PHYSICAL REVIEW LETTERS

VOLUME 74 | 20 FEBRUARY 1995 | NUMBER 8

Optimal Extraction of Information from Finite Quantum Ensembles

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(Received 18 October 1993)

Given only a finite ensemble of identically prepared particles, how precisely can one determine their states? We describe optimal measurement procedures in the case of spin 1/2 particles. Furthermore, we prove that optimal measurement procedures must necessarily view the ensemble as a single composite system rather than as the sum of its components, i.e., optimal measurements cannot be realized by separate measurements on each particle.

PACS numbers: 03.65.Bz

A basic assumption of quantum mechanics is that if an infinite ensemble of identically prepared particles is given the quantum state of the particles can be determined exactly. But in practice one never encounters such infinite ensembles, and very often they are not even large (statistical). Given such a finite ensemble its state can only be determined approximately. How much knowledge can be obtained from such finite ensembles? How quickly does one approach exact knowledge as the system becomes large? What experimental strategies furnish the maximum knowledge? We solve these problems in some particular cases. This is not of academic interest only. The solution to such problems is expected to lead to applications in the fields of quantum information transmission, quantum cryptography, and quantum computation.

A fundamental question related to the above has been raised by Peres and Wootters [1]. Is an ensemble of identically prepared particles, viewed as an entity, more than the sum of its components? That is, could more be learned about the ensemble by performing a measurement on all the constituent particles together than by performing separate measurements on each particle? Peres and Wootters conjectured that this is the case. In the present Letter we prove their conjecture, although not in its letter but in its spirit.

We have answered the above problems in the context of a simple "quantum game." The game consists of many runs. In each run a player receives N spin 1/2 particles, all polarized in the same direction. The player knows that the N spins are parallel. He also knows that in each run they are polarized in another direction, randomly and uniformly distributed in space, and that the Hamiltonian of the particles is the same in each run. The player is allowed to do any measurement he wants and is finally required to guess the polarization direction. (The answer must consist of indicating a direction, i.e., the player is not allowed to say something like "with probability P_1 the particles were polarized along ....") The score of the run is $\cos^2(\alpha/2)$, where α is the angle between the real and guessed directions. The final score is the average of the scores obtained in each run. The aim is to obtain the maximal score.

As it has been defined the score is a number between 0 and 1. If no measurement is performed, but a polarization direction is simply guessed at randomly, the score is 1/2. The improvement over 1/2 actually represents the "information" gain; scores less than 1/2 also correspond to a gain in information, but in this case the guessed direction is systematically opposite to that of the spins. The maximal score (1) corresponds to perfect knowledge of the direction of polarization. In this Letter it is shown that the maximum score obtainable is $(N+1)/(N+2)$, which tends towards 1 as N tends to infinity, i.e., as expected for infinite ensembles the direction of polarization can be determined exactly.

Clearly, the above "game" is only a particular way in which the problem of optimizing measurements on finite ensembles might be formulated. Peres and Wootters,

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for example, used the same rules, but a different score, inspired by information theory, and a different distribution of spin directions.

This Letter is organized as follows. A general formalism describing an experiment is used to obtain the equations an optimal experiment must satisfy. Next we consider the game outlined above and obtain $(N + 1)/(N + 2)$ as an upper bound on the score, and optimal experiments that attain this score are exhibited. Last, the conjecture of Peres and Wootters is proven when the system consists of two parallel spins.

Following von Neumann [2], every measurement can be considered as having two stages. The first stage is the interaction between two quantum systems, the measured system and the measuring device; the second stage consists of "reading" the measuring device.

Let us denote by $\{|i\rangle\}$ an orthonormal basis of the Hilbert space of the measured system, and $|\psi_0\rangle_{\rm MD}$ the initial state of the measuring device. The first stage of the measurement consists of the interaction between the measured system and the measuring device,

$$|i\rangle|\psi_0\rangle_{\rm MD} \rightarrow \sum_f |f\rangle|\psi_f^i\rangle_{\rm MD}\,. \qquad (1)$$

If the measured system started in an arbitrary state $|\phi\rangle$ linearity implies

$$|\phi\rangle|\psi_0\rangle_{\rm MD} \rightarrow \sum_{i,f}\langle i|\phi\rangle|f\rangle|\psi_f^i\rangle_{\rm MD}\,. \qquad (2)$$

To allow for the most general measurements we impose no restrictions on the measuring device nor on the interaction with the measured system. The dimension of the Hilbert space of the measuring device is arbitrary and might be much larger than that of the measured system. The wave functions $|\psi_f^i\rangle_{\rm MD}$ are not necessarily normalized, nor orthogonal to each other. The only constraints they obey are

$$\sum_f\langle\psi_f^i|\psi_f^{i'}\rangle = \delta_{ii'}\,, \qquad (3)$$

which follow from the unitarity of the time evolution describing the interaction with the measured system and the normalization of $|\psi_0\rangle_{\rm MD}$. (To simplify notation, in this formula and throughout the text we drop the subscript MD whenever it is obvious that the state belongs to the Hilbert space of the measuring device.)

The second stage of the experiment consists of reading the state of the measuring device. This is implemented by considering a complete set of orthogonal projectors $\{P_\xi\}$. Different outcomes of the experiment correspond to finding the measuring device in the different eigenspaces of the projectors P_ξ. The probability of the outcome ξ if the initial state were $|\phi\rangle$ is

$$P(\phi,\xi) = \sum_{i,i',f}\langle\phi|i'\rangle\langle i|\phi\rangle_{\rm MD}\langle\psi_f^{i'}|P_\xi|\psi_f^i\rangle_{\rm MD}\,. \qquad (4)$$

Here also, for the sake of generality, the number of possible outcomes ξ of the measurement is left arbitrary and can be larger than the dimension of the Hilbert space of the measured system.

We stress, because of its importance to our purpose, the complete generality of the above formalism. It includes ideal measurements (as described in the postulates of quantum mechanics [2]) but also fuzzy measurements, repeated experiments on the same system, etc. For example, a postitive-operator-valued measure (POVM) [3,4] is described in our formalism by simply considering the ancilla as a part of the measuring device and letting the rest of the measuring device act on both the measured system and the ancilla.

Upon finding the measuring device to be in the state ξ, some "information" is obtained about the state of the system. This information could be expressed as a function $S(\xi,\phi)$. The average value of S is

$$S = \sum_\xi \int \mathcal{D}\phi\, P(\phi,\xi)S(\xi,\phi)\,, \qquad (5)$$

where the sums run over the outcomes ξ of the experiment and the initial states ϕ of the system to be measured, with a measure $\mathcal{D}\phi$ corresponding to their distribution.

The problem at hand is to maximize (5) with respect to the possible measurements and guessing strategies, while respecting the unitary relations (3). Below, this program will be carried out in detail in the case of parallel spins.

Before proceeding we simplify the formalism by choosing the P_ξ's to be one dimensional projection operators onto a basis $\{|e_\xi\rangle\}$ of the Hilbert space of the measuring device. Indeed, by decomposing the original projectors as a sum of one dimensional projectors, that is, by a more accurate reading of the measuring device, the information obtained in the measurement can only increase.

We now turn to the specific problem considered in the introduction. The system to be measured consists of N parallel spins polarized in a random direction, say (θ,φ). Denote this state

$$|N_{\theta,\varphi}\rangle = \underbrace{|\uparrow_{\theta,\varphi}\cdots\uparrow_{\theta,\varphi}\rangle}_{N}\,. \qquad (6)$$

The Hilbert space of the N spins can be decomposed into a sum of subspaces having different total spin S with $S = N/2, N/2 - 1, \ldots.$ Since our system consists of N parallel spins, it will always belong to the subspace of highest spin so we have to specify the measuring interaction only for this subspace. A basis of this subspace is $|m\rangle$, $m = -N/2,\ldots,N/2$, which is shorthand for $|S = N/2, S_z = m\rangle$.

The unitary evolution of the spins plus measuring device is given by

$$|m\rangle|\psi_0\rangle_{\rm MD} \rightarrow |v^m\rangle = \sum_{f=1}^{2^N}|f\rangle|\psi_f^m\rangle_{\rm MD}\,, \qquad (7)$$

where $\{|f\rangle\}$ is a complete base of the Hilbert space of N spins. The probability to obtain the result ξ is

$$P(N_{\theta,\varphi};\xi) = \sum_{m,m'=-N/2}^{N/2} \sum_{f=1}^{2^N} \langle N_{\theta,\varphi}|m\rangle\langle\psi_f^m|e_\xi\rangle \times \langle e_\xi|\psi_f^{m'}\rangle\langle m'|N_{\theta,\varphi}\rangle . \quad (8)$$

Upon finding the measuring device to be in the state ξ, one guesses a direction of polarization θ_ξ, φ_ξ and obtains a score $S = S(\theta,\varphi;\theta_\xi,\varphi_\xi) = \cos^2(\alpha/2)$, as explained in the introduction.

We have finally arrived at the mathematical formulation of our problem. We have to maximize the average score S_N,

$$S_N = \sum_\xi \int \frac{\sin\theta\, d\theta\, d\varphi}{4\pi} P(N_{\theta,\varphi};\xi) S(\theta,\varphi;\theta_\xi,\varphi_\xi) , \quad (9)$$

with the unitary constraints (written in the reading basis $|e_\xi\rangle$)

$$\langle v^m|v^{m'}\rangle = \sum_\xi \sum_{f=1}^{2^N} \langle\psi_f^m|e_\xi\rangle\langle e_\xi|\psi_f^{m'}\rangle = \delta^{mm'} . \quad (10)$$

The variables of this problem are $|\psi_f^m\rangle$ which encode the measuring interaction, $|e_\xi\rangle$ which encode the reading procedure, and θ_ξ, φ_ξ which encode the guessing strategy. It is worth noting that the final states of the measuring device $|\psi_f^m\rangle$ and the reading base vectors $|e_\xi\rangle$ always appear together, via the scalar product $\langle\psi_f^m|e_\xi\rangle$, so we do not have to vary them independently. Clearly, the reason behind this is that, given a particular measuring interaction and reading procedure, one can always find a completely equivalent experiment by changing both the final states of the measuring device and the way the result is read.

Rather than work with the complete set of constraints (10), it is convenient to consider first only the constraint

$$\sum_{m=-N/2}^{N/2} \langle v^m|v^m\rangle = \sum_{m=-N/2}^{N/2} \sum_f \sum_\xi \langle\psi_f^m|e_\xi\rangle\langle e_\xi|\psi_f^m\rangle = N + 1 , \quad (11)$$

which follows immediately from (10). The maximal value of the score obtained by using this single constraint equation (11) is larger or equal to the true maximum, obtained when all the constraints are considered. In our case the two maxima coincide. We shall first find the maximum of the reduced problem and then exhibit a solution of the complete problem that attains the same score.

Upon adding to S_N the constraint (11) multiplied by the Lagrange multiplier λ and varying with respect to $\langle\psi_f^m|e_\xi\rangle$ considered as independent variables, one obtains the following linear equations:

$$\sum_{m'} \langle e_\xi|\psi_f^{m'}\rangle [M_{mm'}(\theta_\xi,\varphi_\xi) - \lambda\delta_{mm'}] = 0 , \quad (12)$$

where

$$M_{mm'}(\theta_\xi,\varphi_\xi) = \int \frac{\sin\theta\, d\theta\, d\varphi}{4\pi} \langle N_{\theta,\varphi}|m\rangle\langle m'|N_{\theta,\varphi}\rangle \times S(\theta,\varphi;\theta_\xi,\varphi_\xi) . \quad (13)$$

Upon multiplying the mth equation (12) by $\langle\psi_f^m|e_\xi\rangle$, summing over m, f, and ξ, and using (11), a concise expression for the external value of S_N is found to be $S_{N\,\text{extremum}} = \lambda(N + 1)$.

Equation (12) has a nontrivial solution if and only if λ is an eigenvalue of $M(\theta_\xi,\varphi_\xi)$ (the trivial solutions correspond to $\langle e_\xi|\psi_f^m\rangle = 0$ for all m, implying that the outcome ξ is never realized). The spherical symmetry inherent to this problem can be used to show that the matrix $M(\theta_\xi,\varphi_\xi)$ transforms according to the adjoint representation of SU(2): $M(\theta_\xi,\varphi_\xi) = U(\theta_\xi,\varphi_\xi)M(\theta_\xi = 0)U^\dagger(\theta_\xi,\varphi_\xi)$ where $U(\theta_\xi,\varphi_\xi)$ is an element of the $N + 1$ dimensional irreducible unitary representation of SU(2) that realizes rotations of the spins, sending the $+z$ direction onto the θ_ξ, φ_ξ direction. It follows that the eigenvalues of $M(\theta_\xi,\varphi_\xi)$ are independent of θ_ξ, φ_ξ. Taking $\theta_\xi = 0$, direct computation shows that M is diagonal and its largest eigenvalue is $\lambda = 1/(N + 2)$. So for this reduced problem the corresponding maximal value of the average score is $S_{N\,\text{extremum}} = (N + 1)/(N + 2)$.

We now exhibit optical experiments that attain the score $S_N = (N + 1)/(N + 2)$, thereby proving that this upper bound on the score can be realized.

In the case $N = 1$, one experiment (among many) that attains the score of 2/3 is realized by measuring the projection of the spin along a given axis, say the z axis (a Stern-Gerlach experiment), and according to whether the spin is found to be polarized along the $+z$ or $-z$ direction, to guess that this is the direction along which it is polarized.

In the case $N = 2$, one possible optimal experiment consists of the standard measurement of a nondegenerate operator that has the following four eigenstates:

$$\frac{1}{2}|S\rangle + \frac{\sqrt{3}}{2}|\uparrow_{\hat{n}_i}\uparrow_{\hat{n}_i}\rangle, \quad i = 1,\ldots,4, \quad (14)$$

where $|S\rangle$ is the singlet state, $\uparrow_{\hat{n}_i}$ represents a spin polarized along the $\hat{n}_i$ direction, and the four directions $\hat{n}_i$ are oriented towards the corners of a tetrahedron. [The phases used in the definition of $\uparrow_{\hat{n}_i}$ are such that the four states (14) are orthogonal.] The only requirement of the corresponding eigenvalues is that they be different from each other so that the measurement can distinguish between all four eigenstates. If the spins are found to be in the ith eigenstate, the guessed direction is $\hat{n}_i$.

In the above optimal measurements the Hilbert space of the measuring device is finite dimensional and the number of possible outcomes of the measurement is finite. By counting the number of parameters it can be shown that such finite dimensional optimal measurements exist in the general case (N spins) but have not been able to construct one explicitly. However, allowing for an infinite set of possible outcomes and using the spherical symmetry inherent to our problem, a measurement that attains the optimal score $S_{N\,\text{extremum}}$ can be constructed [5].

The measuring device that gets correlated to the spins is a particle moving on the surface of a sphere. Reading the measuring device consists of measuring the position of the particle. Upon finding it to be located at θ, φ, one guesses that the spins were aligned along the θ, φ direction. Let the reading basis, corresponding to a particle localized at θ, φ, be denoted $|e_{\theta,\varphi}\rangle$, with the normalization $\langle e_{\theta\phi}|e_{\theta'\phi'}\rangle = 4\pi\delta_{\theta\theta'}\delta_{\phi\phi'}/\sin\theta$.

The experiment is described by the unitary evolution equation (7) with $|\psi_f^m\rangle$ given by

$$| \psi_f^m\rangle = \frac{\sqrt{N+1}}{\sqrt{2^N}} \int \frac{d\theta\, d\varphi \sin\theta}{4\pi} U_{mN/2}(\theta,\varphi)|e_{\theta\phi}\rangle, \tag{15}$$

where $U(\theta,\varphi)$ is the same unitary matrix as before. One readily verifies that the $|\psi_f^m\rangle$ obey the unitary relations and that the average score obtained by this measurement is $(N+1)/(N+2)$.

We now come to the crux of our Letter: Must an optimal measurement on an ensemble of parallel spins necessarily treat the ensemble as an entity, i.e., as a single composite system? We show below that there exist no optimal experiments consisting of separate measurements on each spin, even though the result of one measurement may be used to decide which measurement is to be performed next on the other spin. (For related work on optimizing separable measurements, see [6].) For simplicity we consider the case of two spins.

One first makes an arbitrary measurement on the first spin,

$$\begin{aligned} |\!\uparrow\rangle_1 |\psi_0\rangle_{\mathrm{MD1}} &\to |\!\uparrow\rangle_1 |\psi_\uparrow^+\rangle_{\mathrm{MD1}} + |\!\downarrow\rangle_1 |\psi_\downarrow^+\rangle_{\mathrm{MD1}}, \\ |\!\downarrow\rangle_1 |\psi_0\rangle_{\mathrm{MD1}} &\to |\!\uparrow\rangle_1 |\psi_\uparrow^-\rangle_{\mathrm{MD1}} + |\!\downarrow\rangle_1 |\psi_\downarrow^-\rangle_{\mathrm{MD1}}, \end{aligned} \tag{16}$$

where MD1 denotes the first measuring device. The outcomes of this measurement are obtained by projecting the state of MD1 onto the reading base $|e_{\xi_1}\rangle$. According to the outcome ξ_1, different measurements are carried out on the second spin (i.e., the interaction of the second measuring device with the second spin is parametrized by ξ_1),

$$\begin{aligned} |\!\uparrow\rangle_2 |\phi_0\rangle_{\mathrm{MD2}} &\to |\!\uparrow\rangle_2 |\phi_{\uparrow,\xi_1}^+\rangle_{\mathrm{MD2}} + |\!\downarrow\rangle_2 |\phi_{\downarrow,\xi_1}^+\rangle_{\mathrm{MD2}}, \\ |\!\downarrow\rangle_2 |\phi_0\rangle_{\mathrm{MD2}} &\to |\!\uparrow\rangle_2 |\phi_{\uparrow,\xi_1}^-\rangle_{\mathrm{MD2}} + |\!\downarrow\rangle_2 |\phi_{\downarrow,\xi_1}^-\rangle_{\mathrm{MD2}}, \end{aligned} \tag{17}$$

where MD2 denotes the second measuring device. The outcomes of this measurement are obtained by projecting the state of MD2 onto the reading basis $|g_{\xi_2,\xi_1}\rangle$; the index ξ_1 appears because the way the results of the second measurement are read may also depend on the outcomes ξ_1 of the first measurement. Putting it all together one obtains

$$|\!\uparrow\rangle_1 |\!\uparrow\rangle_2 |\psi_0\rangle_{\mathrm{MD1}} |\phi_0\rangle_{\mathrm{MD2}} \to \sum_{\substack{f=\uparrow,\downarrow \\ f'=\uparrow,\downarrow}} \sum_{\xi_1,\xi_2} |f\rangle_1 |f'\rangle_2 \langle e_{\xi_1}|\psi_f^+\rangle \times \langle g_{\xi_2,\xi_1}|\phi_{f',\xi_1}^+\rangle |e_{\xi_1}\rangle |g_{\xi_2,\xi_1}\rangle \tag{18}$$

and similarly for the other initial states $|\!\uparrow\rangle_1|\!\downarrow\rangle_2$, $|\!\downarrow\rangle_1|\!\uparrow\rangle_2$, $|\!\downarrow\rangle_1|\!\downarrow\rangle_2$. Equation (18) is a particular case of the general evolution (7), the measuring basis $|e_\xi\rangle$ being replaced by the basis $|e_{\xi_1}\rangle|g_{\xi_2,\xi_1}\rangle$. Indeed the two successive measurements considered here correspond in the general formalism to a single measuring device consisting of the two pieces MD1 and MD2, and the action of the human observer who "reads" the result of MD1 and decides accordingly what measurement to do next is replaced by MD2 automatically getting correlated to the final state of MD1, and tuning its interaction with the second spin accordingly.

The unitary relations (10) are now replaced by the unitary relations obeyed by each measuring device separately:

$$\begin{gathered} \sum_{f,\xi_1} a_{f,\xi_1}^+\left(a_{f,\xi_1}^+\right)^* = 1, \quad \sum_{f,\xi_1} a_{f,\xi_1}^-\left(a_{f,\xi_1}^-\right)^* = 1, \\ \sum_{f,\xi_1} a_{f,\xi_1}^+\left(a_{f,\xi_1}^-\right)^* = 0, \end{gathered} \tag{19}$$

$$\begin{gathered} \sum_{f',\xi_2} b_{f',\xi_2,\xi_1}^+\left(b_{f',\xi_2,\xi_1}^+\right)^* = 1, \quad \sum_{f',\xi_2} b_{f',\xi_2,\xi_1}^-\left(b_{f',\xi_2,\xi_1}^-\right)^* = 1, \\ \sum_{f',\xi_2} b_{f',\xi_2,\xi_1}^+\left(b_{f',\xi_2,\xi_1}^-\right)^* = 0, \end{gathered} \tag{20}$$

where, as above, $f, f' = \uparrow, \downarrow$ and

$$\begin{aligned} a_{f,\xi_1}^+ &= \langle e_{\xi_1}|\psi_f^+\rangle, & b_{f',\xi_2,\xi_1}^+ &= \langle g_{\xi_2,\xi_1}|\phi_{f',\xi_1}^+\rangle, \\ a_{f,\xi_1}^- &= \langle e_{\xi_1}|\psi_f^-\rangle, & b_{f',\xi_2,\xi_1}^- &= \langle g_{\xi_2,\xi_1}|\phi_{f',\xi_1}^-\rangle. \end{aligned} \tag{21}$$

After completing these two measurements, one guesses a direction of polarization $\theta_{\xi_1\xi_2}, \varphi_{\xi_1\xi_2}$ which depends of course on both outcomes.

If (18) is to describe an optimal experiment it must satisfy (12) with $\lambda = 1/4$ [since any optimal experiment on two parallel spins must necessarily also be an extremum of the reduced problem with (11) as the only constraint]. Explicitly Eq. (12) takes the form (dropping the indices f, f', ξ_1, ξ_2)

$$\begin{gathered} -2Sa^+b^+ + CE(a^+b^- + a^-b^+) = 0, \\ 2CSE^*a^+b^+ - (a^+b^- + a^-b^+) + 2CSEa^-b^- = 0, \\ SE^*(a^+b^- + a^-b^+) - 2Ca^-b^- = 0, \end{gathered} \tag{22}$$

which must be satisfied for all i, j, ξ_1, ξ_2. We have used the notation $C = \cos(\theta_{\xi_1\xi_2}/2)$, $S = \sin(\theta_{\xi_1\xi_2}/2)$, and $E = e^{i\varphi_{\xi_1\xi_2}}$. Equations (22) solve to yield

$$\frac{a_{f,\xi_1}^+}{a_{f,\xi_1}^-} = \frac{b_{f',\xi_2,\xi_1}^+}{b_{f',\xi_2,\xi_1}^-} = \frac{CE}{S}. \tag{23}$$

Upon inserting this relation into the unitary relations (20) a contradiction is readily obtained, thereby proving that experiments such as (18) cannot be optimal experiments.

We have generalized this proof to the case where a finite number of measurements are carried out alternatively on the two spins. Whether an infinite number of such alternating measurements can reach the optimal score is still an open problem.

It is a pleasure for us to thank P. Bieliavsky for very helpful discussions.

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