State determination: An iterative algorithm

Dardo M. Goyeneche and Alberto C. de la Torre*
Departamento de Física, CONICET, Universidad Nacional de Mar del Plata, Funes 3350, 7600 Mar del Plata, Argentina
(Received 24 December 2007; published 23 April 2008)

An iterative algorithm for state determination, that uses as physical input the probability distributions for the eigenvalues of two or more observables in an unknown state Φ is presented. Starting from an arbitrary state Ψ_0, a succession of states Ψ_n is obtained that converges to Φ or to a Pauli partner. This algorithm for state reconstruction is efficient and robust as is seen in the numerical tests presented and is a useful tool not only for state determination but also for the study of Pauli partners. Its main ingredient is the physical imposition operator that changes any state to have the same physical properties, with respect to an observable, of another state.

DOI: 10.1103/PhysRevA.77.042116 PACS number(s): 03.65.Wj, 02.60.Gf

I. INTRODUCTION

At an early stage in the development of quantum mechanics, Pauli [1] raised the question whether the knowledge of the probability density functions for the position and momentum of a particle were sufficient in order to determine its state. That is, can we determine a unique $\psi(x)$ if we are given $\rho(x)=|\psi(x)|^2$ and $\pi(p)=|\phi(p)|^2$, where $\phi(p)$ is the Fourier transform of $\psi(x)$? Since position and momentum are the unique independent observables of the system, it was, erroneously, guessed that this Pauli problem could have an affirmative answer. This was erroneous because there may be different quantum correlations between position and momentum that are not reflected in the distributions of position and momentum individually. Indeed, many examples of Pauli partners, that is, different states $\psi_1 \neq \psi_2$ with identical probability distributions ρ and π, were found. A review of these issues, with references to the original papers, and the treatment of the problem of state reconstruction for finite and infinite dimension of the Hilbert space, can be found in Refs. [2,3]. The general problem of the determination of a quantum state from laboratory measurements turned out to be a difficult one. In this work, "laboratory measurement" means the complete measurement of an observable, that is, the determination of the probability distribution $\varrho(a_k)$ of the eigenvalues a_k of the operator A associated with the observable. Given a state Φ, the probability distribution (assuming nondegeneracy) is given by $\varrho(a_k)=|\langle\varphi_k,\Phi\rangle|^2$ where φ_k are the eigenvectors of the operator. The state is not directly observable; what can be measured, are the probability distributions of the eigenvalues of the observables and we want to be able to determine the state Φ of the system using these distributions. Besides the academic interest of quantum state reconstruction based on measurements of probability distributions, the issue has gained actuality in the last decade in the possible practical applications of quantum-information theory [4].

In order to clearly state the problem, let us consider a system described in an N-dimensional Hilbert space. The determination of the state requires the determination of $2N-2$ real numbers and a complete measurement of an observable provides $N-1$ equations. With the measurement of two observables (such as position and momentum in the Pauli problem) we have the same number of equations as unknowns. However the equations available are not linear and the system of equations will not have, in general, a unique solution. In many practical cases, a minimal additional information (such as the sign of an expectation value) is sufficient to determine the state. In this work we will not search the minimal extra information required, but instead, we will add a complete measurement of a third observable. One may think that this massive addition of information will make the system over-determined and that with three complete measurements we should always be able to find a unique state. This is wrong; there are pathological cases where the complete measurement of N observables, that is $N(N-1)$ equations, is not sufficient for the determination of a unique set of $2(N-1)$ numbers. In the other extreme, if the state happens to be equal to one of the eigenvectors of the observable measured, then, of course, just one complete measurement is sufficient to fix the state. From these two cases we conclude that the choice of the observables to be measured is crucial for the determination of the state; an observable with a peaked probability distribution provides much more information than an observable with uniform distribution. A pair of observables may provide redundant information and we expect that it is convenient to use observables as different as possible; this happens when their eigenvectors build two unbiased bases as is the case, for example, with position and momentum (two bases $\{\varphi_k\}$ and $\{\phi_r\}$ are unbiased when $|\langle\varphi_k,\phi_r\rangle| = 1/\sqrt{N} \ \forall \ k,r$, that is, every element of one basis has equal "projection" on all elements of the other basis). For this reason, unbiased bases have been intensively studied in the problem of state determination and also in quantum-information theory [5–7]. The number of mutually unbiased bases that one can define in an N-dimensional Hilbert space is not known in general although it can be proved that if N is equal to a power of a prime number, then there are $N+1$ unbiased bases. Unbiased observables, those represented by operators whose eigenvectors build unbiased bases, provide independent information; there are however pathological cases where the measurement of several unbiased observables is useless to determine a unique state: Assume, for

*delatorre@mdp.edu.ar

instance, that the state belongs to a basis that is unbiased to several other mutually unbiased bases associated with the measured observables. In this case all the probability distributions are uniform and the state cannot be uniquely determined because there are at least N different states (corresponding to the N elements of the basis to which the state belongs) all generating uniform distributions for the observables. If N is a power of a prime number we could have up to N observables with uniform distributions for N different states. This is the pathological case mentioned before: if there are $N+1$ mutually unbiased bases and we have M unbiased observables with uniform distributions then we have $N(N+1-M)$ Pauli partners, that is, different states having the same distributions.

If we make complete measurements of two or more observables we should be able to determine the state but it will not always be unique because there may be several different states having the same distributions for the measured observables. If we measure three observables, the mathematical problem would be to solve a set of $3N-3$ nonlinear equations to determine $2N-2$ numbers. One could blindly apply some numerical method to find the solution. Instead of this, we present in this work an iterative method that is physically appealing because it involves the imposition of physical data to Hilbert space elements that are approaching the solution. Another advantage of this algorithm is that it does not involve the solution of a system of equations and therefore when we change the number of observables measured or the dimension of the Hilbert space, we only have to make a trivial change in the algorithm. We will test the algorithm numerically by assuming an arbitrary state and two, three or four arbitrary observables, with them we generate the data corresponding to the distributions of the observables in the chosen state, and then we run the algorithm and we see how efficiently it returns the chosen state.

II. A METRIC FOR STATES

In order to study the convergence of an iterative algorithm for the determination of a state, we will need a concept of distance that can tell us how close we are from the wanted solution. This criteria of approach can be applied in the space of states or in the space of probability distributions. In the first case we want to know how close a particular state is from the state searched, that is, we need a metric in the space of states. In the other case a particular state generates probability distributions for some observables and we want to know how close these distributions are from the corresponding distributions generated by the state searched. In this second case we need a metric in the space of distributions. The relation between these two distances in two different spaces has been studied for several choices of distances [8]. However, the application of some of these "distances" that do not satisfy the mathematical requirements of a "metric" (positivity, symmetry, and triangular inequality) in an iterative algorithm is questionable. In this work we use a metric in the Hilbert space of states in order to study the convergence of the algorithm but we also compare the final probability distributions with the corresponding distributions used as physical input for the algorithm because, as was explained before, there are cases of different states generating the same probability distributions. The usual Hilbert space metric induced by the norm, itself induced by the internal product,

$$\delta(\Psi,\Phi) = \|\Psi - \Phi\| = \sqrt{\langle \Psi - \Phi, \Psi - \Phi \rangle}, \tag{1}$$

is not an appropriate metric for states because the states are not represented by Hilbert space elements but by rays that are sets of Hilbert space elements with an arbitrary phase. That is, a state is given by

$$R_\Psi = \{ e^{i\alpha}\Psi | \ \forall \ \alpha, \|\Psi\| = 1 \}. \tag{2}$$

The Hilbert space element Ψ is a representation of the ray and it is common practice in quantum mechanics to say that the state is given by Ψ. However, when we deal with distance between states we cannot take the induced metric mentioned before, because this metric for two Hilbert space elements, $e^{i\alpha}\phi$ and $e^{i\beta}\phi$, belonging to the same ray, that is, belonging to the same state, does not vanish. A correct concept of distance between states is given by the distance between sets

$$d(R_\Psi, R_\Phi) = \min_{\alpha,\beta} \delta(e^{i\alpha}\Psi, e^{i\beta}\Phi). \tag{3}$$

The minimization can be performed in general and we obtain

$$d(R_\Psi, R_\Phi) = \sqrt{2}\sqrt{1 - |\langle \Psi, \Phi \rangle|}. \tag{4}$$

We compare this result with $\delta(\Psi,\Phi) = \sqrt{2}\sqrt{1 - \mathrm{Re}\langle \Psi, \Phi \rangle}$ that involves only the real part of $\langle \Psi, \Phi \rangle$ and we conclude that $d(R_\Psi, R_\Phi) \leq \delta(\Psi, \Phi)$, and therefore every sequence converging in the induced metric is also convergent in the ray metric used here.

In order to have a rigorous concept of convergence we must check that the distance between states given above in Eqs. (3) and (4) is really a metric (in general, for arbitrary sets, the distance between sets is not always a metric since one can easily find examples that violate the triangle inequality). The requirement of symmetry and positivity are trivially satisfied but to prove that this distance satisfies the triangle inequality is not trivial. However, we can be sure that the distance between states is a metric because, in this particular case where the sets are rays, the distance between rays has the same value as the Hausdorff distance and one can prove that the Hausdorff distance is a metric [9]. The Hausdorff distance between two sets X and Y is defined by

$$d^H(X,Y) = \max\{\sup_{x\in X} d(x,Y), \sup_{y\in Y} d(y,X)\}. \tag{5}$$

As a final comment in this section, notice that the square root in Eq. (4) is a nuisance but it cannot be avoided because expressions such as $1 - |\langle \Psi, \Phi \rangle|$ or $1 - |\langle \Psi, \Phi \rangle|^2$ are not metrics. In order to simplify the notation, in what follows, we will denote the distance between rays $d(R_\Psi, R_\Phi)$ simply by $d(\Psi, \Phi)$.

III. PHYSICAL IMPOSITION OPERATOR

A state, or a Hilbert space element, contains encoded information about all the observables of the system. Given a

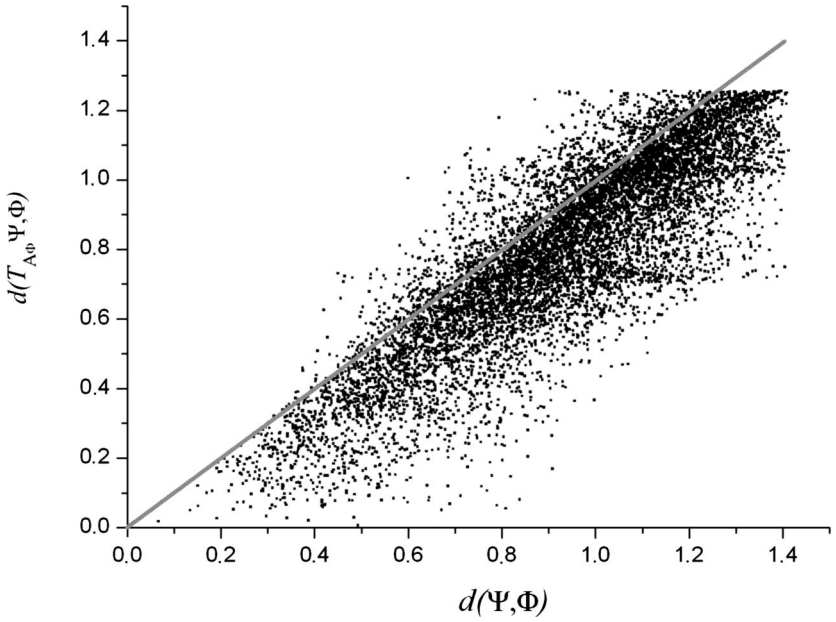

FIG. 1. Scatter plot of the distances $d(\Psi,\Phi)$ and $d(T_{A\Phi}\Psi,\Phi)$ for 8000 random initial states Ψ. Points below the diagonal indicate cases where $T_{A\Phi}$ brings Ψ closer to Φ.

state Φ, the probability distribution for an observable A is given by $\varrho(a_k)=|\langle\varphi_k,\Phi\rangle|^2$, where φ_k are the eigenvectors of the operator A associated with the observable corresponding to the eigenvalue a_k. Given any state Ψ, we can impose to this state the same distribution that the observable A has in the state Φ by means of an operator, the physical imposition operator, $T_{A\Phi}$ that involves the expansion of Ψ in the basis $\{\varphi_k\}$ of A and a change in the modulus of the expansion coefficients. That is,

$$T_{A\Phi}\Psi=\sum_k |\langle\varphi_k,\Phi\rangle|\frac{\langle\varphi_k,\Psi\rangle}{|\langle\varphi_k,\Psi\rangle|}\varphi_k. \tag{6}$$

If $\langle\varphi_k,\Psi\rangle=0$, we assume zero phase, that is $\langle\varphi_k,\Psi\rangle/|\langle\varphi_k,\Psi\rangle|=1$. The moduli of the expansion coefficients are changed in order to impose the distribution of the observable A in the state Φ but the phases are retained and therefore some information of the original state Ψ is kept in the phases. Although the numerical treatment of this operator is straightforward, its mathematical features are not simple. The operator is idempotent $T^2=T$, it has no inverse and it is not linear but $T(c\Psi)=(c/|c|)T(\Psi)$. Furthermore, the operator is bounded because $\|T\Psi\|=\|\Phi\|=1$. The fix points of this nonlinear application is the set of states that have the same distribution for the observable A as the state Φ. Notice that the operator is not only nonlinear but furthermore it cannot even be linearized for small general variations $\Psi\rightarrow\Psi+\delta\Psi$. However, as will be seen later, some sort of approximation can be made for small variations around a fix point that show that the fix points are attractive and their attractive basin are not of null measure. This mathematical complexity is unfortunate because it makes it very difficult to obtain general analytic results in order to justify the efficiency of the numerical algorithm presented later.

We will use this operator in order to develop an iterative algorithm for the determination of a state Φ using as physical input the distribution of several observables in this state. It is therefore interesting to study whether this operator, applied to an arbitrary Hilbert space element Ψ, brings us closer to the state Φ or not. For this we can compare the distance $d(\Psi,\Phi)$ with the distance $d(T_{A\Phi}\Psi,\Phi)$ for some given observable A and some state Φ. Let us then define an observable A by choosing its eigenvectors $\{\varphi_k\}$ (a basis) in a three-dimensional Hilbert space, $N=3$, and in this space let us take an arbitrary state Φ. Now we consider a large number (8000) of randomly chosen states Ψ and draw a scatter plot of the distances of this state to Φ before and after applying the imposition operator $T_{A,\Phi}$. In Fig. 1 we see that there are more points below the diagonal, showing cases where the imposition operator brings us closer to the state but there are also many cases where the operator takes us farther away from the searched state. We will later see that this has the consequence that the iterative algorithm will not converge to the desired state for every starting point.

The imposition operator will shift the state Ψ some distance $d(T_{A\Phi}\Psi,\Psi)$ that is smaller than the total distance to the state $d(\Psi,\Phi)$. That is, there is no "overshoot" that could undermine the convergence of the iterative algorithm. In order to prove this, consider the internal product

$$\begin{aligned}\langle T_{A\Phi}\Psi,\Psi\rangle &= \left\langle \sum_k |\langle\varphi_k,\Phi\rangle|\frac{\langle\varphi_k,\Psi\rangle}{|\langle\varphi_k,\Psi\rangle|}\varphi_k, \sum_r \langle\varphi_r,\Psi\rangle\varphi_r \right\rangle \\ &= \sum_k |\langle\varphi_k,\Phi\rangle||\langle\varphi_k,\Psi\rangle| = \sum_k |\langle\Phi,\varphi_k\rangle\langle\varphi_k,\Psi\rangle| \\ &\geq \left|\sum_k \langle\Phi,\varphi_k\rangle\langle\varphi_k,\Psi\rangle\right| = |\langle\Phi,\Psi\rangle|. \end{aligned} \tag{7}$$

Now, using this inequality in the definition of distance in Eq. (4) we obtain

$$d(T_{A\Phi}\Psi,\Psi)\leq d(\Psi,\Phi). \tag{8}$$

We can notice in Fig. 1 that there is a bound for the distance $d(T_{A\Phi}\Psi,\Phi)$ at some value smaller than the absolute bound for the distance $\sqrt{2}$. We will see that this bound appears when the state Φ is chosen close to one of the eigen-

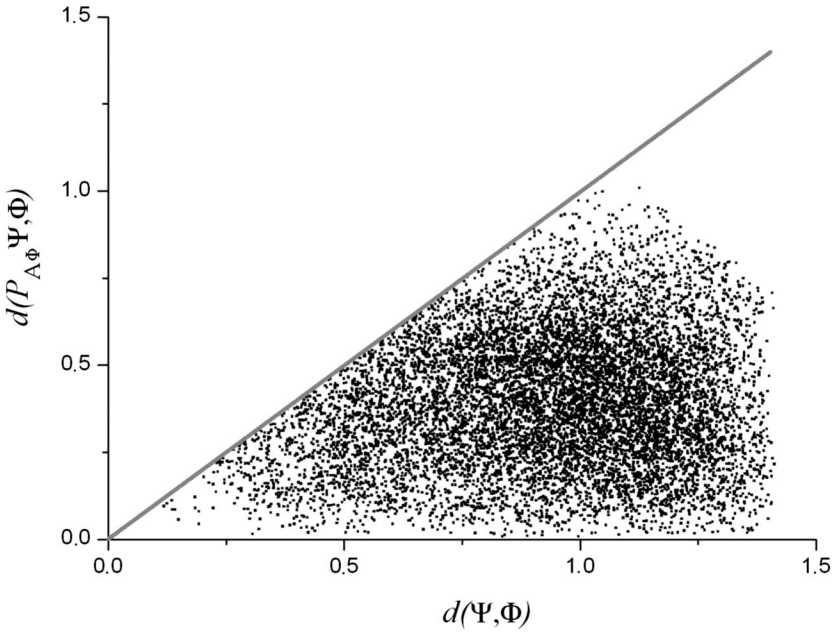

FIG. 2. Scatter plot of the distances $d(\Psi,\Phi)$ and $d(P_{A\Phi}\Psi,\Phi)$ for the same operator and states as in Fig. 1. Notice that the phase imposition operator $P_{A\Phi}$ always approaches the state Φ.

vectors of A. From the definition of the distance and of the imposition operator it follows easily that the distance of $T_{A\Phi}\Psi$ to any element of $\{\varphi_k\}$ is the same as the distance of Φ to the same element. That is,

$$d(T_{A\Phi}\Psi,\varphi_k) = d(\Phi,\varphi_k) \quad \forall \quad k, \tag{9}$$

so that $T_{A\Phi}\Psi$ is something similar to a "mirror image" of Φ reflected on $\{\varphi_k\}$. We can now use this in order to derive the bound mentioned. Consider the triangle inequality $d(T_{A\Phi}\Psi,\Phi) \leq d(T_{A\Phi}\Psi,\varphi_k) + d(\Phi,\varphi_k)$. Using Eq. (9), we obtain $d(T_{A\Phi}\Psi,\Phi) \leq 2d(\Phi,\varphi_k)$. Now we specialize this inequality for the value of k that minimizes the right-hand side, that is, the value of k that maximizes $|\langle\varphi_k,\Phi\rangle|$ or equivalently $\sqrt{\rho(a_k)}$. Then we have

$$d(T_{A\Phi}\Psi,\Phi) \leq 2 \min_k d(\Phi,\varphi_k) = 2\sqrt{2}\sqrt{1-\max_k \sqrt{\rho(a_k)}}. \tag{10}$$

If the state Φ is close enough to one of the eigenvectors of A, the corresponding maximum value of the distribution can be larger than 9/16 and the bound derived is smaller than the absolute bound $\sqrt{2}$. Notice that this bound depends only on the operator A and on the state Φ and is therefore valid for all Ψ regardless how "far" it is from Φ. With increasing dimension N of the Hilbert space, the probability that a randomly chosen state is close to one of the basis elements decreases, making the appearance of the bound less probable.

The physical imposition operator modifies the moduli of the expansion coefficients but leaves the phases unchanged. The reason for choosing this definition is that the moduli of the coefficients are measured in an experimental determination of the probability distribution of the eigenvalues of an observable and therefore this operator provides a way to impose physical properties to a state. It is unfortunate that the phases of the expansion coefficients are not directly accessible in an experiment because we could use the knowledge of the phases in a much more efficient algorithm. In a sense that will become clear later, the phases have more information about the state than the moduli. In order to clarify this let us define a phase imposition operator $P_{A\Phi}$ that leaves the moduli of the expansion coefficients unchanged but imposes the phases of the state Φ. That is

$$P_{A\Phi}\Psi = \sum_k |\langle\varphi_k,\Psi\rangle| \frac{\langle\varphi_k,\Phi\rangle}{|\langle\varphi_k,\Phi\rangle|}\varphi_k. \tag{11}$$

The same as was done before, we study how efficiently this operator approaches to the state Φ. In Fig. 2 we see the corresponding scatter plot for the same operator and states of those in Fig. 1, that shows that in all cases the application of this operator brings us closer to the wanted state. One can indeed prove that $d(P_{A\Phi}\Psi,\Phi) \leq d(\Psi,\Phi)$ considering the internal product

$$\begin{aligned}\langle P_{A\Phi}\Psi,\Phi\rangle &= \left\langle \sum_k |\langle\varphi_k,\Psi\rangle| \frac{\langle\varphi_k,\Phi\rangle}{|\langle\varphi_k,\Phi\rangle|}\varphi_k, \sum_r \langle\varphi_r,\Phi\rangle\varphi_r \right\rangle \\ &= \sum_k |\langle\varphi_k,\Psi\rangle||\langle\varphi_k,\Phi\rangle| = \sum_k |\langle\Psi,\varphi_k\rangle\langle\varphi_k,\Phi\rangle| \\ &\geq \left|\sum_k \langle\Psi,\varphi_k\rangle\langle\varphi_k,\Phi\rangle\right| = |\langle\Psi,\Phi\rangle|. \end{aligned} \tag{12}$$

Using this inequality in the definition of distance in Eq. (4) we obtain the inequality above. As said before, if we had physical information about the phases of the expansion coefficients, we could devise a very efficient algorithm. Unfortunately we do not have experimental access to the phases and this, in principle interesting, operator will not be further studied here.

IV. ALGORITHM FOR STATE DETERMINATION

In this section we will investigate an algorithm for state determination that uses as physical input the knowledge pro-

vided by the complete measurement of several observables. These measurements provide the probability distributions for the eigenvalues in the unknown state Φ. In other words, we assume that we know the physical imposition operators $T_{A\Phi}, T_{B\Phi}, T_{C\Phi}, \ldots$ for several observables. The algorithm basically consists in the iterative application of the physical imposition operators to some arbitrary initial state Ψ_0 randomly chosen.

A. Description of the algorithm

In order to understand the basic mechanism of the algorithm, consider the physical imposition operator $T_{A\Phi}$ applied to some initial state Ψ_0. Even if this takes us closer to Φ (it not always does, as seen in Fig. 1) it is useless to apply $T_{A\Phi}$ again because the operator is idempotent. If we now use the information provided by another independent observable, B, and calculate $(T_{B\Phi}T_{A\Phi})\Psi_0$, we might get even closer to Φ, but the more interesting feature of this combined operator is that it is not idempotent and we may apply it again and again for a closer approach. The algorithm consists then in applying the operator $T_{A\Phi}$ to the initial state Ψ_0, then we use another operator for a closer approach, say $T_{B\Phi}$, and another one afterwards, until all physical information is used; then we start again with $T_{A\Phi}$. That is, we calculate the iterations $\Psi_1, \Psi_2, \Psi_3, \ldots$ given by $\Psi_n = (\cdots T_{C\Phi}T_{B\Phi}T_{A\Phi})^n\Psi_0$ and the convergence $\Psi_n \to \Phi$ is checked comparing the physical input, that is, the distributions associated with the observables $A, B, C, \ldots$ in the state Φ, with the corresponding distributions generated in the state Ψ_n.

In order to check the efficiency of the algorithm numerically, we choose a state Φ at random and with it we generate a compatible set of distributions corresponding to some observables, that we use as input in the algorithm. Calculating the distance $d(\Psi_n, \Phi)$ we study how efficiently the algorithm returns the initial state Φ. There are cases where the algorithm converges to a state Φ' different from Φ but having the same physical distributions, that is, to a Pauli partner of Φ. An interesting feature of the algorithm is that we can span the whole Hilbert space by choosing the starting states Ψ_0 randomly and the algorithm will deliver the Pauli partners. Since the attractive basin of each Pauli partner is not of null measure, as will be proved later, we can detect all Pauli partners by sufficiently large sampling of the Hilbert space with the initial states Ψ_0. In this way, the algorithm presented is not only a numerical tool for state determination but is also a useful tool for the theoretical investigation of the appearance of Pauli partners. An example of this is presented later.

The convergence to the state Φ, or to a Pauli partner, was tested numerically in several Hilbert space dimensions and for different choice of observables. These choices were random in some cases, that is, their associated orthonormal bases are randomly chosen, and in other cases we used physically relevant observables such as angular momentum or position and momentum. Position and momentum observables are usually represented by unbound operators in infinite-dimensional Hilbert spaces; however there are also realizations of these observables in finite dimensions, for instance, in a cyclic lattice, where they are represented by unbiased operators [10,11].

In general the operators $T_{A\Phi}, T_{B\Phi}, \ldots$ do not commute and the iteration of $(\cdots T_{B\Phi}T_{A\Phi})^n$ and $(\cdots T_{A\Phi}T_{B\Phi})^n$ are not necessarily equal. The algorithm was tested with several different choices in the ordering of the noncommuting physical imposition operators and also with random ordering and it turned out that the convergence of the algorithm is not much affected by the different orderings. The algorithm is robust under the noncommutativity of the observables.

B. Restart of the algorithm

The algorithm is very efficient; however, there are some starting states Ψ_0 where the algorithm fails to converge to the generator state Φ or to any of its Pauli partners. It was not surprising to find these failures because, as was suggested in Fig. 1, the physical imposition operator sometimes take us farther away from the wanted state. In case of a failure the algorithm converges to a state that has the correct distribution of only one observable (the one corresponding to the last application of the physical imposition operator). We are informed of this failure because all the distributions used as input are not approached in each iteration. In the case of a failure, we can simply restart the algorithm with a different initial state Ψ_0 or restart with another initial state orthogonal to the one that failed. In this last case, the probability of a repeated failure is much reduced and therefore it is a convenient choice. The appearance of a failure depends strongly on the choice of observables used to determine the state. If we use three unbiased observables we very rarely found a failure, in less than 1% of the cases, but if we use three random observables (see below), 40% of the randomly chosen starting states Ψ_0 fail but only 10% of these fail again if we restart with an orthogonal state. In the case of four angular momentum observables in four arbitrary directions we had to restart the algorithm in some 10% of the cases. The appearance of failures also depends on the shape of the distributions: when one of the distributions is peaked, that is, the maximum value of the distribution $\rho(a_k)$ has a large value for some k, the application of the corresponding imposition operator bring us close to the wanted state as can be seen in Eq. (10), and Fig. 1 shows that then the algorithm has better convergence and no failures are found. This has been confirmed in the numerical tests.

C. Application of the algorithm with two observables

As mentioned before, the physical imposition operator $T_{A\Phi}$ is idempotent so it is useless to apply it more than once (successively) in an attempt to approach the state Φ. Clearly, the complete measurement of just one observable is not sufficient to determine the state, except in the trivial case when the state happens to be equal to one of the eigenvectors of the operator. Therefore, we consider the information provided by two observables A and B (for two unbiased observables, such as X and P, this is precisely the Pauli problem). We studied then the convergence of $\Psi_n = (T_{B\Phi}T_{A\Phi})^n\Psi_0$ toward Φ or to a Pauli partner, for an arbitrary Ψ_0. In a three-dimensional Hilbert space, $N=3$, we applied the algorithm in several cases: for A and B random, unbiased (that is, of the type X and P) and also for angular momentum operators

J_x, J_y. As was expected, in all of these cases the algorithm returned several Pauli partners. Choosing the starting state Ψ_0 randomly (uniform distributed in the Hilbert space) we found that all Pauli partners found are accessed with similar frequency. As was mentioned before, we expect to detect all partners and we may be confident that this is so, because in one particular case, where we can calculate exactly the number of partners, the algorithm returns them all. This particular case is the, so-called, pathological case in N-dimensional Hilbert space (N prime) where we have uniform distributions for M observables that correspond to $N(N+1-M)$ partners. For several combinations of N and M, the algorithm delivered all partners. In this case, where we know theoretically the number of Pauli partners, the algorithm delivers all of them and this gives us the expectation that the same could happen in all cases. However, in order to prove this expectation we should be able to calculate the number of Pauli partners in general for all cases and this has not been done and does not seen to be possible due to the complexity of the problem. A systematic analytic study of Pauli partners for all cases seems to be out of reach but at least, our algorithm provides a numerical tool that may be useful for such a study. As an example of this, we will see later that in the case of angular momentum, the Pauli partners provided by the algorithm showed some regularity that could be later proved analytically.

D. Application of the algorithm with three observables

Next we studied the case with three operators providing physical information to determine the state (also with Hilbert space dimension $N=3$). We studied then the iteration $\Psi_n = (T_{C\Phi} T_{B\Phi} T_{A\Phi})^n \Psi_0$. When two of the observables are unbiased (of the type X and P) we always obtained a unique state, regardless of the choice of the third operator: either unbiased or of the type $X+P$ (biased to the first two), or random. This means that the information provided by two unbiased observables almost fixes the state and any other additional information is sufficient to find a unique state. However, we know that in the, so-called, pathological cases we must find Pauli partners and the algorithm does indeed find them. In these pathological cases, the distributions corresponding to three unbiased operators are all uniform (that is, the generator state Φ is unbiased to all three bases). Spanning the Hilbert space by choosing Ψ_0 randomly as a starting state for the algorithm, we converge to all $N(N-2)=3$ Pauli partners with almost equal probability. The pathological case was also studied with two unbiased observables with uniform distributions. In this case the algorithm also delivered all $N(N-1)=6$ Pauli partners with similar probability.

For biased operators, such as angular momentum operators J_x, J_y, J_z and also for random A, B, C we sometimes found Pauli partners showing that, although we have more equations (six) than unknowns (four), the nonlinearity of the problem may cause nonunique solutions. The appearance of Pauli partners in the angular momentum case is consistent with the result reported by Amiet and Weigert [12]. An inspection of the numerical results for these Pauli partners revealed a symmetry that could also be proved analytically: given a state ϕ (in the basis of J_z) with the corresponding distributions for the observables J_x, J_y, J_z,

$$\phi = \begin{pmatrix} a \\ b \\ c \end{pmatrix} \tag{13}$$

(it is always possible to fix b real an nonnegative) when $b>0$ and $(a^*+c) \neq 0$, if any one of the following conditions on the real (Re), imaginary (Im) part or modulus of the components is satisfied:

$$\mathrm{Re}(a) = -\mathrm{Re}(c), \tag{14}$$

$$\mathrm{Im}(a) = \mathrm{Im}(c), \tag{15}$$

$$|a| = |c|, \tag{16}$$

$$\mathrm{Im}(ac) = 0, \tag{17}$$

then there is a Pauli partner ϕ' given by

$$\phi' = \begin{pmatrix} a' \\ b \\ c' \end{pmatrix}, \tag{18}$$

where

$$a' = a^* \frac{(a+c^*)}{(a^*+c)}, \quad c' = c^* \frac{(a^*+c)}{(a+c^*)}. \tag{19}$$

If $b=0$ we can make a real and positive and then $a'=a$, $c'=c^*$, and finally if $(a^*+c)=0$ then $c'=-a'^*$, where a' can take three values, $-a$, a^*, $-a^*$. Spanning the Hilbert space with generator states ϕ randomly chosen, in some 1% of the cases the algorithm returned the state ϕ and a Pauli partner ϕ' covering all possibilities mentioned above. Notice that the ability of the algorithm to detect Pauli partners is due to the limited precision of the numerical procedure. Among all possible states ϕ of the system, only a few of them have Pauli partners, more precisely, the set of states with Pauli partners has null measure and if we had infinite precision, we would never find partners by random sampling of the Hilbert space. Because of the limited precision of the algorithm, all points in the Hilbert space within a small environment are equivalent and therefore the sets of points with null measure can be accessed in a random sampling of the Hilbert space. We have found indeed that if we become more restrictive with conditions of convergence we need more tries in order to detect partners. Usually the limited precision is considered a drawback, however in this case it is an advantage that allows us to detect sets of null measure.

E. Application of the algorithm with four observables

With the information provided by the complete measurement of four operators A, B, C, D we iterated $\Psi_n = (T_{D\Phi} T_{C\Phi} T_{B\Phi} T_{A\Phi})^n \Psi_0$ and we found unique states, not only

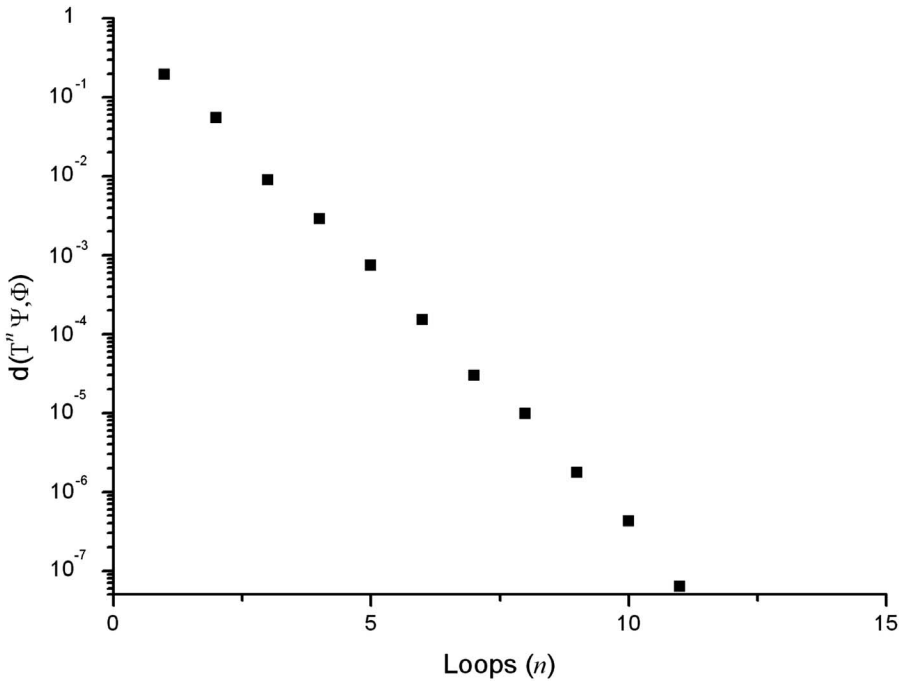

FIG. 3. Distance from the state $\Psi_n=(T_{C\Phi}T_{B\Phi}T_{A\Phi})^n\Psi_0=T^n\Psi_0$ to the state Φ after n iterations, showing exponential convergence of the algorithm for A,B,C unbiased operators in a three-dimensional Hilbert space.

when two of them are unbiased (consistent with the result obtained with three operators), but also in the case of random operators or angular momentum in arbitrary directions J_r,J_s,J_t,J_u. Of course, in this case of excessive physical information we could ignore one of the observables and determine the state with only three of them. However, not all the Pauli partners found with three observables will have the correct distribution for the fourth one and therefore the use of all observables may be needed for a unique determination of the state. In this case the number of equations, eight if $N=3$, uniquely determine the four unknowns in spite of the nonlinearity. Notice that the convergence of the algorithm in this case is not trivial. It is true that we are using much more information than what is needed (except for the pathological cases that can only appear if $N>3$) but we must consider that we are using this excessive information in an iterative and an approximate algorithm and therefore the consistency of the data in the final state does not necessarily cooperate in the iterations. The fact that the over-determined algorithm converges is a sign of its robustness.

F. Convergence and stability

In this work we have used three different criteria of convergence. In the numerical tests of the algorithm, we know the state Φ that was used in order to generate the distributions corresponding to several observables and therefore we use as convergence criteria the distance from this state Φ to the state Ψ_n obtained in each iteration. The generator state Φ is of course not known in the problem of state determination. In this case we can choose as convergence criteria the distance between two successive iterations $d(\Psi_n,\Psi_{n+1})$ (typically we stopped the iterations for distances less than 10^{-8}) or instead of it, we could use the usual distance between distributions given by the Euclidean metric, in order to compare the distributions used as physical input and the distributions generated in each iteration Ψ_n (typically we stopped the iterations for distances less than 10^{-5}).

The algorithm converges in a very efficient way, close to exponential, as we see in Fig. 3 where the distance to the converging state is given as a function of the number of iterations for the case of three unbiased operators with $N=3$. This is a typical example showing the exponential convergence where the distance to the solution is divided by 4.5 in each iteration. However, the speed of convergence, that is, the slope in the figure, is not always the same and depends on the operators used and on the generating state Φ. In many cases, the exponential approach begins after a few iterations and not in the first one, This is due to the effect that, as can be seen in Fig. 1, if the initial state is far from the target we may have some cases where the application of the physical imposition operator does not bring us closer to the target and therefore the first iterations may be of slower approach. For higher Hilbert space dimensions we obtained similar convergence behavior of exponential approach. For three operators with physical relevance, such as angular momentum or unbiased operators, the distance to the target state was divided by 2–3 in each iteration in Hilbert spaces with dimensions up to 20. In the fastest case found, the distance was divided by 126 in each iteration, approaching the solution within 10^{-7} after three iterations. With random operators the approach was not always so fast and in some unfavorable cases up to 100 iterations were required (this took only a fraction of a second in an old PC).

The good numerical convergence of the algorithm suggest that perhaps some analytical proofs of convergence could be obtained. However, the nonlinearity of the operator and the high dimensionality makes this task extremely difficult. Assume, for instance, that we want to determine the attractive basin of a particular solution Φ that is given by $2N$ real parameters (the real and imaginary part of the expansion coefficients in some Hilbert space basis). In this case we must

find the conditions such that the eigenvalues of the $2N \times 2N$ Hessian matrix have modulus less than 1. This is analytically out of reach. We can however prove that the fix points of the physical imposition operator are stable because if we make a variation in a neighborhood of a fix point $\Phi \to \Phi + \delta\Phi$, the application of the nonlinear operator $T_{A\Phi}$ results (to first order) in $\Phi + \delta\Phi'$ with $\delta\Phi' \neq \delta\Phi$ and $\|\delta\Phi'\| \leq \|\delta\Phi\|$, that is, we land closer to Φ (of course the same is true for the product $\cdots T_{C\Phi} T_{B\Phi} T_{A\Phi}$). Since the variation $\delta\Phi$ is arbitrary, the attractive basin of the fix point is not of null measure, as was mentioned before. In order to prove this, consider from the definition of $T_{A\Phi}$ that

$$T_{A\Phi}(\Phi + \delta\Phi) = \sum_k \varphi_k (z_k + \delta z_k) \frac{|z_k|}{|z_k + \delta z_k|}, \tag{20}$$

where

$$z_k = \langle \varphi_k, \Phi \rangle \quad \text{and} \quad \delta z_k = \langle \varphi_k, \delta\Phi \rangle. \tag{21}$$

Here we can assume $z_k \neq 0$ because otherwise the corresponding term vanishes and is excluded in the expansion of Eq. (20). Let us treat now the denominator

$$|z_k + \delta z_k| = \left| \frac{z_k^*}{|z_k|} (z_k + \delta z_k) \right| = \left| |z_k| + \frac{z_k^*}{|z_k|} \delta z_k \right|. \tag{22}$$

Since we can take $|\delta z_k| \ll |z_k|$ the denominator becomes

$$|z_k + \delta z_k| \approx |z_k| + \mathrm{Re}\left(\frac{z_k^*}{|z_k|} \delta z_k \right), \tag{23}$$

and with this, the fraction in Eq. (20) is

$$\frac{|z_k|}{|z_k + \delta z_k|} \approx \frac{1}{1 + \mathrm{Re}\left(\dfrac{\delta z_k}{z_k} \right)} \approx 1 - \mathrm{Re}\left(\frac{\delta z_k}{z_k} \right). \tag{24}$$

Inserting the above equation, we have

$$\begin{aligned} T_{A\Phi}(\Phi + \delta\Phi) &\approx \sum_k \varphi_k (z_k + \delta z_k) \left[1 - \mathrm{Re}\left(\frac{\delta z_k}{z_k} \right) \right] \\ &\approx \sum_k \varphi_k \left[z_k + \delta z_k - z_k \, \mathrm{Re}\left(\frac{\delta z_k}{z_k} \right) \right], \end{aligned} \tag{25}$$

where we have neglected a term of order $(\delta z_k)^2$. Now expressing the real part as a sum of the number plus its conjugate we obtain

$$T_{A\Phi}(\Phi + \delta\Phi) \approx \sum_k \varphi_k \left(z_k + \frac{1}{2} \delta z_k - \frac{1}{2} \frac{z_k}{z_k^*} \delta z_k^* \right). \tag{26}$$

Inserting now the values of Eq. (21) we recognize the expansion of the elements in the basis $\{\varphi_k\}$,

$$T_{A\Phi}(\Phi + \delta\Phi) \approx \Phi + \frac{1}{2} \delta\Phi - \frac{1}{2} \delta\chi = \Phi + \delta\Phi', \tag{27}$$

where $\delta\chi$ is a variation different from $\delta\Phi$ with basis expansion given by

$$\delta\chi = \sum_k \varphi_k \frac{\langle \varphi_k, \Phi \rangle}{\langle \Phi, \varphi_k \rangle} \langle \delta\Phi, \varphi_k \rangle. \tag{28}$$

Notice that the expansion coefficients of this variation are the same coefficients for the expansion of $\delta\Phi$ but complex conjugated and multiplied by a phase. It follows then that $\|\delta\chi\| = \|\delta\Phi\|$ and from the triangle inequality for the norm we obtain the inequality wanted, $\|\delta\Phi'\| = \frac{1}{2}\|\delta\Phi - \delta\chi\| \leq \frac{1}{2}(\|\delta\Phi\| + \|\delta\chi\|) = \|\delta\Phi\|$.

V. CONCLUSION

In this work we defined the physical imposition operator $T_{A\Phi}$ that imposes to any state Ψ the same distribution that the eigenvalues of an observable A have in a state Φ. For this operator we do not need to know the state Φ but we just need the probability distribution for the observable A in this state, that can be obtained from a complete measurement. Considering two or more observables, we applied their corresponding physical imposition operators iteratively to an arbitrary initial state Ψ_0 and obtained a succession of states Ψ_n that converge to the unknown state Φ, or to a Pauli partner having the same distribution for the observables. Varying the initial state we expect to find all Pauli partners because, in the cases where we can know exactly all the Pauli partners, the algorithm finds them all and therefore it becomes a useful tool for the investigation of Pauli partners. This algorithm for state determination was tested numerically for different sets of observables and different dimensions of the Hilbert space and it turned out to be quite an efficient and robust way to determine a quantum state using complete measurements of several observables.

ACKNOWLEDGMENTS

We would like to thank M. Hoyuelos for comments and H. de Pascuale for his help on mathematical questions. This work, part of the Ph.D. thesis of one of the authors (D.M.G.), received partial support from "Consejo Nacional de Investigaciones Científicas y Técnicas" (CONICET).

[1] W. Pauli, "Quantentheorie," *Handbuch der Physik* (Springer, Berlin, 1933), Vol. 24.
[2] S. Weigert, Phys. Rev. A **45**, 7688 (1992).
[3] S. Weigert, Phys. Rev. A **53**, 2078 (1996).
[4] M. Keyl, Phys. Rep. **369**, 431 (2002).
[5] I. D. Ivanovic, J. Phys. A **14**, 3241 (1981).
[6] W. K. Wootters and B. D. Fields, Ann. Phys. **191**, 363 (1989).
[7] S. Bandyopadhyay, P. Boykin, V. Roychowdhury, and F. Vatan, Algorithmica **34**, 512 (2002).
[8] A. Majtey, P. W. Lamberti, M. T. Martin, and A. Plastino, Eur. Phys. J. D **32**, 413 (2005).
[9] E. Lages Lima, *Espaços Métricos*, 3rd ed. (Projeto Euclides,

IMPA, Rio de Janeiro, 2003).
[10] A. C. de la Torre and D. Goyeneche, Am. J. Phys. **71**, 49 (2003).
[11] A. C. de la Torre, H. O. Mártin, and D. Goyeneche, Phys. Rev. E **68**, 031103 (2003).
[12] J. P. Amiet and S. Weigert, J. Phys. A **32**, 2777 (1999).