

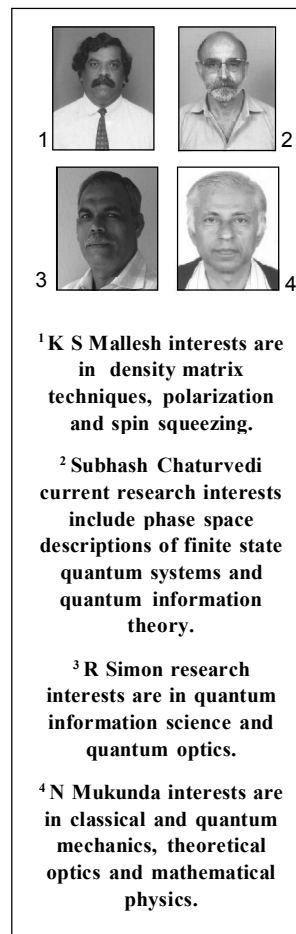
States of Physical Systems in Classical and Quantum Mechanics

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We discuss the descriptions of states of physical systems in classical and quantum mechanics. We show that while it is possible to evolve a terminology common to both, the differences in the underlying mathematical structures lead to significant points of departure between the two descriptions both at mathematical and conceptual levels. We analyse the state spaces associated with physical systems described by two and three dimensional complex Hilbert spaces in considerable detail to illustrate how subtle this question can in general be. We highlight the role the Bargmann invariants play in the passage from the Hilbert space to the ray space, the space of states in quantum mechanics, and also in the context of Wigner's theorem on symmetries in quantum mechanics where they originally appeared.

1. Introduction

The basic mathematical structures encountered in classical and in quantum mechanics are very different from one another, so it is probably surprising that analogies appear at certain points of comparison. In both there is a separation between kinematical and dynamical aspects. The kinematical part in the classical case is rather simple. In quantum mechanics, on the other hand, it is extremely subtle and occupies a very substantial part of the whole theory. Indeed, aspects of quantum kinematics (of composite systems) are of intense current research interest. The discussion in this article will be predominantly kinematical, and restricted to 'single systems' as against composite systems.



Keywords

Classical states, quantum states, pure states, mixed states, superposition principle, density matrix, Bargmann invariants, Wigner's theorem, ray space.

2. States of Classical Systems

We describe a classical mechanical system in the Hamiltonian formalism. The basic mathematical object is the phase space Γ of even dimension, say $2n$. A canonical coordinate system consists of n generalised coordinates $\mathbf{q} = (q_1, q_2, \dots, q_n)$ and their conjugate momenta $\mathbf{p} = (p_1, p_2, \dots, p_n)$. A general dynamical variable representing some physical property is a real-valued function $A(\mathbf{q}, \mathbf{p})$ on Γ . The Hamiltonian $H(\mathbf{q}, \mathbf{p})$ determines the dynamics via the canonical equations of motion

$$\begin{aligned}\dot{q}_j &= \frac{\partial H}{\partial p_j} = \{q_j, H\}, \\ \dot{p}_j &= -\frac{\partial H}{\partial q_j} = \{p_j, H\},\end{aligned}\quad (1)$$

where $\{A, B\}$ is the familiar Poisson Bracket of A with B :

$$\{A, B\} = \sum_k \left\{ \frac{\partial A}{\partial q_k} \frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k} \frac{\partial B}{\partial q_k} \right\}. \quad (2)$$

In this framework a *pure state* is represented by a single point $(\mathbf{q}_0, \mathbf{p}_0) \in \Gamma$. Every dynamical variable A has, in this pure state, a definite numerical value $A(\mathbf{q}_0, \mathbf{p}_0)$ – no spread, no dispersion, and no need or role for probabilities *at the level of pure states*. Such states are cases of maximum possible information.

In contrast, a general or *mixed state* brings in probabilities. Such a state is defined completely by a probability density ρ on the phase space Γ :

$$\begin{aligned}\rho(\mathbf{q}, \mathbf{p}) &\text{ real, } \geq 0; \\ \iint d^n q d^n p \rho(\mathbf{q}, \mathbf{p}) &= 1.\end{aligned}\quad (3)$$

The meaning is that unlike in a pure state, the q 's and p 's do not now have definite values. Rather, different



ranges of values are likely to occur with corresponding probabilities:

Probability that system ‘lies in’ small phase space region

$$d^n q d^n p \text{ around } (\mathbf{q}, \mathbf{p}) = \rho(\mathbf{q}, \mathbf{p}) d^n q d^n p. \quad (4)$$

A general dynamical variable $A(\mathbf{q}, \mathbf{p})$ has an expectation value $\langle A \rangle$ and a spread or dispersion $\langle (\Delta A)^2 \rangle$ computed as follows:

$$\begin{aligned} \langle A \rangle &= \iint d^n q d^n p \rho(\mathbf{q}, \mathbf{p}) A(\mathbf{q}, \mathbf{p}), \\ \langle (\Delta A)^2 \rangle &= \langle (A(\mathbf{q}, \mathbf{p}) - \langle A \rangle)^2 \rangle \\ &= \langle A(\mathbf{q}, \mathbf{p})^2 \rangle - \langle A \rangle^2 \geq 0. \end{aligned} \quad (5)$$

Using the Dirac delta function one can describe a pure state too in terms of a probability distribution,

$$\rho_{\mathbf{q}_0, \mathbf{p}_0}(\mathbf{q}, \mathbf{p}) = \delta^n(\mathbf{q} - \mathbf{q}_0) \delta^n(\mathbf{p} - \mathbf{p}_0), \quad (6)$$

which is an elementary statement. A mixed state can be expressed in an essentially *unique manner* as a *convex sum* or *mixture* of pure states,

$$\rho(\mathbf{q}, \mathbf{p}) = \iint d^n \mathbf{q}_0 d^n \mathbf{p}_0 \rho(\mathbf{q}_0, \mathbf{p}_0) \rho_{\mathbf{q}_0, \mathbf{p}_0}(\mathbf{q}, \mathbf{p}), \quad (7)$$

which is again essentially trivial. It can also be described as a mixture of mixed states; clearly, such an ensemble would not be unique.

The set of all (mixed and pure) states is a *convex set*: if $\rho_j(\mathbf{q}, \mathbf{p})$ for $j = 1, 2, \dots$ are the distributions for any states, and $\{P_j\}$ is any classical system of probabilities, then

$$\rho(\mathbf{q}, \mathbf{p}) = \sum_j P_j \rho_j(\mathbf{q}, \mathbf{p}), \quad P_j > 0, \quad \sum_j P_j = 1, \quad (8)$$

is a possible (mixed) state. Only pure states cannot be so decomposed in a nontrivial manner as convex sum of

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other states, so they are the extremal points (or extremal elements) in the space of all states.

A word about dynamics: the equation of motion for a general state of a Hamiltonian system is the Liouville equation

$$\frac{\partial}{\partial t} \rho(\mathbf{q}, \mathbf{p}; t) + \{\rho(\mathbf{q}, \mathbf{p}; t), H(\mathbf{q}, \mathbf{p}; t)\} = 0, \quad (9)$$

in which the Poisson Bracket of $\rho(\mathbf{q}, \mathbf{p}; t)$ with the Hamiltonian appears. The important difference in sign compared to (1) is to be noted. For a non-Hamiltonian system like an open system more general Liouville equations will be needed, though.

3. States of Quantum Systems

Given a quantum mechanical system, the basic mathematical object now is a Hilbert space \mathcal{H} , a complex linear vector space with hermitian nonnegative inner product. The dimension N of \mathcal{H} may be finite or infinite. Vectors in \mathcal{H} are denoted by $\psi, \phi, \dots, |\psi\rangle, |\phi\rangle, \dots$; they are used to describe states of the system. Dynamical variables – physical properties of the system – are represented by hermitian operators \hat{A}, \hat{B}, \dots acting on \mathcal{H} . The structure, mathematical properties, and physical interpretation of states are all quite intricate, much more so than in the classical case.

3.1 Pure States

Each nonzero vector $|\psi\rangle \in \mathcal{H}$, assumed to be normalized, determines a corresponding pure state, a state with *maximum possible* information. But already for such states, probabilities of a quantum mechanical nature play an essential role:

$$\text{QM probability} \sim |\text{Complex QM probability amplitude}|^2. \quad (10)$$

Let \hat{A} be some dynamical variable, with real eigenvalues $\{a_j\}$ and corresponding orthonormalized eigenvectors

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$\{|\phi_j\rangle\}$. Assume for simplicity that the eigenvalues are discrete and nondegenerate. Then we have the relations

$$\begin{aligned} \hat{A}|\phi_j\rangle &= a_j|\phi_j\rangle, \quad a_j \text{ real}; \\ \{|\phi_j\rangle\} &= \text{an orthonormal basis (ONB) for } \mathcal{H}, \\ \langle\phi_j|\phi_k\rangle &= \delta_{jk}, \quad \sum_k |\phi_k\rangle\langle\phi_k| = \mathbb{I}; \\ \hat{A} &= \sum_j a_j|\phi_j\rangle\langle\phi_j| \text{(spectral resolution)}. \end{aligned} \quad (11)$$

All these are elementary consequences of hermiticity of \hat{A} .

If a measurement of \hat{A} is carried out by an appropriate experimental arrangement the result will always be one of the eigenvalues a_j , each with some probability. In a self-evident notation we have, the initial pure state being the one determined by a normalized $|\psi\rangle$:

$$\text{Pr}(\hat{A} \rightarrow a_j; \psi) = |\langle\phi_j|\psi\rangle|^2 = \langle\phi_j|\psi\rangle\langle\psi|\phi_j\rangle. \quad (12)$$

Here $\text{Pr}(\hat{A} \rightarrow a_j; \psi)$ stands for the probability that an experiment set-up to measure the dynamical variable \hat{A} will return the value a_j , given that the system is in state $|\psi\rangle$. These are *irreducible* QM probabilities, not caused by inadequate knowledge of the condition of the system. So even in pure states we have, in general, expectation values and spreads or dispersions or uncertainties:

$$\begin{aligned} \langle\hat{A}\rangle_\psi &= \sum_j a_j \text{Pr}(\hat{A} \rightarrow a_j; \psi) = \langle\psi|\hat{A}|\psi\rangle \\ &= \text{Tr}(\hat{A}\hat{\rho}(\psi)), \quad \rho(\psi) = |\psi\rangle\langle\psi|; \\ \langle(\Delta A)^2\rangle_\psi &= \langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle_\psi = \langle\hat{A}^2\rangle_\psi - \langle\hat{A}\rangle_\psi^2 \geq 0. \end{aligned} \quad (13)$$

Here we have introduced the projection operator $\hat{\rho}(\psi)$ on to the vector $|\psi\rangle$, called the density operator (or density matrix) associated with the pure state $|\psi\rangle$. So in general any \hat{A} has a spread ΔA unless $|\psi\rangle$ happens to be an

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Even in a state of maximum possible information, probabilities of a QM nature come in for the description of measurement.

eigenstate of \hat{A} . Omitting the argument ψ , pure state density matrices are fully characterized thus:

$$\hat{\rho}^\dagger = \hat{\rho} \geq 0, \text{Tr}\hat{\rho} = 1, \hat{\rho}^2 = \hat{\rho}. \quad (14)$$

Any such $\hat{\rho}$ is $\hat{\rho}(\psi)$ for some (normalized) $|\psi\rangle \in \mathcal{H}$.

3.2 The Superposition Principle of QM

We have seen in (12) that even in a state of maximum possible information, probabilities of a QM nature come in for the description of measurement. As if in compensation for this, and in fact leading to a great simplification, we have a Principle of Superposition of states. We are dealing here of course with pure states. Quoting from Dirac's discussion of this key principle of QM [1]:

“It requires us to assume that between these states there exist peculiar relationships such that whenever the system is definitely in one state we can consider it as being partly in each of two or more other states. The original state must be regarded as the result of a kind of *superposition* of the two or more new states, in a way that cannot be conceived on classical ideas. . . . any two or more states may be superposed to give a new state. . . . *The intermediate character of the state formed by superposition (thus) expresses itself through the probability of a particular result for an observation being intermediate between the corresponding probabilities for the original states, not through the result itself being intermediate between the corresponding results for the original states.*”

At the level of vectors in \mathcal{H} : if ψ_1, ψ_2, \dots are (nonzero, distinct) vectors in \mathcal{H} , each determining after normalisation a corresponding pure state, and if c_1, c_2, \dots are complex numbers, then

$$\psi = c_1\psi_1 + c_2\psi_2 + \dots \in \mathcal{H} \quad (15)$$

is or determines another possible pure state. Note that the ψ_j 's need not be mutually orthogonal; we also assume there are no superselection rules which would limit



the allowed superpositions. In general, given the linear vector level relationship (15),

$$\hat{\rho}(\psi) \neq \text{any expression involving only } \hat{\rho}(\psi_1), \hat{\rho}(\psi_2), \dots \quad (16)$$

There are very subtle features involved here, which we study in some depth later.

3.3 General Mixed States, Density Matrices

These arise from pure states by the same *classical statistical mixing* as in Section 2. Let ψ_1, ψ_2, \dots be distinct normalized, but not necessarily mutually orthogonal, vectors; and let P_1, P_2, \dots be any sequence of classical probabilities. Then the (most) general mixed state of the quantum system is given by

$$\begin{aligned} \hat{\rho} &= P_1 \hat{\rho}(\psi_1) + P_2 \hat{\rho}(\psi_2) + \dots \\ &= \sum_j P_j \hat{\rho}(\psi_j) = \sum_j P_j |\psi_j\rangle\langle\psi_j|. \end{aligned} \quad (17)$$

The complete *defining properties* of such density matrices are:

$$\begin{aligned} \hat{\rho}^\dagger &= \hat{\rho} \geq 0, \text{Tr} \hat{\rho} = 1, \\ \hat{\rho} - \hat{\rho}^2 \geq 0 &: \begin{cases} = 0 & \text{pure case,} \\ \neq 0 & \text{mixed or impure case.} \end{cases} \end{aligned} \quad (18)$$

In such a state, for a dynamical variable \hat{A} :

$$\begin{aligned} \text{Pr}(\hat{A} \rightarrow a_j; \hat{\rho}) &= \langle\phi_j|\hat{\rho}|\phi_j\rangle \\ &= \sum_k P_k \langle\phi_j|\hat{\rho}(\psi_k)|\phi_j\rangle \\ &= \sum_k P_k |\langle\phi_j|\psi_k\rangle|^2. \end{aligned} \quad (19)$$

In each term in the last expression here, the first factor is a classical probability, the second factor a quantum



While the probabilities have both classical and quantum components, there is no unique separation into these components. It is like saying that there is a boundary, but it is movable.

mechanical one. For the expectation value we have

$$\begin{aligned} \langle \hat{A} \rangle_{\hat{\rho}} &= \sum_j a_j \Pr(\hat{A} \rightarrow a_j; \hat{\rho}) \\ &= \sum_k P_k \langle \hat{A} \rangle_{\hat{\rho}(\psi_k)} \\ &= \text{Tr}(\hat{\rho} \hat{A}), \end{aligned} \tag{20}$$

and similarly for $\langle (\Delta A)^2 \rangle_{\hat{\rho}}$.

In the expression (17), the P_j 's and ψ_j 's are generally *not* the eigenvalues and eigenvectors of $\hat{\rho}$. Of course $\hat{\rho}$ does have its own spectrum of eigenvalues and associated eigenvectors, so they do lead to a corresponding representation (the spectral representation) like (17) for $\hat{\rho}$. Unlike the classical equation (7), however, a mixed state $\hat{\rho}$ has infinitely many decompositions of the type (17) in terms of *pure states*, one among which is given by its own eigenvalues and eigenvectors. This enormous multiplicity means that *while the probabilities (19) have both classical and quantum components, there is no unique separation into these components*. It is like saying that there is a boundary, but it is movable.

For any general (pure or mixed) states $\hat{\rho}_1, \hat{\rho}_2, \dots$ and any *classical* probabilities P'_1, P'_2, \dots , the *convexity law* says, as in the classical situation, that

$$\hat{\rho} = P'_1 \hat{\rho}_1 + P'_2 \hat{\rho}_2 + \dots = \sum_j P'_j \hat{\rho}_j \tag{21}$$

is another possible mixed state. The great contrast between this and superposition (15) at the vector level is to be emphasised. So the picture of states in QM is:

$$\begin{aligned} \text{Pure states } \hat{\rho}(\psi) &= |\psi\rangle\langle\psi| \longrightarrow \\ \text{General mixed states} \\ \hat{\rho} &= \sum_j P_j \hat{\rho}(\psi_j), \text{ highly nonunique } \longrightarrow \end{aligned}$$



Convexity law

$$\hat{\rho} = \sum_j P'_j \hat{\rho}_j, \text{ mixed state for any states } \hat{\rho}_j. \quad (22)$$

For a given closed system described by a Hamiltonian operator $\hat{H}(t)$, the equation of motion is the quantum Liouville equation

$$\frac{d\hat{\rho}(t)}{dt} = \frac{i}{\hbar} [\hat{\rho}(t), \hat{H}(t)]. \quad (23)$$

As with the classical case, an evolution equation of this kind holds only for Hamiltonian systems; open systems are described by Liouville equations of a more general kind, usually called ‘master equations’.

4. Two-Level and Three-Level Systems

Let us illustrate all this first in the case of $\dim \mathcal{H} = N = 2$. In this case a vector ψ is a two-component column vector

$$\psi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad \langle \psi | \psi \rangle = |\alpha|^2 + |\beta|^2. \quad (24)$$

Any operator on \mathcal{H} can be expressed as a unique linear combination of the unit matrix \mathbb{I}_2 and the three Pauli matrices σ :

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (25)$$

The σ_i 's are hermitian $\sigma_i^\dagger = \sigma_i$ and obey the commutation and anticommutation relations:

$$\begin{aligned} [\sigma_r, \sigma_s] &= 2i\epsilon_{rst}\sigma_t, \\ \{\sigma_r, \sigma_s\} &= 2\delta_{rs}; \quad r, s, t = 1, 2, 3, \end{aligned} \quad (26)$$

where ϵ_{rst} is the familiar Levi–Civita symbol.



Each mixed (or pure) state corresponds uniquely to one point \mathbf{n} inside (or on) the unit sphere \mathbb{S}^2 in a fictitious three-dimensional Euclidean space.

In particular, for the density operator $\hat{\rho}$, we have

$$\begin{aligned}\hat{\rho} &= a_0 \mathbb{I}_2 + \mathbf{a} \cdot \boldsymbol{\sigma} ; \\ \hat{\rho}^\dagger &= \hat{\rho} \Rightarrow a_0, \mathbf{a} \text{ real} ; \\ \text{Tr} \hat{\rho} &= 1 \Rightarrow a_0 = \frac{1}{2} ;\end{aligned}$$

$$\hat{\rho} \geq 0 \Rightarrow \text{eigenvalues } a_0 \pm |\mathbf{a}| \geq 0 \Rightarrow |\mathbf{a}| \leq \frac{1}{2} . \quad (27)$$

Therefore in general

$$\hat{\rho} = \frac{1}{2}(\mathbb{I}_2 + \mathbf{n} \cdot \boldsymbol{\sigma}), \quad |\mathbf{n}| \leq 1. \quad (28)$$

Thus each mixed (or pure) state corresponds uniquely to one point \mathbf{n} inside (or on) the unit sphere \mathbb{S}^2 in a fictitious three-dimensional Euclidean space:

$$\begin{aligned}\text{Pure case : } \hat{\rho} &= \hat{\rho}^2 \Rightarrow |\hat{\mathbf{n}}| = 1, \\ \hat{\rho} &= \frac{1}{2}(\mathbb{I}_2 + \hat{\mathbf{n}} \cdot \boldsymbol{\sigma}), \quad \hat{\mathbf{n}} \in \mathbb{S}^2 ;\end{aligned} \quad (29a)$$

$$\begin{aligned}\text{Mixed case : } \hat{\rho} - \hat{\rho}^2 &> 0 \Rightarrow |\mathbf{n}| < 1, \\ \hat{\rho} &= \frac{1}{2}(\mathbb{I}_2 + \mathbf{n} \cdot \boldsymbol{\sigma}), \quad \mathbf{n} \in \text{Interior of } \mathbb{S}^2 .\end{aligned} \quad (29b)$$

The sphere \mathbb{S}^2 is the Poincaré or Bloch sphere. As examples of (29a) we have:

$$\begin{aligned}\psi &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} ; \quad \hat{\mathbf{n}} = (0, 0, 1), \quad \text{North Pole} ; \\ \psi &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} ; \quad \hat{\mathbf{n}} = (0, 0, -1), \quad \text{South Pole} ; \\ \psi &= \begin{pmatrix} \cos \theta / 2 \\ e^{i\phi} \sin \theta / 2 \end{pmatrix} ; \\ \hat{\mathbf{n}} &= (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \in \mathbb{S}^2 .\end{aligned} \quad (30)$$

The state corresponding to $\mathbf{n} = 0$, i.e., the one that sits at the centre of the Bloch sphere corresponds to

$$\hat{\rho}_0 = \frac{1}{2} \mathbb{I}_2, \quad (31)$$



the maximally mixed state – the state corresponding to maximal ignorance about the system.

For any two states $\hat{\rho}(\mathbf{n})$, $\hat{\rho}(\mathbf{n}')$ we have:

$$\text{Tr}(\hat{\rho}(\mathbf{n})\hat{\rho}(\mathbf{n}')) = \frac{1}{2}(1 + \mathbf{n} \cdot \mathbf{n}'). \quad (32)$$

Clearly the RHS can vanish only when both $\hat{\rho}(\mathbf{n})$, $\hat{\rho}(\mathbf{n}')$ describe pure states and in that case one finds that two mutually orthogonal pure states correspond to diametrically opposite – or antipodal – points on \mathbb{S}^2 .

The nonuniqueness of the expansion (17) for a given mixed state is very easy to illustrate. The most dramatic case corresponds to $\hat{\rho}_0 = \frac{1}{2}\mathbb{I}_2$, for then:

$$\hat{\rho}_0 = \frac{1}{2}\hat{\rho}(\hat{\mathbf{n}}) + \frac{1}{2}\hat{\rho}(-\hat{\mathbf{n}}), \quad \text{any } \hat{\mathbf{n}} \in S^2. \quad (33)$$

Since a density operator is completely specified by the Bloch vector \mathbf{n} , one may introduce a notion of the ‘distance’ $d(\hat{\rho}(\mathbf{n}), \hat{\rho}(\mathbf{n}'))$ between two density operators as:

$$d^2(\hat{\rho}(\mathbf{n}), \hat{\rho}(\mathbf{n}')) = \frac{1}{2}\text{Tr}((\hat{\rho}(\mathbf{n}) - \hat{\rho}(\mathbf{n}'))^2) \quad (34)$$

$$= \frac{1}{4}(\mathbf{n} - \mathbf{n}')^2 \quad (35)$$

which directly relates to the Euclidean distance between the corresponding Bloch vectors. In particular, the distance between $\hat{\rho}(\mathbf{n})$ and $\hat{\rho}_0$, the ‘origin’ in the set of density operators is given by

$$d^2(\hat{\rho}(\mathbf{n}), \hat{\rho}_0) = \frac{1}{4}\mathbf{n}^2 \quad (36)$$

and can be expressed entirely in terms of the eigenvalues λ_r of $\hat{\rho}(\mathbf{n})$ as

$$d^2(\hat{\rho}(\mathbf{n}), \hat{\rho}_0) = \frac{1}{2}\left(\sum_{r=1}^2 \lambda_r^2 - \frac{1}{2}\right). \quad (37)$$



These results for $N = 2$ have been known for more than a century, first in the realm of classical polarization optics and later in quantum mechanics. An explicit treatment of the case $N = 3$ has been developed much more recently, and we describe it at this point, both to show that it is not very complicated and to show what new features are involved.

In the case of $N = 3$, \mathcal{H} is a 3-dimensional complex space with a hermitian inner product and every pure state $\psi \in \mathcal{H}$ can be written as

$$\psi = \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}, \quad \langle \psi | \psi \rangle = |\alpha|^2 + |\beta|^2 + |\gamma|^2. \quad (38)$$

Further, the roles of $SU(2)$ and the Pauli matrices are respectively played by the group $SU(3)$ defined by

$$SU(3) = \{A = 3 \times 3 \text{ complex matrix} \mid A^\dagger A = 1, \det A = 1\}; \quad (39)$$

and its eight Hermitian and trace orthogonal generators λ_i :

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

$$\lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$



$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \quad (40)$$

The λ 's obey the characteristic commutation and anti-commutation relations:

$$[\lambda_r, \lambda_s] = 2if_{rst}\lambda_t, \quad \{\lambda_r, \lambda_s\} = \frac{4}{3}\delta_{rs} + 2d_{rst}\lambda_t,$$

where f_{ijk} are completely antisymmetric and d_{ijk} are completely symmetric. The independent and nonvanishing f and d symbols are:

$$\begin{aligned} f_{123} &= 1, f_{458} = f_{678} = \frac{\sqrt{3}}{2}, \\ f_{147} &= f_{246} = f_{257} = f_{345} = f_{516} = f_{637} = \frac{1}{2}; \\ d_{118} &= d_{228} = d_{338} = -d_{888} = \frac{1}{\sqrt{3}}, \\ d_{448} &= d_{558} = d_{668} = d_{778} = -\frac{1}{2\sqrt{3}}, \\ d_{146} &= d_{157} = -d_{247} = d_{256} = d_{344} = d_{355} \\ &= -d_{366} = -d_{377} = \frac{1}{2}. \end{aligned} \quad (41)$$

These symbols allow one to define two products $\mathbf{a} \wedge \mathbf{b}$ and $\mathbf{a} \star \mathbf{b}$ among real vectors \mathbf{a} , \mathbf{b} in an eight-dimensional real Euclidean space \mathbb{R}^8 :

$$\begin{aligned} (\mathbf{a} \wedge \mathbf{b})_r &= f_{rst} a_s b_t, \quad \mathbf{a} \wedge \mathbf{b} = -\mathbf{b} \wedge \mathbf{a}; \\ (\mathbf{a} \star \mathbf{b})_r &= \sqrt{3} d_{rst} a_s b_t, \quad \mathbf{a} \star \mathbf{b} = \mathbf{b} \star \mathbf{a}. \end{aligned} \quad (42)$$

The eight λ_r 's together with the unit matrix \mathbb{I}_3 provide a basis in the space of linear operators on \mathcal{H} appropriate to a three-level system. Any density matrix for a three-level system, being hermitian and having unit trace, can therefore be uniquely expressed as a real linear combination of these as

$$\hat{\rho} = \frac{1}{3}(\mathbb{I}_3 + \sqrt{3} c \hat{\mathbf{n}} \cdot \boldsymbol{\lambda}), \quad (43)$$



Every pure state for a three-level system thus corresponds in a one-to-one manner to a unit vector, $\hat{\mathbf{n}} \in \mathbb{S}^7$, the unit seven-sphere in \mathbb{R}^8 , which in addition obeys $\hat{\mathbf{n}} \star \hat{\mathbf{n}} = \hat{\mathbf{n}}$.

where c is a scalar and $\hat{\mathbf{n}}$ is a unit vector in \mathcal{R}^8 .

It is easy to see that if ρ is pure, i.e., $\rho = |\psi\rangle\langle\psi|$ for some $|\psi\rangle \in \mathcal{H}$, then,

$$\hat{\rho}^\dagger = \hat{\rho}^2 = \hat{\rho} \geq 0 \iff c = 1 \quad \text{and} \quad \hat{\mathbf{n}} \cdot \hat{\mathbf{n}} \star \hat{\mathbf{n}} = 1, \\ \text{i.e.,} \quad \hat{\mathbf{n}} \star \hat{\mathbf{n}} = \hat{\mathbf{n}}. \quad (44)$$

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It may also be worth mentioning here that if $\hat{\rho}$ and $\hat{\rho}'$ are two pure states and $\hat{\mathbf{n}}, \hat{\mathbf{n}}'$ are their corresponding 8-dimensional vectors, then,

$$\hat{\rho} = |\psi\rangle\langle\psi|, \hat{\rho}' = |\psi'\rangle\langle\psi'| \Rightarrow \text{Tr}(\hat{\rho}'\hat{\rho}) = |\langle\psi'|\psi\rangle|^2 \\ = \frac{1}{3}(1 + 2\hat{\mathbf{n}}' \cdot \hat{\mathbf{n}}), \\ 0 \leq \text{Tr}(\hat{\rho}'\hat{\rho}) \leq 1 \iff 0 \leq \cos^{-1}(\hat{\mathbf{n}}' \cdot \hat{\mathbf{n}}) \leq \frac{2\pi}{3}, \quad (45)$$

and so mutually orthogonal vectors in \mathcal{H} do not correspond to diametrically opposite points on \mathcal{O} . They correspond to points with a maximum opening angle of $\frac{2\pi}{3}$ radians. In the case of $N = 2$, $\hat{\mathbf{n}} \in \mathbb{S}^2 \Rightarrow -\hat{\mathbf{n}}$ is the vector for the orthogonal state and so $-\hat{\mathbf{n}} \in \mathbb{S}^2$, while in case $N = 3$, if $\hat{\mathbf{n}} \in \mathcal{O}$, then $-\hat{\mathbf{n}} \notin \mathcal{O}$.

Moving to a general density operator, not necessarily describing a pure state, positivity of $\hat{\rho}$ constrains $\hat{\mathbf{n}}$ and c as follows [2]:

$$\hat{\mathbf{n}} \cdot \hat{\mathbf{n}} \star \hat{\mathbf{n}} = -\sin 3\phi, \quad (46)$$

$$c \leq \frac{1}{2} \text{cosec}(\phi + \pi/3), \quad \phi \in [\pi/6, \pi/2]. \quad (47)$$



The subset characterised by

$$c = \frac{1}{2} \operatorname{cosec}(\phi + \pi/3), \quad (48)$$

consists of density operators for which at least one eigenvalue is zero and constitutes the boundary of the full set. The boundary set obviously contains both pure and mixed states. The pure states in the boundary set, i.e, those with only one nonzero eigenvalue, correspond to

$$\phi = \frac{\pi}{2} \quad (49)$$

in which case we have

$$c = 1, \quad \hat{\mathbf{n}} \cdot \hat{\mathbf{n}} \star \hat{\mathbf{n}} = 1, \text{ i.e., } \hat{\mathbf{n}} \star \hat{\mathbf{n}} = \hat{\mathbf{n}} \quad (50)$$

as noted earlier.

The other extreme value of ϕ viz $\pi/6$ corresponds to those density operators which have two equal nonzero eigenvalues and in this case we have

$$c = \frac{1}{2}, \quad \hat{\mathbf{n}} \cdot \hat{\mathbf{n}} \star \hat{\mathbf{n}} = -1, \text{ i.e., } \hat{\mathbf{n}} \star \hat{\mathbf{n}} = -\hat{\mathbf{n}}. \quad (51)$$

Again, as before, if one defines the ‘distance’ $d(\hat{\rho}(\mathbf{n}), \hat{\rho}(\mathbf{n}'))$ between two density operators as

$$d^2(\hat{\rho}(\mathbf{n}), \hat{\rho}(\mathbf{n}')) = \frac{1}{2} \operatorname{Tr} ((\hat{\rho}(\mathbf{n}) - \hat{\rho}(\mathbf{n}'))^2), \quad (52)$$

then, one finds that distance between $\hat{\rho}(\mathbf{n})$ and $\hat{\rho}_0 = \mathbb{I}_3/3$, the ‘origin’ in the set of density operators is given by

$$d(\hat{\rho}(\mathbf{n}), \hat{\rho}_0) = \frac{c}{\sqrt{3}} \quad (53)$$

and further that the states in the boundary set that are farthest from $\hat{\rho}_0 = \mathbb{I}_3/3$ are the pure states, and those on the boundary set closest to $\hat{\rho}_0 = \mathbb{I}_3/3$ are the ones that have only two nonzero and equal eigenvalues. The



It is on account of the normalisation of total probability to unity that we use unit vectors $\psi \in \mathcal{H}$ to describe pure quantum states.

values of the distances in the two cases are $1/\sqrt{3}$ and $1/2\sqrt{3}$ corresponding to $c = 1$ and $c = 1/2$ respectively.

One can extend the study of other concepts too for three-level systems and see several similarities as well as differences with the corresponding ones for two-level systems. As mentioned earlier, such an attempt has been done earlier while trying to obtain the Pancharatnam phase formula for three-level systems [3],[4]. For extensions of the considerations above to arbitrary N and also for other notions of ‘distance’ between density operators, the reader may consult ref [5].

5. Further Features of Pure States

It is on account of the normalisation of total probability to unity that we use unit vectors $\psi \in \mathcal{H}$ to describe pure quantum states. But this is still a *many to one relation* since, as (13) shows, ψ and $e^{i\alpha}\psi$ for any α always determine the same $\hat{\rho}(\psi)$. Let us first define

$$\mathcal{B} = \{ \psi \in \mathcal{H} \mid \langle \psi | \psi \rangle = 1 \} = \text{unit sphere } S^{2N-1} \subset \mathcal{H}, \tag{54}$$

so we can say to begin with:

$$\psi \in \mathcal{B} \xrightarrow{\text{many-to-one}} \text{definite pure state } \hat{\rho}(\psi). \tag{55}$$

Now if we wish to convert this to a one-to-one relation, it is useful to define *rays* and a ray space \mathcal{R} :

$$\begin{aligned} \psi \in \mathcal{B} &\rightarrow \text{ray determined by } \psi : \text{equivalence class} \\ &\text{of unit vectors related by phases} \\ &= \text{collection } \{ e^{i\alpha} \psi \mid \psi \text{ fixed, } 0 \leq \alpha < 2\pi \}. \end{aligned} \tag{56}$$

So each ray consists of a circle or S^1 worth of unit vectors.

Each ray consists of a circle or S^1 worth of unit vectors.

Thus each $\psi \in \mathcal{B}$ defines a definite ray to which it belongs, and we can say:

$$\begin{aligned} \mathcal{R} &\equiv \text{set of all rays} \\ \xleftrightarrow{\text{one-to-one}} &\text{set of all pure quantum states.} \end{aligned} \tag{57}$$



We thus have the sequence

$$\begin{aligned} \mathcal{H} &= \text{linear space of all vectors } \psi \longrightarrow \\ \mathcal{B} &= \text{unit sphere in } \mathcal{H} \longrightarrow \\ \mathcal{R} &= \{ \hat{\rho} = |\psi\rangle\langle\psi| \mid \psi \in \mathcal{B} \} . \end{aligned} \tag{58}$$

Neither \mathcal{B} nor \mathcal{R} is a linear vector space; from \mathcal{B} to \mathcal{R} there is a well-defined *projection map* π :

$$\pi : \mathcal{B} \rightarrow \mathcal{R} : \psi \in \mathcal{B} \rightarrow \pi(\psi) = \hat{\rho}(\psi) = |\psi\rangle\langle\psi| \in \mathcal{R}. \tag{59}$$

These objects and relationships can be depicted (possibly inadequately) as in *Figure 1*.

For $N = 2$, the ray space \mathcal{R} is the Poincaré sphere \mathbb{S}^2 .

Now we introduce *Bargmann Invariants*: these are simple expressions involving inner products of n vectors in \mathcal{B} , but actually defined on \mathcal{R} . With a single vector, $n = 1$, we have nothing interesting as $\langle\psi|\psi\rangle = 1$. Next, for the case of two vectors, we have the two-vertex

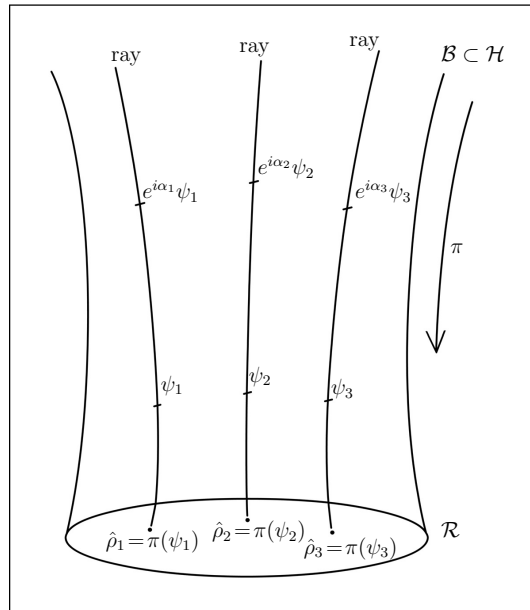


Figure 1. Picture of rayspace, rays, unit vectors in \mathcal{H} , projection π .

This three-vertex Bargmann invariant is cyclically symmetric, invariant under independent phase changes and, most importantly, *complex* in general.

Bargmann invariant:

$$\begin{aligned}
 n = 2 : \quad \psi_1, \psi_2 \in \mathcal{B} : \Delta_2(\psi_1, \psi_2) &= (\psi_1, \psi_2)(\psi_2, \psi_1) \\
 &= |\langle \psi_1 | \psi_2 \rangle|^2 = \text{Tr}(\hat{\rho}_1 \hat{\rho}_2) \\
 &= \text{a quantum mechanical probability,} \\
 &\quad \text{real nonnegative.} \tag{60}
 \end{aligned}$$

Referring to *Figure 1*, we see that $\Delta_2(\psi_1, \psi_2)$ is unchanged under $\psi_1 \rightarrow e^{i\alpha_1}\psi_1, \psi_2 \rightarrow e^{i\alpha_2}\psi_2$, i.e., under *sliding* ψ_1 and ψ_2 on their respective rays, always projecting onto $\hat{\rho}_1, \hat{\rho}_2$ in \mathcal{R} . For three vectors we get something more interesting:

$$\begin{aligned}
 n = 3 : \quad \psi_1, \psi_2, \psi_3 \in \mathcal{B} : \Delta_3(\psi_1, \psi_2, \psi_3) \\
 &= (\psi_1, \psi_2)(\psi_2, \psi_3)(\psi_3, \psi_1) \\
 &= \text{Tr}(\hat{\rho}_1 \hat{\rho}_2 \hat{\rho}_3). \tag{61}
 \end{aligned}$$

This three-vertex Bargmann invariant is cyclically symmetric, invariant under independent phase changes and, most importantly, *complex* in general. For higher orders one has:

$$\begin{aligned}
 n \geq 4 : \Delta_n(\psi_1, \psi_2, \dots, \psi_n) \\
 &= (\psi_1, \psi_2)(\psi_2, \psi_3) \cdots (\psi_{n-1}, \psi_n)(\psi_n, \psi_1) \\
 &= \text{Tr}(\hat{\rho}_1 \hat{\rho}_2 \dots \hat{\rho}_n). \tag{62}
 \end{aligned}$$

It is a simple exercise to show that in general Δ_n for $n \geq 4$ can be reduced to Δ_3 's and Δ_2 's, so the basic Bargmann invariant capturing the presence of complex numbers in quantum mechanics is Δ_3 .

Now let us go back to *Figure 1*. Remember that $\dim \mathcal{H} = N$. Given any n distinct nonzero vectors $\psi_1, \psi_2, \dots, \psi_n \in \mathcal{B}$, they are linearly dependent if for some nontrivial complex coefficients c_1, c_2, \dots, c_n we have

$$c_1 \psi_1 + c_2 \psi_2 + \dots + c_n \psi_n = 0; \tag{63}$$

otherwise they are linearly independent. For $n \leq N$ they may be linearly dependent or independent, while if



$n > N$ they are definitely linearly dependent. In the independent case (so $n \leq N$), every nontrivial linear combination appearing on the left in (63) leads, after normalization, to a new pure state – a superposition of $\psi_1, \psi_2, \dots, \psi_n$. We ask: how is this seen or reflected at the ray space level?

Start with n distinct pure states $\hat{\rho}_1, \hat{\rho}_2, \dots, \hat{\rho}_n \in \mathcal{R}$. Choose any vectors $\psi_1, \psi_2, \dots, \psi_n \in \mathcal{B}$ in the respective rays, or equivalence classes of unit vectors, so that

$$\hat{\rho}_1 = \hat{\rho}(\psi_1), \hat{\rho}_2 = \hat{\rho}(\psi_2), \dots, \hat{\rho}_n = \hat{\rho}(\psi_n). \quad (64)$$

Each of $\psi_1, \psi_2, \dots, \psi_n$ is fixed up to a phase. But whether they are linearly dependent or independent is a phase-change-independent or *gauge-invariant* property! To explore and show this, we form an $n \times n$ matrix of scalar products

$$M(\psi_1, \psi_2, \dots, \psi_n) = \left((\psi_j, \psi_k) \right). \quad (65)$$

That is, the jk th entry of the matrix equals the inner product (ψ_j, ψ_k) . If we make independent phase changes

$$\psi_j \rightarrow \psi'_j = e^{i\alpha_j} \psi_j, \quad j = 1, 2, \dots, n, \quad (66)$$

then clearly

$$\begin{aligned} M(\psi'_1, \psi'_2, \dots, \psi'_n) &= D^\dagger M(\psi_1, \psi_2, \dots, \psi_n) D, \\ D &= \text{diag}(e^{i\alpha_1}, e^{i\alpha_2}, \dots, e^{i\alpha_n}). \end{aligned} \quad (67)$$

For any n , the matrix $M(\psi_1, \psi_2, \dots, \psi_n)$ is hermitian positive semidefinite. Clearly, the signal that the ψ 's are linearly dependent is the singularity of $M(\psi_1, \psi_2, \dots, \psi_n)$, the vanishing of $\det M(\psi_1, \psi_2, \dots, \psi_n)$. But from (67), this is a ray space criterion! We can check this for small values of n :

$$\begin{aligned} n = 2 : \det M(\psi_1, \psi_2) &= \begin{vmatrix} 1 & (\psi_1, \psi_2) \\ (\psi_2, \psi_1) & 1 \end{vmatrix} \\ &= 1 - \text{Tr}(\hat{\rho}_1 \hat{\rho}_2); \end{aligned}$$

Whether they are linearly dependent or independent is a phase-change-independent or *gauge-invariant* property!



$$\begin{aligned}
 n = 3 : \det M(\psi_1, \psi_2, \psi_3) &= \begin{vmatrix} 1 & (\psi_1, \psi_2) & (\psi_1, \psi_3) \\ (\psi_2, \psi_1) & 1 & (\psi_2, \psi_3) \\ (\psi_3, \psi_1) & (\psi_3, \psi_2) & 1 \end{vmatrix} \\
 &= 1 - \text{Tr}(\hat{\rho}_2 \hat{\rho}_3) - \text{Tr}(\hat{\rho}_3 \hat{\rho}_1) - \text{Tr}(\hat{\rho}_1 \hat{\rho}_2) \\
 &\quad + \Delta_3(\psi_1, \psi_2, \psi_3) + \Delta_3(\psi_1, \psi_3, \psi_2). \tag{68}
 \end{aligned}$$

For any n we can see that

$$\begin{aligned}
 \det M(\psi_1, \psi_2, \dots, \psi_n) &= \begin{vmatrix} 1 & (\psi_1, \psi_2) & \dots & (\psi_1, \psi_n) \\ (\psi_2, \psi_1) & 1 & \dots & (\psi_2, \psi_n) \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ (\psi_n, \psi_1) & (\psi_n, \psi_2) & \dots & 1 \end{vmatrix} \\
 &= \epsilon_{k_1 k_2 \dots k_n} (\psi_1, \psi_{k_1}) (\psi_2, \psi_{k_2}) \dots (\psi_n, \psi_{k_n}) \\
 &= n! \text{ terms, each a product of some Bargmann} \\
 &\quad \text{invariants (modulo signature) as each } \psi_j \text{ appears} \\
 &\quad \text{once as ket and once as bra in scalar products} \\
 &= \text{expressible in terms of } \Delta_m \text{'s, } m = 1, 2, \dots, n. \tag{69}
 \end{aligned}$$



We can say, remembering Dirac's words quoted earlier:

Vectors $\psi_1, \psi_2, \dots, \psi_n$ are linearly independent \iff
 $\det M(\psi_1, \psi_2, \dots, \psi_n) > 0 \iff$
 pure states $\hat{\rho}_1, \hat{\rho}_2, \dots, \hat{\rho}_n$ are 'physically independent',
 and necessarily $n \leq N$; (70a)

Vectors $\psi_1, \psi_2, \dots, \psi_n$ are linearly dependent \iff
 Superposition principle is at work here \iff
 $\det M(\psi_1, \psi_2, \dots, \psi_n) = 0 \iff$
 pure states $\hat{\rho}_1, \hat{\rho}_2, \dots, \hat{\rho}_n$ are 'physically dependent',
 necessarily so if $n > N$. (70b)

The important points are that these criteria are entirely expressed via Bargmann invariants which are ray space objects; and in case (70b) there is a 'physical dependence' in the sense of the superposition principle *even though* (in general) none of the $\hat{\rho}$'s can be explicitly expressed in terms of the others. All this is evidence of the subtleties involved in the relationships among the quantum mechanical pure states.

6. The Theorem on Symmetries in QM

This theorem is a remarkable fact concerning pure states of quantum systems and is well worth a careful description even in the absence of a proof. It is a result of a kinematical analysis, with no particular Hamiltonian in mind. We have \mathcal{H} , \mathcal{B} , and \mathcal{R} as indicated in (58). From (60) :

$$\hat{\rho}_1, \hat{\rho}_2 \in \mathcal{R} \rightarrow \text{Tr}(\hat{\rho}_1 \hat{\rho}_2) = \text{a quantum mechanical probability.} \quad (71)$$

Then, a *Wigner Symmetry* (WS) is defined to be a one-to-one onto map $\Omega : \mathcal{R} \rightarrow \mathcal{R}$ which preserves these probabilities, i.e., a pure state map leaving transition



probabilities unchanged:

$$\hat{\rho} \in \mathcal{R} \rightarrow \Omega(\hat{\rho}) \in \mathcal{R} : \\ \text{Tr}\left(\Omega(\hat{\rho}_1) \Omega(\hat{\rho}_2)\right) = \text{Tr}(\hat{\rho}_1 \hat{\rho}_2), \quad \text{all } \hat{\rho}_1, \hat{\rho}_2 \in \mathcal{R}. \quad (72)$$

Any unitary transformation U on \mathcal{H} leads via conjugation to a WS:

$$\mathcal{U}(\hat{\rho}) = U\hat{\rho}U^{-1} : \text{Tr}\left(\mathcal{U}(\hat{\rho}_1)\mathcal{U}(\hat{\rho}_2)\right) \\ = \text{Tr}\left(U\hat{\rho}_1U^{-1}U\hat{\rho}_2U^{-1}\right) = \text{Tr}(\hat{\rho}_1\hat{\rho}_2). \quad (73)$$

It is easy to show that the inverse Ω^{-1} of a WS Ω is another WS. So also the composition $\Omega' \circ \Omega$ of two WS's is another WS.

Wigner's theorem now says: any WS $\Omega: \mathcal{R} \rightarrow \mathcal{R}$ can be 'lifted' to the level of vectors in \mathcal{H} , acting there either as a linear unitary transformation or as an antilinear antiunitary transformation. In any case, given the action of Ω on \mathcal{R} , we can say:

$$\psi \in \mathcal{B} \rightarrow \hat{\rho}(\psi) \in \mathcal{R} \xrightarrow{\Omega} \hat{\rho}' = \Omega(\hat{\rho}(\psi)) = \hat{\rho}(\psi'), \\ \psi' \in \mathcal{B} \text{ determined up to a phase.} \quad (74)$$

The theorem claims that ψ' is determined by ψ basically in one of two possible ways, unitarily or antiunitarily. This may be pictorially depicted as in *Figure 2*.

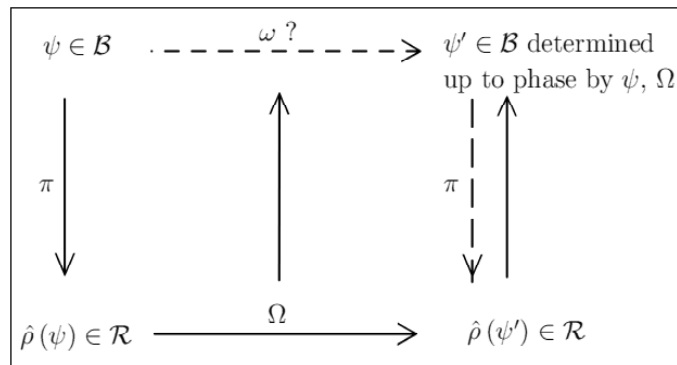


Figure 2. Lifting a Wigner symmetry from \mathcal{R} to \mathcal{B} and \mathcal{H} .



So the basic result is that Ω can always be ‘lifted’ to a map $\omega : \mathcal{B} \rightarrow \mathcal{B}$, which can be extended to act $\mathcal{H} \rightarrow \mathcal{H}$, and then ω is one of the two types mentioned above. Even though this ω is not unique, its nature is! The Bargmann invariants were originally introduced as a way to see immediately which alternative obtains in a particular case, since $\Delta_3(\psi_1, \psi_2, \psi_3)$ is invariant in the unitary case and simply goes into its complex conjugate in the antiunitary case.

The only physically interesting WS which ‘utilises’ the antiunitary choice is time reversal. A consequence is that in quantum mechanics parity is an observable, its eigenvalues can be measured, but time reversal is not!

6. Concluding Comments

The richness of the space of states of quantum systems is quite remarkable; so many new features appear compared to the classical scene which seems so mundane in comparison. For composite systems some specifically new features appear, such as entanglement, which have profound consequences for information theory and quantum computation. We hope to treat these too in a pedagogical fashion comparable to the above, on another occasion!

Suggested Reading

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