Optimal minimal measurements of mixed states

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Abstract

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 averaged fidelity. We do this for up to three copies of the unknown state in a way which leads to the generalization to any number of copies, which we then present and prove.
1 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 to extract more information, although only in the limit of infinitely many copies we acquire complete knowledge of the unknown quantum state. Performing an optimal measurement, the one which 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 which significantly quantify the difficulty of the problem. One of them is the dimension of the Hilbert space which 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, 2, 3]. The averaged, mean fidelity of the optimal measurements performed on \(N\) copies of a pure state is [1]

\[
F_{\text{max}}^{(N)}(\text{pure}) = \frac{N + 1}{N + 2} \quad (1.1)
\]

and the minimal measurements correspond, for \(N = 1\) to 5, to [3]

\[
n_{\text{min}}^{(N)}(\text{pure}) = 2, 4, 6, 10, 12 \quad (1.2)
\]

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 absolutely 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 which 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 x 2 density matrix

\[
\rho(\vec{b}) = \frac{1}{2} \left( I + \vec{b} \cdot \vec{\sigma} \right) = \frac{1 + b}{2} \ket{\hat{b}}\bra{\hat{b}} + \frac{1 - b}{2} \ket{-\hat{b}}\bra{-\hat{b}}, \quad b \equiv \left| \vec{b} \right| \leq 1, \quad (1.3)
\]
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

$$f(b) \geq 0 \quad , \quad 4\pi \int_0^1 db \ b^2 \ f(b) = 1 \ . \quad (1.4)$$

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 which 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 guesses on average lead to the highest fidelity estimation of $\rho(\hat{b})$, 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 which 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 which will be presented for $N = 1$ to 3 copies in the next three sections. In sect. 5 we present and prove our general results for any $N$. The last section briefly recollects our findings and conclusions.

2  \quad N = 1

Let us start with one single copy of $\rho$, $N = 1$, 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

$$\sum_{i=1}^n A_i^\dagger A_i \equiv \sum_{i=1}^n c_i^2 \rho_i = I \quad , \quad \rho_i = \rho_i^\dagger \geq 0 \quad , \quad \text{Tr} \rho_i = 1 \quad (2.1)$$

which implies

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

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

$$c_i^2 \ \text{Tr} \left( \rho(\vec{b}) \rho_i \right) = c_i^2 \frac{1}{2} \left( 1 + \vec{b} \cdot \vec{s}_i \right) \ , \quad (2.3)$$

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

\[ F(\rho, \tilde{\rho}_i) \equiv \left( \text{Tr} \sqrt{\rho^{1/2} \tilde{\rho}_i \rho^{1/2}} \right)^2 = \frac{1}{2} \left( 1 + \tilde{b} \cdot \tilde{r}_i + \sqrt{1 - b^2} \sqrt{1 - r_i^2} \right), \tag{2.4} \]

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

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

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 \( \rho(\tilde{b}) \) weighed with the known probability distribution function \( f(b) \), is readily obtained

\[ \overline{F}^{(N=1)} \equiv \int d\Omega \int_0^1 db \, b^2 \, f(b) F^{(N=1)}(\rho) = \pi \int_0^1 db \, b^2 \, f(b) \sum_{i=1}^{n} c_i^2 \left( 1 + \frac{b^2}{3} \tilde{s}_i \cdot \tilde{r}_i + \sqrt{1 - b^2} \sqrt{1 - r_i^2} \right). \tag{2.6} \]

With the notation

\[ I_\alpha \equiv 4\pi \int_0^1 db \, b^2 \, f(b) \left( \frac{1 - b^2}{4} \right)^\alpha, \quad I_0 = 1, \tag{2.7} \]

(note that \( I_\alpha - 4I_{\alpha+1} \geq 0 \)) the averaged fidelity reads

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

We have now to settle which is the best guess for the unknown initial state based on the result of our measurement, that is the proposed \( \tilde{\rho}_i \) which leads to the highest mean fidelity. Let us first dispose of the case \( 4I_1 = 1 \), which corresponds only to \( f(b) = \frac{1}{4\pi b^2} \lim_{\epsilon \to 0} \delta(b - \epsilon), \epsilon > 0 \). It implies a vanishing Bloch vector and thus \( \rho(\tilde{b}) = \frac{1}{2} I \), 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-up of our results. Then from eq. (2.8) maximization implies that the best guess corresponds to

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

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

\[ \max_{\tilde{r}_i} F^{(N=1)} = \overline{F}^{(N=1)} = \frac{1}{4} \sum_{i=1}^{n} c_i^2 \left( 1 + \frac{1}{3} \sqrt{36I_{1/2}^2 + (1 - 4I_1)^2 s_i^2} \right). \tag{2.10} \]
We now have to determine the best measuring strategy, the one which 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

\[
\max s_i F_m^{(N=1)} = F_{\max}^{(N=1)} = \frac{1}{2} \left( 1 + \frac{1}{3} \sqrt{36 I_i^{1/2} + (1 - 4 I_i)^2} \right). \tag{2.11}
\]

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 \( \rho_i \). 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)

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

it is clear that taking as the guess for \( \rho \) for both outcomes associated to \( |\rho_{i1}\rangle \) and \( |\rho_{i2}\rangle \) precisely \( \tilde{\rho}_i \), one can trade \( \rho_i \) 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 \( F_{\max}^{(N)} \), but it does not allow to analyze optimal measurements which are minimal, which will need a separate treatment.

In the case we are considering here, \( N = 1 \), the outcomes are necessarily associated to rank-one operators and thus, from eq. (2.2), a minimal optimal measurement requires two outcomes, \( n_{\min}^{(N=1)} = 2 \). 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

\[
f(b) = \frac{1}{\sqrt{\pi}} \lim_{b_0 \to 1} \delta(b - b_0), \quad b_0 < 1.
\]

It follows that

\[
F_{\max}^{(N=1)} (\text{pure}) = \frac{2}{3},
\]

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 new 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

\[
F_{\max}^{(N=1)} (\text{random}) = 1,
\]

as it should. One could think that minimizing \( F_{\max}^{(N=1)} \) with respect to \( f(b) \) would lead to \( \tilde{\rho}_i = \rho_i \), as pure states cover the border of the Poincaré sphere and thus maximize the naive distance between the states. This is not so. The probability distribution function

\[
f(b) = \frac{1}{40 \sqrt{\pi}} (\delta(b) + 9 \delta(b - 1))
\]

gives

\[
F_{\max}^{(N=1)} = \frac{1}{2} (1 + \frac{1}{\sqrt{10}}) < \frac{2}{3}
\]

and we believe it to be the absolute minimum.
3 \quad 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 for the first time.

Notice that defining the exchange operator $V$ by

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

we have the following exchange invariance

$$V (\rho \otimes \rho) V = \rho \otimes \rho.$$  \hfill (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

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

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

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

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

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

and, as

$$|\psi_i\rangle \langle \psi_i| + V |\psi_i\rangle \langle \psi_i| V = (1 + \langle \psi_i|V|\psi_i\rangle) |\psi_i\rangle_+ \langle \psi_i|_+ + (1 - \langle \psi_i|V|\psi_i\rangle) |\psi_i\rangle_- \langle \psi_i|_-, $$  \hfill (3.6)

we have another decomposition

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

If the decomposition eq. (3.3) corresponds to an optimal measurement, so does eq. (3.5) just recalling eq. (3.2) and using the same guesses. Furthermore, as the probability of the $i$-th outcome is the sum of the probabilities of the $i_+$ and $i_-$ outcomes of the decomposition of eq. (3.7),

$$c_i^2 \langle \psi_i|\rho \otimes \rho|\psi_i\rangle = \frac{c_i^2}{2} (1 + \langle \psi_i|V|\psi_i\rangle) + \langle \psi_i|\rho \otimes \rho|\psi_i\rangle_+ + \frac{c_i^2}{2} (1 - \langle \psi_i|V|\psi_i\rangle) - \langle \psi_i|\rho \otimes \rho|\psi_i\rangle_- $$  \hfill (3.8)
it is enough to associate again the same guess to 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, and which will be more convenient for $N > 2$, is based on the identity
\[ V = S^2 - I \] (3.9)
relating the exchange operator with the square of the total spin operator,
\[ S \equiv \frac{1}{2}(\vec{\sigma} \otimes I + I \otimes \vec{\sigma}). \] (3.10)
Eq. (3.2) now reads
\[ [S^2, \rho \otimes \rho] = 0 \] (3.11)
and our previous results allow to write eq. (3.3) as
\[ |\sigma\rangle\langle\sigma| + \sum_{i=1}^{n-1} c_i^2 |\tau_i\rangle\langle\tau_i| = I \] (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 $S^2$,
\[ \mathcal{H}^{(N=2)} = \mathcal{H}_A \otimes \mathcal{H}_B = E_0 \oplus E_1, \] (3.13)
where $E_s$ corresponds to the eigenvalue $s(s + 1)$ of $S^2$, 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
\[ \langle\sigma|\rho \otimes \rho|\sigma\rangle = \frac{1 - b^2}{4}. \] (3.14)
For the triplet states we have found it convenient to use the Hilbert-Schmidt parametrization
\[ |\tau_i\rangle\langle\tau_i| = \frac{1}{4} \left( I \otimes I + \hat{t}_i \cdot \vec{\sigma} \otimes I + I \otimes \hat{t}_i \cdot \vec{\sigma} + \hat{t}_i \cdot \vec{\sigma} \otimes \hat{t}_i \cdot \vec{\sigma} \right) \]
\[ + \sqrt{1 - t_i^2} \left( \hat{u}_i \cdot \vec{\sigma} \otimes \hat{u}_i \cdot \vec{\sigma} - \hat{v}_i \cdot \vec{\sigma} \otimes \hat{v}_i \cdot \vec{\sigma} \right) \] (3.15)
where $\hat{t}_i$, $\hat{u}_i$ and $\hat{v}_i$ are $n - 1$ triads of orthonormalized vectors. Notice that $\hat{t}_i$ is the Bloch vector of the reduced density matrix
\[ \text{Tr}_A|\tau_i\rangle\langle\tau_i| = \text{Tr}_B|\tau_i\rangle\langle\tau_i| = \frac{1}{2} \left( I + \hat{t}_i \cdot \vec{\sigma} \right) \equiv \rho_i, \] (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 $\hat{t}_i$ which will not be needed here. The probability that the outcome corresponds to $|\tau_i\rangle$ is
\[
c_i^2 \langle \tau_i | \rho \otimes \rho | \tau_i \rangle = \frac{c^2_i}{4} \left( 1 + 2 \vec{b} \cdot \vec{t}_i + (\vec{b} \cdot \hat{t}_i)^2 + \sqrt{1 - t^2_i} ((\vec{b} \cdot \hat{u}_i)^2 - (\vec{b} \cdot \hat{v}_i)^2) \right) . \tag{3.18}
\]
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
\[
F^{(N=2)}(\rho) = \frac{1}{8} (1 - b^2) \left( 1 + \vec{b} \cdot \vec{r}_n + \sqrt{1 - b^2} \sqrt{1 - r_n^2} \right)
+ \frac{1}{8} \sum_{i=1}^{n-1} c_i^2 \left( 1 + 2\vec{b} \cdot \vec{t}_i + (\vec{b} \cdot \hat{t}_i)^2 + \sqrt{1 - t^2_i} ((\vec{b} \cdot \hat{u}_i)^2 - (\vec{b} \cdot \hat{v}_i)^2) \right)
\left( 1 + \vec{b} \cdot \vec{r}_i + \sqrt{1 - b^2} \sqrt{1 - r_i^2} \right) . \tag{3.19}
\]
The mean fidelity is obtained after averaging over the state space with the probability distribution function and reads
\[
\overline{F}^{(N=2)} = \frac{1}{2} \left( I_1 + 2I_{3/2} \sqrt{1 - r_n^2} \right)
+ \frac{1}{6} \sum_{i=1}^{n-1} c_i^2 \left( 1 - I_1 + \frac{1}{2} (1 - 4I_1) \vec{t}_i \cdot \vec{r}_i + 2(I_{1/2} - I_{3/2}) \sqrt{1 - r_i^2} \right) . \tag{3.20}
\]
From here the best guesses are readily obtained
\[
r_n = 0 \text{ (except for } f(b) = \frac{1}{4\pi} \delta(b - 1) \text{ when } r_n \text{ is not determined)}
\[
\vec{r}_i = \frac{(1 - 4I_1)}{\sqrt{16(I_{1/2} - I_{3/2})^2 + (1 - 4I_1)^2 t_i^2}} \vec{t}_i \quad i = 1, \ldots, n-1 \tag{3.21}
\]
As before for $N = 1$, again $\tilde{\rho}_i \neq \rho_i$ is a function of $\rho_i$, in fact a mixture of $\rho_i$ and the completely random state. Substituting the best guesses we obtain
\[
\overline{F}_m^{(N=2)} = \frac{1}{2} I_1 + I_{3/2} + \frac{1}{6} \sum_{i=1}^{n-1} c_i^2 \left( 1 - I_1 + \frac{1}{2} \sqrt{16(I_{1/2} - I_{3/2})^2 + (1 - 4I_1)^2 t_i^2} \right) . \tag{3.22}
\]
The best measurement strategy is obtained for $t_i = 1$, so that $\rho_i$ 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 that 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. But 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

\[
F_{\text{max}}^{(N=2)} = \frac{1}{2} + I_{3/2} + \frac{1}{4} \sqrt{16(I_{1/2} - I_{3/2})^2 + (1 - 4I_1)^2}
\] (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 \( f(b) = \frac{1}{4\pi} \delta(b-1) \). Also for the completely random state \( F_{\text{max}}^{(2)}(\text{random}) = 1 \). One can also check from the comparison of \( (F_{\text{max}}^{(i)} - \frac{1}{2})^2 \) for \( i = 1 \) and 2 that, as it should,

\[
F_{\text{max}}^{(N=2)} \geq F_{\text{max}}^{(N=1)}
\] (3.24)

Let us now analyze optimal measurements which 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 five. This is because in the 3-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 not symmetric nor antisymmetric. Obviously the best guess associated to \( V|\psi\rangle\langle\psi|V \) 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. But this is impossible, as we saw that the best guess associated to the antisymmetric state is the completely random state, while the one associated to the symmetric state has a non-vanishing Bloch vector (see eq. (3.21), and thus the best guesses cannot be equal.

The very same reasoning forbids to have 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 which 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, \( n_{\text{min}}^{(N=2)} = 5 \). 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 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
four a von Neumann measurement has four outcomes. We have seen that optimal measurements with four outcomes only exist 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. first of eq. (3.21)) $r_n$ is arbitrary. It is thus a legitimate question. Its answer is yes, for $N = 2$. The answer for $N > 2$ is not known.

Let us briefly go back to the situation in which we had one copy (section 2), 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

\[
\rho(\vec{b}) \rightarrow \rho_c^{(2)} \equiv \frac{1}{4}(I \otimes I + \eta(\vec{b} \cdot \vec{\sigma} \otimes I + I \otimes \vec{b} \cdot \vec{\sigma}) + t_{ij}\sigma_i \otimes \sigma_j), \quad t_{ij} = t_{ji}, \quad (3.25)
\]

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

\[
\frac{1}{4}(1 \pm 2b\eta + t), \quad \frac{1}{4}(1 + t), \quad \frac{1}{4}(1 - 3t)
\]

lie between 0 and 1. Of course measuring on $\rho_c^{(2)}$ will allow to learn the most about $\vec{b}$ for the largest $\eta$ 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 following results,

\[
\langle \sigma | \rho_c^{(2)} | \sigma \rangle = 0, \quad \langle \tau_i | \rho_c^{(2)} | \tau_i \rangle = \frac{1}{3} \left(1 + \vec{b} \cdot \vec{t}_i\right), \quad (3.27)
\]

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

\[
F_c^{(2)}(\rho) = \frac{1}{6} \sum_{i=1}^{n-1} c_i^2 \left(1 + \vec{b} \cdot \vec{r}_i\right) \left(1 + \vec{b} \cdot \vec{r}_i + \sqrt{1 - b^2} \sqrt{1 - r_i^2}\right) \quad (3.28)
\]

This expression, together with eq. (3.17), is identical to eq. (2.3), 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 byproduct 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 the first of eq. (3.27): the optimally cloned state lives in the triplet space. This is not surprising, as the singlet space cannot carry any information about the original cloned state.
Consider now three copies of the unknown state, $\rho \otimes \rho \otimes \rho$. Let us recall its exchange invariances

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

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

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

where the partial and total spin operators are

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

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

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

where $p_N(x)$ is a polynomial in $x$ of degree $N$. The second 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 which are simultaneous eigenstates of $\vec{S}^2$ and $\vec{S}_{AB}^2$. Moreover these states should again be eigenstates of $\vec{S} \cdot \vec{n}$ for some $\vec{n}$ with maximal eigenvalue. Using the notation $|s, s_{AB}, \vec{n}\rangle$, this leads immediately to the following states in terms of which the optimal operator sum decomposition can be built:

$$|\frac{3}{2}, 1, \vec{n}\rangle = |\vec{n}\rangle|\vec{n}\rangle|\vec{n}\rangle,$$

$$|\frac{1}{2}, 0, \vec{n}\rangle = |\sigma\rangle|\vec{n}\rangle,$$

$$|\frac{1}{2}, 1, \vec{n}\rangle = \frac{1}{\sqrt{3}} (V_{AC} - V_{BC}) |\sigma\rangle|\vec{n}\rangle.$$

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 the first one of eq. (4.5) 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 following optimal operator sum decomposition

$$\sum_{i=1}^{6} (|\vec{n}_i\rangle \langle \vec{n}_i|)^{\otimes 3} + |\sigma\rangle \langle \sigma| \otimes |\vec{n}\rangle \langle \vec{n}| + |\sigma\rangle \langle \sigma| \otimes | - \vec{n}\rangle \langle - \vec{n}|$$

$$+ \frac{1}{3} (V_{AC} - V_{BC}) |\sigma\rangle \langle \sigma| \otimes |\vec{n}\rangle \langle V_{AC} - V_{BC}|$$

$$+ \frac{1}{3} (V_{AC} - V_{BC}) |\sigma\rangle \langle \sigma| \otimes | - \vec{n}\rangle \langle - \vec{n}| (V_{AC} - V_{BC}) = I.$$

(4.6)
This result recalls the decomposition into eigenspaces $E_{s,s,AB}$ of $\tilde{S}^2$ and $\tilde{S}_2^2$,
\begin{equation}
\mathcal{H}^{(N=3)} \equiv \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C = E_{2,1} \oplus E_{2,0} \oplus E_{2,1}
\end{equation}
and that under permutations $E_{2,0}$ can be transformed into $E_{2,1}$. (Let us note here that the correctness of eq. (4.6) has been confirmed by a brute force assumption-free computation which we performed in early stages of this work). Because of the isotropy of the probability distribution $f(b)$ we just need to compute the following probabilities
\begin{align}
\langle \hat{n} | \hat{n} | \rho \otimes \rho \otimes \rho | \hat{n} \rangle | \hat{n} \rangle &= \langle \hat{n} | \rho | \hat{n} \rangle^3 = \frac{1}{8} \left( 1 + \hat{b} \cdot \hat{n} \right)^3 \\
\langle \sigma | \hat{n} | \rho \otimes \rho \otimes \rho | \sigma \rangle | \hat{n} \rangle &= \langle \sigma | \rho \otimes \rho | \sigma \rangle | \rho | \rho | \hat{n} \rangle = \frac{1 - \hat{b}^2}{8} \left( 1 + \hat{b} \cdot \hat{n} \right) \\
\frac{1}{3} \langle \sigma | \hat{n} | (V_{AC} - V_{BC}) \rho \otimes \rho \otimes \rho | \sigma \rangle | \hat{n} \rangle &= \langle \sigma | \hat{n} | \rho \otimes \rho \otimes \rho | \sigma \rangle | \hat{n} \rangle
\end{align}
where the last expression is obtained from
\begin{equation}
\frac{1}{3} (V_{AC} - V_{BC})^2 | \sigma \rangle | \hat{n} \rangle = | \sigma \rangle | \hat{n} \rangle.
\end{equation}

Putting all the pieces together we obtain (from eq. (2.3))
\begin{align}
F^{(N=3)}(\rho) &= \frac{1}{4} (1 - \hat{b}^2)(1 + \hat{b} \cdot \hat{n}) \left( 1 + \hat{b} \cdot \vec{r}_m + \sqrt{1 - \hat{b}^2} \sqrt{1 - r_m^2} \right) \\
&\quad + \frac{1}{4} (1 + \hat{b} \cdot \hat{n})^3 \left( 1 + \hat{b} \cdot \vec{r}_s + \sqrt{1 - \hat{b}^2} \sqrt{1 - r_s^2} \right),
\end{align}
where $\vec{r}_m$ and $\vec{r}_s$ are the Bloch vectors of the proposed guesses of $\rho$ corresponding to the mixed symmetry and completely symmetric projectors respectively. Angular integration over $\hat{b}$ leads to
\begin{align}
\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} \\
&\quad + (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,
\end{align}
from which the optimal guesses are obtained for
\begin{align}
\vec{r}_m &= \frac{(I_1 - 4I_2)}{\sqrt{36I_{3/2}^2 + (I_1 - 4I_2)^2}} \hat{n} \\
\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}.
\end{align}
Substitution into eq. (4.10) leads to our final result for $N = 3$,
\begin{align}
F^{(N=3)}_{\text{max}} &= \frac{1}{2} + \frac{1}{3} \sqrt{36I_{3/2}^2 + (I_1 - 4I_2)^2} \\
&\quad + \frac{1}{10} \sqrt{100(I_{1/2} - 2I_{3/2})^2 + (3 - 14I_1 + 8I_2)^2}.
\end{align}
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 come to those optimal measurements which are minimal. Up to now we have an optimal measurement with 10 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 7-th and 9-th terms of eq. (4.6) are the same and given by the first of eq. (4.12), and the ones corresponding to the 8-th and 10-th terms of eq. (4.6) are also the same and given by the first of eq. (4.12), but with opposite sign. Thus the minimal optimal measurement has eight outcomes, \( n_{\text{min}}^{(3)} = 8 \). The corresponding positive operators \( O_{N,s,i} \) and guesses \( \rho_{N,s,i} \) for \( N = 3 \) are (cf. eq. (4.6)) six for the space \( E_{3/2} \):

\[
O_{3,3/2,i} = \frac{2}{3} |\hat{n}_i\rangle \langle \hat{n}_i|^{\otimes 3}, \quad \rho_{3,3/2,i} = \frac{1}{2} (I + r_s \hat{n}_i \cdot \vec{\sigma}),
\] (4.14)

and two for the space \( E_{1/2,0} \oplus E_{1/2,1} \):

\[
O_{3,1/2,1} = |\sigma\rangle \langle \sigma| \otimes |\hat{n}\rangle \langle \hat{n}| + \frac{1}{3} (V_{AC} - V_{BC}) |\sigma\rangle \langle \sigma| \otimes |\hat{n}\rangle \langle \hat{n}| (V_{AC} - V_{BC})
\]

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

\[
O_{3,1/2,2} = |\sigma\rangle \langle \sigma| \otimes |\hat{n}\rangle \langle \hat{n}| + \frac{1}{3} (V_{AC} - V_{BC}) |\sigma\rangle \langle \sigma| \otimes |\hat{n}\rangle \langle \hat{n}| (V_{AC} - V_{BC})
\]

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

This is the first time in which 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, 2, 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 \( F_{\text{max}}^{(N)} \) and \( n_{\text{min}}^{(N)} \) for any \( N \) with relative ease in the next section.

### 5 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 \( F_{\text{max}}^{(N)} \) one can obtain on average by performing such collective measurements over \( \rho^{\otimes N} \), together with the minimal number \( n_{\text{min}}^{(N)} \) of outcomes an optimal generalized measurement can have. For any \( N \) we provide also a generalized measurement which 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:

\[
F_{\text{max}}^{(N)} = \frac{1}{2} + \sum_{s=s_0}^{N/2} \frac{(2s+1)^2}{N + s + 1} \left( \frac{N}{2} + s \right) \sqrt{g_1(N,s)^2 + g_2(N,s)^2},
\]

where

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

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

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

\[
n_{\text{min}}^{(N)} = \sum_{s=s_0}^{N/2} n_{\text{ps}}^{(2s)} ,
\]

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

\[
n_{\text{min}}^{(N)} = 2, 5, 8, 15, 20.
\]

For \(N > 5\) the minimal \(n_{\text{ps}}^{(N)}\) relies on a conjecture proposed in [3], and this is therefore also the case of \(n_{\text{min}}^{(N)}\) 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 \(f(b) = \frac{1}{4\pi} \delta(b - 1)\) (pure states).

The optimal and minimal generalized measurements consists of the following decomposition of the identity operator in the space \(H^{(N)} = C^{2\otimes N}\) of the \(N\) copies in terms of positive operators \(O_{N,s,i}\) and the corresponding guesses \(\rho_{N,s,i}\): for each \(s \in [s_0, s_0 + 1, ..., \frac{N}{2} - 1, \frac{N}{2}]\), our optimal and minimal generalized measurement contains \(n_{\text{ps}}^{(2s)}\) positive operators of the form

\[
O_{N,s,i} = c_{s,i}^2 \frac{(2s+1)}{N + s + 1} \left( \frac{N}{2} + s \right) \frac{1}{N!} \sum_{V \in S_N} V \left( |\sigma\rangle \langle \sigma|^{\otimes \frac{N}{2} - s} \right. \otimes \left. |\hat{n}_{s,i}\rangle \langle \hat{n}_{s,i}|^{\otimes 2s} \right) V^\dagger,
\]

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

\[
\sum_{s=s_0}^{N/2} \sum_{i=1}^{n_{\text{ps}}^{(2s)}} O_{N,s,i} = I.
\]

The corresponding guesses are

\[
\rho_{N,s,i} = \frac{1}{2} (I + r_{N,s} \hat{n}_{s,i} \cdot \vec{\sigma}),
\]
where
\[ r_{N,s} = \frac{g_2(N,s)}{\sqrt{g_1(N,s)^2 + g_2(N,s)^2}}. \] (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
\[ \sum_{i=1}^{n_{ps}^{(2s)}} c_{s,i}^2 \hat{n}_{s,i} = 0 , \quad \sum_{i=1}^{n_{ps}^{(2s)}} c_{s,i}^2 = 2s + 1. \] (5.9)

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

For \( N = 4 \) our results can be explicitly written as
\[ F_{\max}^{(N=4)} = \frac{1}{2} + 2I_5/2 + \frac{1}{6} \sqrt{(2 - 11I_1 + 12I_2)^2 + 36 (I_{1/2}/I_{3/2} + I_{5/2})^2} \]
\[ + \frac{3}{4} \sqrt{(I_1 - 4I_2)^2} + 16 (I_{3/2} - I_{5/2})^2 \] (5.10)

and
\[ n_{\min}^{(N=4)} = 15. \] (5.11)

The positive operator sum decomposition reads
\[ I = O_{4,0} + \sum_{i=1}^{4} O_{4,1,i} + \sum_{i=1}^{10} O_{4,2,i} , \] (5.12)

where to the rank-two projector
\[ O_{4,0} = \frac{1}{12} \sum_{V \in S_4} V |\sigma\rangle \langle \sigma| \otimes |\sigma\rangle \langle \sigma| V^\dagger \] (5.13)

there corresponds the guess
\[ \rho_{4,0} = \frac{1}{2} I \quad (r_{4,0} = 0) . \] (5.14)

The 4 rank-three positive operators
\[ O_{4,1,i} = \frac{3}{32} \sum_{V \in S_4} V |\sigma\rangle \langle \sigma| \otimes |\hat{n}_{1,i}\rangle \langle \hat{n}_{1,i}| \otimes^2 V^\dagger , \quad i = 1, \ldots, 4 \] (5.15)

have associated guesses
\[ \rho_{4,1,i} = \frac{1}{2} (I + r_{4,1} \ \hat{n}_{1,i} \cdot \vec{\sigma}) , \quad r_{4,1} = \frac{I_1 - 4I_2}{\sqrt{(I_1 - 4I_2)^2 + 16 (I_{3/2} - I_{5/2})^2}} \] (5.16)
(here the $\hat{n}_{1,i}$ are distributed according to a regular tetrahedron \[3\]), and the 10 rank-one positive operators
\[ O_{4,2,i} = c_{x,i}^2 |\hat{n}_{2,i}\rangle\langle \hat{n}_{2,i}| \otimes^4, \quad i = 1, \ldots, 10 \tag{5.17} \]
have associated guesses
\[ \rho_{4,2,i} = \frac{1}{2}(I + r_{4,2} \hat{n}_{2,i} \cdot \vec{\sigma}), \quad r_{4,2} = \frac{(2 - 11I_1 + 12I_2)^2}{\sqrt{(2 - 11I_1 + 12I_2)^2 + 36(I_{1/2} - 3I_{3/2} + I_{5/2})^2}} \tag{5.18} \]
(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 which we have obtained along the previous sections and which we now put together in their generalized version:

1. Permutation invariance

For any element $V$ of the permutation group of $N$ elements, $S_N$,
\[ [V, \rho^{\otimes N}] = 0, \quad \forall V \in S_N. \tag{5.19} \]

2. Spin invariance

With the following notation for the composite Hilbert space,
\[ \mathcal{H}^{(N)} \equiv \mathcal{H}_A \otimes \mathcal{H}_B \otimes \ldots \mathcal{H}_N, \tag{5.20} \]
for the corresponding local spin operators,
\[ \vec{S}_A \equiv \frac{1}{2} \vec{\sigma} \otimes I^{\otimes N-1}, \]
\[ \vec{S}_B \equiv \frac{1}{2} I \otimes \vec{\sigma} \otimes I^{\otimes N-2}, \]
\[ \vec{S}_N \equiv \frac{1}{2} I^{\otimes N-1} \otimes \vec{\sigma}, \tag{5.21} \]
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
\[ [\vec{S}^2, \rho^{\otimes N}] = [\vec{S}_{(M)}^2, \rho^{\otimes N}] = [\vec{S}_A^2, \rho^{\otimes N}] = 0. \tag{5.23} \]
They are an immediate consequence of the following relatively straightforward result,

$$\rho(\vec{b}) \otimes N = p_N (\vec{S} \cdot \vec{b}) ,$$  \hspace{1cm} (5.24)

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

3. Direct sum decomposition

Since

$$\left[\vec{S}^2, \vec{S}^2_{(M)}\right] = \left[\vec{S}^2_{(M)}, \vec{S}^2_{(L)}\right] = 0 \quad \forall M, L$$  \hspace{1cm} (5.25)

the total Hilbert space can be written as a direct sum

$$\mathcal{H}^{(N)} = \bigoplus_{s,\{s_{(M)}\}} E_{s,\{s_{(M)}\}}$$  \hspace{1cm} (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 $s(s+1), \{s_{M}(s_{M} + 1)\}$ ordered with decreasing $M$, respectively. For instance, for $N = 4$,

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 which we retain for our proof as reference space is the one with the maximal number of vanishing partial spins,

$$E_{s,s-s-\frac{1}{2},s-\frac{1}{2},0,...,0}_{s-\frac{1}{2},0} \quad \text{(with } \frac{N}{2} - s \text{ zeros)}.$$  \hspace{1cm} (5.28)

There are as many of these equivalent spaces as the dimension of the irreducible representation of $S_N$ in a space of total spin $s$.

$$d_N(s) = \left(\frac{N}{2} + s\right) \frac{2s + 1}{\frac{N}{2} + s + 1}.$$  \hspace{1cm} (5.29)

One can check the dimensional consistency of the previous expression from eq. (5.26),

$$2^N = \sum_{s=s_0}^{\frac{N}{2}} (2s + 1) d_N(s) \quad s_0 = 0 \text{ or } \frac{1}{2}$$  \hspace{1cm} (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
\[ |\sigma\rangle \otimes N^{s} \otimes |\psi\rangle, \quad |\psi\rangle \in \mathbb{C}^{2 \otimes 2^s} \] (5.31)
the best measuring strategy turns out to be the one corresponding to \(2^s\) copies of an unknown pure state \([1, 2, 3]\), and thus projects onto states of the form
\[ |\sigma\rangle \otimes N^{s} \otimes |\tilde{n}\rangle \otimes 2^s \] (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. (5.3) are of rank \(d_N(s)\).

We are now ready to perform the final computation of
\[ F_{\text{max}}^{(N)} = \sum_{s=s_0}^{N} \sum_{i=1}^{n_{\text{bps}}} \int d\Omega \int_0^1 db \, b^2 f(b) \text{Tr} \left( O_{N,s,i} \rho^{\otimes N} \right) F(\rho, \rho_{N,s,i}). \] (5.33)
From
\[ \text{Tr} \left( O_{N,s,i} \rho^{\otimes N} \right) = c_{s,i}^2 d_N(s) \left( 1 - b^2 \right)^{N-s} \left( \frac{1 + b \cdot \hat{n}_{s,i}}{2} \right)^{2s}, \] (5.34)
which is obtained from eq. (4.8), (5.5) and (5.29), eq. (5.33) can be written as
\[ F_{\text{max}}^{(N)} = \sum_{s=s_0}^{N} (2s + 1)d_N(s) \int d\Omega \int_0^1 db \, b^2 f(b) \left( 1 - b^2 \right)^{N-s} \left( \frac{1 + b \cdot \hat{n}}{2} \right)^{2s} \]
\[ \frac{1}{2} \left( 1 + r_{N,s} \hat{b} \cdot \hat{n} + \sqrt{1 - b^2} \sqrt{1 - \hat{r}_{N,s}^2} \right) \] (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 where 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 our point 5 above.

6 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. They are:

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

2) 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 to relate them with optimal measurements corresponding to a smaller number of copies of unknown pure states.

3) Optimal measurements which are minimal have, beyond two copies, outcomes associated with positive operators of rank larger than one and, beyond three copies, less 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.

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.

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