Reconstructing the density matrix of a spin *s* through Stern - Gerlach measurements

1998 J. Phys. A: Math. Gen. 31 L543

(http://iopscience.iop.org/0305-4470/31/31/001)

J. Phys. A: Math. Gen. **31** (1998) L543–L548. Printed in the UK PII: S0305-4470(98)93767-2

LETTER TO THE EDITOR

Reconstructing the density matrix of a spin s through Stern–Gerlach measurements

Jean-Pierre Amiet and Stefan Weigert

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

Received 29 April 1998, in final form 19 May 1998

Abstract. The Pauli problem is solved for a spin of length s prepared in an arbitrary (unnormalized) mixed state which has $(2s+1)^2$ free real parameters. The reconstruction of its density operator ρ is possible if one knows the probabilities of the $(2s+1)$ spin components along each of $(2s+1)$ directions in space. These probabilties are directly accessible through measurements performed with a Stern–Gerlach apparatus. A multipole expansion of the density operator establishes the link between the matrix elements of ρ and the measured intensities.

Repeated measurements on an ensemble of identically prepared systems allow one to reconstruct the density operator of a particle [1]. The methods to solve this *inverse* problem—originally formulated by Pauli [2] for pure particle states—simplifies considerably if one performs *redundant* measurements. Experimentally, reconstruction schemes have been shown to work for light [3], vibrating molecules [4] and ions in a trap [5] (see [6] for a review). The state of atoms in motion has been reconstructed recently [7]. It is difficult, however, to decide on the *minimum* number of expectation values in order to determine unambiguously a pure or mixed state since the particle Hilbert-space is of infinite dimension.

The Hilbert space of a spin s being of finite dimension, one expects the Pauli problem to be easier to handle. Indeed, various answers to the problem have been obtained for mixed spins of arbitrary length and for pure states with $s = \frac{1}{2}, 1$, as reviewed in [8]. The density matrix of a spin s has been shown to be fixed through $(4s+1)$ measurements performed with a Stern–Gerlach apparatus [9]. Using *Feynman filters*, a phase-sensitive version of a Stern–Gerlach apparatus [10], one can determine directly moduli and (relative) phases of the individual matrix elements of the density operator [11] for spin s. If normalized, it depends on $(2s+1)^2 - 1 = 4s(s+1)$ real parameters. Furthermore, as shown in [12], the expectations of $4s(s+1)$ linearly independent spin multipoles do fix a unique density operator; however, no method has indicated how to determine experimentally these values. Alternatively, the discrete version of a Wigner function associated with finite-dimensional Hilbert spaces allows for experimental reconstruction of quantum states [13] as exemplified in the determination of a single quantized cavity mode [14].

In this letter, it will be shown that the mixed state of a spin s can be reconstructed while respecting the following two constraints:

(i) the measurements are performed with a standard Stern–Gerlach apparatus only;

(ii) no redundant information is acquired.

These two requirements are natural in the sense that they correspond (i) to an especially simple experimental procedure and (ii) to the most effective one. In particular, the use of *Feynman filters* involving delicate interference experiments is avoided. In addition, the method is *constructive*: the measured data are not only shown to single out a *unique* quantum state but the matrix elements of ρ are expressed *explicitly* in terms of expectation values.

The states of a spin of magnitude s belong to a Hilbert space $\mathcal{H}_s$ of complex dimension $(2s+1)$, carrying an irreducible representation of the group $SU(2)$. The components of the spin operator $\vec{S} \equiv \hbar\vec{s}$ with standard commutation relations $[s_x, s_y] = \mathrm{i}s_z, \ldots$ generate rotations about the corresponding axes. The standard basis of the space $\mathcal{H}_s$ is given by the eigenvectors of the z component of the spin, denoted by $|\mu\rangle, -s \leqslant \mu \leqslant s$. The phases of the states are fixed by the transformation under the anti-unitary time reversal T operator: $T|\mu\rangle = (-1)^{s-\mu}|-\mu\rangle$, and the ladder operators $s_\pm = s_x \pm \mathrm{i}s_y$ act as usual in this basis:

$$s_\pm|\mu\rangle = \sqrt{s(s+1) - \mu(\mu\pm 1)}|\mu \pm 1\rangle. \tag{1}$$

The complexified algebra $\mathcal{A}_s$ of *observables* in the space $\mathcal{H}_s$ has complex dimension $(2s+1)^2$. It consists of all polynomials in the operators s_x, s_y and s_z with complex coefficients and of degree $2s$ at most. A monomial of a degree higher than $2s$ can be expressed as a linear combination of monomials of lower degree.

It is convenient to use a basis consisting of *multipole* operators associated with the group $SU(2)$ (cf [15]):

$$K_{lm} = \sqrt{2s+1} \sum_{\mu\mu'=-s}^{s} (-1)^{s-\mu} (lm|s\mu', s-\mu)|\mu'\rangle\langle\mu| \qquad 0 \leqslant l \leqslant 2s,\ -l \leqslant m \leqslant l \tag{2}$$

where $(lm|s\mu', s-\mu)$ is the standard Clebsch–Gordan coefficient. The ensemble of all operators K_{lm} forms an *irreducible tensorial* set. The $(2s+1)^2$ *Hermitian* ($K_{lm}^\dagger = (-1)^m K_{l-m}$) multipole operators are orthogonal to each other:

$$\frac{1}{2s+1}\,\mathrm{Tr}(K_{l'm'}^\dagger K_{lm}) = \delta_{ll'}\delta_{mm'}. \tag{3}$$

The multiplication table of multipole operators K_{lm} and their commutators are given in the appendix.

As tensorial sets, the multipoles transform under an element of $SU(2)$ according to

$$U(\vec{\omega})K_{lm}U(\vec{\omega})^\dagger = \sum_{m'=-l}^{l} K_{lm'} D_{m'm}^{(l)}(\vec{\omega}) \tag{4}$$

where rotations about an axis $\vec{e}_\omega$ by an angle $|\vec{\omega}|$ are represented as follows:

$$U(\vec{\omega}) = \mathrm{e}^{\mathrm{i}\vec{\omega}\cdot\vec{s}} \qquad \text{and} \qquad D^{(l)}(\vec{\omega}) = \mathrm{e}^{\mathrm{i}\vec{\omega}\cdot\vec{L}_{(l)}} \tag{5}$$

and the angular momentum operator $\vec{L}_{(l)}$ acts in a subspace of dimension $(2l+1)$.

A statistical (mixed) spin state is given by a Hermitian operator, the density matrix ρ, which is an element of the algebra $\mathcal{A}_s$. Thus, it can be expanded in the basis of multipoles:

$$\rho = \frac{1}{2s+1}\sum_{lm} \rho_{lm}^* K_{lm} \tag{6}$$

with coefficients ρ_{lm}^* given through (3) as expectation values of the operators K_{lm}:

$$\rho_{lm} = \mathrm{Tr}(\rho K_{lm}) = (-1)^m \rho_{l-m}^*. \tag{7}$$

Explicitly, one has

$$\rho_{lm} = \sqrt{2s+1}\sum_{\mu\mu'}(-1)^{s-\mu}(lm|s\mu', s-\mu)\langle\mu|\rho|\mu'\rangle. \tag{8}$$

Using the orthogonality of the Clebsch–Gordan coefficients [15], one can express the matrix elements of the density matrix in terms of the coefficients in the expansion (6):

$$\langle\mu|\rho|\mu'\rangle = \frac{(-1)^{s-\mu}}{\sqrt{2s+1}}\sum_{lm}(s\mu', s-\mu|lm)\rho_{lm} \tag{9}$$

and equation (7) implies that the diagonal elements of ρ are real. Clearly, both the collection of all $\langle\mu|\rho|\mu'\rangle$ and of all ρ_{lm} each depend on $(2s+1)^2$ real parameters—if, for convenience, the density operator ρ is *not* normalized to one but $\mathrm{Tr}\,\rho = \rho_{00} > 0$ only is required. According to equation (9), the reconstruction of a density matrix has been achieved if one is able to express the coefficents ρ_{lm} in terms of expectation values.

As indicated earlier, the measurements are to be performed with a Stern–Gerlach apparatus only. Therefore, the experimentally accessible quantities are given by the intensities $p_\mu(\theta, \varphi)$, representing the probability to find the system in an eigenstate $|\mu; \theta, \varphi\rangle$ of the spin operator $\vec{n}\cdot\vec{s}$ along direction $\vec{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$. The probabilities are diagonal elements of the density operator ρ:

$$p_\mu(\theta, \varphi) = \langle\mu; \theta, \varphi|\rho|\mu; \theta, \varphi\rangle \tag{10}$$

where

$$|\mu; \theta, \varphi\rangle \equiv \exp[-\mathrm{i}\varphi \boldsymbol{s}_z]\exp[-\mathrm{i}\theta \boldsymbol{s}_y]|\mu\rangle = \sum_{\nu=-l}^{l}|\nu\rangle\langle\nu|U^\dagger(0, \theta, \varphi)|\mu\rangle. \tag{11}$$

Upon introducing the multipole expansion (6) of ρ into (10), one obtains

$$\begin{aligned} p_\mu(\theta, \varphi) &= \frac{1}{2s+1}\sum_{lm}\rho^*_{lm}\langle\mu|U(0, \theta, \varphi)K_{lm}U^\dagger(0, \theta, \varphi)|\mu\rangle \\ &= \frac{1}{2s+1}\sum_{lmm'}\rho^*_{lm}\langle\mu|K_{lm'}|\mu\rangle D^{(l)}_{m'm}(0, \theta, \varphi) \end{aligned} \tag{12}$$

and the second equality follows from the transformation property of the basis K_{lm} under rotations, equation (4). It is useful to replace the measured intensities p_μ by $(2s+1)$ linear combinations:

$$\Pi_l(\theta, \varphi) = \sqrt{2s+1}\sum_{\mu=-l}^{l}(-1)^{s-\mu}(s\mu, s-\mu|l0)p_\mu(\theta, \varphi). \tag{13}$$

A linear relation between measurable quantities and the multipole coefficients of the spin state follows if the probabilities p_μ are expressed as in equation (12):

$$\Pi_l(\theta, \varphi) = \left(\frac{4\pi}{2l+1}\right)^{\frac{1}{2}}\sum_{m=-l}^{l}Y_{lm}(\theta, \varphi)\rho^*_{lm} \tag{14}$$

where the functions $Y_{lm}(\theta, \varphi)$ are the spherical harmonics:

$$\left(\frac{4\pi}{2l+1}\right)^{\frac{1}{2}}Y_{lm}(\theta, \varphi) = d^{(l)}_{0m}(\theta)\mathrm{e}^{\mathrm{i}m\varphi} = D^{(l)}_{0m}(0, \theta, \varphi). \tag{15}$$

In order to express the density matrix in terms of measurable quantities, now one has to determine an appropriate set of directions in space such that it becomes possible to invert the fundamental relation, equation (14). As a matter of fact there are many possibilities to extract the $(2s+1)^2$ components of the state ρ from measured data (recall that the density operator ρ is not normalized to one). In the following, four approaches are presented which require less and less measurements.

(i) If one were able to measure the probabilities $p_\mu(\theta,\varphi)$ for *all* angles $\theta \in [0,\pi)$, $\varphi \in [0,2\pi)$, one could use the orthogonality of the spherical harmonics to extract the unknowns by an integration over the surface of the unit sphere:

$$\rho_{lm} = \left(\frac{4\pi}{2l+1}\right)^{\frac{1}{2}} \int_0^{2\pi}\int_0^{\pi} \mathrm{d}\varphi\,\mathrm{d}\theta\ \sin\theta\, Y_{lm}(\theta,\varphi)\Pi_l^*(\theta,\varphi). \tag{16}$$

In view of the *finite* number of unknown parameters, this procedure involves a highly redundant (and physically unrealistic) set of measurements.

(ii) What does a discretized version of this approach look like? Measure the probabilities for $(2s+1)^2$ pairs of angles (θ_j,φ_k) distributed 'homogeneously' over the sphere in such a way that the square matrix

$$\mathcal{Y}_{(lm)(jk)} \equiv Y_{lm}(\theta_j,\varphi_k) \tag{17}$$

is invertible. A possible choice of directions $\vec{n}(\theta_j,\varphi_k)$ is given by $\varphi_k = k2\pi/(2s+1)$, $k=1,\ldots,2s+1$, and $\theta_j = j\pi/(2s+2)$, $j=1,\ldots,2s+1$, for example [16]. Note that this method works for arbitrary states since the matrix $\mathcal{Y}_{(lm)(jk)}$ is independent of the density operator ρ. Altogether, the values of $(2s+1)^3$ real numbers have to be determined, thus still exceeding considerably the number of independent parameters.

For a further reduction of the number of measurements, the explicit form of the spherical harmonics is used:

$$Y_{lm}(\theta,\varphi) = \mathrm{e}^{\mathrm{i}m\varphi}\mathcal{P}_{lm}(\theta) \tag{18}$$

where $\mathcal{P}_{lm}(\theta) = N_{lm}P_l^m(\cos\theta)$ with P_l^m being a Legendre function of first kind multiplied by a numerical factor N_{lm}. Using $\mathcal{P}_{l-m} = (-1)^m\mathcal{P}_{lm}$ and equation (7), one obtains for any pair of angles (θ_j,φ_k)

$$\Pi_l(\theta_j,\varphi_k) = \mathcal{P}_{l0}(\theta_j)\rho_{l0} + \sum_{m=1}^{l}\mathcal{P}_{lm}(\theta_j)(\cos(m\varphi_k)\mathrm{Re}\,\rho_{lm} + \sin(m\varphi_k)\mathrm{Im}\,\rho_{lm}). \tag{19}$$

(iii) For directions $\varphi_0 = 0$, $\varphi_1 = 2\pi/(2s+1)$, $\theta_j = j\pi/(2s+1)$ with $j=0,\ldots,2s$ on two half-circles, one obtains a set of $2(2s+1)^2$ linear equations from equation (19):

$$\Pi_l(\theta_j,0) = \mathcal{P}_{l0}(\theta_j)\rho_{l0} + \sum_{m=1}^{l}\mathcal{P}_{lm}(\theta_j)\mathrm{Re}\,\rho_{lm} \tag{20}$$

$$\Pi_l(\theta_j,\varphi_1) = \mathcal{P}_{l0}(\theta_j)\rho_{l0} + \sum_{m=1}^{l}\mathcal{P}_{lm}(\theta_j)(\cos(m\varphi_1)\mathrm{Re}\,\rho_{lm} + \sin(m\varphi_1)\mathrm{Im}\,\rho_{lm}). \tag{21}$$

When checking the case $l=2s$, one realizes that indeed all $2(2s+1)^2$ equations are needed to solve for the unknown real and imaginary parts of ρ_{lm}, requiring the matrices $\mathcal{P}_{lm}(\theta_j)$ to be invertible for all θ_j.

(iv) The most economical scheme is to measure the probabilities at a fixed angle $\theta_j = \theta_M$, and angles $\varphi_k = k\,2\pi/(2s+1)$, $k=0,\ldots,2s$, corresponding to $(2s+1)$ directions located on a cone about the z axis. Knowing the values $\Pi_l(\theta_M,\varphi_k)$, and using the orthogonality relation $\sum_k \exp\mathrm{i}(m-m')\varphi_k = (2s+1)\delta_{mm'}$ $(-s \leqslant m, m' \leqslant s)$, one has

$$\rho_{lm} = \frac{1}{(2s+1)\mathcal{P}_{lm}(\theta_M)}\sum_{k=0}^{2s}\mathrm{e}^{-\mathrm{i}m\varphi_k}\Pi_l(\theta_M,\varphi_k). \tag{22}$$

The multipole amplitudes ρ_{lm} are just proportional to the Fourier transforms of $\Pi_l(\theta_M, \varphi_k)$. This methods works if $\mathcal{P}_{lm}(\theta_M) \neq 0$ for all (l, m) which can be achieved always. Now using equation (9), the matrix elements $\langle\mu|\rho|\mu'\rangle$ are given in terms of measurable quantities. As a matter of fact, exactly $(2s+1)^2$ real numbers have to be determined for a reconstruction of the operator ρ. One might suspect that for a generic density operator a natural generalization of this results holds: one may select other appropriate $(2s+1)$ spatial directions to define the measurements.

The method presented here also applies to pure states with a density matrix $\rho = |\psi\rangle\langle\psi|$. If $|\psi\rangle$ is not normalized, $2(2s+1)$ real parameters are unknown. In principle, the knowledge of ρ_{l0} and ρ_{l1}, $0 \leqslant l \leqslant 2s$, is sufficient to reconstruct the state as follows from equation (9):

$$\psi_\mu^* \psi_\mu = \frac{(-1)^{s-\mu}}{\sqrt{2s+1}} \sum_l (s\mu, s-\mu|l0)\rho_{l0} \tag{23}$$

$$\psi_\mu^* \psi_{\mu+1} = \frac{(-1)^{s-\mu}}{\sqrt{2s+1}} \sum_l (s\mu+1, s-\mu|l1)\rho_{l1}. \tag{24}$$

The first set of equations allows one to extract the moduli of the coefficients, and the second one can be used subsequently to determine the relative phases. It is not clear, however, what kind of Stern–Gerlach measurement would determine ρ_{l0} and ρ_{l1} alone. Thus, even the most economic procedure for mixed states is necessarily redundant for pure states. The problem of defining nonredundant measurements for a pure spin state can be solved by a different method [17].

To sum up, the multipole expansion of the density operator for a spin s is a useful tool in order to reconstruct the quantum state by measurements with a Stern–Gerlach apparatus. The most efficient approach requires to measure the $(2s+1)$ intensities along $(2s+1)$ directions on a cone about some axis in space determining all $(2s+1)^2$ free parameters of the density matrix ρ.

Appendix

The multiplication table of multipole operators in $\mathcal{A}_s$ is given by

$$K_{lm}K_{l'm'} = \sum_{l''m''} \rho(ll'l''s)(lm, l'm'|l''m'')K_{l''m''} \tag{25}$$

where the number $\rho(ll'l''s)$ is essentially a Racah $6j$-coefficient [15]:

$$\rho(ll'l''s) = (-1)^{2s+l''}\sqrt{(2s+1)(2l+1)(2l'+1)} \begin{Bmatrix} l & l' & l'' \\ s & s & s \end{Bmatrix}. \tag{26}$$

The Lie-algebra composition law of basis elements reads

$$[K_{lm}, K_{l'm'}] = \frac{\mathrm{i}}{\sqrt{s(s+1)}} \sum_{l''m''} \sigma(ll'l''s)(lm, l'm'|l''m'')K_{l''m''} \tag{27}$$

where

$$\sigma(ll'l''s) = -\mathrm{i}\sqrt{s(s+1)}[1-(-1)^{l+l'+l''}]\rho(ll'l''s). \tag{28}$$

References

[1] Raymer M G 1997 *Contemp. Phys.* **38** 343

[2] Pauli W 1933 *Handbuch der Physik* vol XXIV, part 1, ed Geiger and Scheel (Reprinted 1958 *Encyclopedia of Physics* vol V, part I (Berlin: Springer))

[3] Smithey D T, Beck M, Raymer M G and Faridani A 1993 *Phys. Rev. Lett.* **70** 1244
[4] Dunn T J, Walmsley I A and Mukamel S 1995 *Phys. Rev. Lett.* **74** 884
[5] Leibfried D, Meekhof D, King B E, Monroe C, Itano W M and Wineland D J 1996 *Phys. Rev. Lett.* **77** 4281
[6] Leonhardt U 1997 *Measuring the Quantum State of Light* (Cambridge: Cambridge University Press)
[7] Kurtsiefer C, Pfau T and Mlynek J 1997 *Nature* **386** 150
[8] Weigert St 1992 *Phys. Rev.* A **45** 7688
[9] Newton R G and Young B 1968 *Ann. Phys., NY* **49** 393
[10] Feynman R P, Leighton R B and Sands M 1965 *The Feynman Lectures on Physics* vol III (Reading, MA: Addison-Wesley) ch 5
[11] Gale W, Guth E and Trammell G T 1968 *Phys. Rev.* **165** 1414
[12] Park J L and Band W 1971 *Found. Phys.* **1** 211
Park J L and Band W 1971 *Found. Phys.* **1** 339
[13] Leonhardt U 1995 *Phys. Rev. Lett.* **74** 4101
[14] Walser R, Cirac J I and Zoller P 1996 *Phys. Rev. Lett.* **77** 2658
[15] Fano U and Racah G 1959 *Irreducible Tensorial Sets* (New York: Academic)
[16] Amiet J-P unpublished
[17] Amiet J-P and Weigert St submitted