}{2}$. Then the coefficient of w for this choice is

$$2n + 1 - x^2$$

and (86) follows.

The confluent hypergeometric functions are solutions of the DE

$$x\frac{d^2y}{dx^2} + (c - x)\frac{dy}{dx} - ay = 0 \tag{91}$$

and one of the solutions is given by $\Psi(a, c; x)$ [21, II, p. 248].

(91) amounts to Whittaker's standard form

$$\frac{d^2w}{dx^2} + \left(-\frac{1}{4} + \frac{\varkappa}{x} + \frac{\frac{1}{4} - \mu^2}{x^2}\right)w = 0 \tag{92}$$

where $a = \frac{1}{2} - \varkappa + \mu$, $c = 1 + 2\mu$.

Proof. We determine the constants α, β so that by the change of variable

$$y = x^\alpha e^{\beta x}w \tag{93}$$

(91) reduces to the one without $\frac{dw}{dx}$. We have

$$\frac{dy}{dx} = x^{-\frac{c}{2}}e^{\frac{1}{2}x}\left(\left(\frac{\alpha}{x} + \beta\right)w + \frac{dw}{dx}\right)$$

and

$$\frac{d^2y}{dx^2} = x^\alpha e^{\beta x}\left(\frac{d^2w}{dx^2} + 2\left(\frac{\alpha}{x} + \beta\right)\frac{dw}{dx} + \left(\frac{\alpha^2 - \alpha}{x^2} + \frac{2\alpha\beta}{x} + \beta^2\right)w\right)$$

Substituting these and dividing by $x^\alpha e^{\beta x}$, we see that (91) reads

$$x\frac{d^2w}{dx^2} + \left(2(\alpha + \beta x) + c - x\right)\frac{dw}{dx} \tag{94}$$

$$+\left(\frac{\alpha^2 - \alpha + c\alpha}{x} + 2\alpha\beta - \alpha + c\beta - a + \beta(\beta - 1)x\right)w = 0.$$

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For the coefficient of $\frac{dw}{dx}$ to vanish, we choose $\alpha = -\frac{c}{2}$, $\beta = \frac{1}{2}$. Then the coefficient of w for this choice is

$$\frac{-\frac{c^2}{4}+\frac{c}{2}}{x}+\frac{c}{2}-a-\frac{1}{4}x.$$

Dividing (94) by x leads to (92).

(91) reduces to (84) and (86).

Proof. We write the variable x by x in (91) and put

$$z = \alpha x^2 \tag{95}$$

to obtain

$$\frac{dy}{dx} = 2\alpha x\frac{dy}{dz}, \quad \frac{dy}{dz} = \frac{1}{2\alpha x}\frac{dy}{dx}.$$

Hence

$$\frac{d^2y}{dx^2} = 2\alpha\frac{dy}{dz}+2\alpha x\frac{d}{dx}\frac{dy}{dz} = \frac{1}{x}\frac{dy}{dx}+(2\alpha x)^2\frac{d^2y}{dz^2}$$

or

$$\frac{d^2y}{dz^2} = \frac{1}{4\alpha^2x^2}\left(\frac{d^2y}{dx^2}-\frac{1}{x}\frac{dy}{dz}\right).$$

Substituting in (91), we deduce that

$$\frac{\alpha}{4\alpha^2}\left(\frac{d^2y}{dx^2}-\frac{1}{x}\frac{dy}{dz}\right)+(c-\alpha x^2)\frac{1}{2\alpha x}\frac{dy}{dx}-ay = 0$$

or

$$\frac{d^2y}{dx^2}+\left(c-\frac{\alpha}{2}\right)\frac{1}{2\alpha x}\frac{dy}{dx}-2\alpha x\frac{dy}{dx}-4\alpha ay = 0.$$

Letting $c = \frac{\alpha}{2}\alpha$, we arrive at

$$\frac{d^2y}{dx^2}-2\alpha x\frac{dy}{dx}-4\alpha ay = 0. \tag{96}$$

Hence (96) with $\alpha = 1$ (whence $c = \frac{1}{2}$) and $a = -\frac{1}{2}n$ amounts to (84).

Proposition 3.1: *For the Hermite polynomial (87) we have ([21, II, p.194 (16)]*

$$H_n(x) = 2^n\Psi\left(-\frac{1}{2}n,\frac{1}{2};x^2\right) \tag{97}$$

and [21, I, p. 267 (32)]

$$H_n(x) = 2^n x\Psi\left(\frac{1}{2}-\frac{1}{2}n,\frac{3}{2};x^2\right). \tag{98}$$

amounts to (97).

Proof. Recall the asymptotic formula [21, I, p. 278 (1)]

$$\Psi(a,c;x) = \sum_{m=0}^{N}(-1)^m\frac{(a)_m(a-c+1)_m}{m!}x^{-a-m}+O\left(|x|^{-a-N-1}\right), \tag{99}$$

where

$$N = 0,1,2,\cdots, \quad -\frac{3}{2}\pi < \arg x < \frac{3}{2}\pi, \quad |x|\to\infty.$$

Comparing the leading coefficients of (87) and (99), we conclude (97).

To show that (98) amounts to (97) we recall [21, I, p. 267 (6)]

$$\Psi(a,c;x) = x^{1-c}\Psi(a-c+1,2-c:x), \tag{100}$$

(100) with $a = -\frac{n}{2}$, $c = \frac{1}{2}$, $x\leftrightarrow x^2$ establishes (98).

Using Proposition 3.1, Theorem 3.2 reads

Theorem 3.3 *Under the assumption of (??), eigenfunctions corresponding to eigenvalues* $E_n = \left(n+\frac{1}{2}\right)\hbar\omega$ *are*

$$\Psi_n(x) = \sqrt{\frac{2^n}{n!}\sqrt{\frac{m\omega}{\pi\hbar}}}\Psi\left(-\frac{1}{2}n,\frac{1}{2};\frac{m\omega}{\hbar}x\right)e^{-\frac{m\omega}{2\hbar}x^2}, \tag{101}$$

where the left-hand side resp. right-hand side Ψ means the wave function resp. confluent hypergeometric function.

A slightly more general class of functions are that of parabolic cylinder functions, [21, pp. 115-132] (in which the header on p. 131 should read “parabolic cylinder functions”).

Finally we state the following extreme case which is important in molecular orbital theory. Cf. [22, pp. 16-22].

Example 3.1: *We consider the extreme case where the quantum state* $\boldsymbol{\Psi} = \boldsymbol{\Psi}(t)$ *varies with time variable* t *only according to the Schrödinger equation (28), If* $H\boldsymbol{\Psi}(t) = E\boldsymbol{\Psi}(t)$ *and the eigenvalue E is real called the* energy levels *of the system, cf. the first equation in (47). The solution of this equation is called the stationary state on the ground that its expectation does not change with time. The energy level means the values of the energy which the stationary state can assume. (28) amounts to*

$$\frac{d}{dt}\boldsymbol{\Psi}(t) = \frac{-iE}{\hbar}\boldsymbol{\Psi}(t) \tag{102}$$

and the solution given by (42) amounts to

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$$\Psi(t) = e^{-\frac{iEt}{\hbar}}\Psi(0). \tag{103}$$

Quantum information

Given two wave-functions ψ_m, ψ_n, their inner product (ψ_m, ψ_n) is usually defined as in (27) by

$$(\psi_m, \psi_n) = \int \overline{\psi_m}\psi_n \, dx. \tag{104}$$

We show in (112) below that

$$(\psi_m, \psi_n) = \langle \psi_m \mid \psi_n \rangle \tag{105}$$

in the Dirac notation [23].

Let $\{u_i\}$ be an ONB (e.g. (83) in infinite dimensional case). Then an arbitrary wave-function may be expressed as

$$\psi_m = \sum_i c_{im} u_i, \tag{106}$$

where $c_{im} = (\psi_m, u_i) \in \mathbb{C}$ such that

$$\sum_i |c_{im}|^2 = 1. \tag{107}$$

We define the ket vector $|\psi_m\rangle$ by

$$|\psi_m\rangle = \begin{pmatrix} c_{1m} \\ c_{2m} \\ \vdots \end{pmatrix} \tag{108}$$

and the **bra vector** $\langle \psi_m |$ by

$$\langle \psi_m | = |\psi_m\rangle^* = \left(\overline{c_{1m}}, \ \overline{c_{2m}}, \ \cdots\right), \tag{109}$$

Cf. Table 1.

Table 1: Notation in linear algebra and quantum theory.

Subject	Lin. alg.	Quantum (ftn'al analysis)
system	vector space, matrices	Hilbert space, linear operators
complex conj.	$\overline{A}$	T^*
transpose	${}^tA$	T^T
conj. transpose	A^*	$T^\dagger$
Hermitian	$A^* = A$	$T^\dagger = T$
unitary	$U^* = U^{-1}$	$U^\dagger = U^{-1}$
vector	column $\mathtt{a}$	ket $\lvert\psi\rangle$
vector	row $\mathtt{a}'$	bra $\langle\psi\rvert\ (=\lvert\psi\rangle^*)$
inner prod.	$(\mathtt{a}, \mathtt{b}) = \mathtt{b}^*\mathtt{a}$	$\langle\psi_1 \mid \psi_2\rangle = \lvert\psi_1\rangle^* \mid \psi_2\rangle$

Here the scalar product hψ1|ψ2i is as in (105)

(108) reads for the element μ_i of the ONB,

$$|u_i\rangle = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} = \mathtt{e}_i, \tag{110}$$

the i th fundamental unit vector. (107) implies that

$$\| \psi_m \rangle | = 1. \tag{111}$$

Substituting (107) into (104), we find that

$$(\psi_m, \psi_n) = \sum_i \sum_j \overline{c_{im}} c_{jn} (u_i u_j) = \sum_i \sum_j \overline{c_{im}} c_{jn} \delta_{ij} \tag{112}$$

$$= \sum_i \overline{c_{im}} c_{in} = (\langle \psi_m \mid, \mid \psi_n \rangle),$$

i.e. the matrix product of the bra- and the ket-vectors, which we express as $\langle \psi_m \mid \psi_n \rangle$ following Dirac's convention [23, p. 19, ll. 15-16 from below] of contracting two vertical lines into one. Hence (112) leads to (105). Up here the Hilbert spaces comprising of wave functions is of infinite dimensional and is referred to as continuous-variable quantum information. The ket vectors and matrices are of infinite degree, which are rather classical, as stated in § 1. For modern theory cf. e.g. [24].

In what follows we shall confine ourselves to qubits where the associated Hilbert spaces H are finite dimensional complex vector spaces which we may view as C^N (as mentioned in § 2. $N = 2^\nu$, cf. (119)). Hence a ket vector is an N-dimensional column vector and a Hermitian operator is a Hermite matrix. Since qubits are (N-dimensional) unit vectors, unitary matrices are essential because they are *isometries*: $|U \mid \psi\rangle| = \| \psi\rangle|$. It will turn out that qubits are generated from single qubits $\phi\rangle, \psi\rangle$ by Kronecker product $\phi\rangle \otimes \psi\rangle = \phi\psi\rangle$ which are then processed by unitary matrices. This is expressed by saying that a qubit $\psi\rangle$ is input into a quantum gate U and output is $U\psi\rangle$.

From here to the end of this section we partly refer to [12,25] some materials are taken from there with more detailed and lucid expoundation using more well-known symbols from linear algebra. It is standard to start from the 2-dimensional complex vector space $\mathcal{H} \simeq \mathbb{C}^2 = \mathbb{C}\mathtt{e}_1 \oplus \mathbb{C}\mathtt{e}_2$ (the totality of all single qubits). It is customary to denote the unit basis vectors as two special states $|0\rangle, |1\rangle$ known as *computational basis states*. In the notation of (110)

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \mathtt{e}_1, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \mathtt{e}_2. \tag{113}$$

These correspond to the spin-up and spin-down states of a particle such as an electron or a proton. All the elements $a \mid 0\rangle + b \mid 1\rangle$, $|a|^2 + |b|^2 = 1$ in $\mathcal{H} \simeq \mathbb{C}^2$ are called (single) qubits (quantum bits) or a 1-qubit. When qubits are *observed*

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(or measured), the value is determined either to be 0 or 1 with probability $|a|^2$ and $|b|^2$, respectively. Measurement is formally conducted by applying the measurement operators in Definition 6 and the coefficients $|a|^2$ and $|b|^2$ may be thought of as probabilities (cf. Remark 1).

Single qubits are extended to ν-qubits by way of tensor products. Cf. e.g. [14,26].

Definition 3: For two free C-modules M,N (i.e. C-vector spaces) with bases $\{u_\mu\}$, $\{v_\nu\}$, their tensor product $M \otimes N$ is the totality of all linear combinations of $u_\mu \otimes v_\nu$, which is again a free C-module. For matrices, we specify the tensor product to be the Kronecker product in Definition 4.

Every state of a quantum system is expressed by a ket vector $|\psi\rangle$ which is a wave function and satisfies the Schrödinger equation (28):

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle.$$

If $|\psi\rangle$ is only timedependent, then Example 28 gives an explicit expression as an exponential phenomenon:

$$|\psi(t)\rangle = e^{\frac{iHt}{\hbar}} |\psi(0)\rangle \tag{114}$$

which is called the time evlolved state.

The state space of a composite quantum system is the tensor product of the state spaces of the component systems. If $|\psi_j\rangle$, $1 \le j \le n$ are the states of the component systems (N_j -qubit), then the joint state of the total system is the Kronecker product $|\psi_1\rangle \otimes \cdots \otimes |\psi_n\rangle$, which is an $N = N_1 \cdots N_n$ -qubit in $\mathbb{C}^N$. For the length of this vector is $\| |\psi_1\rangle | \cdots \| |\psi_n\rangle | = 1$ in view of (124).

Hence 2-qubits are all the unit vectors in the state space $\mathbb{C}^2 \otimes \mathbb{C}^2$. Then we define ν-qubits inductively as unit vectors in (116) below.

For linear maps $f : M \to M'$, $g : N \to N'$, there exits a unique linear map denoted $f \otimes g$ such that

$$(f \otimes g)(x \otimes y) = f(x) \otimes g(y). \tag{115}$$

ν -qubits are all the unit vectors in the Hilbert space (state space)

$$\mathcal{H} \simeq \underbrace{\mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2}_{\nu}, \tag{116}$$

i.e. they are of the form

$$a_1 e_1 + \cdots + a_\nu e_N \tag{117}$$

with normalization

$$\sum_{k=1}^{N} |a_k|^2 = 1, \tag{118}$$

where

$$e_1 = |0 \cdots 0\rangle, \cdots, e_N = |1 \cdots 1\rangle$$

and

$$N = 2^\nu. \tag{119}$$

E.g. $|0 \cdots 0\rangle = \underbrace{|0\rangle \otimes \cdots \otimes |0\rangle}_{\nu}$ is the Kronecker product of ν $|0\rangle$'s. Since $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, we have $|0 \cdots 0\rangle = {}^t(1, 0, \cdots, 0)$ by (123).

Definition 4: *For any matrices* $A = (a_{ij})_{1 \le i \le m, 1 \le j \le n}$ *and* $B = (b_{k\ell})_{1 \le k \le p, 1 \le \ell \le q}$ *their* Kronecker product *(or tensor product)* $A \otimes B$ *is defined by*

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1n}B \\ & \cdots & \\ a_{m1}B & \cdots & a_{mn}B \end{pmatrix} = (a_{ij} b_{k\ell}) \tag{120}$$

and this extends linearly in both variables. In particular for two ket vectors

$$|\varphi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{pmatrix} \in \mathbb{C}^m, \quad |\psi\rangle = \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{pmatrix} \in \mathbb{C}^n \tag{121}$$

their Kronecker product is

$$|\varphi\rangle \otimes |\psi\rangle = (c_i d_j) = \begin{pmatrix} c_1 d_1 \\ \vdots \\ c_1 d_n \\ \\ \vdots \\ c_m d_1 \\ \vdots \\ c_m d_n \end{pmatrix}, \tag{122}$$

which we usually express in the transposed row vector form

$${}^t(c_1 d_1, \cdots, c_1 d_n, \cdots, c_m d_1, \cdots, c_m d_n).$$

The left-hand side of (122) is abbreviated as:

$$|\varphi\rangle |\psi\rangle = |\varphi\psi\rangle = |\varphi\rangle \otimes |\psi\rangle = (c_i d_j), \tag{123}$$

This satisfies

$$\| |\varphi\rangle \otimes |\psi\rangle | = \| |\varphi\rangle | \, \| |\psi\rangle | \, . \tag{124}$$

The outer product $|\psi\rangle\langle\phi|$ is the Kronecker product $|\varphi\rangle^* \otimes |\psi\rangle$ given by

$$|\psi\rangle\langle\varphi| = |\varphi\rangle^* \otimes |\psi\rangle = (\overline{c}_1, \cdots, \overline{c}_m) \otimes \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{pmatrix} = \begin{pmatrix} \overline{c}_1 d_1 & \cdots & \overline{c}_m d_1 \\ & \cdots & \\ \overline{c}_1 d_n & \cdots & \overline{c}_m d_n \end{pmatrix}, \tag{125}$$

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It is convenient to view it as a linear map $C^m \to C^n$

$$|\psi\rangle\langle\varphi|(|\varphi'\rangle) = |\psi\rangle\langle\varphi|\varphi'\rangle = \langle\varphi|\varphi'\rangle|\psi\rangle. \quad (126)$$

If $\{e_j\}$ be an ONB, then we have

$$|e_i\rangle\langle e_j| = E_{ij}, \quad (127)$$

where E_{ij} is a matrix unit consisting of all 0's except for the (i, j)-entry which is 1. In particular,

$$P_k = |e_k\rangle\langle e_k| = E_{kk} \quad (128)$$

is called a projector, cf. [17, p. 173] for a projector in a Hilbert space. They have properties stated in (135).

It is instructive to know the source of the Kronecker product.

Theorem 4.1: *Suppose M, M', N, N' are f.g. free K-modules. Then $M^* = \mathrm{Hom}_J(M, J)$ denoting the dual of M, we have*

$$(M \otimes N)^* \cong M^* \otimes N^* \quad (129)$$

in general. (129) and

$$\mathrm{Hom}_R(M \otimes N, M' \otimes N') \cong \mathrm{Hom}_R(M, M') \otimes \mathrm{Hom}_R(N, N') \quad (130)$$

are equivalent. (130) gives a motivation for the tensor product of maps in Definition 4.

Suppose $M = \oplus_{i=1}^n Ku_i$, $M' = \oplus_{j=1}^{n'} Ku'_j$, $N = \oplus_{k=1}^m Kv_k$, and $N' = \oplus_{\ell=1}^{m'} Rv'_\ell a$ and that the matrices corresponding to $f = f_A \in \mathrm{Hom}_K(M, M')$ and $g = g_B \in \mathrm{Hom}_K(N, N')$ are as in Theorem 2.1. Then the matrix corresponding to the tensor product $f \otimes g$ with respect to the bases $\{u_i \otimes v_k\}$, $\{u'_j \otimes v'_\ell\}$ is the Kronecker product $A \otimes B$:

$$(f \otimes g)(u_i \otimes v_k) = (u'_j \otimes v'_\ell) A \otimes B. \quad (131)$$

Example 4.1: *v-qubits can represent 2^v states:*

$$|n\rangle = e_{n+1}, \quad (132)$$

where the left-hand side means the nth member of the sequence of v digits numbers in dyadic expansion arranged in increasing order and the right means the nth 2^v-dimensional fundamental unit vector.

E.g. for $N = 3$, we have by (123) and (122)

$$|6\rangle = |110\rangle = |1\rangle|1\rangle|0\rangle = |1\rangle\otimes|1\rangle\otimes|0\rangle \quad (133)$$

$$= \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix} = {}^t(0,0,0,0,0,0,1,0) = e_7.$$

Here the first notation is the decimal number 6 viewed as its dyadic expansion $2^2 + 1\cdot 2 + 0$.

Proposition 4.1: *(125) and (126) are equivalent. Let $\{e_j\}$ be an ONB satisfying $\langle e_i | e_j\rangle = \delta_{ij}$. Then the completeness condition*

$$\sum_{i=1}^n |e_i\rangle\langle e_i| = E. \quad (134)$$

as well as

$$P_k^2 = P_k, \quad \langle P_k\varphi_1|\varphi_2\rangle = \langle\varphi_1|P_k\varphi_2\rangle, \quad P_kP_\ell = 0 \quad (k \neq \ell) \quad (135)$$

are satisfied, where P_k is the projector defined by (128).

Proof. Let $|\varphi'\rangle = \begin{pmatrix} c'_1 \\ c'_2 \\ \vdots \\ c'_m \end{pmatrix}$. Then noting $\langle\varphi|\varphi'\rangle = \sum_{i=1}^m \bar{c}_i c'_i$, we see the equivalence by multiplying $|\varphi'\rangle$ by the matrix (125).

The second assertion follows from (127). Finally the second equality in (135) holds since both sides are $\langle e_k|\varphi_1\rangle\langle e_k|\varphi_2\rangle$.

We prove that the totality of all Kronecker products of single qubits $|a\rangle|b\rangle$ does not exhaust the totality of 2-qubits states.

Proof. 2-qubits are of the form

$$a_1|00\rangle + a_2|01\rangle + a_3|10\rangle + a_4|11\rangle \quad (136)$$

with $\sum_{k=1}^4 |a_k|^2 = 1$.

On the other hand, by (132),

$$|a\rangle\otimes|b\rangle = (a_1|0\rangle + a_2|1\rangle)\otimes(b_1|0\rangle + b_2|1\rangle) = {}^t(a_1b_1, a_1b_2, a_2b_1, b_1b_2), \quad (137)$$

which cannot exhaust (136).

E.g.

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}} = {}^t\left(\frac{1}{\sqrt{2}}, 0, 0, \frac{1}{\sqrt{2}}\right) \quad (138)$$

cannot be expressed in the form (137).

But since the totality of all N-qubits arising from the Kronecker products of component N_j-qubits have restrictions on the coefficients, it does not exhaust all N-qubits. In qubit theory one says that a state of a composite system which cannot be written as a product of states of its component systems is an entangled state. The state (138) is an entangled state.

The following theorem is the special case of Theorem 2.3 for a compact operator as stated toward the end of § 2.

Theorem 4.2: *Let A be a Hermite matrix of degree n with eigenvalues λ_k and the corresponding eigenvectors $|\lambda_k\rangle$, $1 \le k \le n$ forming an ONB. Then the spectral decomposition*

$$A = \sum_{k=1}^n \lambda_k P_k = \sum_{k=1}^n \lambda_k |\lambda_k\rangle\langle\lambda_k| \quad (139)$$

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holds true, where P_k is the projector in (128). If $f(z) = \Sigma_{k=0}^{\infty} a_k z^k$ is an analytic function with power series convergent in a disc, then

$$f(A) = \sum_{k=1}^{n} f(\lambda_k) \mid \lambda_k \rangle\langle \lambda_k \mid \tag{140}$$

and in particular,

$$e^A = \sum_{k=1}^{n} e^{\lambda_k} \mid \lambda_k \rangle\langle \lambda_k \mid \tag{141}$$

Proof. This is a special case of Lemma 2.1 with a Hermite matrix. Indeed, writing

$$A = UDU^* = \sum_{k=1}^{n} \lambda_k U E_{kk} U^*, \tag{142}$$

we see that this amounts to (139).

We may directly prove this by operating A resp. $\Sigma_{k=1}^{n} \lambda_k P_k$ on an arbitrary $\mid a\rangle = \Sigma_{\ell=1}^{n} a_\ell \mid \lambda_\ell \rangle$. We have

$$A \mid a\rangle = \sum_{k=1}^{n} a_k A \mid \lambda_k \rangle = \sum_{k=1}^{n} a_k \lambda_k \mid \lambda_k \rangle$$

and

$$\sum_{k=1}^{n} \lambda_k P_k \mid a\rangle = \sum_{k=1}^{n} \lambda_k \mid \lambda_k \rangle\langle \lambda_k \mid \sum_{\ell=1}^{n} a_\ell \mid \lambda_\ell \rangle = \sum_{k,\ell} a_\ell \lambda_k \mid \lambda_k \rangle\langle \lambda_k \mid \lambda_\ell \rangle = \sum_{k=1}^{n} a_k \lambda_k \mid \lambda_k \rangle$$

by orthogonality, whence (139) follows.

Proposition 4.2: *Let*

$$\sigma_y = \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{143}$$

be one of three three Pauli matrices. Then prove that

$$e^{i\gamma\sigma_y} = \begin{pmatrix} \cos\gamma & -\sin\gamma \\ \sin\gamma & \cos\gamma \end{pmatrix} \tag{144}$$

which is the matrix of rotation by γ

Proof. It is easy to see that the eigenvalues and the corresponding eigenspaces of σ_y are $\lambda_1 = 1, \lambda_2 = -1$, $E_{\sigma_y}(1) = \mathbb{C}\begin{pmatrix} -i \\ 1 \end{pmatrix}$, $E_{\sigma_y}(-1) = \mathbb{C}\begin{pmatrix} i \\ 1 \end{pmatrix}$. With $\mid \lambda_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -i \\ 1 \end{pmatrix}$, $\mid \lambda_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} i \\ 1 \end{pmatrix}$, we have

$$\mid \lambda_1\rangle\langle\lambda_1 \mid = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}, \quad \mid \lambda_2\rangle\langle\lambda_2 \mid = \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}. \tag{145}$$

Substituting this in (141), we conclude (144).

Information processing (IP) *f* is a process by which an input data is processed by *f* and an output data is released. This has been done by classical computers whose circuits consist of wires and logical gates, where the former carry information around the circuit and the latter perform manipulations of information from one form to another. A Parallel Information Processing (PIP) is the case where there are several processors f_i working on an input to give an output, where processors are not necessarily independent. Quantum Information Processing (QIP) is similar in spirit to PIP in that instead of several processors one uses only one processor—a (programmed) unitary operator as in (42) and the logical gate performing this *operation of multiplying by a unitary matrix* is called a **quantum gate**:

$$\mid \Psi_{out}\rangle = U_f \mid \Psi_{in}\rangle, \quad U_f = e^{-\frac{i}{\hbar} H_f t}, \tag{146}$$

where H_f is the Hamiltonian corresponding to the processor *f*. The quantum computer to be defined in Definition 7 drastically reduces the number of computational steps by means of the generated entanglement.

It is noticeable that quantum physics, esp. quantum entanglement has a close connection with the Riemann zeta-function, esp. the Riemann-Siegel formula [27-31] etc. This will be studied elsewhere.

Example 4.2: *The NOT gate acting on single qubits is the one which changes* $\mid 0\rangle$ *and* $\mid 1\rangle$ *and can be represented by the matrix*

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{147}$$

which is a unitary matrix and one of Pauli matrices denoted $\sigma_1 = \sigma_x = X$.

Let *U* be a unitary matrix of degree2. Then the controlled *U*-gate acting on 2-qubits is the one which transforms the second bit (target bit) by *U* only when the first bit (the control bit) is $\mid 1\rangle$. In the special case where the unitary matrix *U* is given by

$$U_{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} E_2 & O \\ O & X \end{pmatrix}, \tag{148}$$

the controlled *U* -gate is called the CNOT (controlled NOT gate). I.e. CNOT gate acts on 2-qubits and changes $\mid xy\rangle$ into $\mid x(x+y) \bmod 2\rangle$, i.e. it changes the target bit—the second bit by the other one only when the control bit—the first bit is 1.

For any unitary matrices used *U1*, *U2*, the conditional transformation

$$U = \mid 0\rangle\langle 0 \mid \otimes U_1 + \mid 1\rangle\langle 1 \mid \otimes U_2 \tag{149}$$

is also unitary. For

$$UU^* = (\mid 0\rangle\langle 0 \mid \otimes U_1 + \mid 1\rangle\langle 1 \mid \otimes U_2)(\mid 0\rangle\langle 0 \mid \otimes U_1^* + \mid 1\rangle\langle 1 \mid \otimes U_2^*)$$

reduces to $\mid 0\rangle\langle 0 \mid \otimes E_2 + \mid 1\rangle\langle 1 \mid \otimes E_2 = E_2 \otimes E_2 = E_4$ since

$$E_{ii} E_{jj} = \delta_{ij} E_{ij}. \tag{150}$$

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Since

$$\begin{pmatrix} E_2 & O \\ O & X \end{pmatrix} = \begin{pmatrix} E_2 & O \\ O & O \end{pmatrix} + \begin{pmatrix} O & O \\ O & X \end{pmatrix} = E_{11} \otimes E_2 + E_{22} \otimes X = |0\rangle\langle 0| \otimes E_2 + |1\rangle\langle 1| \otimes X, \tag{151}$$

it follows that the matrix U_{CNOT} in (148) is a conditional transformation and *a fortiori* is a unitary matrix.

Example 4.3: *The Hadamard gate H is defined by*

$$H|x\rangle = \frac{1}{\sqrt{2}} \sum_{y=0}^{1} (-1)^{xy} |y\rangle. \tag{152}$$

Hence it sends $|0\rangle$ (resp. $|1\rangle$) to $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ (resp. $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$) and is represented by the matrix $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$. Since $H^2 = E_2$ we have

$$HH|0\rangle = |0\rangle, \quad HH|1\rangle = |1\rangle. \tag{153}$$

Consider the CNOT gate with the control and target bits are squeezed by two Hadamard gates. Then if the first input bit is $|1\rangle$, then by the conditional negation, the second input bit is interchanged, i.e. the second input bit after the controlled negation becomes $H|1\rangle$ (resp. $H|0\rangle$) if the second input bit is $H|0\rangle$ (resp. $H|1\rangle$). Then this is processed by the last Hadamard gate to become $H|1\rangle$ (resp. $H|0\rangle$), i.e. this circuit has the same effect as the up-side-down CNOT gate.

We have also

$$H \otimes H|00\rangle = H \otimes H|0\rangle \otimes 0\rangle = H|0\rangle \otimes H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle). \tag{154}$$

Let

$$U = \begin{pmatrix} E_2 & O \\ O & \tilde{U} \end{pmatrix} \tag{155}$$

where

$$\tilde{U} = \begin{pmatrix} a & \circ & b \\ \circ & E_4 & \circ \\ c & \circ & d \end{pmatrix} \tag{156}$$

where $a, b, c, d \in \mathbb{C}$ satisfy the conditions under which $\tilde{U}$ is unitary. Let

$$\tilde{\tilde{U}} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{157}$$

U acts non-trivially only on the 3rd qubit $\alpha|010\rangle$ and the 8 th q-bit $\beta|111\rangle$ of a 3-qubit giving rise to

$${}^t(0, 0, a\alpha + b\beta, 0, 0, 0, 0, c\alpha + d\beta).$$

We interpret this as an action of $\tilde{U}$. A Grey code connecting $|010\rangle$ and $|111\rangle$ is

$$g_1 = |010\rangle \to g_2 = |011\rangle \to g_3 = |111\rangle. \tag{158}$$

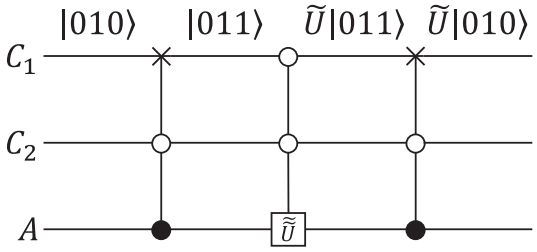

Figure 1: Circuit implementing U in (155).

Since g_2 and g_3 are different only at the first qubit, we think of them as contracted to $\alpha|0\rangle + \beta|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ and multiply it by $\tilde{\tilde{U}}$ and then pull back the first entry $a\alpha + b\beta$ to the 3rd qubit $|010\rangle$ -position as shown in Figure 1.

In Figure 1, $ac_2c_1\rangle$ is input to the gate AC_2C_1. The cross symbol means the NOT gate and so $010\rangle$ is output as $011\rangle$. Then after operation by $\tilde{U}$, $\tilde{U}011\rangle$ is output as $\tilde{U}010\rangle$.

It can be shown that any unitary matrix U can be expressed as the product of level 2-matrices. This is a step toward the proof of Theorem 4.3 at the end. For its proof we refer to [25].

The theory of finite Fourier transforms (or discrete Fourier transform) has been developed in [32] in the case of periodic functions and in [17, pp. 109-114] in the case of a finite group. Cf. also [33, 8.1], [22, 4.1, 4.3].

Definition 5: *Let*

$$\varepsilon_j(x) = e^{2\pi i x/N}, \quad 1 \le j \le N, \tag{159}$$

where x is an integer variable and N is defined by (119). Then the set $\{\varepsilon_j(x) \mid 1 \le j \le N\}$ forms a basis of the vector space $C(N)$ of all periodic arithmetic functions with period N, where an arithmetic function is one defined only for integer arguments. We define the discrete Fourier transform (DFT) $\hat{f}$ (or the y th Fourier coefficient) of f by

$$\hat{f}(y) = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} \varepsilon_y(-x) f(x). \tag{160}$$

Then the Fourier inversion or Fourier expansion formula holds true:

$$f(x) = \sum_{y=0}^{N-1} \hat{f}(y) \varepsilon_y(-x). \tag{161}$$

Note that (161) is the expression of f with respect to the basis $\{\varepsilon_j\}$.

Example 4.4: *The case N = 2 of (160) amounts to the Hadamard gate. This is so since* $\varepsilon_j(x) = (-1)^{xj}$ *and the quantum gate realizing the DFT (N = 2) coincides with (152).*

Definition 6: *Let*

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$$u_1, \cdots, u_N \qquad (N = 2^\nu) \tag{162}$$

be an ONB of H and le $$|\psi\rangle = \sum_{m=1}^{N} a_m |u_m\rangle, \tag{163}$$

where $a_m = \langle \psi | u_m \rangle$. Then we define the measurement operator M_m by

$$M_m |\psi\rangle = a_m |u_m\rangle. \tag{164}$$

After the measurement by M_m, the probability that the result involves $|u_m\rangle$ is

$$p(m) = \langle \psi | M_m^* M_m |\psi\rangle = (M_m |\psi\rangle, M_m |\psi\rangle) = \left| M_m |\psi\rangle \right|^2. \tag{165}$$

Normalizing the vector in (164), we see that the state after the measurement is to be

$$\frac{M_m |\psi\rangle}{\sqrt{p(m)}} = \frac{a_m}{\sqrt{p(m)}} |u_m\rangle \tag{166}$$

whose right-hand side is sometimes abbreviated as $|m\rangle$ to indicate that the state after the measurement is the mth basis element, so that more information is contained here than (132).

Remark 1 *Since*

$$\langle \psi | M_m^* = |\psi\rangle^* M_m^* = (M_m |\psi\rangle)^* = (a_m |u_m\rangle)^* = \overline{a}_m |u_m\rangle \tag{167}$$

by (164), it follows that

$$p(m) = |a_m|^2 \langle u_m | u_m \rangle = |a_m|^2. \tag{168}$$

This explains the statement after (113) about the probability of a qubit $a|0\rangle + b|1\rangle$.

(34) is viewed as the probability, which is the inner product $\langle \psi | \psi \rangle$. Since (165) is also an inner product $\langle M_m \psi | M_m \psi \rangle$ by (165), it is reasonable to view (165) as the probability.

Example 4.5: (i) *By (127),*

$$M_1 = M_{|0\rangle} = |0\rangle\langle 0|, \quad M_2 = M_{|1\rangle} = |1\rangle\langle 1| \tag{169}$$

work as measurement operators on 1-qubits: If $|\psi\rangle = a|0\rangle + b|1\rangle$ then $p(0) = |a|^2, p(1) = |b|^2$, so that the state after the measurement (166) reads

$$\frac{M_{|0\rangle} |\psi\rangle}{|a|} = \frac{a}{|a|} |0\rangle, \quad \frac{M_{|1\rangle} |\psi\rangle}{|b|} = \frac{b}{|b|} |1\rangle. \tag{170}$$

(ii) Similarly, the measurement operators acting on the first qubit of a 2-qubit given by (136) are

$$M_1 = |0\rangle\langle 0| \otimes E_2 = \begin{pmatrix} E_{11} & O \\ O & E_{11} \end{pmatrix}, \quad M_2 = |1\rangle\langle 1| \otimes E_2 = \begin{pmatrix} E_{22} & O \\ O & E_{22} \end{pmatrix}. \tag{171}$$

Expressing (136) as

$$|\psi\rangle = |0\rangle \otimes (a_1 |0\rangle + a_2 |1\rangle) + |1\rangle \otimes (a_3 |0\rangle + a_4 |1\rangle). \tag{172}$$

we obtain

$$M_1 |\psi\rangle = \left(|0\rangle\langle 0| \otimes E_2 \right) \left(|0\rangle \otimes (a_1 |0\rangle + a_2 |1\rangle) \right) \tag{173}$$

$$= |0\rangle\langle 0| \left(|0\rangle \right) \otimes E_2 \left(a_1 |0\rangle + a_2 |1\rangle \right)$$

$$= |0\rangle \otimes \left(a_1 |0\rangle + a_2 |1\rangle \right)$$

with $p(0) = |a_1|^2 + |a_2|^2$. Hence the state after the measurement (166) reads

$$\frac{M_1 |\psi\rangle}{\sqrt{p(0)}} = |0\rangle \otimes \left(\frac{a}{\sqrt{p(0)}} |0\rangle + \frac{b}{\sqrt{p(0)}} |1\rangle \right) \tag{174}$$

and similarly for $\frac{M_1 |\psi\rangle}{\sqrt{p(1)}}$. The measurement operators acting on the second qubit can be introduced verbatim.

Definition 7 *Let H be the state space of a quantum system, i.e. the Hilbert space in (116), U be a unitary operator acting on H and let $\{M_m\}$ be a set of measurement operators. The triple $(H,U,\{M_m\})$ is called a* quantum computer. *In this context, H is called a register and U an algorithm.*

Theorem 4.3 (Barenco, et al.) *The set of single qubit gates and the* CNOT *gate is universal, i.e. any quantum circuit or any unitary matrix can be constructed by them.*

There are a few well-known quantum algorithms which enable to accomplish computation not possible by conventional computers in polynomial time. For well-known Shor or Glover algorithms, cf. e.g. [25].

Now that the reader has acquired some sense and is to be ready for browsing through the bnewest research papers with less psycological barrier, e.g. [34] and those in the website https://arxiv.org/archive/quant-ph.

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