Quantum Time Evolution in Terms of Nonredundant Probabilities

Stefan Weigert*

Institut de Physique, Université de Neuchâtel, Rue A.-L. Breguet 1, CH-2000 Neuchâtel, Switzerland

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Each scheme of state reconstruction comes down to parametrize the state of a quantum system by expectation values or probabilities directly measurable in an experiment. It is argued that the time evolution of these quantities provides an unambiguous description of the quantal dynamics. This is shown explicitly for a single spin s, using a quorum of expectation values which contains no redundant information. The quantum mechanical time evolution of the system is rephrased in terms of a closed set of linear first-order differential equation coupling $(2s + 1)^2$ expectation values. This new representation of the dynamical law refers neither to the wave function of the system nor to its statistical operator.

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For a quantum system with statistical operator $\hat{\rho}$, it is straightforward to determine the expectation value of an operator $\hat{A}$ according to

$$\langle \hat{A} \rangle_\rho = \mathrm{Tr}[\hat{A}\hat{\rho}]. \tag{1}$$

Methods of *state reconstruction* [1] solve the inverse problem: the unknown state $\hat{\rho}$ of the quantum system is expressed as a function of the expectation values of properly chosen observables $\hat{\mathcal{Q}}^j$, which constitute a *quorum* $\mathcal{Q}$. The resulting equivalences,

$$\hat{\rho} \Leftrightarrow \{\langle \hat{\mathcal{Q}}^j \rangle, j \in I\}, \qquad \hat{\mathcal{Q}}^j \in \mathcal{Q}, \tag{2}$$

with j taking on values from a discrete or continuous set I of labels, are more than mathematical beauties—they have been used in the laboratory to reconstruct correctly states of various quantum systems [2]. For example, the state of an ion in a Paul trap has been identified [3] by a method realizing (2) on the basis of Wigner functions.

The purpose of this paper is to point out that the parametrization (2) of a density matrix by expectation values suggests a conceptually interesting way to describe the time evolution of a quantum system *without* invoking its density matrix or wave function. Instead, only *expectation values* of Hermitian operators are used which can be measured directly contrary to the wave function. The argument will be given in general terms first, specifying neither the system at hand nor a particular method of state reconstruction. In the main part of this paper the example of a single spin s is worked out explicitly. The discussion at the end puts the results into perspective.

The *von Neumann* equation,

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}], \tag{3}$$

describes the time evolution of a quantum system with Hamiltonian operator $\hat{H}$ and statistical operator $\hat{\rho}$. The state $\hat{\rho}_0$ at time t_0 is transported to $\hat{\rho}_1$ at time t_1 along a smooth path in state space. Suppose that the operators $\{\hat{\mathcal{Q}}^j\}$ provide a quorum $\mathcal{Q}$ for all possible states of the system at hand. Then, each state $\hat{\rho}_t$ on the path between $\hat{\rho}_0$ and $\hat{\rho}_1$ is characterized uniquely by the set of expectation values $\{\langle \hat{\mathcal{Q}}^j \rangle_t\}$. In other words, the path $\hat{\rho}_t$ in state space has an unambiguous image in the *space of expectations* $\{\langle \hat{\mathcal{Q}}^j \rangle\}$. This path is expected to arise as the solution of a dynamical law in this space [4]:

$$\frac{d}{dt}\langle \hat{\mathcal{Q}}^j \rangle_t = \mathcal{D}^j_{\hat{H}}(\{\langle \hat{\mathcal{Q}}^j \rangle_t\}), \tag{4}$$

where the function $\mathcal{D}$ depends on both the Hamiltonian $\hat{H}$ of the system and the quorum $\mathcal{Q}$. Subsequently, time dependent expectation values of *arbitrary* operators $\hat{A}$ can be expressed in terms of the $\{\langle \hat{\mathcal{Q}}^j \rangle_t\}$ simply by using Eq. (2) to eliminate $\hat{\rho}_t$ in favor of the elements of the quorum.

In the following, an explicit form of Eq. (4) will be derived for a spin s using a nonredundant quorum. Quantum mechanically, the spin is described by a vector operator $\hat{\mathbf{S}} \equiv \hbar\hat{\mathbf{s}}$, the components of which satisfy the commutation relations of the algebra $su(2)$: $[\hat{s}_x, \hat{s}_y] = i\hat{s}_z, \ldots$. These operators act irreducibly in a complex Hilbert space $\mathcal{H}_s$ of dimension $(2s + 1)$. The standard basis of the space $\mathcal{H}_s$ is given by the eigenvectors of the z component of the spin, $\hat{S}_z = \mathbf{n}_z \cdot \hat{\mathbf{S}}$, and they are denoted by $|m, \mathbf{n}_z\rangle$, $m = -s, \ldots, s$ [5].

Observables are represented by Hermitian operators, $\hat{A}^\dagger = \hat{A}$, all of which are linear combinations of polynomials in the operators $\hat{s}_x$, $\hat{s}_y$, and $\hat{s}_z$ of degree $2s$ at most. The ensemble of all Hermitian operators acting on $\mathcal{H}_s$ can be considered as a vector space $\mathcal{A}_s$ of dimension $N_s = (2s + 1)^2$. It is convenient [6] to introduce a basis of $\mathcal{A}_s$ consisting of Hermitian operators $\hat{K}_\nu = \hat{K}^\dagger_\nu$, $\nu = 1, \ldots, N_s$ which are orthogonal with respect to a scalar product defined as a trace taken in Hilbert space, $\mathcal{H}_s$,

$$\frac{1}{2s + 1}\mathrm{Tr}[\hat{K}_\nu \hat{K}_{\nu'}] = \delta_{\nu\nu'}. \tag{5}$$

Then each (Hermitian) operator $\hat{A}$ has an expansion

$$\hat{A} = \frac{1}{2s + 1}\sum_{\nu=1}^{N_s} \alpha_\nu \hat{K}_\nu, \qquad \alpha_\nu = \mathrm{Tr}[\hat{A}\hat{K}_\nu], \tag{6}$$

with a unique set of (real) coefficients α_ν. For a spin $1/2$, the Pauli matrices $\sigma_k, k = x, y, z$, combined with the unit

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matrix provide a well-known example of such a basis. One can write a general density matrix in the form

$$\hat{\rho} = \tfrac{1}{2}(1 + \vec{e} \cdot \vec{\sigma}), \tag{7}$$

where $\vec{e}$ is any vector within a ball of radius one, the Bloch sphere.

Here the purpose is to express the dynamical evolution of a quantum spin in terms of *specific* expectation values which are easily accessible in an experiment. Denote the eigenstate of the operator $\mathbf{n} \cdot \hat{\mathbf{s}}$ along the direction $\mathbf{n} = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta)$ and with eigenvalue s by

$$|\mathbf{n}\rangle \equiv \exp[-i\vartheta\mathbf{m}(\varphi)\cdot\hat{\mathbf{s}}]\,|s, \mathbf{n}_z\rangle, \tag{8}$$

where $\mathbf{m}(\varphi) = (-\sin\varphi, \cos\varphi, 0)$: the state $|\mathbf{n}\rangle$ is obtained from rotating the state $|s, \mathbf{n}_z\rangle$ about the axis $\mathbf{m}(\varphi)$ in the xy plane by an angle ϑ. In this way, a *coherent state* $|\mathbf{n}\rangle$ is attached to each point of the surface of the unit sphere [7]. The ensemble of all coherent states provides an overcomplete basis of the Hilbert space $\mathcal{H}_s$.

The density matrix $\hat{\rho}$ of a spin s is determined unambiguously if one performs appropriate measurements with a traditional Stern-Gerlach apparatus. Now randomly select N_s unit vectors $\mathbf{n}_\nu, \nu = 1, \ldots, N_s$, and measure the relative frequencies $p_s(\mathbf{n}_\nu) = \langle\mathbf{n}_\nu|\hat{\rho}|\mathbf{n}_\nu\rangle$, that is, the expectation values of the statistical operator $\hat{\rho}$ in the coherent states $|\mathbf{n}_\nu\rangle$ associated with the direction $\mathbf{n}_\nu$ [8]. These N_s positive numbers do fix (in almost all cases) a unique (unnormalized) statistical operator—in other words, the projection operators,

$$\hat{Q}_\nu = |\mathbf{n}_\nu\rangle\langle\mathbf{n}_\nu|, \qquad \nu = 1, \ldots, N_s, \tag{9}$$

constitute a quorum $\mathcal{Q}$ for a spin s. This fact, when used for state reconstruction, defines an *optimal* method since exactly N_s numbers have to be determined experimentally which equals the number of free (real) parameters of the (unnormalized) Hermitian density matrix $\hat{\rho}$.

The set of all unnormalized Hermitian density matrices for a spin s is a subset (of the same dimension) among all Hermitian operators acting on the Hilbert space $\mathcal{H}_s$ so that the quorum $\mathcal{Q}$ also provides a basis of the space of operators $\mathcal{A}_s$. However, the operators $\hat{Q}_\nu$ are not orthogonal: $\mathrm{Tr}[\hat{Q}_\nu\hat{Q}_{\nu'}] = |\langle\mathbf{n}_\nu \mid \mathbf{n}_{\nu'}\rangle|^2 \neq 0$, except for $\mathbf{n}_{\nu'} = -\mathbf{n}_\nu$. Nevertheless, there is a generalization of (6) for a *nonorthogonal* basis,

$$\hat{A} = \frac{1}{2s+1}\sum_{\nu=1}^{N_s} A^\nu \hat{Q}_\nu, \qquad A^\nu = \mathrm{Tr}[\hat{A}\hat{Q}^\nu], \tag{10}$$

where now the expansion coefficients A^ν involve a second set of operators $\hat{Q}^\nu$ *dual* to the elements of the original basis. The existence of the operators $\hat{Q}^\nu$ is guaranteed [9] if the $\hat{Q}_\nu$ are linearly independent, and they are entirely determined by the relations

$$\frac{1}{2s+1}\mathrm{Tr}[\hat{Q}_\nu\hat{Q}^{\nu'}] = \delta_\nu^{\nu'}, \qquad \nu, \nu' = 1, \ldots, N_s. \tag{11}$$

The quorum and its dual provide a biorthogonal basis of the space $\mathcal{A}_s$ consisting of a covariant and a contravariant basis which suggests the use of lower and upper labels. A second expansion for Hermitian operators is available due to the symmetry between $\mathcal{Q}$ and its dual:

$$\hat{A} = \frac{1}{2s+1}\sum_{\nu=1}^{N_s} A_\nu\hat{Q}^\nu, \qquad A_\nu = \mathrm{Tr}[\hat{A}\hat{Q}_\nu]. \tag{12}$$

Let us now consider the properties of the statistical operator $\hat{\rho}$ when expanded in the dual basis,

$$\hat{\rho} = \frac{1}{2s+1}\sum_{\nu=1}^{N_s} P_\nu\hat{Q}^\nu, \tag{13}$$

where the coefficients $P_\nu = \mathrm{Tr}[\hat{\rho}\hat{Q}_\nu] \equiv \langle\mathbf{n}_\nu|\hat{\rho}|\mathbf{n}_\nu\rangle$ satisfy

$$0 \leq P_\nu \leq 1, \qquad n = 1, \ldots, N_s. \tag{14}$$

Each of the N_s numbers P_ν has a value less or equal to 1 due to the normalization of the density matrix, $\mathrm{Tr}[\hat{\rho}] = 1$, and since $\hat{\rho}$ is a positive operator, the P_ν are *non-negative* throughout. This is a unique and essential feature of the dual basis $\{\hat{Q}^\nu\}$—the expansion coefficients of $\hat{\rho}$ with respect to neither the original basis $\{\hat{Q}_\nu\}$ nor a randomly chosen set of orthogonal operators $\{\hat{K}_\nu\}$ satisfying (5), have this property. The interpretation of the coefficients P_ν—to measure the value s along the axis $\mathbf{n}_\nu$—is clearly compatible with (14). It is important to note that, although each of the P_ν *is* a probability, they do *not* sum up to unity:

$$0 < \sum_{\nu=1}^{N_s} P_\nu < N_s. \tag{15}$$

This is due to the fact that they all refer to *different orientations* of the Stern-Gerlach apparatus, being thus associated with the measurement of *incompatible* observables,

$$[\hat{Q}_\nu, \hat{Q}_{\nu'}] \neq 0, \qquad \nu, \nu' = 1, \ldots, N_s. \tag{16}$$

The sum in (15) cannot take the value N_s since this would require a common eigenstate of all the operators $\hat{Q}_\nu$ which does not exist due to (16). By an appropriate choice of the directions $\mathbf{n}_\nu$ (all in the neighborhood of one single direction $\mathbf{n}_0$, say), the sum can be arbitrarily close to $(2s+1)^2$ for states "peaked" about $\mathbf{n}_0$. Similarly, the sum of all P_ν cannot be zero since this would require the density matrix to vanish. Considered as a sum of *expectation values*, however, there is no need for the numbers P_ν to sum up to unity. Nevertheless, they are not completely independent when arising from a statistical operator: its normalization implies that

$$\mathrm{Tr}[\hat{\rho}] = \frac{1}{2s+1}\sum_{\nu=1}^{N_s}\mathrm{Tr}[\hat{Q}^\nu]P_\nu = 1, \tag{17}$$

which turns one of the probabilities into a function of the $N_s - 1 = 4s(s+1)$, leaving us with the correct number of free real parameters needed to specify a density matrix.

It is useful to visualize the description of a density matrix by the numbers P_ν in geometrical terms. Consider the linear space $\mathcal{A}_s$ of dimension N_s, each axis being associated with one projector $\hat{Q}^\nu$ and a coefficient P_ν. Since $\mathrm{Tr}[\hat{Q}_\nu \hat{Q}_{\nu'}] = |\langle \mathbf{n}_\nu \mid \mathbf{n}_{\nu'}\rangle|^2 \neq 0$, this is not an orthonormal basis of $\mathcal{A}_s$, and neither is its dual $\{\hat{Q}^\nu\}$. According to (13) and (14) each statistical operator determines a point $\vec{P}$ with components P_ν in an N_s-dimensional parallelepiped [9]. Equation (17) may be understood as a scalar product of $\vec{P}$ and the vector $\vec{E}$ with components $E^\nu = \mathrm{Tr}[\hat{E}\hat{Q}^\nu] = \mathrm{Tr}[\hat{Q}^\nu]$, where $\hat{E}$ denotes the unit operator in $\mathcal{A}_s$. Thus, the points $\vec{P}$ which correspond to normalized density matrices are necessarily located in the *intersection* $\mathcal{R}$ [having dimension $4s(s+1)$] of the parallelepiped with a hyperplane in $\mathcal{A}_s$. However, not all points in $\mathcal{R}$ are associated with a density matrix. To see this, imagine the quantum system to be in an eigenstate $|s, \mathbf{n}_{\nu_0}\rangle$ of the projection operator $\hat{Q}_{\nu_0}$, say. Then, the corresponding probability P_{ν_0} has the value 1, and all of the others are smaller than 1. This is the *only* point of the unit cube with $P_{\nu_0} = 1$ associated with a density matrix while one constructs easily other points satisfying (17) but not associated with a density matrix.

Let us turn to the dynamics of the quantum system expressed by the probabilities P_ν. Their time derivative, $dP_\nu/dt = \langle \mathbf{n}_\nu | d\hat{\rho}/dt | \mathbf{n}_\nu\rangle$, is determined unambiguously by Eq. (3). Using expansion (13) it is easy to express the resulting equations in the form (4). A *closed* set of equations for the variables $P_\nu(t)$ follows from plugging (13) into the right-hand side of Eq. (3) and taking the expectation value in the state $|\mathbf{n}_\nu\rangle$:

$$\frac{d}{dt} P_\nu(t) = \frac{i}{\hbar} \sum_{\nu'=1}^{N_s} \langle \mathbf{n}_\nu | [\hat{Q}^{\nu'}, \hat{H}] | \mathbf{n}_\nu \rangle P_{\nu'}(t) . \qquad (18)$$

Thus, the spin dynamics has been expressed entirely in terms of the N_s variables P_ν: this equation, the explicit form of (4) for a single spin s, provides the main result of this paper. The dynamics is consistent with (17): multiply (18) by $\mathrm{Tr}[\hat{Q}^\nu]$ and sum over all values of ν:

$$\sum_{\nu=1}^{N_s} \mathrm{Tr}[\hat{Q}^\nu] \frac{d}{dt} P_\nu = \sum_{\nu'=1}^{N_s} \mathrm{Tr}[\hat{Q}^{\nu'}, \hat{H}]$$
$$P_{\nu'} = \frac{i}{\hbar} \mathrm{Tr}[[\hat{\rho}, \hat{H}]] = 0 , \qquad (19)$$

using (18) and expanding the identity as $\hat{E} = \sum_\nu \mathrm{Tr}[\hat{Q}^\nu]\hat{Q}_\nu$. Consequently, the time evolution of the quantum system can be represented by a point moving in the domain $\mathcal{R}$, with a trajectory determined by (18). Equation (18) will be called the "expectation-value representation" of the equation of motion (3).

Let us point out some properties of the time evolution of the spin s when given in the expectation-value representation. The dynamical law (18) is a *closed* set of *linear* equations for the N_s real variables P_ν: the time derivatives dP_ν/dt at time t are expressed entirely in terms of the probabilities P_ν at that time. Introduce a real $(N_s \times N_s)$ matrix M with entries

$$\mathsf{D}_\nu^{\nu'} = \frac{i}{\hbar} \langle \mathbf{n}_\nu | [\hat{Q}^{\nu'}, \hat{H}] | \mathbf{n}_\nu \rangle$$
$$= \frac{i}{\hbar} \mathrm{Tr}[\hat{H}[\hat{Q}_\nu, \hat{Q}^{\nu'}]] = (\mathsf{D}_\nu^{\nu'})^* , \qquad (20)$$

using the cyclic property of the trace. Then, one can rewrite the dynamics (18) and the constraint (17) as

$$\frac{d\vec{P}(t)}{dt} = \mathsf{D}\vec{P}(t) , \qquad \vec{P}(t_0) \cdot \vec{E} = 1 . \qquad (21)$$

Therefore, the quantum dynamics of a spin s is equivalent to that of a *classical dynamical system* with N_s degrees of freedom, constrained to move in a certain region $\mathcal{R}$ to be considered as its phase space. For an eigenstate of the Hamiltonian $\hat{H}$ with eigenvalue ϵ_k and density matrix $\hat{\rho}^{(k)} = |\epsilon_k\rangle\langle\epsilon_k|$, one has $[\hat{\rho}^{(k)}, \hat{H}] = 0$; hence, the flow generated by D in $\mathcal{R}$ is zero on a $(2s)$-dimensional hyperplane spanned by the eigenstates of the Hamiltonian.

The function $\mathcal{D}$ introduced in (4) is *linear* in the variables P_ν which, in turn, are *linear* functions of the density matrix $\hat{\rho}$. Therefore, the *convexity* of the state space, $\hat{\rho}^{(\lambda)} = (1-\lambda)\hat{\rho}^{(a)} + \lambda\hat{\rho}^{(b)}$, $0 \leq \lambda \leq 1$, turns into

$$\vec{P}^{(\lambda)} = \vec{P}^{(a)} + \lambda(\vec{P}^{(b)} - \vec{P}^{(a)}) , \qquad (22)$$

tracing out a straight line in the space of expectations.

Conceptually, the "realization" introduced here differs from other formulations of quantum mechanics "without wave function" such as the familiar phase-space representation through Wigner functions for a particle [10], for example. Both the continuous and the discrete version of a Wigner function associated with finite-dimensional Hilbert spaces [11] do not allow for a probabilistic interpretation in the familiar sense. The occurrence of *negative* values is characteristic of "quasiprobability" distributions *à la* Wigner, and it reflects the impossibility that position and momentum simultaneously have definite values. The expectation-value representation allows one to rephrase the quantal dynamics entirely in terms of *directly* observable and *non-negative* quantities, defined on $(2s+1)^2$ points of the sphere. This construction can be thought of as discretizing the phase space of the classical spin and associating probabilities (which, however, do *not* sum up to unity) to the individual points.

Furthermore, there is a link to the "probability representation" for both quantum particles and spins [12] which is based on positive smooth distributions on the classical phase space of the underlying system. It provides, however, a highly redundant description, while the expectation-value representation works with nonredundant information only.

From a general point of view, Eqs. (10) and (12) provide the basis for a *symbolic calculus* comparable

to the Wigner formalism [13] or to the coherent state representation [14] of quantum mechanics. Once the vector $\vec{P}(t_0)$ associated with a quantum state $\hat{\rho}(t_0)$ is known, one can extract the time evolution of arbitrary observables $\hat{A}(t)$ from $\vec{P}(t)$ without ever invoking $\hat{\rho}(t)$. The details of this calculus based on the expectation-value representation will be developed elsewhere. Furthermore, it is not difficult to generalize the present approach to *nonautonomous* quantum systems described by explicitly time dependent Hamiltonian operators $\hat{H}(t)$. Similarly, this representation could be used to reexpress the nonunitary time evolution of an open quantum system described by a Lindblad operator [15].

The difference between the *statistical* and the *individual* interpretation of quantum theory [16] is particularly blatant in the expectation-value representation. On the one hand, a parametrization in terms of probabilities $\vec{P}$ strongly suggests that a state $\hat{\rho}$ is associated with an *ensemble* of identically prepared systems. On the other hand, the vector $\vec{P}$ will also be used to describe an *individual* quantum system in a well-defined state such as results from measuring an observable.

In summary, the expectation-value representation of quantum mechanics, as derived from (13), is equivalent to any other representation. It is based on expanding operators in a specific basis of Hermitian but nonorthogonal operators. The statistical operator $\hat{\rho}$ of a quantum spin s is represented by a point on a manifold in an N_s-dimensional space parametrized by probabilities or, equivalently, expectation values. Its time evolution [Eq. (18) or (21)] is governed by a linear and autonomous classical flow. Therefore, one can describe the quantum dynamics as a smooth trajectory in the space of expectation values. With all unobservable elements eliminated from the theory, the expectation-value representation provides an appealing explicit realization of Schrödinger's remark [17] to consider the wave function as a "Katalog der Erwartung."

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*Electronic address: stefan.weigert@iph.unine.ch

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