Optimal minimal measurements of mixed states

G. Vidal,* J. I. Latorre, P. Pascual, and R. Tarrach
Departament d'Estructura i Constituents de la Matèria, Universitat de Barcelona, Diagonal 647, E-08028 Barcelona, Spain
and IFAE, Universitat de Barcelona, Diagonal 647, E-08028 Barcelona, Spain
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The optimal and minimal measuring strategy is obtained for a two-state system prepared in a mixed state with a probability given by any isotropic *a priori* distribution. We explicitly construct the specific optimal and minimal generalized measurements, which turn out to be independent of the *a priori* probability distribution, obtaining the best guesses for the unknown state as well as a closed expression for the maximal mean-average fidelity. We do this for up to three copies of the unknown state in a way that leads to the generalization to any number of copies, which we then present and prove. [S1050-2947(99)06206-X]

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I. INTRODUCTION

A measurement allows us to extract only a small amount of the information needed to specify a quantum state. If our preparing device produces several identical copies of the unknown state, then measurements allow us to extract more information, although only in the limit of infinitely many copies do we acquire complete knowledge of the unknown quantum state. Performing an optimal measurement, the one that extracts the maximal possible amount of information about the state, and among these a minimal measurement, the one with the minimal number of outcomes, is always a priority, especially if the process leading to the state is rare or costly. It is also the broad subject of this paper.

There are two aspects that significantly quantify the difficulty of the problem. One of them is the dimension of the Hilbert space that corresponds to the physical system we are considering. We will take the lowest one, two. The second is the *a priori* probability distribution function of the unknown state. If the state is known to be pure, the problem has been solved [1–3]. The average, mean fidelity of the optimal measurements performed on N copies of a pure state is [1]

$$\overline{F}^{(N)}_{max}(\text{pure})=\frac{N+1}{N+2} \tag{1.1}$$

and the minimal measurements correspond, for $N=1$–5, to [3]

$$n^{(N)}_{min}(\text{pure})=2,4,6,10,12 \tag{1.2}$$

outcomes. The aim of this paper is to solve this problem when we enlarge the *a priori* probability distribution function to include mixed states: more specifically, when one assumes that it is isotropic and otherwise arbitrary, but known.

On the other hand, the difficult and heavily discussed issue about which is the abolutely unbiased probability distribution in the space of density matrices is not settled and it might even not have an unbiased solution. In any case an unbiased distribution will be isotropic in the three-dimensional Poincaré sphere covered by the Bloch vector that parametrizes the unknown density matrix and thus our results will be valid for any author's preferred candidate for an unbiased probability distribution. We will not discuss this issue further.

Let us now outline the strategy defining optimal minimal measurements. We consider the simplest possible quantum system, a two-state system. It might be the spin of an electron, the polarization of a photon, an atom at very low temperatures so that only the two lowest hyperfine states matter, a linearly trapped ion for which only the ground and the first excited vibrational states are important, etc. This state is described by a 2×2 density matrix

$$\rho(\vec{b})=\frac{1}{2}(I+\vec{b}\cdot\vec{\sigma})=\frac{1+b}{2}|\hat{b}\rangle\langle\hat{b}|+\frac{1-b}{2}|-\hat{b}\rangle\langle-\hat{b}|,$$
$$b\equiv|\vec{b}|\leqslant1, \tag{1.3}$$

where $\vec{b}$ is the Bloch vector and $|\hat{b}\rangle$ and $|-\hat{b}\rangle$ are the eigenstates of $\rho(\vec{b})$. These density matrices are prepared according to a known, isotropic, *a priori* probability distribution function given by

$$f(b)\geqslant0,\quad 4\pi\int_0^1 db\, b^2 f(b)=1. \tag{1.4}$$

Let us point out here that all our results are independent of the specific integration measure we have chosen in Eq. (1.4). This is because in all our expressions the integration measure dbb^2 and the distribution function $f(b)$ always go together and one can thus redefine the latter so as to absorb any change in the former.

We will analyze the generalized measurements performed on the state corresponding to N copies of $\rho(\vec{b})$, that is, $\rho(\vec{b})^{\otimes N}$, and determine which ones are optimal. There are two aspects to an optimal measurement: which are the positive operators correlated to the different outcomes and which are the guesses that one makes, given an outcome, about the unknown state (which we shall call $\tilde{\rho}_i$). Optimal measurements have to answer both questions by demanding that the

*Electronic address: guifre@ecm.ub.es

guesses on average lead to the highest fidelity estimation of $\rho(\vec{b})$, after averaging over the known probability distribution function $f(b)$. We will then determine which of these optimal measurements are minimal, i.e., have the minimal number of outcomes. For more than one copy $N>1$, measurements may be collective and thus may involve entanglement. We will have something to say also about the relation between optimality and entanglement. The role of cloning as part of an optimal measurement will also be studied. We will also show that for more than two copies optimal measurements that are minimal are not complete, i.e., they involve positive operators with rank larger than one (and yet are optimal).

These are the main issues that will be presented for $N=1$–3 copies in Secs. II–IV. In Sec. V we present and prove our general results for any N. Section VI briefly recollects our findings and conclusions.

II. $N=1$

Let us start with one single copy of ρ, $N=1$, and use this example to present some of the systematics of our approach. We will first perform a generalized measurement [4] on $\rho(\vec{b})$ with n outcomes, given by the operator sum decomposition

$$\sum_{i=1}^{n}\sum_{j} A_{ij}^{\dagger}A_{ij}\equiv\sum_{i=1}^{n} c_i^2\rho_i=I, \quad \rho_i=\rho_i^{\dagger}\geqslant 0, \quad \mathrm{Tr}\,\rho_i=1, \tag{2.1}$$

which implies

$$\sum_{i=1}^{n} c_i^2=2, \quad \sum_{i=1}^{n} c_i^2\vec{s}_i=0, \tag{2.2}$$

where $\vec{s}_i$ is the Bloch vector of ρ_i. If the outcome i is obtained, which happens with probability

$$c_i^2\mathrm{Tr}[\rho(\vec{b})\rho_i]=c_i^2\frac{1}{2}(1+\vec{b}\cdot\vec{s}_i), \tag{2.3}$$

one proposes $\tilde{\rho}_i$ as a guess for the unknown state $\rho(\vec{b})$. The fidelity, i.e., the measure of the goodness for a proposed guess, is quantified by [5]

$$F(\rho,\tilde{\rho}_i)\equiv(\mathrm{Tr}\sqrt{\rho^{1/2}\tilde{\rho}_i\rho^{1/2}})^2=\frac{1}{2}(1+\vec{b}\cdot\vec{r}_i+\sqrt{1-b^2}\sqrt{1-r_i^2}), \tag{2.4}$$

where $\vec{r}_i$ is the Bloch vector of $\tilde{\rho}_i$. Thus the fidelity averaged over all outcomes is

$$F^{(N=1)}(\rho)\equiv\frac{1}{4}\sum_{i=1}^{n} c_i^2(1+\vec{b}\cdot\vec{s}_i)(1+\vec{b}\cdot\vec{r}_i+\sqrt{1-b^2}\sqrt{1-r_i^2}), \tag{2.5}$$

where the superscript reminds us that we are dealing with only one copy. From here the mean fidelity, i.e., the fidelity averaged over all unknown states $\rho(\vec{b})$ weighed with the known probability distribution function $f(b)$, is readily obtained

$$\begin{aligned}\overline{F}^{(N=1)}&\equiv\int d\Omega\int_0^1 db\, b^2 f(b)F^{(N=1)}(\rho)\\&=\pi\int_0^1 db\, b^2 f(b)\sum_{i=1}^{n} c_i^2\\&\quad\times\left(1+\frac{b^2}{3}\vec{s}_i\cdot\vec{r}_i+\sqrt{1-b^2}\sqrt{1-r_i^2}\right).\end{aligned} \tag{2.6}$$

With the notation

$$I_\alpha\equiv 4\pi\int_o^1 db\, b^2 f(b)\left(\frac{1-b^2}{4}\right)^{\alpha}, \quad I_0=1 \tag{2.7}$$

(note that $I_\alpha-4I_{\alpha+1}\geqslant 0$), the average fidelity reads

$$\overline{F}^{(N=1)}=\frac{1}{4}\sum_{i=1}^{n} c_i^2\left(1+\frac{1}{3}(1-4I_1)\vec{s}_i\cdot\vec{r}_i+2I_{1/2}\sqrt{1-r_i^2}\right). \tag{2.8}$$

We now have to settle which is the best guess for the unknown initial state based on the result of our measurement, which is the proposed $\tilde{\rho}_i$ that leads to the highest mean fidelity. Let us first dispose of the case $4I_1=1$, which corresponds only to $f(b)=(1/4\pi b^2)\lim_{\epsilon\to 0}\delta(b-\epsilon)$, $\epsilon>0$. It implies a vanishing Bloch vector and thus $\rho(\vec{b})=\frac{1}{2}I$, the completely random state. Since the unknown state is necessarily the completely random state, the state is known without performing any measurement whatsoever. We will thus always assume $4I_1<1$ and only use $4I_1=1$ as a check of our results. Then from Eq. (2.8) maximization implies that the best guess corresponds to

$$\vec{r}_i=\frac{(1-4I_1)\vec{s}_i}{\sqrt{36I_{1/2}^2+(1-4I_1)^2s_i^2}}. \tag{2.9}$$

Notice that $\tilde{\rho}_i\neq\rho_i$, but $\tilde{\rho}_i$ is a known function of ρ_i, as its coefficients depend only functionally on $f(b)$. As $f(b)$ is known, Eq. (2.9) determines the optimal guess in terms of ρ_i. Substituting one obtains

$$\begin{aligned}\max_{\vec{r}_i}\overline{F}^{(N=1)}\equiv\overline{F}_m^{(N=1)}&=\frac{1}{4}\sum_{i=1}^{n} c_i^2\\&\quad\times\left(1+\frac{1}{3}\sqrt{36I_{1/2}^2+(1-4I_1)^2s_i^2}\right).\end{aligned} \tag{2.10}$$

We now have to determine the best measuring strategy, the one that leads to the largest possible fidelity. It is obviously given by $s_i=1$, i.e., by outcomes associated with rank-one projectors, and gives

$$\max_{\vec{s}_i}\overline{F}_m^{(N=1)}=\overline{F}_{max}^{(N=1)}=\frac{1}{2}\left(1+\frac{1}{3}\sqrt{36I_{1/2}^2+(1-4I_1)^2}\right). \tag{2.11}$$

This is our result for one single copy of the physical system in state $\rho(\vec{b})$ with *a priori* probability distribution $f(b)$.

Notice that we have found that optimal measurements require necessarily an operator sum decomposition in terms of rank-one projectors. It is of course obvious that one can always perform an optimal measurement with rank-one projectors. Suppose, for instance, that we have some optimal operator sum decomposition with one operator of rank two, say ρ_i. Then from its spectral decomposition

$$\rho_i = p_i |\rho_{i1}\rangle\langle\rho_{i1}| + (1-p_i)|\rho_{i2}\rangle\langle\rho_{i2}| \tag{2.12}$$

and from Eq. (2.3)

$$c_i^2 \mathrm{Tr}[\rho(\vec{b})\rho_i] = c_i^2 p_i \mathrm{Tr}[\rho(\vec{b})|\rho_{i1}\rangle\langle\rho_{i1}|] + c_i^2(1-p_i)\mathrm{Tr}[\rho(\vec{b})|\rho_{i2}\rangle\langle\rho_{i2}|], \tag{2.13}$$

it is clear that taking as the guess for ρ for both outcomes associated with $|\rho_{i1}\rangle$ and $|\rho_{i2}\rangle$ precisely $\tilde{\rho}_i$, one can trade ρ_i for its two rank-one eigenprojectors, having thus a measurement with only rank-one projectors. This result can be trivially generalized to N copies and is of course well known [6]. We will use it without further comments in obtaining $\overline{F}^{(N)}_{max}$, but it does not allow us to analyze optimal measurements that are minimal, which will need a separate treatement.

In the case we are considering here, $N=1$, the outcomes are necessarily associated with rank-one operators and thus, from Eq. (2.2), a minimal optimal measurement requires two outcomes $n^{(N=1)}_{min}=2$. This corresponds to a standard von Neumann measurement, which is a result unique for $N=1$. For $N>1$ optimal measurements are generalized measurements.

A limit of interest corresponds to considering pure states, which is obtained by taking $f(b)=(1/4\pi b^2)\lim_{b_0\to 1}\delta(b-b_0)$, $b_0<1$. It follows that $\overline{F}^{(N=1)}_{max}(\text{pure})=\frac{2}{3}$, which is the known result given in Eq. (1.1). Notice that in this case $\tilde{\rho}_i=\rho_i$ and thus the guess is precisely the pure state corresponding to the projector, while we have found that for mixed states the guess $\tilde{\rho}_i$ is a mixed state, different, though related, to the pure state corresponding to the projector. This is a different feature of optimal measurements. The two guesses correspond to two points in the interior of the Poincaré sphere and symmetric with respect to its center. In the other extreme, discussed after Eq. (2.8), when one knows that $\rho(\vec{b})$ is the completely random state, we obtain $\overline{F}^{(N=1)}_{max}(\text{random})=1$, as it should.

III. $N=2$

We will now study the situation in which two copies of the unknown state $\rho(\vec{b})$ are available, i.e., we have the state $\rho(\vec{b})\otimes\rho(\vec{b})$. As we shall see, collective measurements appear here.

Notice that by defining the exchange operator V by

$$V|\varphi\rangle\otimes|\psi\rangle = |\psi\rangle\otimes|\varphi\rangle, \quad V=V^\dagger=V^{-1}, \tag{3.1}$$

we have the exchange invariance

$$V(\rho\otimes\rho)V=\rho\otimes\rho. \tag{3.2}$$

We will consider generalized measurements for which outcomes correspond to rank-one projectors, as our purpose now is to build an optimal measurement. Thus the operator sum decomposition will be written as

$$\sum_{i=1}^{n} c_i^2 |\psi_i\rangle\langle\psi_i| = I, \quad |\psi_i\rangle \in C^2\otimes C^2. \tag{3.3}$$

Given one decomposition, one can obtain other decompositions as follows. First, obviously,

$$\sum_{i=1}^{n} c_i^2 V|\psi_i\rangle\langle\psi_i|V = I. \tag{3.4}$$

Then, introducing the eigenstates of V built from $|\psi_i\rangle$ and $V|\psi_i\rangle$,

$$|\psi_i\rangle_\pm \equiv \frac{1}{\sqrt{2}\sqrt{1\pm\langle\psi_i|V|\psi_i\rangle}}(|\psi_i\rangle \pm V|\psi_i\rangle), \tag{3.5}$$

and, as

$$|\psi_i\rangle\langle\psi_i| + V|\psi_i\rangle\langle\psi_i|V = (1+\langle\psi_i|V|\psi_i\rangle)|\psi_i\rangle_{++}\langle\psi_i| + (1-\langle\psi_i|V|\psi_i\rangle)|\psi_i\rangle_{--}\langle\psi_i|, \tag{3.6}$$

we have another decomposition

$$\frac{1}{2}\sum_{i=1}^{n} c_i^2[(1+\langle\psi_i|V|\psi_i\rangle)|\psi_i\rangle_{++}\langle\psi_i| + (1-\langle\psi_i|V|\psi_i\rangle)|\psi_i\rangle_{--}\langle\psi_i|] = I. \tag{3.7}$$

If the decomposition (3.3) corresponds to an optimal measurement, so does Eq. (3.7) just recalling Eq. (3.2) and using the same guesses. Furthermore, as the probability of the ith outcome is the sum of the probabilities of the i_+ and i_- outcomes of the decomposition of Eq. (3.7),

$$c_i^2\langle\psi_i|\rho\otimes\rho|\psi_i\rangle = \frac{c_i^2}{2}(1+\langle\psi_i|V|\psi_i\rangle)\,{}_+\langle\psi_i|\rho\otimes\rho|\psi_i\rangle_+ + \frac{c_i^2}{2}(1-\langle\psi_i|V|\psi_i\rangle)\,{}_-\langle\psi_i|\rho\otimes\rho|\psi_i\rangle_-, \tag{3.8}$$

it is enough to associate again the same guess with the i_+ and i_- outcomes to make the measurement of Eq. (3.7) optimal too. Thus optimal measurements can always be obtained by projecting on eigenstates of V.

An equivalent way of presenting these results, which will be more convenient for $N>2$, is based on the identity

$$V=\vec{S}^2 - I \tag{3.9}$$

relating the exchange operator with the square of the total spin operator

$$\vec{S} \equiv \frac{1}{2}(\vec{\sigma}\otimes I + I\otimes\vec{\sigma}). \tag{3.10}$$

Equation (3.2) now reads

$$[\vec{S}^2,\rho\otimes\rho]=0 \tag{3.11}$$

and our previous results allow us to write Eq. (3.3) as

$$|\sigma\rangle\langle\sigma|+\sum_{i=1}^{n-1} c_i^2|\tau_i\rangle\langle\tau_i|=I, \tag{3.12}$$

where $|\sigma\rangle$ is the singlet or antisymmetric state and $|\tau_i\rangle$ are triplet or symmetric states. This is an important result. It states that decomposing the Hilbert space of the two copies A and B into a direct sum of eigenspaces of $\vec{S}^2$,

$$\mathcal{H}^{(N=2)}\equiv\mathcal{H}_A\otimes\mathcal{H}_B=E_0\oplus E_1, \tag{3.13}$$

where E_s corresponds to the eigenvalue $s(s+1)$ of $\vec{S}^2$, it is enough to find optimal measurements in each of the spin eigenspaces for obtaining an optimal measurement in the whole space. The generalization of this result to $N>2$ will be essential. It will then also be convenient to use both spin and exchange invariances simultaneously.

We are ready to resume our general strategy for performing optimal measurements. First, the probability that the outcome corresponds to the singlet state is

$$\langle\sigma|\rho\otimes\rho|\sigma\rangle=\frac{1-b^2}{4}. \tag{3.14}$$

For the triplet states we have found it convenient to use the Hilbert-Schmidt parametrization

$$|\tau_i\rangle\langle\tau_i|=\frac{1}{4}[I\otimes I+\vec{t}_i\cdot\vec{\sigma}\otimes I+I\otimes\vec{t}_i\cdot\vec{\sigma}+\hat{t}_i\cdot\vec{\sigma}\otimes\hat{t}_i\cdot\vec{\sigma} + \sqrt{1-t_i^2}(\hat{u}_i\cdot\vec{\sigma}\otimes\hat{u}_i\cdot\vec{\sigma}-\hat{v}_i\cdot\vec{\sigma}\otimes\hat{v}_i\cdot\vec{\sigma})], \tag{3.15}$$

where $\hat{t}_i$, $\hat{u}_i$, and $\hat{v}_i$ are $n-1$ triads of orthonormalized vectors. Notice that $\vec{t}_i$ is the Bloch vector of the reduced density matrix

$$\mathrm{Tr}_A|\tau_i\rangle\langle\tau_i|=\mathrm{Tr}_B|\tau_i\rangle\langle\tau_i|=\frac{1}{2}(I+\vec{t}_i\cdot\vec{\sigma})\equiv\rho_i, \tag{3.16}$$

where we use subscripts A and B to earmark the Hilbert space over which the trace is performed. Furthermore, from Eq. (3.12) we have

$$\sum_{i=1}^{n-1} c_i^2=3, \quad \sum_{i=1}^{n-1} c_i^2\vec{t}_i=0, \tag{3.17}$$

and further restrictions on $\hat{u}_i$, $\hat{v}_i$, and $\hat{t}_i$ that will not be needed here. The probability that the outcome corresponds to $|\tau_i\rangle$ is

$$c_i^2\langle\tau_i|\rho\otimes\rho|\tau_i\rangle=\frac{c_i^2}{4}\{1+2\vec{b}\cdot\vec{t}_i+(\vec{b}\cdot\hat{t}_i)^2 + \sqrt{1-t_i^2}[(\vec{b}\cdot\hat{u}_i)^2-(\vec{b}\cdot\hat{v}_i)^2]\}. \tag{3.18}$$

Once outcome i is obtained one proposes $\tilde{\rho}_i$ as a guess of the unknown state $\rho(\vec{b})$. From Eq. (2.4) one obtains for the fidelity averaged over outcomes

$$F^{(N=2)}(\rho)=\frac{1}{8}(1-b^2)(1+\vec{b}\cdot\vec{r}_n+\sqrt{1-b^2}\sqrt{1-r_n^2}) + \frac{1}{8}\sum_{i=1}^{n-1} c_i^2\{1+2\vec{b}\cdot\vec{t}_i+(\vec{b}\cdot\hat{t}_i)^2 + \sqrt{1-t_i^2}[(\vec{b}\cdot\hat{u}_i)^2-(\vec{b}\cdot\hat{v}_i)^2]\} \times(1+\vec{b}\cdot\vec{r}_i+\sqrt{1-b^2}\sqrt{1-r_i^2}). \tag{3.19}$$

The mean fidelity is obtained after averaging over the state space with the probability distribution function and reads

$$\overline{F}^{(N=2)}=\frac{1}{2}(I_1+2I_{3/2}\sqrt{1-r_n^2})+\frac{1}{6}\sum_{i=1}^{n-1} c_i^2\left(1-I_1+\frac{1}{2}(1-4I_1)\vec{t}_i\cdot\vec{r}_i+2(I_{1/2}-I_{3/2})\sqrt{1-r_i^2}\right). \tag{3.20}$$

From here the best guesses are readily obtained

$$r_n=0 \tag{3.21a}$$

[except for $f(b)=(1/4\pi)\delta(b-1)$ when r_n is not determined]

$$\vec{r}_i=\frac{1-4I_1}{\sqrt{16(I_{1/2}-I_{3/2})^2+(1-4I_1)^2t_i^2}}\vec{t}_i, \quad i=1,\ldots,n-1. \tag{3.21b}$$

As before, for $N=1$, again $\tilde{\rho}_i\neq\rho_i$ is a function of ρ_i, in fact a mixture of ρ_i, and the completely random state. Substituting the best guesses, we obtain

$$\overline{F}_m^{(N=2)}=\frac{1}{2}I_1+I_{3/2}+\frac{1}{6}\sum_{i=1}^{n-1} c_i^2 \times\left(1-I_1+\frac{1}{2}\sqrt{16(I_{1/2}-I_{3/2})^2+(1-4I_1)^2t_i^2}\right). \tag{3.22}$$

The best measurement strategy is obtained for $t_i=1$, so that ρ_i is a pure state and $|\tau_i\rangle$ is a product state, without entanglement. This is a reasonable result since $\rho\otimes\rho$ has neither entanglement nor classical correlations, so it would be surprising that projecting on entangled states would lead to an optimal measuring strategy. Notice also that this result of no entanglement, which we will reencounter later for $N>2$, is independent of $f(b)$. In fact, once the specification of the operator sum decomposition does not depend on $f(b)$, it has to correspond to an optimal measurement strategy valid for pure states. However, this is known [1,2] to precisely require product states. For the singlet, which is a maximally entangled state, there are no alternatives and thus the previous argument is irrelevant. The final result is

$$\overline{F}_{max}^{(N=2)}=\frac{1}{2}+I_{3/2}+\frac{1}{4}\sqrt{16(I_{1/2}-I_{3/2})^2+(1-4I_1)^2}. \tag{3.23}$$

This final result reproduces the known limits. Indeed, the pure state result of Eq. (1.1) is readily obtained from Eq. (3.23) when $f(b)=(1/4\pi)\delta(b-1)$. Also for the completely random state $\overline{F}_{max}^{(2)}(\text{random})=1$. One can also check from the comparison of $(\overline{F}_{max}^{(i)}-\frac{1}{2})^2$ for $i=1$ and 2 that, as it should,

$$\overline{F}_{max}^{(N=2)}\geqslant\overline{F}_{max}^{(N=1)}. \tag{3.24}$$

Let us now analyze optimal measurements that are minimal. With the constraints we have been using for obtaining optimal measurements, i.e., an operator sum decomposition in terms of rank-one symmetric or antisymmetric projectors, the minimal n is 5. This is because in the three-dimensional symmetric (triplet) space a resolution of the identity in terms of symmetric product states needs four of them [3], which together with the singlet makes five. When the unknown state is known to be pure, the outcome corresponding to the singlet never happens and one can do with just four projectors. Let us now prove that one cannot do with less.

Suppose we have an optimal measurement such that one of the rank-one projectors of its operator sum decomposition $|\psi\rangle\langle\psi|$, with associated best guess $\tilde{\rho}$, is neither symmetric nor antisymmetric. Obviously the best guess associated with $V|\psi\rangle\langle\psi|V$ is also $\tilde{\rho}$. One can then build, following the arguments of Eqs. (3.5)–(3.8), an optimal measurement with $|\psi\rangle_{++}\langle\psi|$ and $|\psi\rangle_{--}\langle\psi|$ with associated best guesses $\tilde{\rho}$ for both of them. However, this is impossible, as we saw that the best guess associated with the antisymmetric state is the completely random state, while the one associated with the symmetric state has a nonvanishing Bloch vector [see Eq. (3.21b)] and thus the best guesses cannot be equal.

The very same reasoning forbids an optimal measurement with an operator sum decomposition for which one of the operators has rank larger than one, as the associated rank-one projectors that appear in its spectral decomposition will have necessarily different best guesses. The upshot of all this is that for $N=2$ minimal optimal measurements correspond to operator sum decompositions of rank-one symmetric or antisymmetric projectors and thus have five outcomes $n_{min}^{(N=2)}=5$. We will see that for $N>2$ the result that minimal measurements correspond to rank-one projectors does not hold. Notice that the five guesses are situated with one at the center of the Poincaré sphere and the other four on a concentric shell in its interior forming a regular tetrahedron.

A related question to which we turn briefly is whether circumstances exist for which von Neumann measurements can be minimal and optimal. As $C^2\otimes C^2$ is of dimension 4, a von Neumann measurement has four outcomes. We have seen that optimal measurements with four outcomes exist only when we know that the unknown state is pure. The question then is if the four triplet states, which are certainly not orthogonal, can be made orthogonal by adding them coherently to the singlet state. Notice that these states would not have a well-defined symmetry, but our previous proof that such states cannot be part of an optimal measurement fails precisely only for pure states, as then [cf. Eq. (3.21a)] r_n is arbitrary. It is thus a legitimate question. Its answer is "yes" for $N=2$ [1]. The answer for $N>2$ is not known.

Let us briefly return to the situation in which we had one copy (Sec. II) and let us clone it with a state-independent universal quantum cloner [7–11]. The conditions of strong [12] symmetry and isotropy of a universal 1-to-2 quantum cloner imply

$$\rho(\vec{b})\rightarrow\rho_c^{(2)}\equiv\frac{1}{4}[I\otimes I+\eta(\vec{b}\cdot\vec{\sigma}\otimes I+I\otimes\vec{b}\cdot\vec{\sigma})+t_{ij}\sigma_i\otimes\sigma_j],$$

$$t_{ij}=t_{ji}, \tag{3.25}$$

where η is the shrinking factor and t_{ij} depends only on the vector $\vec{b}$ and the invariant tensor δ_{ij}. Linearity, which originates in state independence, and the absence of measurements in optimal cloning [13] forbid the quadratic dependence on b_i, so that eventually $t_{ij}=t\delta_{ij}$. It is also linearity that allows us to clone straightforwardly for $N=1$ a mixed state by just mixing statistically the clones of the pure states that realize the mixed state. The values of the real parameters η and t have to be such that $\rho_c^{(2)}$ is a density matrix, i.e., such that its eigenvalues

$$\frac{1}{4}(1\pm2b\eta+t),\quad\frac{1}{4}(1+t),\quad\frac{1}{4}(1-3t) \tag{3.26}$$

lie between 0 and 1. Of course measuring on $\rho_c^{(2)}$ will allow us to learn the most about $\vec{b}$ for the largest η possible. This is precisely what optimal cloning does: $\eta=\frac{2}{3}$ and thus $t=\frac{1}{3}$. We can now perform an optimal measurement on the optimal clone $\rho_c^{(2)}$, following closely the study of the $N=2$ case, as $V\rho_c^{(2)}V=\rho_c^{(2)}$. From the results

$$\langle\sigma|\rho_c^{(2)}|\sigma\rangle=0, \tag{3.27a}$$

$$\langle\tau_i|\rho_c^{(2)}|\tau_i\rangle=\frac{1}{3}(1+\vec{b}\cdot\vec{t}_i), \tag{3.27b}$$

the expression equivalent to Eq. (3.19), after dropping an irrelevant part, is

$$F_c^{(2)}(\rho)=\frac{1}{6}\sum_{i=1}^{n-1}c_i^2(1+\vec{b}\cdot\vec{t}_i)(1+\vec{b}\cdot\vec{r}_i+\sqrt{1-b^2}\sqrt{1-r_i^2}). \tag{3.28}$$

This expression, together with Eq. (3.17), is identical to Eq. (2.5) when Eq. (2.2) is recalled. We thus recover the result of Eq. (2.11). In words, optimal cloning can be part of an optimal measurement. As a by-product we have checked that indeed $\rho_c^{(2)}$, with $t=\frac{1}{3}$ and $\eta=\frac{2}{3}$, is the optimal clone of $\rho(\vec{b})$.

Notice also the result shown in Eq. (3.27a): The optimally cloned state exists in the triplet space. This is not surprising, as the singlet space cannot carry any information about the original cloned state.

IV. $N=3$

Consider now three copies of the unknown state $\rho\otimes\rho\otimes\rho$. Let us recall its exchange invariances

$$[V_{AC},\rho\otimes\rho\otimes\rho]=[V_{BC},\rho\otimes\rho\otimes\rho]=0, \tag{4.1}$$

where A, B, and C are the subindices labeling the copies that are exchanged, and its spin invariances

$$[\vec{S}^2,\rho\otimes\rho\otimes\rho]=[\vec{S}^2_{AB},\rho\otimes\rho\otimes\rho]=0, \tag{4.2}$$

where the partial and total spin operators are

$$\vec{S}_{AB}\equiv\frac{1}{2}(\vec{\sigma}\otimes I\otimes I+I\otimes\vec{\sigma}\otimes I),\quad \vec{S}\equiv\vec{S}_{AB}+\frac{1}{2}I\otimes I\otimes\vec{\sigma}. \tag{4.3}$$

The first equality of Eq. (4.2) is obvious if one convinces oneself first that

$$\rho\otimes\rho\otimes\rho=p_3(\vec{S}\cdot\vec{b}), \tag{4.4}$$

where $p_N(x)$ is a polynomial in x of degree N. The second equality of Eq. (4.2) follows then immediately. With the adequate generalizations in going from $N=2$ to $N=3$, it can be seen that in order to obtain optimal measurements it is enough to consider operator sum decompositions whose elements are of rank one and project on states that are simultaneous eigenstates of $\vec{S}^2$ and $\vec{S}^2_{AB}$. Moreover, these states should again be eigenstates of $\vec{S}\cdot\hat{n}$ for some $\hat{n}$ with maximal eigenvalue. Using the notation $|s,s_{AB},\hat{n}\rangle$, this leads immediately to the following states in terms of which the optimal operator sum decomposition can be built:

$$\left|\frac{3}{2},1,\hat{n}\right\rangle=|\hat{n}\rangle|\hat{n}\rangle|\hat{n}\rangle, \tag{4.5a}$$

$$\left|\frac{1}{2},0,\hat{n}\right\rangle=|\sigma\rangle|\hat{n}\rangle, \tag{4.5b}$$

$$\left|\frac{1}{2},1,\hat{n}\right\rangle=\frac{1}{\sqrt{3}}(V_{AC}-V_{BC})|\sigma\rangle|\hat{n}\rangle. \tag{4.5c}$$

The first state also corresponds to the completely symmetric representation of the permutation group generated by the exchange operators and the other two correspond to the two-dimensional mixed symmetry representation of the same group. We may recall from Ref. [3] that six states of the type of Eq. (4.5a) a pointing into the six directions of the vertices of a regular octahedron resolve the identity in the four-dimensional maximal spin space $s=\frac{3}{2}$. Therefore, we obtain the optimal operator sum decomposition

$$\frac{2}{3}\sum_{i=1}^{6}(|\hat{n}_i\rangle\langle\hat{n}_i|)^{\otimes 3}+|\sigma\rangle\langle\sigma|\otimes|\hat{n}\rangle\langle\hat{n}|+|\sigma\rangle\langle\sigma|\otimes|-\hat{n}\rangle\langle-\hat{n}|$$
$$+\frac{1}{3}(V_{AC}-V_{BC})|\sigma\rangle\langle\sigma|\otimes|\hat{n}\rangle\langle\hat{n}|(V_{AC}-V_{BC})$$
$$+\frac{1}{3}(V_{AC}-V_{BC})|\sigma\rangle\langle\sigma|\otimes|-\hat{n}\rangle\langle-\hat{n}|(V_{AC}-V_{BC})=I. \tag{4.6}$$

This result recalls the decomposition into eigenspaces $E_{s,s_{AB}}$of $\vec{S}^2$ and $\vec{S}^2_{AB}$,

$$\mathcal{H}^{(N=3)}\equiv\mathcal{H}_A\otimes\mathcal{H}_B\otimes\mathcal{H}_C=E_{3/2,1}\oplus E_{1/2,0}\oplus E_{1/2,1} \tag{4.7}$$

and that under permutations $E_{1/2,0}$ can be transformed into $E_{1/2,1}$. [Let us note here that the correctness of Eq. (4.6) has been confirmed by a brute-force assumption-free computation that we performed in the early stages of this work.] Because of the isotropy of the probability distribution $f(b)$ we just need to compute the probabilities

$$\langle\hat{n}|\langle\hat{n}|\langle\hat{n}|\rho\otimes\rho\otimes\rho|\hat{n}\rangle|\hat{n}\rangle|\hat{n}\rangle=\langle\hat{n}|\rho|\hat{n}\rangle^3=\frac{1}{8}(1+\vec{b}\cdot\hat{n})^3, \tag{4.8a}$$

$$\langle\sigma|\langle\hat{n}|\rho\otimes\rho\otimes\rho|\sigma\rangle|\hat{n}\rangle=\langle\sigma|\rho\otimes\rho|\sigma\rangle\langle\hat{n}|\rho|\hat{n}\rangle$$
$$=\frac{1-b^2}{8}(1+\vec{b}\cdot\hat{n}), \tag{4.8b}$$

$$\frac{1}{3}\langle\sigma|\langle\hat{n}|(V_{AC}-V_{BC})\rho\otimes\rho\otimes\rho(V_{AC}-V_{BC})|\sigma\rangle|\hat{n}\rangle$$
$$=\langle\sigma|\langle\hat{n}|\rho\otimes\rho\otimes\rho|\sigma\rangle|\hat{n}\rangle \tag{4.8c}$$

where expression (4.8c) is obtained from

$$\frac{1}{3}(V_{AC}-V_{BC})^2|\sigma\rangle|\hat{n}\rangle=|\sigma\rangle|\hat{n}\rangle. \tag{4.9}$$

Putting all the pieces together, we obtain [from Eq. (2.3)]

$$F^{(N=3)}(\rho)=\frac{1}{4}(1-b^2)(1+\vec{b}\cdot\hat{n})$$
$$\times(1+\vec{b}\cdot\vec{r}_m+\sqrt{1-b^2}\sqrt{1-r_m^2})$$
$$+\frac{1}{4}(1+\vec{b}\cdot\hat{n})^3(1+\vec{b}\cdot\vec{r}_s+\sqrt{1-b^2}\sqrt{1-r_s^2}), \tag{4.10}$$

where $\vec{r}_m$ and $\vec{r}_s$ are the Bloch vectors of the proposed guesses of ρ corresponding to the mixed symmetry and completely symmetric projectors, respectively. Angular integration over $\hat{b}$ leads to

$$\overline{F}^{(N=3)}=\frac{1}{2}+\frac{1}{3}(I_1-4I_2)\hat{n}\cdot\vec{r}_m+2I_{3/2}\sqrt{1-r_m^2}+(I_{1/2}-2I_{3/2})\sqrt{1-r_s^2}+\frac{1}{10}(3-14I_1+8I_2)\hat{n}\cdot\vec{r}_s, \tag{4.11}$$

from which the optimal guesses are obtained for

$$\vec{r}_m=\frac{(I_1-4I_2)}{\sqrt{36I_{3/2}^2+(I_1-4I_2)^2}}\hat{n}, \tag{4.12a}$$

$$\vec{r}_s=\frac{3-14I_1+8I_2}{\sqrt{100(I_{1/2}-2I_{3/2})^2+(3-14I_1+8I_2)^2}}\hat{n}. \tag{4.12b}$$

Substitution into Eq. (4.10) leads to our final result for $N=3$,

$$\overline{F}_{max}^{(N=3)}=\frac{1}{2}+\frac{1}{3}\sqrt{36I_{3/2}^2+(I_1-4I_2)^2}+\frac{1}{10}\sqrt{100(I_{1/2}-2I_{3/2})^2+(3-14I_1+8I_2)^2}. \tag{4.13}$$

This result reproduces the pure state result of Eq. (1.1) and gives 1 for the completely random state, as in previous cases.

Let us finally discuss those optimal measurements that are minimal. Up to now we have an optimal measurement with ten outcomes. Remember that the only possibility of grouping together two rank-one projectors of the operator sum decomposition happens when the two different outcomes correspond to the same guess. Now from our results it is clear that this happens twice, that is, the guesses corresponding to the seventh and ninth terms of Eq. (4.6) are the same and given by Eq. (4.12a) and the ones corresponding to the eighth and tenth terms of Eq. (4.6) are also the same and given by Eq. (4.12a), but with opposite sign. Thus the minimal optimal measurement has eight outcomes $n_{min}^{(3)}=8$. The corresponding positive operators $\mathcal{O}_{N,s,i}$ and guesses $\rho_{N,s,i}$ for $N=3$ are [cf. Eq. (4.6)] six for the space $E_{3/2,1}$,

$$\mathcal{O}_{3,3/2,i}=\frac{2}{3}|\hat{n}_i\rangle\langle\hat{n}_i|^{\otimes 3},\quad \rho_{3,3/2,i}=\frac{1}{2}(I+r_s\hat{n}_i\cdot\vec{\sigma}), \tag{4.14}$$

and two for the space $E_{1/2,0}\oplus E_{1/2,1}$,

$$\mathcal{O}_{3,1/2,1}=|\sigma\rangle\langle\sigma|\otimes|\hat{n}\rangle\langle\hat{n}|+\frac{1}{3}(V_{AC}-V_{BC})|\sigma\rangle\langle\sigma|\otimes|\hat{n}\rangle\times\langle\hat{n}|(V_{AC}-V_{BC}),$$

$$\rho_{3,1/2,1}=\frac{1}{2}(I+r_m\hat{n}\cdot\vec{\sigma}),$$

$$\mathcal{O}_{3,1/2,2}=|\sigma\rangle\langle\sigma|\otimes|-\hat{n}\rangle\langle-\hat{n}|+\frac{1}{3}(V_{AC}-V_{BC})|\sigma\rangle\langle\sigma|\otimes|-\hat{n}\rangle\times\langle-\hat{n}|(V_{AC}-V_{BC}),$$

$$\rho_{3,1/2,2}=\frac{1}{2}(I-r_m\hat{n}\cdot\vec{\sigma}). \tag{4.15}$$

Here a minimal optimal measurement has operators of rank two in its decomposition. The Bloch vectors of the corresponding guesses are situated on two concentric shells in the interior of the Poincaré sphere.

Notice that again the measuring strategy, i.e., Eq. (4.6), is independent of $f(b)$ and thus determined actually by what is known from [1–3]: For each s the pure state strategy for $2s$ copies is the optimal strategy. This will allow us to prove the general expression for $\overline{F}_{max}^{(N)}$ and $n_{min}^{(N)}$ for any N with relative ease in the next section.

V. GENERAL RESULTS FOR $N>3$

We will analyze in this section optimal and minimal generalized measurements when a generic number N of copies of the unknown state are available. We present here the maximal fidelity $\overline{F}_{max}^{(N)}$ one can obtain on average by performing such collective measurements over $\rho^{\otimes N}$, together with the minimal number $n_{min}^{(N)}$ of outcomes an optimal generalized measurement can have. For any N we provide also a generalized measurement that is both optimal and minimal. Explicit results for the case $N=4$ are worked out in order to illustrate the general expressions.

We first display our final, general results

$$\overline{F}_{max}^{(N)}=\frac{1}{2}+\sum_{s=s_0}^{N/2}\frac{(2s+1)^2}{\frac{N}{2}+s+1}\binom{N}{\frac{N}{2}+s}\sqrt{g_1(N,s)^2+g_2(N,s)^2}, \tag{5.1}$$

where

$$g_1(N,s)\equiv\int d\Omega\int_0^1 db\, b^2 f(b)\left(\frac{1-b^2}{4}\right)^{(N+1)/2-s}\left(\frac{1+b_z}{2}\right)^{2s},$$

$$g_2(N,s)\equiv\int d\Omega\int_0^1 db\, b^2 f(b)\left(\frac{1-b^2}{4}\right)^{N/2-s}\left(\frac{1+b_z}{2}\right)^{2s}\frac{b_z}{2}, \tag{5.2}$$

b_z is the third component of $\vec{b}$, and s_0 is 0 (1/2) for even (odd) N. As for $n_{min}^{(N)}$ we have found that

$$n_{min}^{(N)}=\sum_{s=s_0}^{N/2} n_{ps}^{(2s)}, \tag{5.3}$$

where we define $n_{ps}^{(N)}\equiv n_{min}^{(N)}(\text{pure})$, $n_{ps}^{(0)}\equiv 1$. For $N=1$–5 this reads (using [3])

$$n_{min}^{(N)}=2,5,8,15,20. \tag{5.4}$$

For $N>5$ the minimal $n_{ps}^{(N)}$ relies on a conjecture proposed in [3] and this is therefore also the case of $n_{min}^{(N)}$ for $N>5$.

For some very specific *a priori* probability distributions $f(b)$ this number can be reduced. This, though, corresponds only to cases in which there is an accidental degeneracy in the proposed guesses, as in the case $f(b)=(1/4\pi)\delta(b-1)$ (pure states).

The optimal and minimal generalized measurements consists of the following decomposition of the identity operator in the space $\mathcal{H}^{(N)}=C^{2\otimes N}$ of the N copies in terms of positive operators $\mathcal{O}_{N,s,i}$ and the corresponding guesses $\rho_{N,s,i}$: For each $s\epsilon[s_0,s_0+1,\ldots,N/2-1,N/2]$, our optimal and minimal generalized measurement contains $n_{ps}^{(2s)}$ positive operators of the form

$$\mathcal{O}_{N,s,i}=c_{s,i}^2\frac{(2s+1)}{\frac{N}{2}+s+1}\binom{N}{\frac{N}{2}+s}\frac{1}{N!}\times\sum_{V\epsilon S_N}V(|\sigma\rangle\langle\sigma|^{\otimes(N/2)-s}\otimes|\hat{n}_{s,i}\rangle\langle\hat{n}_{s,i}|^{\otimes 2s})V^{\dagger},\tag{5.5}$$

where S_N is the group of the $N!$ possible permutations of N elements acting on the Hilbert space of the N copies and $c_{s,i}^2$ is such that

$$\sum_{s=s_0}^{N/2}\sum_{i=1}^{n_{ps}^{(2s)}}\mathcal{O}_{N,s,i}=I.\tag{5.6}$$

The corresponding guesses are

$$\rho_{N,s,i}=\frac{1}{2}(I+r_{N,s}\hat{n}_{s,i}\cdot\vec{\sigma}),\tag{5.7}$$

where

$$r_{N,s}=\frac{g_2(N,s)}{\sqrt{g_1(N,s)^2+g_2(N,s)^2}}.\tag{5.8}$$

The $n_{ps}^{(2s)}$ vectors $\hat{n}_{s,i}$ are distributed according to their counterparts of the $N=2s$ case of optimal estimation of pure states as described in [3] and the coefficients $c_{s,i}^2$ satisfy

$$\sum_{i=1}^{n_{ps}^{(2s)}}c_{s,i}^2\hat{n}_{s,i}=0,\quad\sum_{i=1}^{n_{ps}^{(2s)}}c_{s,i}^2=2s+1.\tag{5.9}$$

For $s=\frac{1}{2},1,\frac{3}{2},\frac{5}{2}$ they are independent of i: $c_{s,i}^2=(2s+1)/n_{ps}^{(2s)}$. All these results are essentially unique.

For $N=4$ our results can be explicitly written as

$$\bar{F}_{max}^{(N=4)}=\frac{1}{2}+2I_{5/2}+\frac{1}{6}\sqrt{(2-11I_1+12I_2)^2+36(I_{1/2}-3I_{3/2}+I_{5/2})^2}+\frac{3}{4}\sqrt{(I_1-4I_2)^2+16(I_{3/2}-I_{5/2})^2}\tag{5.10}$$

and

$$n_{min}^{(N=4)}=15.\tag{5.11}$$

The positive operator sum decomposition reads

$$I=\mathcal{O}_{4,0}+\sum_{i=1}^{4}\mathcal{O}_{4,1,i}+\sum_{i=1}^{10}\mathcal{O}_{4,2,i},\tag{5.12}$$

where to the rank-two projector

$$O_{4,0}=\frac{1}{12}\sum_{V\epsilon S_4}V|\sigma\rangle\langle\sigma|\otimes|\sigma\rangle\langle\sigma|V^{\dagger}\tag{5.13}$$

corresponds the guess

$$\rho_{4,0}=\frac{1}{2}I\quad(r_{4,0}=0).\tag{5.14}$$

The four rank-three positive operators

$$\mathcal{O}_{4,1,i}=\frac{3}{32}\sum_{V\epsilon S_4}V|\sigma\rangle\langle\sigma|\otimes|\hat{n}_{1,i}\rangle\langle\hat{n}_{1,i}|^{\otimes 2}V^{\dagger},\quad i=1,\ldots,4,\tag{5.15}$$

have associated guesses

$$\rho_{4,1,i}=\frac{1}{2}(I+r_{4,1}\hat{n}_{1,i}\cdot\vec{\sigma}),\qquad r_{4,1}=\frac{I_1-4I_2}{\sqrt{(I_1-4I_2)^2+16(I_{3/2}-I_{5/2})^2}}\tag{5.16}$$

(here the $\hat{n}_{1,i}$ are distributed according to a regular tetrahedron [3]) and the ten rank-one positive operators

$$\mathcal{O}_{4,2,i}=c_{2,i}^2|\hat{n}_{2,i}\rangle\langle\hat{n}_{2,i}|^{\otimes 4},\quad i=1,\ldots,10,\tag{5.17}$$

have associated guesses

$$\rho_{4,2,i}=\frac{1}{2}(I+r_{4,2}\hat{n}_{2,i}\cdot\vec{\sigma}),\qquad r_{4,2}=\frac{(2-11I_1+12I_2)^2}{\sqrt{(2-11I_1+12I_2)^2+36(I_{1/2}-3I_{3/2}+I_{5/2})^2}}\tag{5.18}$$

(a concrete solution for $\hat{n}_{2,i}$ and $c_{2,i}^2$ is given in [3]).

Let us now outline the proof of the above expressions. The proof will be based on a series of results that we have obtained in the previous sections, which we now put together in their generalized version.

1. Permutation invariance. For any element V of the permutation group of N elements S_N,

$$[V,\rho^{\otimes N}]=0 \quad \forall \quad V \epsilon S_N. \tag{5.19}$$

2. Spin invariance. With the following notation for the composite Hilbert space:

$$\mathcal{H}^{(N)} \equiv \mathcal{H}_A \otimes \mathcal{H}_B \otimes \cdots \mathcal{H}_N, \tag{5.20}$$

for the corresponding local spin operators

$$\vec{S}_A \equiv \frac{1}{2}\vec{\sigma}\otimes I^{\otimes N-1},$$

$$\vec{S}_B \equiv \frac{1}{2} I \otimes \vec{\sigma} \otimes I^{\otimes N-2}, \tag{5.21}$$

$$\vec{S}_N \equiv \frac{1}{2} I^{\otimes N-1} \otimes \vec{\sigma}$$

and for the partial and total spin operators

$$\vec{S}_{(M)} \equiv \sum_{x=A}^{M} \vec{S}_x, \quad A < \forall M < N, \quad \vec{S} \equiv \vec{S}_{(N)}, \tag{5.22}$$

the spin invariances read

$$[\vec{S}^2,\rho^{\otimes N}]=[\vec{S}^2_{(M)},\rho^{\otimes N}]=[\vec{S}^2_A,\rho^{\otimes N}]=0. \tag{5.23}$$

They are an immediate consequence of the relatively straightforward result

$$\rho(\vec{b})^{\otimes N}=p_N(\vec{S}\cdot\vec{b}), \tag{5.24}$$

where $p_N(x)$ is a polynominal of degree N in x.

3. Direct sum decomposition. Since

$$[\vec{S}^2,\vec{S}^2_{(M)}]=[\vec{S}^2_{(M)},\vec{S}^2_{(L)}]=0 \quad \forall \quad M,L, \tag{5.25}$$

the total Hilbert space can be written as a direct sum

$$\mathcal{H}^{(N)}=\oplus_{s,\{s_{(M)}\}} E_{s,\{s_{(M)}\}}, \tag{5.26}$$

where $E_{s,\{s_{(M)}\}}$ are the eigenspaces of $\vec{S}^2$ and $\vec{S}^2_{(M)}, N > \forall M > A$, with eigenvalues $s(s+1)$ and $\{s_M(s_M+1)\}$ ordered with decreasing M, respectively. For instance, for $N=4$,

$$\mathcal{H}^{(N=4)}=E_{2,3/2,1} \quad (s=2)$$
$$\oplus E_{1,3/2,1}\oplus E_{1,1/2,1}\oplus E_{1,1/2,0} \quad (s=1) \tag{5.27}$$
$$\oplus E_{0,1/2,1}\oplus E_{0,1/2,0} \quad (s=0).$$

Of course only those eigenvalues consistent with the spin composition rules appear.

4. Permutation group equivalence. For a given $s < N/2$ all the spaces $E_{s,\{s_{(M)}\}}$ corresponding to it can be obtained from one of them with the help of the elements of the permutation group. The one that we retain for our proof as reference space is the one with the maximal number of vanishing partial spins,

$$E_{s,s-1/2,s-1,\ldots 0,1/2,0} \tag{5.28}$$

(with $N/2-s$ zeros). There are as many of these equivalent spaces as the dimension of the irreducible representation of S_N in a space of total spin s,

$$d_N(s)=\begin{pmatrix} N \\ \frac{N}{2}+s \end{pmatrix} \frac{2s+1}{\frac{N}{2}+s+1}. \tag{5.29}$$

From this result one can check the dimensional consistency of expression (5.26),

$$2^N=\sum_{s=s_0}^{N/2}(2s+1)d_N(s), \quad s_0=0 \text{ or } \frac{1}{2}. \tag{5.30}$$

5. Optimal pure state measuring strategy. In each of the reference spaces of the type of Eq. (5.28), where any vector is of the form

$$|\sigma\rangle^{\otimes N/2-s}\otimes|\psi\rangle, \quad |\psi\rangle=V|\psi\rangle \in C^{2\otimes 2s} \quad \forall \quad V\in S_{2s}, \tag{5.31}$$

the best measuring strategy turns out to be the one corresponding to $2s$ copies of an unknown pure state [1–3] and thus projects onto states of the form

$$|\sigma\rangle^{\otimes N/2-s}\otimes|\hat{n}\rangle^{\otimes 2s}. \tag{5.32}$$

Notice that the singlets act as an identity in the reference space of Eq. (5.28) and that the states (5.32) are the ones in Eq. (5.31) with less entanglement. From here, and recalling Eq. (5.29), one readily obtains Eqs. (5.5) and (5.6). The fact that the guesses of Eq. (5.7) can be grouped together due to the permutation equivalence and thus have to be made only for the reference space has been taken into account already in writing Eq. (5.5). Notice that the operators of Eq. (5.5) are of rank $d_N(s)$.

We are now ready to perform the final computation of

$$\overline{F}^{(N)}_{max}=\sum_{s=s_0}^{N/2}\sum_{i=1}^{n^{(2s)}_{ps}}\int d\Omega \int_0^1 db\, b^2 f(b)$$
$$\times \mathrm{Tr}(O_{N,s,i}\rho^{\otimes N})F(\rho,\rho_{N,s,i}). \tag{5.33}$$

From

$$\mathrm{Tr}(O_{N,s,i}\rho^{\otimes N})=c^2_{s,i}d_N(s)\left(\frac{1-b^2}{4}\right)^{N/2-s}\left(\frac{1+\vec{b}\cdot\hat{n}_{s,i}}{2}\right)^{2s}, \tag{5.34}$$

which is obtained from Eqs. (4.8a), (5.5), and (5.29), Eq. (5.33) can be written as

$$\overline{F}^{(N)}_{max}=\sum_{s=s_0}^{N/2}(2s+1)d_N(s)\int d\Omega\int_0^1 db\, b^2 f(b)$$
$$\times\left(\frac{1-b^2}{4}\right)^{N/2-s}\left(\frac{1+\vec{b}\cdot\hat{n}}{2}\right)^{2s}\frac{1}{2}$$
$$\times(1+r_{N,s}\vec{b}\cdot\hat{n}+\sqrt{1-b^2}\sqrt{1-r^2_{N,s}}), \tag{5.35}$$

where we have used Eq. (5.9), as the contributions corresponding to different i are the same, Eq. (2.4) for the fidelity, and the subindices of $\hat{n}_{s,i}$ have been dropped, given their irrelevance at this stage of the computation. In Eq. (5.35) the first term gives $\frac{1}{2}$ and the other two depend on $r_{N,s}$, which is fixed by maximization. Choosing $\hat{n}$ in the direction of the z axis and with the definitions of Eq. (5.2), one immediately obtains Eq. (5.8) and finally our main result Eq. (5.1). The result referring to the number of outputs of minimal measurements, Eq. (5.3), follows from point 5 above.

VI. CONCLUSIONS

We have built the optimal and minimal measuring strategy for N copies of an unknown mixed state prepared according to a known, isotropic, but otherwise arbitrary probability distribution. The strategy is universal, i.e., independent of the probability distribution. Except for one single copy, optimal measurements have to be generalized measurements. We have obtained a closed expression for the maximal averaged mean fidelity and the associated minimal number of outcomes. In obtaining these expressions some interesting windfall results emerged.

(i) Best guesses are not universal. They are pure states only if the unknown state is known to be pure.

(ii) Optimal measurements require projecting onto total spin eigenspaces and within each such subspace onto total spin eigenstates with maximal total spin component in some direction. This allows us to relate them with optimal measurements corresponding to a smaller number of copies of unknown pure states.

(iii) Optimal measurements that are minimal have, beyond two copies, outcomes associated with positive operators of rank larger than one and, beyond three copies, fewer outcomes than dimensions of the Hilbert space. These optimal measurements are thus incomplete. Completing them is useless.

Our results also set the limits to optimal cloning of mixed states. The techniques developed here for dealing with copies of mixed states will be useful for solving related problems.

Note added. After finishing this work we learned from Ignacio Cirac that he has done, together with Artur Ekert and Chiara Macchiavello, somewhat similar work using basically the same techniques [14].

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