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An effective iterative method to build the Naimark extension of rank-n POVMs

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We revisit the problem of finding the Naimark extension of a probability operator-valued measure (POVM), i.e. its implementation as a projective measurement in a larger Hilbert space. In particular, we suggest an iterative method to build the projective measurement from the sole requirements of orthogonality and positivity. Our method improves existing ones, as it may be employed also to extend POVMs containing elements with rank larger than one. It is also more effective in terms of computational steps.

Keywords: Naimark extension; Naimark theorem; POVM.

1. Introduction

Any (generalized) measurement performed on a physical system is described by a probability operator-valued measure (POVM) acting on the Hilbert space of the system. Naimark theorem[1–5] ensures that any POVM may be implemented as a projective measurement in a larger Hilbert space, which is usually referred to as the *Naimark extension* of the POVM. As a matter of fact, there are infinite Naimark extensions and the theorem also ensures that a *canonical extension* exists, i.e. an implementation as an indirect measurement, where the system under investigation is coupled to an independently prepared probe system[6] and then only the probe is subject to a (projective) measurement.[7–9]

The problem of finding the Naimark extensions of a POVM is indeed a central one in quantum technology. On the one hand, it provides a concrete model to realize the measurement,[10,11] and thus to assess entanglement cost[12] and/or implementations on different platforms.[13–18] On the other hand, it permits to evaluate the post-measurement state and thus to investigate the tradeoff between information gain and measurement disturbance,[19–25] as well as any procedure aimed at quantum control.[26]

Let us consider a set of operators $\{\Pi_m\}$ that constitute a POVM for the physical system S described by the Hilbert space $\mathcal{H}_S$, i.e.

$$\sum_{m=1}^{M} \Pi_m = I_S, \quad \Pi_m = \Pi_m^\dagger, \quad \Pi_m \geq 0. \tag{1}$$

The elements of the set are not necessarily projectors, $\Pi_n \Pi_m \neq \Pi_n \delta_{n,m}$. The Naimark theorem states that it is possible to *extend* each POVM elements to a larger (product) Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_S$ (see Appendix A) such that the extended measurement operators are projectors in the product space. In particular, it is possible to define the auxiliary Hilbert space $\mathcal{H}_A$ such that the system Hilbert space $\mathcal{H}_S$ is isomorphic to a subspace in $\mathcal{H}_A \otimes \mathcal{H}_S$, where the density operator ρ defined on $\mathcal{H}_S$ corresponds to the density operator $|e_1\rangle\langle e_1| \otimes \rho$ defined on $\mathcal{H}_A \otimes \mathcal{H}_S$. The state $|e_1\rangle$ may be chosen as the state corresponding to the first vector of the canonical basis of $\mathcal{H}_A$. Naimark theorem states that we can find projectors $\{E_m\}$

$$E_m E_n = E_m \delta_{m,n}, \quad E_m = E_m^\dagger, \quad E_m \geq 0, \tag{2}$$

each of them corresponding to a POVM element Π_m in the following sense. The distributions of the mth outcome, as obtained from $\{E_m\}$ and $\{\Pi_m\}$ on the states $|e_1\rangle\langle e_1| \otimes \rho$ and ρ, respectively, are the same, i.e.

$$\mathrm{Tr}_A[\Pi_m \rho] = \mathrm{Tr}_{AS}[(|e_1\rangle\langle e_1| \otimes \rho)E_m]. \tag{3}$$

At the operatorial level, this is expressed by the following set of relations

$$\Pi_m = \mathrm{Tr}_A[(|e_1\rangle\langle e_1| \otimes \mathbb{I}_S)E_m], \tag{4}$$

which, solved for the E_m given the Π_m, provide the desired Naimark extension of the POVM.

As it was originally suggested by Helstrom[4] the projectors $\{E_m\}$ may be built by placing a copy of Π_m in the upper-left block position of the matrix representation of $\{E_m\}$ (corresponding to the element 1 in the matrix $e_1 \cdot e_1^T$). At the same time, no explicit recipes had been provided on how to find the remaining blocks. The aim of this paper is to describe an iterative method for effectively building those blocks upon exploiting the sole requirements of orthogonality and positivity.

The problem has been addressed before,[27,28] and constructive methods to find the projective measurement have been suggested. In short, these methods amount to set up and solve a linear problem which gives the coefficients of the projectors in the canonical basis of the enlarged Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_S$. However, the focus has been on solving the problem for rank-1 POVM elements. Our iterative method is also based on solving a linear problem, shows two main advantages compared to existing techniques. On the one hand, it is more efficient in terms of computational steps and, on the other hand, it may be applied also to POVMs containing elements with rank greater than one.

The paper is structured as follows. In the next section, we introduce the iterative method, first illustrating the basic idea and then, in Secs. 2.1 and 2.2, describing in details its two building blocks, i.e. the constrained building of an idempotent matrix and the constrained building of a matrix orthogonal to a given one. In Sec. 2.3, we put everything together and illustrate the overall algorithm to build the Naimark extension of a generic rank-n POVM. In Sec. 3, we illustrate few examples of application, whereas Sec. 4 closes the paper with some concluding remarks.

2. An Iterative Method to Build the Naimark Extension of Rank-n POVMs

In the following, we will write projectors as matrices of suitable sizes composed by blocks. The first step in building the projectors E_m is analogue to the original Helstrom recipe, i.e. we define the upper-left block in the matrix of E_m equal to Π_m. The algorithm then builds the projectors one at a time, upon defining their blocks iteratively. As we will see soon, initially the blocks of the first projector are mostly zero, and the building of the following projectors populates other blocks. In this sense, the amount of nonzero rows and columns grows during the building of the projectors, and the size of the necessary auxiliary Hilbert space $\mathcal{H}_A$ is obtained only at the end of the procedure.

The algorithm initially builds the blocks of E_1 in order to satisfy the constraints (2) on itself, i.e.

$$E_1 \cdot E_1 = E_1, \quad E_1 = E_1^\dagger, \quad (E_1 \geq 0), \tag{5}$$

where the third condition (positivity) actually follows from the first two, idempotency and hermiticity. Then, we build *some blocks* of E_2 in order to satisfy the orthogonality with E_1,

$$E_1 \cdot E_2 = 0 \tag{6}$$

and then imposing the other constraints

$$E_2 \cdot E_2 = E_2, \quad E_2 = E_2^\dagger, \quad (E_2 \geq 0), \tag{7}$$

we define the remaining blocks. As we will see, this second step do not modify the previously defined blocks of E_2.

Analogously, the algorithm builds E_3 (if any) imposing its orthogonality with E_1, E_2, and then imposing that $E_3 \cdot E_3 = E_3$. The generalization is straightforward, the element E_m is built in order to satisfy at first the orthogonality with the previously built projectors, and then imposing the condition $E_m \cdot E_m = E_m$. The algorithm is thus an iterative one, since it employs the projectors already found, until all the elements are built.

The algorithm requires basically two steps repeated several times: building a matrix with some assigned blocks such that it is orthogonal to another matrix, and the completion of the matrix in order to make it idempotent, that is, satisfying

$$E_m \cdot E_m = E_m.$$

These steps are analyzed in some details in the following two sections, whereas the overall algorithm is summarized in Sec. 2.3.

2.1. *Building an idempotent matrix*

At first, let us consider the problem of building an idempotent matrix when some of its blocks are assigned. This is the case of the evaluation of E_1, which has the block Π_1 in the upper-left position. If Π_1 is already idempotent, we can just put Π_1 in the corner and set the remaining blocks to zero. If this is not the case, we can define the blocks around Π_1 such that $E_1 \cdot E_1 = E_1$, possibly employing the minimum amounts of blocks, and setting the others to zero. In what follows, we ignore the subscripts that refers to the mth element. The general problem becomes to find the adjacent blocks of the upper-left corner in order to make the matrix E idempotent.

As we will see in the following, it is enough to assume the following matrix structure for E

$$E = \begin{pmatrix} \Pi & A & 0 & \dots \\ A^\dagger & B & 0 & \dots \\ 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{8}$$

with Π a given block, while $A,\ B$ are blocks to find ($A^\dagger$ and $B \geq 0$ have been used so that $E = E^\dagger$). In the case $\Pi^2 = \Pi$, we can omit A, B since the matrix is already idempotent. Otherwise, we have to add the blocks $A, A^\dagger, B$ and the matrix E grows in sizes. The constraint

$$E \cdot E = \begin{pmatrix} \Pi & A \\ A^\dagger & B \end{pmatrix} \cdot \begin{pmatrix} \Pi & A \\ A^\dagger & B \end{pmatrix} = \begin{pmatrix} \Pi & A \\ A^\dagger & B \end{pmatrix} = E, \tag{9}$$

gives the following equations:

$$\Pi^2 + AA^\dagger = \Pi, \tag{10}$$

$$\Pi A + AB = A, \tag{11}$$

$$A^\dagger A + B^2 = B. \tag{12}$$

Equation (10) can be solved exploiting the singular value decomposition (SVD) for $\Pi = V\Lambda V^\dagger$ and $A = USW^\dagger$. Setting $U = V, W = I, S = \sqrt{\Lambda(I - \Lambda)}$ leads to $A = V\sqrt{\Lambda(I - \Lambda)}$. Assuming for the moment a full rank matrix Π, with eigenvalues strictly included in the range $(0, 1)$, Eq. (11) allows us to find $B = I - \Lambda$.

Finally, Eq. (12) is verified with the above solutions, and the blocks of E can be built as

$$E = \begin{pmatrix} \Pi & A & 0 & \dots \\ A^\dagger & B & 0 & \dots \\ 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \begin{pmatrix} V\Lambda V^\dagger & V\sqrt{\Lambda(I-\Lambda)} & 0 & \dots \\ \sqrt{\Lambda(I-\Lambda)}V^\dagger & I-\Lambda & 0 & \dots \\ 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{13}$$

A different route may be also employed upon exploiting positivity of the elements of the POVM. Indeed, for positive semi-definite Π, we have the Choleski decomposition $\Pi = YY^\dagger$ (with Y having no particular properties), which is generally less demanding than the SVD in terms of computational time. Note that if Π is not full rank, the decomposition is still available, with Y being a rectangular matrix with the same rank.

With this decomposition, Eq. (10) is solved by

$$A = Y\sqrt{I - Y^\dagger Y}, \quad A^\dagger = \sqrt{I - Y^\dagger Y}\, Y^\dagger \tag{14}$$

and $B = I - Y^\dagger Y$ follows. Finally, Eq. (12) is verified by re-writing $A^\dagger A = \sqrt{B}(I - B)\sqrt{B}$.

For rectangular Y, Eq. (14) still holds upon defining Y^{-1} as the Penrose inverse of Y, that is, the rectangular matrix satisfying $Y^{-1}Y = I$ on the support of Y. In addition, the decomposition $E = ZZ^\dagger$ is also readily available from Y,

$$E = \begin{pmatrix} YY^\dagger & Y\sqrt{I-Y^\dagger Y} & 0 & \dots \\ \sqrt{I-Y^\dagger Y}\,Y^\dagger & I-Y^\dagger Y & 0 & \dots \\ 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{15}$$

$$= \begin{pmatrix} Y \\ \sqrt{I-Y^\dagger Y} \\ 0 \\ \vdots \end{pmatrix} \cdot \begin{pmatrix} Y^\dagger & \sqrt{I-Y^\dagger Y} & 0 & \dots \end{pmatrix} = ZZ^\dagger. \tag{16}$$

2.2. *Building a matrix orthogonal to a given one*

In this section, we consider the problem of building a matrix (with some assigned blocks) such that it is orthogonal to a given one. This occurs in building, e.g. E_2, which has the upper-left block equal to Π_2 and must verify $E_1 \cdot E_2 = 0$. If we have $\Pi_1 \cdot \Pi_2 = 0$, it is enough to set the blocks adjacent to Π_2 equal to zero. In the most general case, this does not hold, and to satisfy the orthogonality condition, we have to explicitly determine the blocks around Π_2. The expression

$$E_1 \cdot E_2 = \begin{pmatrix} Y_1 Y_1^\dagger & Y_1\sqrt{I - Y_1^\dagger Y_1} \\ \sqrt{I - Y_1^\dagger Y_1}\, Y_1^\dagger & I - Y_1^\dagger Y_1 \end{pmatrix} \cdot \begin{pmatrix} \Pi_2 & A \\ A^\dagger & B \end{pmatrix} = 0, \tag{17}$$

where $\Pi_1 = Y_1 Y_1^\dagger$, provides the constraints

$$Y_1 Y_1^\dagger \Pi_2 + Y_1\sqrt{I - Y_1^\dagger Y_1} A^\dagger = 0, \tag{18}$$

$$Y_1 Y_1^\dagger A + Y_1\sqrt{I - Y_1^\dagger Y_1} B = 0, \tag{19}$$

$$\sqrt{I - Y_1^\dagger Y_1} Y_1^\dagger A + (I - Y_1^\dagger Y_1)B = 0. \tag{20}$$

Equation (18) allows us to find $A = -\Pi_2 Y_1\sqrt{I - Y_1^\dagger Y_1}$, whereas Eq. (19) provides the expression $B = \left(\sqrt{I - Y_1^\dagger Y_1}\right)^{-1} Y_1^\dagger \Pi_2 Y_1 \sqrt{I - Y_1^\dagger Y_1}$. The third Eq. (20), is indeed verified by these solutions.

At this stage, upon imposing the orthogonality with E_1, we found that E_2 has the structure

$$E_2 = \begin{pmatrix} \Pi_2 & -\Pi_2 Y_1\sqrt{I - Y_1^\dagger Y_1} & * & \cdots \\ -\left(\sqrt{I - Y_1^\dagger Y_1}\right)^{-1} Y_1^\dagger \Pi_2 & \left(\sqrt{I - Y_1^\dagger Y_1}\right)^{-1} Y_1^\dagger \Pi_2 Y_1\sqrt{I - Y_1^\dagger Y_1} & * & \cdots \\ * & * & * & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{21}$$

where the blocks indicated by $*$ are left unused and may be exploited to impose other conditions on E_2. If a decomposition $\Pi_2 = XX^\dagger$ is available, the big block just defined in (21) has a simple decomposition,

$$\begin{aligned} &\begin{pmatrix} XX^\dagger & -XX^\dagger Y_1\sqrt{I - Y_1^\dagger Y_1} \\ -\left(\sqrt{I - Y_1^\dagger Y_1}\right)^{-1} Y_1^\dagger XX^\dagger & \left(\sqrt{I - Y_1^\dagger Y_1}\right)^{-1} Y_1^\dagger XX^\dagger Y_1\sqrt{I - Y_1^\dagger Y_1} \end{pmatrix} \\ &\quad = \begin{pmatrix} X \\ -\left(\sqrt{I - Y_1^\dagger Y_1}\right)^{-1} Y_1^\dagger X \end{pmatrix} \cdot \begin{pmatrix} X^\dagger & -X^\dagger Y_1\sqrt{I - Y_1^\dagger Y_1} \end{pmatrix} = Y_2 \cdot Y_2^\dagger. \end{aligned} \tag{22}$$

Note that the blocks just defined depend on Π_1 (via its decomposition) and upon Π_2. If we have to impose the orthogonality of matrix E_m with E_1, only the nonzero blocks in E_1 would be involved. Thus, the solution would be the same substituting $\Pi_m = X_m X_m^\dagger$ in place of $\Pi_2 = X_2 X_2^\dagger$.

2.3. *The algorithm*

The algorithm builds the projectors one at a time, using the previously built projectors. For each projector E_m, two steps are performed: first the *orthogonal construction* of Sec. 2.2, which defines some blocks of E_m such that the projector is orthogonal to all the projectors previously evaluated. In the second step, leveraging the *idempotent construction* illustrated in Sec. 2.1, some other blocks are defined so that $E_m^2 = E_m$. Before applying the orthogonal or idempotent construction, it is checked whether E_m is already orthogonal to the other projectors or idempotent. If this is the case, the step is simply skipped.

The algorithm starts building E_1 with the idempotent construction, as the orthogonal one is not necessary. Π_1 is copied in the upper-left block of E_1 and the solution (15) is evaluated with $Y = Y_1,\ Y_1 Y_1^\dagger = \Pi_1$, where Y_1 has been obtained for instance from the SVD of $\Pi_1 = V_1 \Lambda_1 V_1^\dagger$, giving $Y_1 = V_1 \sqrt{\Lambda_1}$. If Π_1 is full rank, the projector E_1 has a nonzero 2×2 blocks in the upper-left corner. The remaining blocks are zero. The matrix representation reads

$$E_1 = \left(\begin{array}{cc|c} Y_1 Y_1^\dagger & Y_1\sqrt{I - Y_1^\dagger Y_1} & 0 \\ \# & I - Y_1^\dagger Y_1 & \\ \hline \multicolumn{2}{c|}{0} & 0 \end{array}\right)$$

with $\#$ the off-diagonal element such that $E_1 = E_1^\dagger$. The projector E_2 is then built using the two steps. The block Π_2 is copied in the upper-left corner, a decomposition $\Pi_2 = X_2^{(1)} X_2^{(1)\dagger}$ is evaluated (by SVD if needed) and the three blocks around are defined as in (21) leveraging on the decomposition $\Pi_1 = Y_1 Y_1^\dagger$ previously evaluated. At this point, the big block just defined has a decomposition $Y_2 Y_2^\dagger$ as in (22), and if not idempotent, the adjacent blocks need to be evaluated accordingly employing the idempotent construction of Eq. (15).

$$E_2 = \left(\begin{array}{c|c} \overbrace{\begin{matrix} \Pi_2 & -\Pi_2 Y_1 \left(\sqrt{I - Y_1^\dagger Y_1}\right)^{-1} \\ \# \left(\sqrt{I - Y_1^\dagger Y_1}\right)^{-1} & Y_1^\dagger \Pi_2 Y_1 \left(\sqrt{I - Y_1^\dagger Y_1}\right)^{-1} \end{matrix}}^{Y_2 Y_2^\dagger} & Y_2\sqrt{I - Y_2^\dagger Y_2} \\ \hline \# & I - Y_2^\dagger Y_2 \end{array}\right).$$

Note that in this case in the original matrix E_2 the 4×4 blocks in the upper left corner are defined, for a total of $4D$ rows and $4D$ columns (if Π_1, Π_2 are full rank), with D being the dimension of the system Hilbert space. In the evaluation of E_3, the same orthogonal and idempotent construction are repeated, with the difference that the first must be repeated twice to get the orthogonality with E_1 ed E_2. As usual, first the block $\Pi_3 = X_3^{(1)} X_3^{(1)\dagger}$ is copied in the upper left corner. The first blocks around Π_3 are evaluated with (21).

The newly defined big block has decomposition $X_3^{(2)} X_3^{(2)\dagger}$ obtained from (22) where $X = X_3^{(1)}$, $Y_2 = X_3^{(2)}$. The orthogonal construction (21) is repeated to get the orthogonality with E_2, employing the block $X_3^{(2)} X_3^{(2)\dagger}$ and the term Y_2 previously defined in the idempotent construction of E_2. A new bigger block is obtained with decomposition $Y_3 Y_3^{\dagger}$ as in (22).

The idempotent construction is then used employing $Y = Y_3$ as in Eq. (15). Finally, we get the matrix (note that not all the blocks have the same size)

$$E_3 = \left(\begin{array}{c|c} \overbrace{\begin{array}{c|c} \overbrace{\begin{array}{cc} \Pi_3 & -\Pi_3 \; Y_1 R_1^{-1} \\ \# & R_1^{-1} Y_1^{\dagger} \; \Pi_3 \; Y_1 R_1^{-1} \end{array}}^{X_3^{(2)} X_3^{(2)\dagger}} & -X_3^{(2)} X_3^{(2)\dagger} \; Y_2 R_2^{-1} \\ \hline \# & R_2^{-1} Y_2^{\dagger} \; X_3^{(2)} X_3^{(2)\dagger} \; Y_2 R_2^{-1} \end{array}}^{Y_3 Y_3^{\dagger}} & Y_3 R_3 \\ \hline \# & I - Y_3^{\dagger} Y_3 \end{array}\right)$$

with $R_1 = \sqrt{I - Y_1^{\dagger} Y_1}$, $R_2 = \sqrt{I - Y_2^{\dagger} Y_2}$, $R_3 = \sqrt{I - Y_3^{\dagger} Y_3}$. Note that the expression of E_3 depends upon the decompositions $Y_1 Y_1^{\dagger}, Y_2 Y_2^{\dagger}$ of the upper-left blocks of the preceding projectors. This holds for each projector E_m.

The method used to evaluate E_3 may be iterated for any subsequent projector. First, the block $\Pi_m = X_m^{(1)} X_m^{(1)\dagger}$ is copied in the upper left corner. The adjacent blocks are defined imposing the orthogonality with E_1, following the orthogonal construction. The just defined block has decomposition $X_m^{(2)} X_m^{(2)\dagger}$, and the orthogonal construction is repeated using Y_n, which is the term used in the idempotent construction of $E_n, n < m$. At the end of each orthogonal constructions, the newly defined big block is decomposed as $X_m^{(i)} X_m^{(i)\dagger}, i < m$, and the orthogonal construction is repeated until i reach m. The term $X_m^{(m)} = Y_m$ is then used in the idempotent construction to get the final block structure of E_m.

At this stage, upon following the procedure leading to E_m, a recursive construction may be also obtained for its decomposition $E_m = Z_m Z_m^{\dagger}$. For further details, see Appendix B. If all the Π_m are full rank and with eigenvalues in the range $[0, 1]$, then the size of the projectors grows exponentially. In fact, the projector E_1 has in this case 2×2 nonzero blocks, for a total of two-dimensional 2D rows and 2D columns; the projector E_2 populates 4×4 blocks, the projector E_3 has 8×8 nonzero blocks, and so on. An exception occurs if some of the blocks already satisfy the orthogonality conditions. For instance, if Π_2 is already orthogonal to Π_1, there is no need to use the adjacent blocks to obtain its orthogonality. This is also the case if the block is idempotent, since the adjacent blocks may left unused.

3. Examples

Here, we apply our procedure to obtain the Naimark extension of POVMs already presented in the literature. In this way, we are able to show the main features of the algorithm, and its advantages compared to existing ones.

3.1. *Three elements POVM*

Helstrom considered the example a three-elements POVM $\{\Pi_1, \Pi_2, \Pi_3\}$, $\Pi_1 + \Pi_2 + \Pi_3 = \mathbb{I}_S$, defined by $\Pi_k = \frac{2}{3}|\psi_k\rangle\langle\psi_k|, k = 1, 2, 3$, where[4]

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\pi/3} \\ e^{i\pi/3} \end{pmatrix}, \quad |\psi_3\rangle = -\frac{1}{\sqrt{2}}\begin{pmatrix} e^{i\pi/3} \\ e^{-i\pi/3} \end{pmatrix}. \tag{23}$$

i.e.

$$\Pi_1 = \frac{1}{3}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \Pi_2 = \frac{1}{3}\begin{pmatrix} 1 & e^{-2i\pi/3} \\ e^{2i\pi/3} & 1 \end{pmatrix}, \quad \Pi_3 = \frac{1}{3}\begin{pmatrix} 1 & e^{2i\pi/3} \\ e^{-2i\pi/3} & 1 \end{pmatrix}. \tag{24}$$

The extension originally obtained by Helstrom was based on a 2D auxiliary Hilbert space with basis $|v_1\rangle = (1, 0)^T$, $|v_2\rangle = (0, 1)^T$, and it is given by $E_k^H = |\xi_k\rangle\langle\xi_k|$, $k = 1, \ldots, 4$, where

$$|\xi_1\rangle = \sqrt{2/3}|v_1\rangle|\psi_1\rangle + \sqrt{1/3}|v_2\rangle|\psi_3\rangle, \tag{25}$$

$$|\xi_2\rangle = \sqrt{2/3}|v_1\rangle|\psi_2\rangle - \sqrt{1/3}|v_2\rangle|\psi_3\rangle, \tag{26}$$

$$|\xi_3\rangle = \sqrt{2/3}|v_1\rangle|\psi_3\rangle + \sqrt{1/3}|v_2\rangle|\psi_3\rangle, \tag{27}$$

$$|\xi_4\rangle = |v_2\rangle|\psi_3'\rangle, \tag{28}$$

$$|\psi_3'\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -e^{i\pi/3} \\ e^{-i\pi/3} \end{pmatrix}. \tag{29}$$

The iterative algorithm in this case is particularly efficient since the orthogonality construction gives also idempotent matrices. Overall, a 2D auxiliary Hilbert space is still required, but only the upper left 3-by-3 corner has nonzero coefficients.

$$E_1 = \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad E_2 = \frac{1}{3}\begin{pmatrix} 1 & e^{-\frac{2i\pi}{3}} & e^{\frac{2i\pi}{3}} & 0 \\ e^{\frac{2i\pi}{3}} & 1 & e^{-\frac{2i\pi}{3}} & 0 \\ e^{-\frac{2i\pi}{3}} & e^{\frac{2i\pi}{3}} & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{30}$$

$$E_3 = \frac{1}{3}\begin{pmatrix} 1 & e^{\frac{2i\pi}{3}} & e^{-\frac{2i\pi}{3}} & 0 \\ e^{-\frac{2i\pi}{3}} & 1 & e^{\frac{2i\pi}{3}} & 0 \\ e^{\frac{2i\pi}{3}} & e^{-\frac{2i\pi}{3}} & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{31}$$

The correctness of both solutions is verified by checking the properties of orthogonality, idempotence, and the upper left corner equal to the original POVM.

The extension proposed by Helstrom gives 4-by-4 matrices with no zero coefficients, and therefore differs for the block adjacent to the left upper corner. Here, we report the matrix expression of E_1^H for comparison with E_1 in Eq. (30)

$$E_1^H = \frac{1}{3}\begin{pmatrix} 1 & 1 & \frac{e^{\frac{2i\pi}{3}}}{\sqrt{2}} & \frac{e^{-\frac{2i\pi}{3}}}{\sqrt{2}} \\ 1 & 1 & \frac{e^{\frac{2i\pi}{3}}}{\sqrt{2}} & \frac{e^{-\frac{2i\pi}{3}}}{\sqrt{2}} \\ \frac{e^{-\frac{2i\pi}{3}}}{\sqrt{2}} & \frac{e^{-\frac{2i\pi}{3}}}{\sqrt{2}} & \frac{1}{2} & -\frac{1}{2}e^{-\frac{i\pi}{3}} \\ \frac{e^{\frac{2i\pi}{3}}}{\sqrt{2}} & \frac{e^{\frac{2i\pi}{3}}}{\sqrt{2}} & -\frac{1}{2}e^{\frac{i\pi}{3}} & \frac{1}{2} \end{pmatrix}. \tag{32}$$

3.2. *Four elements POVM*

Helstrom also considered a four-elements POVM $\{\Pi_1, \Pi_2, \Pi_3, \Pi_4\}$, with[4]

$$\Pi_k = \frac{1}{2}|\psi_k\rangle\langle\psi_k|, \quad |\psi_k\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i(k-1)\frac{\pi}{4}} \\ e^{i(k-1)\frac{\pi}{4}} \end{pmatrix}, \quad k = 1, 2, 3, 4,$$

i.e.

$$\Pi_1 = \frac{1}{4}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \Pi_2 = \frac{1}{4}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}, \quad \Pi_3 = \frac{1}{4}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad \Pi_4 = \frac{1}{4}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}. \tag{33}$$

Again, the iterative algorithm easily finds the extension since the orthogonal construction directly gives idempotent matrices, without the need of the idempotent construction.

$$E_1 = \frac{1}{4}\begin{pmatrix} 1 & 1 & \sqrt{2} & 0 \\ 1 & 1 & \sqrt{2} & 0 \\ \sqrt{2} & \sqrt{2} & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad E_2 = \frac{1}{4}\begin{pmatrix} 1 & -i & -e^{-\frac{i\pi}{4}} & e^{-\frac{i\pi}{4}} \\ i & 1 & -e^{\frac{i\pi}{4}} & e^{\frac{i\pi}{4}} \\ -e^{\frac{i\pi}{4}} & -e^{-\frac{i\pi}{4}} & 1 & -1 \\ e^{\frac{i\pi}{4}} & e^{-\frac{i\pi}{4}} & -1 & 1 \end{pmatrix}. \tag{34}$$

$$E_3 = \frac{1}{4}\begin{pmatrix} 1 & -1 & 0 & i\sqrt{2} \\ -1 & 1 & 0 & -i\sqrt{2} \\ 0 & 0 & 0 & 0 \\ -i\sqrt{2} & i\sqrt{2} & 0 & 2 \end{pmatrix}, \quad E_4 = \frac{1}{4}\begin{pmatrix} 1 & i & -e^{\frac{i\pi}{4}} & -e^{\frac{i\pi}{4}} \\ -i & 1 & -e^{-\frac{i\pi}{4}} & e^{\frac{3i\pi}{4}} \\ -e^{-\frac{i\pi}{4}} & -e^{\frac{i\pi}{4}} & 1 & 1 \\ e^{\frac{3i\pi}{4}} & -e^{\frac{i\pi}{4}} & 1 & 1 \end{pmatrix}. \tag{35}$$

3.3. *Rank-2 POVMs*

In a more recent paper, rank-2 POVM elements have been introduced to describe generalized measurements involving sets of Pauli quantum observables chosen at random, the so-called *quantum roulettes*.[29] More precisely, quantum roulettes are generalized measurements obtained by selecting the observable σ_k with a probability $\{z_k\}$ in the set of nondegenerate and isospectral observables $\{\sigma_k\}$. The POVM elements are defined as linear combination of the projectors associated with the observables outcomes.

In Ref. 29, the *canonical* Naimark extension is sought, i.e. the implementation of the generalized measurement in a larger Hilbert space using a projective indirect measurement on the ancillary system after its coupling with the system. In this scenario, Eq. (3) is rewritten as

$$\mathrm{Tr}_A[\Pi_m \rho] = \mathrm{Tr}_{AS}[(|\omega_A\rangle\langle\omega_A| \otimes \rho)U^\dagger(P_m \otimes \mathbb{I}_S)U],$$

where $|\omega_A\rangle$ is the ancillary state, U describes the coupled evolution between the systems, and P_m is the projective measurement in the ancillary system. A first example of POVM is that of a roulette obtained from the Pauli operators $\{\sigma_1, \sigma_3\}$ with probabilities $\{z, 1-z\}, z \in (0,1)$, giving the elements

$$\Pi_1 = \frac{1}{2}\begin{pmatrix} 2-z & z \\ z & z \end{pmatrix}, \quad \Pi_{-1} = \frac{1}{2}\begin{pmatrix} z & -z \\ -z & 2-z \end{pmatrix}.$$

The solution proposed uses the ancillary state $|\omega_A\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\phi}|1\rangle)$, the projectors

$$P_1 = \frac{1}{2}\begin{pmatrix} 2-z & \sqrt{z(2-z)} \\ \sqrt{z(2-z)} & z \end{pmatrix}, \quad P_{-1} = \mathbb{I} - P_1,$$

and the unitary

$$U = \begin{pmatrix} f & 0 & 0 & 0 \\ 0 & 0 & if^* & 0 \\ 0 & if^* & 0 & 0 \\ 0 & 0 & 0 & f \end{pmatrix}, \quad f = \sqrt{\sqrt{\frac{2-2z}{2-z}} + i\sqrt{\frac{z}{2-z}}}.$$

On the other hand, upon applying the iterative algorithm gives these solutions straightaway,

$$E_1 = \begin{pmatrix} 1-\frac{z}{2} & \frac{z}{2} & \frac{\sqrt{(1-z)z}}{\sqrt{2}} & 0 \\ \frac{z}{2} & \frac{z}{2} & 0 & \frac{\sqrt{(1-z)z}}{\sqrt{2}} \\ \frac{\sqrt{(1-z)z}}{\sqrt{2}} & 0 & \frac{z}{2} & -\frac{z}{2} \\ 0 & \frac{\sqrt{(1-z)z}}{\sqrt{2}} & -\frac{z}{2} & 1-\frac{z}{2} \end{pmatrix}, \quad E_{-1} = \mathbb{I}_{AS} - E_1,$$

which is equivalent to the canonical one up to a rotation in the ancillary state.

The paper presents also another example with rank-2 diagonal POVM elements,

$$\Pi_1 = \begin{pmatrix} \frac{1}{2}+f & 0 \\ 0 & \frac{1}{2}-f \end{pmatrix}, \quad \Pi_{-1} = \mathbb{I} - \Pi_1.$$

The proposed extension employs the ancillary state $|\omega_A\rangle = |e_1\rangle$, the projectors of the observable σ_3, i.e. $P_1 = |e_1\rangle\langle e_1|, P_{-1} = |e_2\rangle\langle e_2|$, and the unitary

$$U = \begin{pmatrix} \sqrt{\frac{1}{2}+f} & 0 & 0 & i\sqrt{\frac{1}{2}-f} \\ 0 & \sqrt{\frac{1}{2}-f} & i\sqrt{\frac{1}{2}+f} & 0 \\ 0 & i\sqrt{\frac{1}{2}+f} & \sqrt{\frac{1}{2}-f} & 0 \\ i\sqrt{\frac{1}{2}-f} & 0 & 0 & \sqrt{\frac{1}{2}+f} \end{pmatrix},$$

which gives

$$U^\dagger(P_1 \otimes \mathbb{I}_S)U = \begin{pmatrix} \frac{1}{2}+f & 0 & 0 & \frac{1}{2}i\sqrt{1-4f^2} \\ 0 & \frac{1}{2}-f & \frac{1}{2}i\sqrt{1-4f^2} & 0 \\ 0 & -\frac{1}{2}i\sqrt{1-4f^2} & \frac{1}{2}+f & 0 \\ -\frac{1}{2}i\sqrt{1-4f^2} & 0 & 0 & \frac{1}{2}-f \end{pmatrix}. \quad (36)$$

In this case, the iterative algorithm is particularly easy to apply since we have diagonal POVM elements, and it gives the solution

$$E_1 = \begin{pmatrix} \frac{1}{2}+f & 0 & \frac{1}{2}\sqrt{1-4f^2} & 0 \\ 0 & \frac{1}{2}-f & 0 & \frac{1}{2}\sqrt{1-4f^2} \\ \frac{1}{2}\sqrt{1-4f^2} & 0 & \frac{1}{2}-f & 0 \\ 0 & \frac{1}{2}\sqrt{1-4f^2} & 0 & \frac{1}{2}+f \end{pmatrix},$$

which is equivalent to (36) since in both cases, we can see Π_1 in the upper left bock.

4. Conclusions

In this paper, we have addressed the problem of finding the Naimark extension of a probability operator-valued measure, i.e. its implementation as a projective measurement in a larger Hilbert space. As a matter of fact, the extension of a POVM is not unique and we have exploited this degree of freedom to introduce an iterative method to build the projective measurement from the sole requirements of orthogonality and positivity. Our method improves existing ones, as it is more effective in terms of computational steps needed to determine the POVM extension. Even more importantly, our method may be employed also to extend POVMs containing elements with rank larger than one.

Since a Naimark extension provides a concrete model to realize the generalized measurement, we foresee applications of our method to assess technological solutions on different platforms and to investigate the tradeoff between information gain and measurement disturbance in generalized measurements.

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Appendix A. Kronecker Product Convention

The product space is usually defined as $\mathcal{H}_S \otimes \mathcal{H}_A$, with the system Hilbert space $\mathcal{H}_S$ on the left. However, given the definition of Kronecker product

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{pmatrix},$$

the opposite convention, i.e. describing the composite system by the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_S$, makes it easier to graphically visualize the product matrix. For instance, for a matrix given by the product of the first element of the canonical basis only one block is nonzero

$$(e_1 \cdot e_1^T) \otimes B = \begin{pmatrix} B & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}.$$

The standard convention would make the notation more cumbersome.

Appendix B. Building the Decomposition of E_m

The procedure explained in Sec. 2.3 suggests a recursive construction to directly obtain the decomposition $E_m = Z_m Z_m^\dagger$. In order to evaluate Z_m, we initially need a decomposition $\Pi_m = X_m^{(1)} X_m^{(1)\dagger}$, obtained for instance from its SVD. Then, the orthogonal construction (22) is applied with $X = X_m^{(i)}, Y_1 = Y_i$ to evaluate $Y_2 = X_m^{(i+1)}$. This step is repeated for $i = 1$ to m. The last block calculated, $X_m^{(m)}$, is defined as Y_m and used in the idempotent construction (16) employing $Y = Y_m$ to get $Z = Z_m$.

This construction can be summarized by the following matrix (in general rectangular)

$$Z_m = \begin{pmatrix} \left.\begin{array}{c} \left.\begin{array}{c} \left.\begin{array}{c} \left.\begin{array}{c} X_m^{(1)} \\ -\left(\sqrt{I - Y_1^\dagger Y_1}\right)^{-1} Y_1^\dagger X_m^{(1)} \end{array}\right\} X_m^{(2)} \\ -\left(\sqrt{I - Y_2^\dagger Y_2}\right)^{-1} Y_2^\dagger X_m^{(2)} \end{array}\right\} X_m^{(i)} \\ -\left(\sqrt{I - Y_i^\dagger Y_i}\right)^{-1} Y_i^\dagger X_m^{(i)} \end{array}\right\} X_m^{(i+1)} \\ \vdots \\ -\left(\sqrt{I - Y_{m-1}^\dagger Y_{m-1}}\right)^{-1} Y_{m-1}^\dagger X_m^{(m-1)} \end{array}\right\} X_m^{(m)} = Y_m \\ \sqrt{I - Y_m^\dagger Y_m} \end{pmatrix} \tag{B.1}$$

Note that to obtain the term Z_m the decomposition X_m of Π_m is used, as well as all the terms $Y_1, Y_2, \ldots, Y_{m-1}$ used in the preceding idempotent constructions. This is an efficient procedure, since the terms such as $\left(\sqrt{I - Y_i^\dagger Y_i}\right)^{-1} Y_i^\dagger, i < m$ are used in the later evaluation of the projectors, without the need to evaluate them at each iteration. Note that also in this procedure we should check whether the matrices $X_m^{(i)} X_m^{(i)\dagger}$ are orthogonal to E_i or if $Y_m Y_m^\dagger$ is idempotent. In this cases, there is no need to perform the orthogonal or idempotent construction of the algorithm.

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