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Observable Characteristics of Pure Quantum States

John Bohn

Department of Physics and James Franck Institute, The University of Chicago, Chicago, Illinois 60637

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A pure state of a quantum-mechanical system, like a completely polarized state of light, is specified by the results of a few well-chosen experiments. We present a method for selecting such experiments, with applications to low-j angular momentum states.

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The standard notations identifying a quantum-mechanical pure state, such as $|\psi\rangle$ or $\langle i|\psi\rangle$, generally pertain to vectors in a Hilbert space rather than to observable features of the state. Nevertheless, purity of a state implies extensive interrelations among measurements made on the state. In this Letter we outline the appearance of a pure state in physical instead of Hilbert space.

If $|\psi\rangle$ represents a pure state as a vector in an N-dimensional Hilbert space with orthonormal basis $\{|i\rangle\}$, then $|\psi\rangle$ is characterized by the coefficients $\langle i|\psi\rangle$ in the expansion

$$|\psi\rangle=\sum_{i=1}^{N}|i\rangle\langle i|\psi\rangle\,. \tag{1}$$

Since $|\psi\rangle$ is normalized to unity, and since its overall phase is physically irrelevant, the magnitudes and phases of $N-1$ ratios among the $\langle i|\psi\rangle$ characterize $|\psi\rangle$ by $2(N-1)$ real parameters. Observable properties of $|\psi\rangle$ consist of the expectation values of Hermitian operators Ω, namely,

$$\langle\Omega\rangle=\langle\psi|\Omega|\psi\rangle=\sum_{i,j}\langle\psi|i\rangle\langle i|\Omega|j\rangle\langle j|\psi\rangle\,. \tag{2}$$

The operator Ω is a vector in the N^2-dimensional Liouville representation,[1] with basis $\{|i\rangle\langle j|\}$, in which a state is specified by its density matrix ρ. In general, ρ depends on N^2 independent measurements $\langle\Omega^\alpha\rangle$, or rather N^2-1 ignoring the trivial identity operator. A pure state is grossly overdetermined by these N^2-1 measurements. We wish to determine which $2(N-1)$ observables are most appropriate for parametrizing $|\psi\rangle$, as well as the observable consequences of the $(N^2-1)-2(N-1)$ dependency relations.

A step was recently taken in this direction[2] for the case of angular momentum eigenstates, where $N=2j+1$. The essential feature in the analysis of Ref. 2 was the relation

$$\mathrm{Tr}(\rho^2)=\mathrm{Tr}(\rho)=1\,, \tag{3}$$

which is a necessary and sufficient condition for the state ρ to be pure. In this case ρ factors into the dyadic $\rho=|\psi\rangle\langle\psi|$ and the amplitudes $\langle i|\psi\rangle$ are easily recovered from the $\langle\Omega^\alpha\rangle$. While Ref. 2 found explicit formulas for the $\langle i|\psi\rangle$ using only $2(N-1)$ observables, the whole set of N^2-1 was needed implicitly to verify the relation (3). Here we will exploit the entire operator relation

$$\rho^2=|\psi\rangle\langle\psi|\psi\rangle\langle\psi|=\rho \tag{4}$$

rather than just the trace condition (3).

To do this, we introduce a set of N^2 operators $\Omega^0,\Omega^1,\ldots,\Omega^{N^2-1}$, which are orthonormal and complete in the sense that[3]

$$\mathrm{Tr}(\Omega^{\alpha\dagger}\Omega^\beta)=\delta_{\alpha\beta}\,, \tag{5}$$

$$\sum_\alpha(\Omega^{\alpha\dagger})_{ij}(\Omega^\alpha)_{kl}=\delta_{il}\delta_{jk}\,. \tag{6}$$

We set aside Ω^0 to be a multiple of the identity operator, $\Omega^0=I/\sqrt{N}$. Expectation values $\langle\Omega^\alpha\rangle$ of these operators are the expansion coefficients in[3]

$$\rho=\sum_\alpha\mathrm{Tr}(\rho\Omega^\alpha)\Omega^{\alpha\dagger}=\sum_\alpha\langle\Omega^\alpha\rangle\Omega^{\alpha\dagger}\,. \tag{7}$$

In this notation our key condition (4) reads

$$\sum_{\alpha\beta}\langle\Omega^{\alpha}\rangle\langle\Omega^{\beta}\rangle\Omega^{\alpha\dagger}\Omega^{\beta\dagger}=\sum_{\delta}\langle\Omega^{\delta}\rangle\Omega^{\delta\dagger}. \tag{8}$$

Projecting now on any Ω^{γ} yields

$$\sum_{\alpha\beta}\langle\Omega^{\alpha}\rangle\langle\Omega^{\beta}\rangle\mathrm{Tr}(\Omega^{\alpha\dagger}\Omega^{\beta\dagger}\Omega^{\gamma})=\langle\Omega^{\gamma}\rangle. \tag{9}$$

The left-hand side of (9) represents a reduction of the direct product of the set of observables, which could be carried out for any state, pure or mixed. The hallmark of a pure state is that nothing new is generated by this reduction. Equation (9) suggests that after a certain "core" of essential observables has been measured, the rest can be recovered. Notice also that if $\gamma=0$, then $\Omega^0=I/\sqrt{N}$ reduces (9) to the trace condition (3).

For illustration, we now specialize to the case of an eigenstate of total angular momentum j. Then as our base kets we take $\{|jm\rangle,\ -j\le m\le j\}$, and as operators the multipole operators T^K_Q with matrices

$$\langle jm'|T^K_Q|jm\rangle=(-1)^{j-m}\langle jm',j-m|KQ\rangle, \tag{10}$$

$$0\le K\le 2j,\quad -K\le Q\le K,$$

as in Eq. (4.2.5) of Ref. 1. Although these operators are not Hermitian, they have useful transformation properties; for observables, one may take the real and imaginary parts of $\langle T^K_Q\rangle$ with $Q\ge 0$. Representing actual measurements would require us to multiply the matrix element in (10) by the appropriate reduced matrix element, which depends only on K and carries the correct units. Here, however, we are interested only in geometrical effects. In this example T^0_0 serves as Ω^0, and $\langle T^0_0\rangle=(2j+1)^{-1/2}$ fixes normalization.

Cast in these terms, Eq. (9) becomes

$$\sum_{\substack{K_1\ne 0,Q_1\\K_2\ne 0,Q_2}}\langle T^{K_1}_{Q_1}\rangle\langle T^{K_2}_{Q_2}\rangle\langle K_1Q_1,K_2Q_2|KQ\rangle(-1)^{2j+K}(2K_1+1)^{1/2}(2K_2+1)^{1/2}\begin{Bmatrix}K_1 & K_2 & K\\ j & j & j\end{Bmatrix}=\left[1-\frac{2}{2j+1}\right]\langle T^K_Q\rangle \tag{11}$$

whose left-hand side is the familiar recoupling of tensor operators.[4] Since no multipole with $K>2j$ exists for this state, no such multipole can be constructed on the left-hand side of (11); this is the significance of the 6-j symbol. (Terms proportional to $\langle T^0_0\rangle\langle T^K_Q\rangle$ have been moved to the right-hand side, so that only nontrivial products are reduced on the left.)

Parity plays a role in the analysis of (11). The summand is invariant under the exchange $(K_1,Q_1)\leftrightarrow(K_2,Q_2)$, except for the Wigner coefficient, which picks up a factor $(-1)^{K_1+K_2+K}$. Thus, upon summing, only terms with *even* values of K_1+K_2+K survive. This parity-favoredness condition says that no axial tensor constructed on the left-hand side of (11) contributes to the polar tensor on the right. To take an example, the set of $\langle T^K_Q\rangle$ with $K=1$ is equivalent to the mean angular momentum $\langle\mathbf{J}\rangle$ of the system. Thus the combination $K_1=K_2=K=1$ refers to the vector component of the direct product $\{\langle J_i\rangle\langle J_j\rangle\}$, i.e., to the vanishing vector product $\langle\mathbf{J}\rangle\times\langle\mathbf{J}\rangle$. The parity-favored character of the product in (11) implies that higher-rank analogs of the vector product also vanish, while only higher-rank analogs of the scalar product contribute.

Let us examine the meaning of (11) for a few small values of j. For $j=\frac{1}{2}$, there is little to say; the only observable is the mean angular momentum vector $\langle\mathbf{J}\rangle$, proportional to the magnetic dipole moment of the system. For a pure state $|\langle\mathbf{J}\rangle|=\frac{1}{2}$, and the spherical angles (θ,ϕ) identifying the direction of $\langle\mathbf{J}\rangle$ completely identify the state. Values of $|\langle\mathbf{J}\rangle|<\frac{1}{2}$ identify mixed states, represented by incoherent superpositions of two pure states, weighted by the factors $\frac{1}{2}(1\pm 2|\langle\mathbf{J}\rangle|)$.[5]

A pure state with $j=1$ is identified by its dipole ($K=1$) and electric quadrupole ($K=2$) moments. We simplify the analysis by laying the z axis along the direction of $\langle\mathbf{J}\rangle$, thus forcing $\langle T^1_{\pm1}\rangle=0$ and $\langle T^1_0\rangle=|\langle\mathbf{J}\rangle|$. Setting $K=Q=1$ in (11), we see that only terms containing the products $\langle T^2_2\rangle\langle T^1_{-1}\rangle$, $\langle T^2_1\rangle\langle T^1_0\rangle$, and $\langle T^2_0\rangle\langle T^1_1\rangle$ contribute to the sum, but in the chosen reference frame, only the second of these terms survives. Laying aside for the moment the degenerate case $\langle T^1_0\rangle=0$, this forces $\langle T^2_{\pm1}\rangle=0$. This condition may be realized by confining the quadrupole to the x-y plane, leading to the first observable characteristic: A pure state with $j=1$ has its *dipole* moment *orthogonal* to a symmetry plane of the quadrupole.

A second characteristic follows from (11) with $K=1$, $Q=0$, which reduces simply to

$$(\sqrt{2}/\sqrt{3})\langle T^2_0\rangle\langle T^1_0\rangle=\tfrac{1}{3}\langle T^1_0\rangle. \tag{12}$$

Thus, in this reference frame, $\langle T^2_0\rangle$ has the *fixed* value $1/\sqrt{6}$, regardless of the pure state involved. This value of $\langle T^2_0\rangle$ is consistent with $|\psi\rangle$ containing no $m=0$ component, i.e., with a quadrupole confined to the x-y plane.

Finally, using the above results, Eq. (11) with $K=2$, $Q=0$ reduces to an expression connecting the dipole and quadrupole moments:

$$4|\langle T^2_2\rangle|^2+2\langle T^1_0\rangle^2=1. \tag{13}$$

Equation (13) invites us to introduce a parameter λ, defined by

$$\cos 2\lambda = \sqrt{2}\langle T_0^1\rangle, \quad \sin 2\lambda = 2|\langle T_2^2\rangle|^2, \tag{14}$$

which governs the relative strength of dipole and quadrupole excitations. The remaining equations, (11) with $K=2$ and $Q\neq 0$, either vanish or reproduce the results above. Now the case $\langle T_0^1\rangle = 0$, excluded above, is achieved when $\lambda = \pi/4$.

So far we have utilized only three parameters—two spherical angles locating the z axis, plus λ—whereas a pure state with $j=1$ requires four. The final parameter is the azimuthal angle between the semimajor axis of the quadrupole and the x axis. Rotating the coordinate frame to make this angle zero allows us to model the quadrupole simply as a cross consisting of point charges: four negative charges at the origin, and positive charges at $(\pm a,0,0)$ and $(0,\pm b,0)$. The lengths a and b are not free parameters, being determined by

$$\langle T_0^2\rangle = \sqrt{2}(a^2+b^2) = 1/\sqrt{6}, \quad \langle T_2^2\rangle = \sqrt{6}(a^2-b^2), \tag{15}$$

along with (13) and the normalization (3).

The wave function (1) now follows easily from this characterization of its observables. Reference 2 points out that the expansion coefficients $a_m \equiv \langle jm|\psi\rangle$ are recovered from

$$a_{m'}^* a_m = \sum_{KQ} \langle T_Q^K\rangle \langle KQ|jm',j-m\rangle(-1)^{j-m}. \tag{16}$$

In the present case this yields $a_1 = \cos\lambda$, $a_0 = 0$, $a_{-1} = \sin\lambda$, reproducing an earlier result.[6]

The case $j=\frac{3}{2}$ also introduces the magnetic octupole moment ($K=3$). Borrowing from our experience with $j=1$, we choose the z axis orthogonal to the quadrupole plane, and the x axis along an axis of the quadrupole. This exhausts three of the six free parameters, and sets $\langle T_{\pm1}^2\rangle = \mathrm{Im}\langle T_{\pm2}^2\rangle = 0$. We shall not go through the algebra here, but merely report the results. The shape of the quadrupole is determined by a parameter μ,

$$\langle T_0^2\rangle = -\tfrac{1}{2}\cos 2\mu, \quad \langle T_2^2\rangle = (1/2\sqrt{2})\sin 2\mu, \tag{17a}$$

reflecting the fact that the magnitude of the quadrupole, $\sum_Q |\langle T_Q^2\rangle|^2$, has the *fixed* value $\frac{1}{4}$. The magnitudes of charge and current multipoles are decoupled here, in contrast to $j=1$, where one parameter splits the difference between them.

Two parameters are left with which to describe the system of currents. One is the phase ϕ in

$$\langle T_3^3\rangle = |\langle T_3^3\rangle| \exp(i\phi/3), \tag{18}$$

where ϕ represents an overall angle of rotation of the octupole about the z axis. To simplify further results, it is convenient to define the following orthogonal combinations of multipoles with $Q=\pm1$:

$$x = (\sqrt{6}/2)\langle T_1^1\rangle + \langle T_1^3\rangle, \quad y = \langle T_1^1\rangle - (\sqrt{6}/2)\langle T_1^3\rangle. \tag{19}$$

Then the sixth parameter ν mediates the difference between multipoles of current with even and odd values of Q:

$$\langle T_0^1\rangle = -(1/\sqrt{5})(\tfrac{1}{2} - \cos 2\mu)\cos 2\nu, \tag{17b}$$

$$\langle T_0^3\rangle = -(1/\sqrt{5})(1+\tfrac{1}{2}\cos 2\mu)\cos 2\nu, \tag{17c}$$

$$\langle T_2^3\rangle = (1/2\sqrt{2})\sin 2\mu \cos 2\nu, \tag{17d}$$

$$x = (\sqrt{5}/4)\sin 2\mu \sin 2\nu \exp(i\phi/3), \tag{17e}$$

$$y = (\sqrt{5}/4\sqrt{2})(1+\cos 2\mu)\sin 2\nu \exp(-i\phi/3), \tag{17f}$$

$$\langle T_3^3\rangle = \tfrac{1}{4}(1-\cos 2\mu)\sin 2\nu \exp(i\phi/3). \tag{17g}$$

Notice that μ governs the moduli of these multipoles, as it must, since by parity considerations in (11), a current must be constructed by the pairing of charge and current multipoles.

As before, this parametrization also affords an easy representation in Hilbert space. Applying (16), we find, in our coordinate frame,

$$a_{3/2} = \sin\mu \sin\nu \exp(i\phi/6), \tag{20a}$$

$$a_{1/2} = \cos\mu \cos\nu \exp(-i\phi/6), \tag{20b}$$

$$a_{-1/2} = \cos\mu \sin\nu \exp(i\phi/6), \tag{20c}$$

$$a_{-3/2} = \sin\mu \cos\nu \exp(-i\phi/6). \tag{20d}$$

Two additional constructions should prove useful in visualizing this parametrization in specific cases. One is the Majorana representation[7] in which a pure state of spin j is modeled by a "star" consisting of the polarization vectors of $2j$ spin-$\frac{1}{2}$ systems. The $2j$ sets of spherical angles (θ_i,ϕ_i) giving the directions of these vectors correspond to the $4j$ parameters identifying the state, and are determined by the roots of a certain polynomial of degree $2j$.[7] In the present case one would remove three parameters by laying the coordinate axes along the principal axes of the star.

A second construction, due to Maxwell and Sylvester, provides a means of visualizing the multipoles by collections of dipole fields.[8] Specifically, the contribution from the Q component of the 2^K-pole field is represented by $K-Q$ dipoles pointing up along the z axis, along with Q dipoles arranged symmetrically in the x-y plane; these fields are then weighted by the amplitudes $\langle T_Q^K\rangle$. Reference 8 then presents an algebraic procedure for replacing the effect of the entire 2^K-pole field by a collection of just K dipoles, whose directions pick out significant axes of the field. Both this procedure and the Majorana procedure appear analytically cumbersome in the generality of this paper, and are presented for possible use in applications.

The problem remains of connecting these results to specific experiments. Reference 6 presents an instrument consisting of a quadrupole condenser and a dipole coil sharing a common axis. Given the proper orientation and the proper ratio of quadrupole to dipole fields (i.e., the proper λ), the device can select any pure state with $j=1$ as one of its stationary states. The method in the current work can be used, in principle, to design similar experiments for higher j. Any pure state will then be characterized by a type of generalized Stern-Gerlach experiment in which only a properly oriented and balanced combination of electric and magnetic fields will pass a particular polarized beam with 100% transmission. Beyond this lies the possibility of passing an unpolarized beam through several such devices, to decompose the corresponding *mixed* state into a weighted sum of pure states. Such an experiment would constitute an empirical diagonalization of a general density matrix.

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