RECONSTRUCTION OF QUANTUM STATES AND ITS CONCEPTUAL IMPLICATIONS

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State reconstruction for quantum systems is reviewed. Emphasis is on nontomographic approaches for spin states which are based on measurements performed with a Stern-Gerlach apparatus. Two consequences of successfully implemented state reconstruction are pointed out. First, it allows one to determine experimentally the expectation value of an arbitrary operator *without* a device measuring it. Second, state reconstruction suggests a reformulation of Schrödinger's equation in terms of expectation values only, without explicit reference to a wave function or a density operator.

1 Introduction

In a footnote of his article on quantum mechanics for the "Handbuch der Physik," Pauli hides a question which, apparently, he does not know to answer:

> Die mathematische Frage, ob bei gegebenen Funktionen $W(x)$ und $W(p)$ die Wellenfunktion ψ stets eindeutig bestimmt ist, wenn es eine solche zugehörige Wellenfunktion überhaupt gibt, (d. h. wenn $W(x)$ und $W(p)$ physikalisch vereinbar sind), ist noch nicht allgemein untersucht worden.[1]

Knowledge of the probability distributions $W(x) \equiv |\psi(x)|^2$ und $W(p) \equiv |\psi(p)|^2$ for position and momentum is equivalent to knowing all moments $\langle\psi|\hat{x}^n|\psi\rangle$ and $\langle\psi|\hat{p}^n|\psi\rangle$, $n = 1, 2, \ldots$, which are measurable in experiments, at least in principle. Therefore, one can immediately rephrase Pauli's question as follows: Is it possible to reconstruct the state $|\psi\rangle$ (of a particle in a potential $V(x)$ on the real line, say) on the basis of a collection of expectation values, i.e.,

$$\{\langle\psi|\hat{x}^n|\psi\rangle, \langle\psi|\hat{p}^n|\psi\rangle, n = 1, 2, \ldots\} \Rightarrow |\psi\rangle\,? \tag{1}$$

As it stands, this question must be answered in the negative: the *Pauli data* on the left-hand-side of (1) do not *always* single out a unique state $|\psi\rangle$. A wave function $\psi(x) = \psi_r(x) + i\psi_i(x)$ with linearly independent real and imaginary parts,

$$\alpha\,\psi_r(x) + \beta\,\psi_i(x) = 0 \Leftrightarrow \alpha = \beta = 0\,, \tag{2}$$

and with definite odd parity,

$$\psi(x) = -\psi(-x)\,, \tag{3}$$

provides a simple counterexample.[2] The state $\Psi(x) = \psi^*(x)$, obtained by complex conjugation of the wave function $\psi(x)$, is linearly independent of $\psi(x)$. It represents a *Pauli partner* of the original state since it leads to the same probability distributions:

$$|\Psi(x)|^2 = |\psi(x)|^2 \quad \text{and} \quad |\Psi(p)|^2 = |-\psi^*(p)|^2 = |\psi(p)|^2\,. \tag{4}$$

According to Ref. [3], families of *Pauli non-unique* states (not necessarily of definite parity) exist which are dense in the one-particle Hilbert space.

However, a coherent state $|\alpha\rangle$, that is, an eigenstate of the annihilation operator a, is easily seen to be defined completely by the probability distributions of position and momentum. In fact, the expectation values of the operators $\hat{x}$ and $\hat{p}$ are already sufficient,

$$\langle\alpha|a|\alpha\rangle = \alpha = \sqrt{\frac{m\omega}{2\hbar}}\langle\alpha|\hat{x}|\alpha\rangle + \frac{i}{\sqrt{2m\omega\hbar}}\langle\alpha|\hat{p}|\alpha\rangle\,, \tag{5}$$

since they determine the complex number α and thus the state $|\alpha\rangle$.

2 General setting of state reconstruction

Let us rephrase the problem of state reconstruction from a more general point of view. Consider a quantum mechanical system $\mathcal{S}_{QM}$ described by a Hamiltonian operator $\widehat{H}$ acting in a Hilbert space $\mathcal{H}$. The states of the system may be pure ones or mixed ones, in both cases described conveniently by a density matrix $\hat{\rho}$. *Given* a state with density matrix $\hat{\rho}$, it is straightforward to predict the expectation values of hermitean operators $\widehat{\mathcal{O}}_a = \widehat{\mathcal{O}}_a^\dagger$ in the algebra $\mathcal{A}$ of operators acting on $\mathcal{H}$:

$$\langle\widehat{\mathcal{O}}_a\rangle_{\hat{\rho}} = \mathrm{Tr}\left(\widehat{\mathcal{O}}_a\,\hat{\rho}\right)\,, \quad \widehat{\mathcal{O}}_a \in \mathcal{A}\,. \tag{6}$$

These numbers can be compared directly with the outcome of appropriate measurements performed on the physical system $\mathcal{S}_{QM}$.

Suppose now that the state $\hat{\rho}$ of the system is unknown, while the values of various expectation values[a] have been measured:

$$\left\{\langle\widehat{O}_j\rangle\,,\, j \in J\right\} \overset{?}{\Rightarrow} \hat{\rho}\,, \tag{7}$$

where the index j, taking values in some set J, labels hermitean operators. The problem of state reconstruction is seen now to define an *inverse* problem, conceptually similar to a scattering problem. Given a scattering potential, it is straightforward to calculate the cross section, to infer the underlying potential from scattering data, however, is highly complicated.

From the outset it is not obvious which data should be collected experimentally in order to reconstruct the state of the quantum system. For example, position and momentum probability distributions (as proposed by Pauli) do not completely characterize the unknown pure state of a particle in one dimension. In other words, the selection of a set of observables to be measured is by no means trivial. Therefore, it is not surprising that many different solutions to Pauli's problem can be found.

- Suppose that the expectation values of *all* hermitean operators $\widehat{O} \in \mathcal{A}$ were known at some instant of time.[b] This should be sufficient information to determine the density matrix $\hat{\rho}$ since all the information one would ever want to extract from $\hat{\rho}$ is already given. Nevertheless, even in this case it is not obvious how to actually *calculate* the density operator as a function of the measured expectation values.

- The notion of a 'quorum' $\mathcal{Q}$ denotes a set of operators *sufficient* to be measured in order to extract the underlying quantum state.[5] As follows from counting the free parameters of the density matrix of a spin s (cf. below), a quorum of operators $\widehat{O}_q \in \mathcal{Q}$ will indeed be a *subset* $\mathcal{Q} \subset \mathcal{A}$ of all the operators which act on the Hilbert space $\mathcal{H}$ of the system. An ideal quorum of operators consists of the *minimal* number of a set operators for which an experimentally *feasible* measuring prescription is known.

- Instead of measuring many expectation values at a fixed time, one might follow the time evolution of a few observables over some interval of time. This approach has led to the result[6] that one can reconstruct a particle state in a known one-dimensional potential by following the probability distribution of position, $|\psi(x,t)|^2$, over the interval $-\infty < t < \infty$.

- State reconstruction is highly sensitive to the conditions which are imposed from the beginning. Knowing from the outset that the system under study is in a pure state, one can reduce considerably the amount of data needed for a successful reconstruction. Suppose that the probability distribution, $|\psi(x,t_0)|^2$, measured at time t_0 has no nodes for finite values of x. Then the state $|\psi\rangle$ is uniquely determined[7] by a second measurement of the position probability distribution at an infinitesimal time Δt later, $|\psi(x,t_0+\Delta t)|^2$. In the non-generic case of a pure state with N nodes (this requires both the real *and* the imaginary part of the wave function to vanish simultaneously at N points), these data are compatible with a continuous manifold of states isomorphic to an N-dimensional torus. This is due to the fact that N nodes divide the real line into $(N+1)$ compartments with wave functions the relative phases of which remain undetermined. In addition, N expectation values are necessary in order to determine their values. The multi-dimensional version of this result[8] casts doubts on the proposed equivalence of Madelung's hydrodynamic formulation of quantum mechanics[9] with Schrödinger's standard formulation.

- *Tomographic* methods of state reconstruction turn out to be particularly elegant. These approaches are based on two ingredients. In a phase-space formulation of quantum mechanics there is a one-to-one relation between a quantum state and a quasi-probability or Wigner function.[10] Its marginals are accessible experimentally, and an (inverse) Radon transformation[11,12] allows one to reconstruct the phase-space distribution associated with the unknown quantum state. This method has been applied to various physical systems: quantum states of vibrating molecules,[13] of trapped ions,[14] as well as the state of atoms in motion[15] have been reconstructed successfully in the laboratory. Similarly, quantum optical experiments[16] have been performed. Reviews can be found in Refs. [17] and [18].

The question of how to reconstruct quantum states also arises naturally for spin systems. The essential difference to particle systems is its setting in a *finite-dimensional* Hilbert space. Therefore, one might expect that the problem of state reconstruction simplifies. From now on, the focus will be on the Pauli problem for a single spin with quantum number s.

[a] For simplicity, the standard formulation of (nonrelativistic) quantum mechanics will be assumed here, including the idealizations that the preparation of the states to be measured is *perfect*, that *completely* reliable detectors exist, and that one is able to handle *infinite* ensembles in order to extract expectation values. The modifications required for a realistic experimental setup have been studied in Ref. [4], for example.

[b] Clearly, this assumption is debatable due to the difficulty of associating a measurement procedure with arbitrary hermitean operators—cf. the last part of this paper.

3 Reconstructing a mixed spin state

The Hilbert space of a spin s has $(2s+1)$ complex dimensions. Therefore, the most general (unnormalized) density matrix $\hat{\rho}$ is a $(2s+1)\times(2s+1)$ hermitean matrix with $(2s+1)^2$ real parameters. Various methods have been proposed to determine $\hat{\rho}$.

- The expectations of $4s(s+1)$ linearly independent spin multipoles do fix a unique (normalized) density operator.[19] However, no method is outlined which would indicate how to determine their values experimentally.

- If a *Feynman filter*[20] were available, a phase sensitive version of a Stern-Gerlach apparatus, one could determine directly moduli and (relative) phases of the individual matrix elements of the density operator.[21] It is, however, not obvious whether such an apparatus can be build in the laboratory.

- In order to establish a down-to-earth approach, it is natural to restrict the measurements to those performed with a standard Stern-Gerlach apparatus, the quantization axis of which can be oriented arbitrarily in space. In this spirit, the density matrix of a spin s has been shown to be fixed through $(4s+1)$ measurements using a Stern-Gerlach apparatus.[22] All the directions involved are assumed to be located on a cone about some fixed axis in space. Clearly, this will not be the most efficient method since the number of experimentally determined parameters $(=(4s+1)(2s+1))$ exceeds the number of free parameters.

- It has been shown in Ref. [23] that it is possible to parameterize an (unnormalized) density matrix in terms of $(2s+1)^2$ intensities,

$$\hat{\rho} \Leftrightarrow \{p_s(\mathbf{n}_{qr}),\ 0 \le q, r \le 2s\}\,, \tag{8}$$

  with $p_s(\mathbf{n}_{qr})$ being the probability to obtain the value s when the spin is measured along the direction $\mathbf{n}_{qr}$. The $(2s+1)^2$ directions are located on $(2s+1)$ cones about the z axis with different opening angles such that the set of the $(2s+1)$ axes on each cone is invariant under a rotation about z by an angle $2\pi/(2s+1)$.

The fourth approach is particularly satisfactory since it pertains to a minimal quorum of observables all of which are easily accessible in an experiment.

4 Reconstructing a pure spin state

Suppose now that the spin state to be reconstructed is known to be prepared in a (normalized) *pure* state which has $4s$ free parameters. This number is *linear* in s while the data needed for state reconstruction presented above grows *quadratically* with s. Especially for large values of s, one would like to systematically reduce the amount of data needed to reconstruct a pure state. Three methods are presented which solve this problem using Stern-Gerlach type measurements only.

- The first approach involves the measurement of intensities along *three* axes, two of which are infinitesimally close to each other, while the third one is perpendicular to the plane spanned by the other two.[24] It is possible to make explicit the set of Pauli partners compatible with the intensities associated with the two nearby axes. Their number is 2^{2s}, growing thus exponentially with the spin quantum number s. Effectively, on has to solve $2s$ *quadratic* equations for the $2s$ unknown phases; this leaves $2s$ signs undetermined giving rise to 2^{2s} possible combinations. The third measurement provides $2s$ additional real numbers which can be used to select the correct state among the 2^{2s} partners. Hence, a total of $6s$ numbers has to be measured. If the state in question is generic, one is able to single out the correct state among the 2^{2s} partner by measuring a *single* additional expectation value.

- The second approach[25] is more realistic than the first one because it is not necessary to perform measurements along infinitesimally close axes. Generically, any three axes not in a plane will do:

$$\hat{\rho} \equiv |\psi\rangle\langle\psi| \Leftrightarrow \{p_m(\mathbf{n}_k), -s \le m \le s,\ k = 1,2,3\}\,, \tag{9}$$

  where the index k labels three unit vectors $\mathbf{n}_k$ satisfying $\mathbf{n}_1\cdot(\mathbf{n}_2\times\mathbf{n}_3)\neq 0$. As before, this amounts to measuring more expectation values than there are free parameters in the pure state but here it is not obvious to reduce the required number of measurements. Furthermore, this approach is not constructive.

As far as the mathmematics is concerned, the second method is completely different from the first one. As a matter of fact, it is much simpler to derive the result for two infinitesimally close axes than for the general case. It does not seem possible to extend the argument which holds for infinitesimally close axes to a situation with finite angles between the axes.

It is worth while to rephrase the problem solved here in algebraic form.[25] Consider a faithful $(2s+1)$ dimensional representation of the group $SU(2)$

acting on the Hilbert space $\mathcal{H}_s$, and a fixed normalized (generic) state $|\psi\rangle$. Then, the following statement holds:

$$e^{if(\hat{s}_x)}|\psi\rangle = e^{ig(\hat{s}_y)}|\psi\rangle = e^{ih(\hat{s}_z)}|\psi\rangle \Leftrightarrow \hat{f} = \hat{g} = \hat{h} = \text{const} , \quad (10)$$

where the functions $f(x), g(x)$ and $h(x)$ are polynomials of degree $2s$, $f(x)=\sum_{\sigma=0}^{2s} f_\sigma x^\sigma$, etc. For simplicity, the axes in (10) are associated with an orthogonal set of unit vectors $\mathbf{n}_k$. If there is a Pauli partner $|\Psi\rangle$ of the original state $|\psi\rangle$ at all, it must have the form given by the left-hand-side of (10). For $\mathbf{n}_z$, e.g., one has

$$|\Psi\rangle = e^{ih(\hat{s}_z)}|\psi\rangle = \sum_{m_z=-s}^{s} |m_z\rangle e^{ih(m_z)}\langle m_z|\psi\rangle , \quad (11)$$

which implies

$$|\langle m_z|\Psi\rangle|^2 = |e^{ih(m_z)}\langle m_z|\psi\rangle|^2 = |\langle m_z|\psi\rangle|^2 , \quad (12)$$

and similarly for the two remaining directions. Thus, the states $|\Psi\rangle$ and $|\psi\rangle$ give rise to the *same* intensities along the three axes of quantization. The only consistent and nontrivial choice of the operators $\hat{f}, \hat{g}$, and $\hat{h}$ indicated on the right-hand-side of (10) leads, however, to a state $|\Psi\rangle$ which is just a multiple of $|\psi\rangle$ – hence, $|\psi\rangle$ does not have a Pauli partner.

- A third simple and effective method makes use of spin coherent states.[26] A Stern-Gerlach apparatus is used to measure $(4s+1)$ expectations of projection operators on appropriate coherent states in the unknown state, $p_s(\mathbf{n}_\nu)$, $\nu = 0, 1, \ldots, 4s$. These measurements are compatible with a finite number of states which can be distinguished, in the generic case, by measuring one more probability. Furthermore, this technique shows that the zeroes of a Husimi distribution do have an *operational* meaning since they can be identified through measurements with a Stern-Gerlach apparatus. This result comes down to saying that it is possible to resolve experimentally structures in quantum phase-space which are smaller than $\hbar$.

5 Indirect measurement of arbitrary operators

In quantum mechanics, physical observables are described by self-adjoint operators acting in the Hilbert space of the system. How about the inverse of this statement? One is tempted to claim that all hermitean operators could be promoted to observables:

> In practice it may be very awkward or perhaps even beyond the ingenuity of the experimenter to devise an apparatus which could measure some particular operator, but the theory always allows one to imagine that the measurement can be made.[27]

Nevertheless, one often reserves the notion "observable" for those operators which are known to be measured by some well-defined experimental setup. This requires an apparatus which, upon measuring $\widehat{\mathcal{O}}$, "projects" the original state into an eigenstate of the measured operator. On the basis of repeated measurements one would then be able to determine the expectation value of $\widehat{\mathcal{O}}$, to be compared with the calculated value, $\text{Tr}(\widehat{\mathcal{O}}\,\hat{\rho})$. Without an apparatus measuring the operator $\widehat{\mathcal{O}}$, its expectation values seem to be out of reach. This state of affairs is judged as unsatisfactory:

> There is, however, no rule which would tell us which self-adjoint operators are truly observables, nor is there any prescription known how the measurements are to be carried out, what apparatus to use, etc. In a theory with a positivistic undertone, this is a serious gap.[28]

Successful schemes of state reconstruction, be it for particle or spin systems, provide 'half' an answer to the problem to relate self-adjoint operators and observables in quantum mechanics since a working scheme of state reconstruction makes it possible to determine the expectation value of *any* operator $\widehat{\mathcal{O}}$ *without* measuring it. All one has to do is to reconstruct the (pure or mixed) state of the system at hand. This provides then a parametrization of its density matrix in terms of a well-defined quorum $\mathcal{Q}$ of experimentally accessible expectation values $\langle\widehat{\mathcal{O}}_q\rangle$,

$$\hat{\rho} = \hat{\rho}\left(\{\langle\widehat{\mathcal{O}}_q\rangle\}\right) . \quad (13)$$

Subsequently, it is straightforward to *calculate* the expection value of $\widehat{\mathcal{O}}$ according to the rules of quantum mechanics giving

$$\langle\widehat{\mathcal{O}}\rangle_{\hat{\rho}} = \text{Tr}\left(\widehat{\mathcal{O}}_a\hat{\rho}\left(\{\langle\widehat{\mathcal{O}}_q\rangle\}\right)\right) = \langle\widehat{\mathcal{O}}\rangle_{\hat{\rho}}\left(\{\langle\widehat{\mathcal{O}}_q\rangle\}\right) . \quad (14)$$

Thus, the expectation values of operators without practicable measuring apparatus are accessible experimentally—the operators do not even have to be hermitean. ¿From this point of view, one might consider the Stern-Gerlach apparatus as a *universal measuring device* for spin systems: in combination with a scheme of state reconstruction, it enables one to extract all expectation values one can ever dream of. This argument can be turned around in order to 'test' the predictions of quantum mechanics.[29] The expectation value of an observable with known measuring device can now be determined in *two* independent ways, using either the apparatus or the indirect method with a quorum $\mathcal{Q}$ of measurable operators. Comparison of the results checks the consistency of quantum mechanics. In a spin system, for example, this test is easily realized by looking at the expectation value of a spin component along some axis *not* used for the quorum.

6 Quantum mechanics in terms of expectation values

Each scheme of state reconstruction provides a new way to represent the time evolution of a quantum system. As indicated earlier, one parametrizes the density matrix $\hat{\rho}$ of a mixed or pure state via

$$\hat{\rho} \Leftrightarrow \{\langle \widehat{\mathcal{O}}_q \rangle\}\,, \quad \widehat{\mathcal{O}}_q \in \mathcal{Q}\,, \tag{15}$$

where the operators $\widehat{\mathcal{O}}_q$ are assumed to provide a quorum $\mathcal{Q}$ for the system at hand. The time evolution of the system is governed by the 'quantum mechanical Liouville' equation,[30]

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\widehat{H}\,, \hat{\rho}]\,, \tag{16}$$

which transports $\hat{\rho}(t_0)$ at time t_0 along a path in the space of operators to $\hat{\rho}(t)$ at some later time t. In view of the one-to-one relation (15), it is obvious that the traversed path has an unambiguous image in the *space of expectation values.* Therefore, a closed set of equations of motion for the elements of the quorum must exist,

$$\frac{d}{dt}\langle \widehat{\mathcal{O}}_q \rangle = \mathcal{D}_q\left(\widehat{H}, \{\langle \widehat{\mathcal{O}}_q \rangle\}\right)\,, \tag{17}$$

where the function $\mathcal{D}_q$ generates the correct transformation of the expectation values. It depends in a subtle way on both the quorum and the Hamiltonian $\widehat{H}$, and its detailed properties remain to be explored.

In Ref. [31], Eq. (17) has been derived explicitly for a spin s, using the quorum introduced in Ref. [23]. The quantum mechanical time evolution of the system is rephrased in terms of a closed set of linear first-order differential equations coupling the $(2s+1)^2$ expectation values $\langle \widehat{\mathcal{O}}_q \rangle$. This 'realization' of the dynamical law indeed refers neither to the wavefunction of the system nor to its statistical operator.

The resulting 'expectation-value representation' of quantum mechanics is equivalent to any other representation. The time evolution of the system is represented as the motion of a point on a manifold in a space with axes corresponding to expectation values (or probabilities). This representation

has the interesting property that it refers to measurable quantities only (in the form of expectation values): the wave function completely drops out. Conceptually, this approach differs truly from other formulations of quantum mechanics 'without wave function' such as the phase-space representation in terms of Wigner functions, be it for particles[10] or spin.[32] The novelty of the representation introduced here is due to the fact that the quantal dynamics is expressed entirely in terms of *directly* observable quantities.

7 Conclusion

State reconstruction for mixed and pure spin states has been reviewed. In both cases, measurements performed with a Stern-Gerlach apparatus are sufficient for a realistic quorum. Any working scheme of reconstruction has two interesting consequences. On the one hand, it becomes possible to access experimentally the expectation values of arbitrary operators. This provides a partial solution to the problem of associating self-adjoint operators with observables: even if no measuring device for some operator $\widehat{\mathcal{O}}$ is known, one can determine its expectation value. On the other hand, new representations of the quantum dynamics follow from reliable reconstruction methods. In this framework, the time evolution of a quantum state corresponds to the trajectory of a point in a space of expectation values. Such a representation of quantum mechanics has the noteworthy feature to eliminate all unobservable elements from the theory. This provides a new and unexpected way to draw consequences of Schrödinger's idea[33] to think of the wave function as a "Katalog der Erwartung."

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Time Asymmetry and Decay

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