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A REAL FORMULA FOR TRANSITION PROBABILITIES

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1. INTRODUCTION

According to quantum theory (Isham, 1995; Peres, 1995; Sakurai 1994), quantum systems behave on two different levels: the microscopic one, in which they live and evolve in a deterministic way, and the macroscopic one, in which they jump when they meet a macroscopic device, as for instance a measurement apparatus. At the moment of the interaction with the macroscopic world, something completely random happens to the quantum system, so that its deterministic evolution breaks down and its state irreversibly changes. The outside world in some way records the change. Thus the result of a quantum measurement, i.e. of an experiment performed on a quantum system by means of a macroscopic device, is a random variable whose probability distribution depends on the state of the system before the interaction and on the measurement itself. Since states and measurements are described by vectors in complex Hilbert spaces, the probability distributions depend on *complex* vectors.

In this paper, we show that in two dimensional quantum systems, the probability that measuring a system in a state w turns the system in a state u (transition probability from w to u) can be written as a function of *real* vectors in the three dimensional Euclidean space. The proof is based on the Bloch or Poincarè or Riemann sphere representation (Preskill, 1998; Scott et al. 1999; Penrose, 1999; respectively) of two dimensional complex Hilbert spaces by means of unit vectors in real three dimensional Euclidean spaces. Such representation is well known among physicists and mathematicians, but not as well among statisticians and probabilists, to whom the paper is mainly directed: for this reason it is described in all details.

The paper is organised as follows. Basic quantum probability is reviewed in section 2; section 3 deeply develops the geometry of two dimensional quantum systems. Transition probabilities as functions of real vectors are derived in section 4. Brief comments with references for further developments are in section 5.

Notation: any column vector will be indicated as $\underline{u}$ if it is real or as $|u\rangle$ if it is complex (according to Dirac "bra-ket" notation); corresponding row vectors will

be the transpose of $\underline{u}$, namely $\underline{u}^T$, and the Hermitian transpose of $|u\rangle$ that is $\langle u|$. Because of the isomorphism between any two dimensional complex Hilbert space $\mathbf{H}_2$ and the Euclidean space $\mathbf{C}^2$, we will refer to the latter and we will equivalently talk about selfadjoint operator and Hermitian matrices.

2. QUANTUM PROBABILITY

In quantum statistics (Barndorff-Nielsen, Gill and Jupp, 2001; Holevo, 1982; Helstrom, 1976), the probability distribution of a random variable $X:(\Omega,\mathcal{F},P) \rightarrow (\mathbf{G},\mathcal{G},P_X)$ is given by the *trace rule for probability*

$$P_X(G) = \mathrm{tr}\{\rho \mathrm{M}(G)\} \tag{1}$$

where ρ is a *density matrix*, i.e. a nonnegative, selfadjoint and trace-one linear operator representing the state of a system in an n-dimensional Hilbert space $\mathbf{H}_n$, while M is a *probability operator-valued measure* (POM), i.e. a set of nonnegative and selfadjoint linear operators defined on a measure space $(\mathbf{G},\mathcal{G})$ and acting on $\mathbf{H}_n$, such that $M(\mathbf{G})=\mathbf{I}_n$, the identity operator in $\mathbf{H}_n$, $M(\varnothing)=\mathbf{O}_n$, the null operator in $\mathbf{H}_n$, and $M\left(\bigcup_{h=1}^{\infty} G_h\right) = \sum_{h=1}^{\infty} M\left(G_h\right)$ if $G = \bigcup_{h=1}^{\infty} G_h$, $G_h \cap G_k = \varnothing, \forall h \neq k$.

If ρ is of the form $|w\rangle\,|w\rangle$ where $|w\rangle$ is a unit vector in $\mathbf{C}^2$, then it is a *pure state*. The probability that a measurement M: $(\mathbf{G},\mathcal{G}) \rightarrow \mathbf{C}^{2x2}$, $\mathbf{C}=\{1,0\}$, throws the pure state $|w\rangle\langle w|$ in the new state $|u\rangle\langle u|$ where $|u\rangle$ is also a unit vector in $\mathbf{C}^2$, can be computed by setting $X(\{\omega =$ the new state is $|u\rangle\})=1$, $X(\{\omega =$ the new state is orthogonal to $|u\rangle\})=0$, and

$$\mathrm{M}(\{1\}) = |u\rangle\langle u|, \mathrm{M}(\{0\}) = \mathbf{I}_2 - |u\rangle\langle u| \tag{2}$$

such that

$$P_X(\{1\}) = \mathrm{tr}\{|w\rangle\langle w||u\rangle\langle u|\} = |\langle w||u\rangle|^2 .$$

The latter is called *transition probability* from $|w\rangle$ to $|u\rangle$ and (2) is a *von Neumann measurement* (von Neumann, 1955; Davies and Lewis, 1970).

In the following we will show how to represent state vectors and von Neumann measurements acting on $\mathbf{C}^2$ by means of unit vectors in $\mathbf{R}^3$. In this way, transition probabilities can also be written in function of real vectors.

3. GEOMETRY OF QUANTUM SYSTEMS IN $\mathbf{C}^2$

Consider the vector space $S_2 \subset \mathbf{C}^{2x2}$ of Hermitian matrices acting on $\mathbf{C}^2$ in which the Hilbert-Schmidt inner product is defined as $\langle A,B\rangle := \mathrm{tr}\{A^H B\}, \forall A,B \in S_2$. The set $\{\mathbf{I}_2, \sigma_x, \sigma_y, \sigma_z\}$ where $\mathbf{I}_2$ is the 2×2 identity matrix and

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix},\ \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

are the *Pauli matrices*, constitutes an orthogonal basis for S_2, dim S_2=4; every Hermitian matrix S can be uniquely written as a linear combination of the matrices $\mathbf{I}_2, \sigma_x, \sigma_y, \sigma_z$ with real coefficients u,x,y,z:

$$S = \frac{1}{2}\begin{bmatrix} u+z & x-iy \\ x+iy & u-z \end{bmatrix}, \forall\ u,x,y,z \in \mathbf{R} \tag{3}$$

Any density matrix ρ is of the form (3), provided that it has (i) unitary trace and (ii) non negative determinant. Condition (i) implies that $u_1=1/2$ in such a way that (3) becomes

$$S = \frac{1}{2}\begin{bmatrix} 1+z & x-iy \\ x+iy & 1-z \end{bmatrix} \tag{4}$$

while condition (ii) is equivalent to $x^2+y^2+z^2 \le 1$. It follows that the state of a system can be written as

$$\rho(\underline{w}) = \frac{1}{2}(\mathbf{I}_2 + \langle \underline{w}, \underline{\sigma} \rangle) \tag{5}$$

where $\underline{w}^T = [x \quad y \quad z] \in \mathbf{R}^3$ and $\|w\| \le 1$ while $\underline{\sigma}$ is the three dimensional vectors of 2×2 Pauli matrices, i.e. $\underline{\sigma}^T = [\sigma_x \quad \sigma_y \quad \sigma_z]$ in such a way that $\langle \underline{w}, \underline{\sigma} \rangle = \underline{w}^T \underline{\sigma} = \sum_{V=x,y,z} w_V \sigma_V$.

Relation (5) allows to represent the space of density matrices as the closed unit ball in $\mathbf{R}^3$ (*Poincarè* or *Riemann* or *Bloch sphere*); the surface of the sphere corresponds to the set of pure states since $\rho(\underline{w})^2 = \rho(\underline{w}) \Leftrightarrow \|\underline{w}\|^2 = 1$, as one gets by deriving $\rho(\underline{w})^2$ from (5) and by the following properties of Pauli matrices:

$$\sigma_U \sigma_V = -\sigma_V \sigma_U \ \text{ if } u \ne v \ \text{ and } \ \sigma_U \sigma_V = 1 \ \text{ if } u \ne v\,. \tag{6}$$

Hence, if $\underline{u} = \dfrac{\underline{w}^2}{\|w\|} \in \mathbf{R}^3$ is a unit vector, then $\rho(\underline{u}) = \dfrac{1}{2}(\mathbf{I}_2 + \langle \underline{u}, \underline{\sigma} \rangle)$ is an orthogonal projection matrix and its spectrum is the set {0,1}. It follows by the spectral

theorem that $\rho(\underline{u})$ can be written as[1] $\rho(|u\rangle)=|u\rangle\ \langle u|$, where $|u\rangle \in \mathbf{C}^2$ is an eigenvector of $\rho(\underline{u})$ corresponding to the eigenvalue 1. It can be simply obtained by normalising any column vector of $\rho(\underline{u})$. In fact, let $\mathbf{E}_0$ and $\mathbf{E}_1$ be eigenspaces corresponding to the eigenvalues 0 and 1 respectively and let $\mathbf{R}_{\rho(\underline{u})}$ and $\mathbf{C}_{\rho(\underline{u})}$ be the row and column space of $\rho(\underline{u})$ respectively. Denoting with $S^{\perp}$ the orthogonal complement with respect to $\mathbf{C}^2$ of a subspace $S \subseteq \mathbf{C}^2$, we have $\mathbf{E}_0 = \mathbf{E}_1^{\perp}$ and $\mathbf{N}_{\rho(\underline{u})} = \mathbf{R}_{\rho(\underline{u})}^{\perp}$. It follows from $\mathbf{E}_0 \equiv \mathbf{N}_{\rho(\underline{u})}$ that $\mathbf{E}_1 \equiv \mathbf{R}_{\rho(\underline{u})}$. Since $\rho(\underline{u})$ is Hermitian, $\mathbf{E}_1 \equiv \mathbf{C}_{\rho(\underline{u})} = \mathrm{span}\{|u\rangle\}$.

The orthogonal projection matrix onto $\mathbf{E}_0$ is therefore given by

$$\mathbf{I}_2 - \rho(\underline{u}) = \mathbf{I}_2 - \frac{1}{2}(\mathbf{I}_2 + \langle \underline{u}, \underline{\boldsymbol{\sigma}} \rangle) = \frac{1}{2}(\mathbf{I}_2 + \langle -\underline{u}, \underline{\boldsymbol{\sigma}} \rangle) = \rho(-\underline{u}).$$

Summarising: $\underline{u}$ and $-\underline{u}$ are unit vectors in $\mathbf{R}^3$ and one is the opposite of the other; they respectively correspond to the pure states $\rho(\underline{u})$ and $\rho(-\underline{u})$ that orthogonally project the state vectors of $\mathbf{C}^2$ onto the one dimensional subspaces spanned by the vectors $|u\rangle$ and $|u\rangle$ which are mutually orthogonal (and not opposite[2]).

Considering non pure states, if $\underline{w} \in \mathbf{R}^3$, $\|w\| \leq 1$, then, by the spectral theorem and by the unitary trace constraint for the density matrix $\rho(\underline{w})$,

$$\rho(\underline{w}) = \alpha\rho(\underline{u}) + (1-\alpha)\,\rho(-\underline{u}) \tag{7}$$

with $\alpha \in [0,1]$ where $\alpha = \frac{1}{2} - \frac{1}{2}\|\underline{w}\|$ and $1-\alpha = \frac{1}{2} + \frac{1}{2}\|\underline{w}\|$ are eigenvalues of $\rho(\underline{w})$ with eigenvectors $|u\rangle$ and $|-u\rangle$ while $\underline{u}$ is a unit vector in $\mathbf{R}^3$. Observe that excluding $\mathbf{I}_2$ and $\mathbf{O}_2$ that project any vector of $\mathbf{C}^2$ onto its improper subspaces ($\mathbf{C}^2$ and the null vector), given a unit vector $\underline{u} \in \mathbf{R}^3$, $\rho(\underline{u})$ and $\rho(-\underline{u})$ are the unique two density matrices that project onto one dimensional proper subspaces of $\mathbf{C}^2$ orthogonal to each other. It follows that, in $\mathbf{C}^2$, the density matrices can be represented as a mixture of matrices $\rho(\underline{u})$ and $\rho(-\underline{u})$. Note that (7) is equivalent to $\underline{w} = \alpha\underline{u} + (1-\alpha)(-\underline{u})$.

In the following, we will show that von Neumann measurement acting on $\mathbf{C}^2$ can be represented by unit vectors of $\mathbf{R}^3$ in such a way that the transition probability between pure states can be equivalently written as a function of two unit vectors of $\mathbf{R}^3$ (instead of two state vectors in $\mathbf{C}^2$).

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[1] Observe that $\rho(\underline{u})$ and $\rho(|u\rangle)$ represent the *same* matrix, provided that is built on the vector $\underline{u} \in \mathbf{R}^3$, i.e. $\rho(\underline{u}) = \frac{1}{2}(\mathbf{I}_2 + \langle \underline{u}, \underline{\boldsymbol{\sigma}} \rangle)$, or on the vector $|u\rangle \in \mathbf{X}^2 |u\rangle\ \langle u|$, i.e. $\rho(|u\rangle) = |u\rangle\langle u|$.

[2] Dirac notation emphasises the geometric meaning of state vectors instead of their algebraic connotation.

4. TRANSITION PROBABILITIES OVER $\mathbf{R}^3$

Measurement (2) can be written as

$$\mathrm{M}(\{1\}) = \frac{1}{2}(\mathbf{I}_2 + \langle \underline{u}, \underline{\boldsymbol{\sigma}} \rangle), \mathrm{M}(\{0\}) = \frac{1}{2}(\mathbf{I}_2 - \langle \underline{u}, \underline{\boldsymbol{\sigma}} \rangle) \tag{8}$$

and we can now compute the probability that, given a system in state $\rho(\underline{w})$, it collapses in the state $\rho(\underline{u})$ after being measured by M. The transition probability is

$$\mathrm{P_u} = \mathrm{P}(\{u\}) = \frac{1}{2} + \frac{1}{2}\langle \underline{w}, \underline{u} \rangle \tag{9}$$

as follows by the trace rule for probability $\mathrm{P_u} = \mathrm{tr}\{\rho(\underline{w})\mathrm{M_u}\}$, replacing (5) for $\rho(\underline{w})$ and (8) for $\mathrm{M_u}$ to obtain $\mathrm{P_u} = \mathrm{tr}\left\{\frac{1}{2}(\mathbf{I}_2 + \langle \underline{w}, \underline{\boldsymbol{\sigma}} \rangle)\frac{1}{2}(\mathbf{I}_2 + \langle \underline{w}, \underline{\boldsymbol{\sigma}} \rangle)\right\}$ and then using (6) and the linearity of the trace operator. By (1), it is immediate to see that if $\rho(\underline{w})$ is a pure state with corresponding eigenstate $|w\rangle$ relation (9) is equivalent to

$$\mathrm{P}_u = \mathrm{tr}\{\rho(\underline{w})\mathrm{M}_u\} = \mathrm{tr}\{|w\rangle\langle w||u\rangle\langle u|\} = \langle u||w\rangle\langle w||u\rangle = |\langle u||w\rangle|^2 . \tag{10}$$

On the other hand, if $\rho(\underline{w})$ is not a pure state, the above relation becomes $\mathrm{P_u} = \mathrm{tr}\{\rho(\underline{w})\mathrm{M_u}\} = \mathrm{tr}\{\alpha\rho(\underline{u}) + (1-\alpha)\rho(-\underline{u})\ \rho(\underline{u})\} = \mathrm{tr}\{\alpha\rho(\underline{u}\ )\} = \alpha$ and equivalently (9) gives $P_u = \frac{1}{2} + \frac{1}{2}\langle \underline{w}, \underline{u} \rangle = \frac{1}{2} + \frac{1}{2}\langle \alpha\,\underline{u} + (1-\alpha)(-\underline{u}), \underline{u} \rangle = \alpha$.

For instance, a spin-1/2 system (see Beltrametti and Cassinelli, 1981) in the pure state

$$\rho(\eta, \phi) = \begin{bmatrix} \cos^2\left(\frac{\eta}{2}\right) & \cos\left(\frac{\eta}{2}\right)\sin\left(\frac{\eta}{2}\right)e^{-i\phi} \\ \cos\left(\frac{\eta}{2}\right)\sin\left(\frac{\eta}{2}\right)e^{i\phi} & \sin^2\left(\frac{\eta}{2}\right) \end{bmatrix} \tag{11}$$

with $\eta \in]0, \pi[$, $\phi \in [0, 2\pi[$ can be equivalently represented by the coherent eigenstate (Peres, 1995)

$$|w(\eta, \phi)\rangle = \begin{bmatrix} \cos\left(\frac{\eta}{2}\right)e^{-i\phi} \\ \sin\left(\frac{\eta}{2}\right) \end{bmatrix} \in \mathbf{C}^2 \tag{12}$$

such that $\rho(\eta, \phi) = |w(\eta, \phi)\rangle\langle w(\eta, \phi)|$ or by

$$\underline{w}(\eta,\phi)=\begin{bmatrix}\sin\eta\cos\phi\\ \sin\eta\sin\phi\\ \cos\eta\end{bmatrix}\in\mathbf{R}^3 \tag{13}$$

such that $\rho(\eta,\phi)=\frac{1}{2}(\mathbf{I}_2+\langle\underline{w}(\eta,\phi),\underline{\boldsymbol{\sigma}}\rangle)$, as one can derive by comparing (4) and (11). Transition probability from $|w(\eta,\phi)\rangle$ to, say, $|u(\eta,\phi)\rangle$, such that $\mathrm{M}_{u(\eta,\phi)}=|u(\eta,\phi)\rangle\langle u(\eta,\phi)|$ can be obtained by (12) through (10) or by (13) through (9).

5. COMMENTS

We illustrated a representation of transition probabilities in two-state quantum systems based on real tridimensional instead of complex bidimensional vectors.

On a theoretical viewpoint, the present study is part of a wider research in quantum statistics with special reference to Fisher information in pure and mixed states (see Luati 2001, 2004). Readers who are familiar to this topic could employ the present perspective in viewing state vectors and transition probabilities for developments concerning the geometry of spin-1/2 systems, asymptotic quantum statistics and measurement problems (Barndorff-Nielsen and Gill, 2000; Gill, 1999; Gill and Massar, 2000 respectively, and references therein).

A recent research area in which unit sphere representation of *qubits* (quantum bits), as two-state systems are there called, is quantum computing (Brooks, 1999; Steane, 1998; Williams and Clearwater, 1998).

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SUMMARY

A real formula for transition probabilities

Transition probabilities between states in two dimensional quantum systems are derived as functions of unit vectors in $\mathbf{R}^3$ instead of state vectors in $\mathbf{C}^2$. This can be done once represented states and von Neumann measurements acting on $\mathbf{C}^2$ by means of vectors on the unit sphere of $\mathbf{R}^3$.

RIASSUNTO

Una formula reale per le probabilità di transizione

Le probabilità di transizione tra stati in sistemi quantistici di dimensione 2 sono ottenute come funzioni di vettori unitari in $\mathbf{R}^3$ anziché di vettori unitari in $\mathbf{C}^2$. Ciò è reso possibile dalla rappresentazione di stati e misure di von Neumann che operano su $\mathbf{C}^2$ attravero vettori nella sfera unitaria di $\mathbf{R}^3$.