Dealing with entanglement of continuous variables:
Schmidt decomposition with discrete sets of orthogonal functions

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We propose a method for obtaining the Schmidt decomposition of bipartite systems with continuous variables. It approximates the modes to the prescribed accuracy by well known orthogonal functions. We give some criteria for the control of errors. We illustrate the method comparing its results with the already published analysis for entanglement of biphotons. The agreement is excellent.

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I. INTRODUCTION

Bipartite and multipartite entanglement is one of the features that give rise to many of the developments of quantum computation and information, like quantum teleportation [1] [2] and quantum cryptography [3] [4], among others [5]. The evaluation of the entanglement of a composite state is thus a main task to be done. For this purpose, the Schmidt decomposition [6] [7] has proven to be a valuable tool, for systems with just two components.

In this paper we consider the case of continuous variables entanglement. For us, these variables may be \{a+a, i(a-a)\} which commute as phase space variables do. We also refer to continuous variable entanglement in systems described by momentum and/or energy observables. Precisely, the entanglement of continuous variables stems from the original EPR article [8]. However, the treatment of systems with continuous variables is far from straightforward. Until now, Schmidt decomposition in the continuous case required solving the corresponding integral equations [9] [10] [11] [12] [13]. They had to be discretized, losing the continuous dependence of the initial state. Here we propose a method to perform the Schmidt decomposition for this case, to the accuracy desired, keeping the continuous character of the variables. This method consists of two steps:

1) We decompose the bipartite system wave function, \( f(p,q) \), by using two discrete and complete sets of orthogonal functions, \( \{O_n^{(1)}(p)\}, \{O_n^{(2)}(q)\} \), of \( L^2 \), in the form:

\[
 f(p,q) = \sum_{m,n} C_{mn} O_n^{(1)}(p) O_n^{(2)}(q) \quad (1)
\]

The purpose of this step is to transform the continuous problem into a discrete one (a necessary step for the numerical computation), while preserving the continuous dependence of \( f(p,q) \).

2) Then we apply the (finite dimensional) Schmidt procedure to (1) in order to write the wave function \( f(p,q) \) as diagonal sum of biorthogonal terms:

\[
 f(p,q) = \sum_n \sqrt{\lambda_n} \psi_n^{(1)}(p) \psi_n^{(2)}(q) \quad (2)
\]

The orthogonal functions \( \psi_n^{(1)}(p), \psi_n^{(2)}(q) \) -the modes- will be some particular linear combinations of \( O_n^{(1)}(p) \), \( O_n^{(2)}(q) \), respectively. Notice that we are using the Schmidt procedure for discrete systems to obtain the decomposition for the continuous case. This is much more tractable, as it implies diagonalizing matrices instead of solving integral equations.

The rationale for this procedure is the expectation that only a few \( O_n \) will suffice: A handful of appropriate orthogonal functions will approximate \( f(p,q) \) to the desired accuracy. We finish by pointing out some properties of this method, namely

a) We obtain complete analytic characterization of the modes \( \psi_n^{(1)}(p), \psi_n^{(2)}(q) \) to the desired precision. Our method surpasses the standard numerical procedures in that keeps the continuous features present in \( f(p,q) \).

b) We remark the portability of the attained modes \( \psi_n^{(1)}(p), \psi_n^{(2)}(q) \) that are ready for later uses.

c) For the physical system analyzed in this paper (biphoton), we found that with \( 26 \times 26 \ C_{mn} \) matricies the error was of around 2\%, that is, the number of \( O_n \) functions required is small. For other systems studied that we do not include here, the convergence was even better: For the case of two electrons which interact electrostatically, the obtained error with \( 12 \times 12 \) matrices was of 0.7\% (Schmidt number \( K = 2.4 \)).

In this paper we begin with a detailed exposition of our method in Sect. 11. Then, in Sect. 1II we apply it to a relevant case: the entanglement of two photons created by parametric down-conversion. We compare our results (leading to well known, continuous functions) with those computed by numerical methods [14] that produce sets of points: discrete functions. Both methods agree remarkably well. Finally, in Sect. 1V we decompose the Dirac delta, a case of physical and mathematical interest.
II. SCHMIDT DECOMPOSITION WITH DISCRETE SETS OF ORTHOGONAL FUNCTIONS

We consider a bipartite quantum system formed by two subsystems $S_1$ and $S_2$. Some examples are two photons entangled by parametric down-conversion, a photon emitted by an excited atom and as a result entangled with it or two charged particles which interact electrically. This system is described by the vector state

$$|\psi\rangle = \int dp dq f(p, q) a_{(1)}^\dagger(p) a_{(2)}^\dagger(q) |0, 0\rangle$$

$$\langle|f(p, q)|^2 \equiv \int dp dq |f(p, q)|^2 < \infty$$

where $a_{(1)}^\dagger(p)$, $a_{(2)}^\dagger(q)$ are the creation operators of a particle associated to the subsystems $S_1$ and $S_2$. $p$ and $q$ are continuous variables associated to $S_1$ and $S_2$ respectively, which can represent momenta, energies, frequencies, or the like. In general, the analysis is made in an ad hoc kinematical situation in which $p$ and $q$ turn out to be one-dimensional variables, $p \in (a_1, b_1)$, $q \in (a_2, b_2)$. In the following we assume this is the case. In addition, there can be discrete variables (like the spin) to be treated with the Schmidt method, that we do not include here to avoid unwieldy notation.

Our method works as follows:

We consider two denumerable, complete sets of orthogonal $L^2$ functions $\{O_{n}^{(1)}(p)\}$, $\{O_{n}^{(2)}(q)\}$ $n = 0, 1, \ldots, \infty$, each one associated to each particular subsystem $S_\alpha$ ($\alpha = 1, 2$). These functions obey

$$\int_{a_\alpha}^{b_\alpha} dk O_m^{(\alpha^*)}(k) O_n^{(\alpha)}(k) = \delta_{mn}$$

$$\sum_n O_m^{(\alpha^*)}(k) O_n^{(\alpha)}(k') = \delta(k - k')$$

1) Our first step is to expand the wave function $f(p, q)$ as a linear combination of the $O_n^{(\alpha)}$, translating the continuous problem into a discretized one. Thus we work with the discrete coefficients of the linear combination, though the continuous character of the state is preserved in the $k$ dependence of the $O_n^{(\alpha)}$ functions. The expansion reads:

$$f(p, q) = \sum_{m, n = 0}^{\infty} C_{mn} O_n^{(1)}(p) O_n^{(2)}(q)$$

where the coefficients $C_{mn}$ are given by

$$C_{mn} = \int_{a_1}^{b_1} dp O_m^{(1)^*}(p) \int_{a_2}^{b_2} dq O_n^{(2)^*}(q) f(p, q)$$

2) Our second step is to apply the Schmidt decomposition to the discretized bipartite state $|\psi\rangle$, as is usually done for finite dimension Hilbert spaces (diagonalizing matrices, instead of solving integral equations). In order to do this, it is necessary to truncate the expansion $|\psi\rangle$, something that is possible to a certain accuracy due to the fact that $\int dp dq |f(p, q)|^2 < \infty$ ($f(p, q)$ is in principle normalizable), and the expansion is in orthogonal functions, so the coefficients $C_{mn}$ go to 0 with increasing $m, n$ (see below).

We truncate the series at $m = m_0$, $n = n_0$, with $m_0 \leq n_0$, without loss of generality. The Schmidt procedure leads to [2], where

$$\psi_i^{(1)}(p) = \sum_{m = 0}^{m_0} V_{im} O_n^{(1)}(p)$$

$$\psi_i^{(2)}(q) = \frac{1}{\sqrt{N}} \sum_{m = 0}^{m_0} \sum_{n = 0}^{n_0} V_{im} C_{mn} O_n^{(2)}(q)$$

Here the matrix $V$ is the (transposed) eigenvectors matrix of $M_{ij} = M_{ij}^* \equiv \sum_{n = 0}^{n_0} C_{in}^* C_{jn}$.

$$\sum_{m = 0}^{m_0} M_{im} V_{jm} = \lambda_j V_{ji}$$

and $\{\lambda_i\}_{i=0,\ldots,m_0}$ are the eigenvalues of $M$.

There are two sources of error in this procedure:

a) Truncation error: This is the largest source of error in our method. Inescapably, the series must end at some finite $m, n$ when attempting to obtain some specific result. This step is possible to a certain accuracy because the function $f(p, q)$ is square-integrable and we are expanding it into orthogonal functions, so $\sum_{m = 0}^{\infty} \sum_{n = 0}^{\infty} |c_{mn}|^2 < \infty$ and thus $C_{mn} \to 0$ when $m, n \to \infty$.

The particular choice of the orthogonal functions $O_n^{(\alpha)}$ will affect how fast the $C_{mn}$ go to zero. Hence, the choice of these functions for a particular physical problem will be a delicate task. To reach the same accuracy with different sets $\{O_n^{(\alpha)}\}$ it will be necessary in general to consider a different pair of cut-offs $\{m_0, n_0\}$ for each of the sets.

b) Numerical error: This is a better controlled source. It includes the error in calculating the coefficients $C_{mn}$ via (4) and the one produced when diagonalizing the matrix $M = CC^\dagger$.

The suitable quantity to control the convergence for a particular $f(p, q)$ and a specific set $\{O_n^{(\alpha)}\}$ is the well known (squared) distance $d_{m_0, n_0}^2$ between the function $f(p, q)$ and the Schmidt decomposition obtained with cut-offs $\{m_0, n_0\}$ (mean square error):
this expression gives the truncation error. It will go to zero with increasing cut-offs according to the specific \( \{O^{(\alpha)}\} \) chosen.

Another easily computable, less precise way of controlling the convergence is given by the fact that (with no cut-offs) \( \sum_{m=0}^{\infty} \lambda_m = ||f(p, q)||^2 \) and thus

\[
d_{m_0,n_0}^2 \equiv 1 - \sum_{m=0}^{m_0} \lambda_m/||f(p, q)||^2
\]  

(12)

is another measure of the truncation error, where here \( \lambda_m \) is calculated with cut-offs \( \{m_0, n_0\} \). Would we compute the \( \lambda_m \) exactly, then \( d^1 = d^2 \). In practice this cannot be done because our \( \lambda_m \) are the eigenvalues of the \( m_0 \times m_0 \) matrix \( M_{ij} \), that depend slightly on \( m_0, n_0 \). Both distances behave in a very similar way, as we show in Fig. 1 and Fig. 2, though \( d^2 \) is more easily computable than \( d^1 \).

The election of the two sets of orthogonal functions for a particular physical problem, \( \{O^{(\alpha)}\}_\alpha \), can be approached from two different points of view, according to the feature one desires to emphasize: fundamental or practical.

### A. Fundamental point of view

The election of the orthogonal functions in a particular problem can be done according to the specific intervals in which the variables \( p, q \) take values for that case. Typical examples of discrete sets of orthogonal functions are the orthogonal polynomials, defined in a variety of intervals. For example, a possible choice to describe one dimensional momenta \( p \in (\pm \infty, \infty) \), are the Hermite polynomials, \( O^{(1)}_n(p) \sim H_n(p) \). The equivalence sign indicates here that the polynomial must be accompanied by the square root of the weight function in order to be correctly orthonormalized, and normalization factors must be included. If, on the other hand, the variable of interest in a specific problem is bounded from below, like the energy of a free massless particle \( p \in (0, \infty) \), then the election could be Laguerre polynomials, \( O^{(1)}_n(p) \sim L_n(p) \).

The criterion for choosing the orthogonal functions \( O^{(\alpha)} \) according to the intervals in which \( p, q \) are defined has a fundamental character. For example, the localizability in configuration space of the Fourier transforms of the modes \( \omega \), depends critically on the intervals in which these modes are defined. Only if we choose the functions \( O^{(\alpha)} \) to be defined exactly in the same intervals as the amplitude \( f(p, q) \), may the Fourier transforms of the modes have the right localization properties. In spite of that, this point of view may not be the most suitable one, as it may give slower convergence than the point of view presented below.

### B. Practical point of view

In this case, the election is approached with the goal of improving the convergence. The \( O^{(\alpha)} \) are chosen here according to the functional form of \( f(p, q) \). The closer the lowest modes are to \( f \) the lesser the number of them necessary to obtain the required accuracy. What we are looking for here are \( O^{(\alpha)} \) that maximize \( \int_{a_1}^{b_1} dp \int_{a_2}^{b_2} dq |f(p, q)|^2 \) for low \( m, n \).

In some cases this practical point of view will be more useful than the fundamental one. For example, suppose the amplitude for a particular problem is of the form \( f(p, q) = g(p, q) e^{-\alpha^2/2} e^{-\beta^2/2} \), with \( g(p, q) \) a slowly varying function of \( p, q \). In this particular case it is reasonable to choose the functions \( O^{(\alpha)} \) as Hermite polynomials, because their weight functions are indeed gaussians. This leads to \( O^{(1)}_n(p) \sim H_n(p) e^{-p^2/2} \), and similarly for \( O^{(2)}_n(q) \).

We call this approach practical because the convergence is reached faster. There is a price: the information relevant to localization might be lost.

### III. ENTAILMENT OF CONTINUOUS VARIABLES IN PARAMETRIC DOWN-CONVERSION

In this section we consider a realistic case of biphotons already studied in the literature \([11, 12]\): two photons entangled in frequency through parametric down-conversion. We apply our method to this physical system in order to obtain the Schmidt decomposition and the structure of modes without losing the analytic character within the target accuracy.

The system under study is a biphoton state generated by parametric down-conversion (PDC) of an ultrashort pump pulse with type-II phase matching. The amplitude in this particular case takes the form

\[
f(\omega_0, \omega_c) = \exp[-(\omega_0 + \omega_c - 2\omega)^2/\sigma^2] \times \text{sinc}(L[(\omega_0 - \omega)(k'_c - k)] + (\omega_c - \omega)(k'_c - k)]/2)
\]  

(13)

where \( \omega_0, \omega_c \in (0, \infty) \) are the frequencies associated to the ordinary and extraordinary fields respectively, \( k'_c \) and \( k'_c \) are the inverse of group velocities at the frequency \( \omega \), \( \tilde{k} \) is the inverse group velocity at the pump frequency \( 2\omega \), \( L \) is the PDC crystal length and \( \sigma \) is the width of the initial pulse. Typical values for these parameters are \( \tilde{k} = 0.213 \text{ps}^{-1} \), \( \tilde{k} = 0.061 \text{ps}^{-1} \), \( \omega = 2700 \text{ps}^{-1} \), \( L = 0.8 \text{mm} \) and \( \sigma = 35 \text{ps}^{-1} \).

We perform now the following change of variables
We choose as orthogonal functions Hermite polynomials, because their weights are gaussians and a gaussian normalized) according to section II, in the following way:

\[ \begin{align*}
    p &= \frac{\omega_0 - \bar{\omega}}{\sigma}; \quad L_p = (k - k_0) L \sigma \\
    q &= \frac{\omega_e - \bar{\omega}}{\sigma}; \quad L_q = (k - k_0) L \sigma
\end{align*} \]

and thus obtain

\[ f(p, q) = e^{-(p+q)^2} \text{sinc}[(L_p p + L_q q)/2] \tag{16} \]

We have applied our method to the function (16) (once normalized) according to section II. We have computed \( O^{(\alpha)}_n(k) = (\sqrt{\pi}2^n n!)^{-1/2} H_n(k)e^{-k^2/2} \alpha = 1, 2 \tag{17} \)

This choice of polynomials is suitable for the practical approach (subsection II), taking into account that \( \bar{\omega} \gg \sigma \) and thus the interval of definition of \( f(\omega_0, \omega_e) \) can be restricted to a region centered in \( \bar{\omega} \) of width \( \sim \sigma \) in \( \omega_0, \omega_e \). We did a careful analysis of this, that for brevity we do not show here. Notice that our conclusions would not apply in the case \( L_p = L_q \).

We have considered cut-offs \( m_0 = n_0 \) taking values \( \{5-25\} \) and followed the steps of Sect. II. We have computed the eigenvalues \( \lambda_n \) of the Schmidt decomposition (2) for each pair \( \{m_0, n_0\} \). We have also computed the modes (3) and (4).

In Fig. 1 we plot the distance \( d_{m_0,n_0}^1 \) as a function of \( m_0 = n_0 \) to show how fast the convergence is. With \( m_0 = n_0 = 25 \) the truncation error is of 2%. We also plot in Fig. 2 the distance \( d_{m_0,n_0}^2 \), which serves as another measure of the convergence, as a function of \( m_0 = n_0 \). We obtained \( d_{25,25}^2 = 2\% \).

Regarding now the most precise case considered, \( m_0 = n_0 = 25 \), we plot in Fig. 3 the eigenvalues \( \lambda_n \) for different values of \( n \), observing good agreement with the results existing in the literature (10). For this case we also plot in Fig. 1 the modes (8) and (9) for \( i = 0, 1, 2, 3 \), confirming the validity of the method when comparing with (10).

The modes are given explicitly by:

\[ \psi_m^{(\alpha)}(k) = e^{-k^2/2} \sum_{n=0}^{25} (\sqrt{\pi}2^n n!)^{-1/2} A_m^{(\alpha)} H_n(k) \tag{18} \]

\[ m = 0, ..., 25 \quad \alpha = 1, 2 \]

where the values of the coefficients \( A_m^{(\alpha)} \) are obtained through (8) and (9). The actual properties of the modes (15) depend on these values. In fact, the parity and number of nodes is determined by them, taking into account that \( H_n \) is a polynomial of degree \( n \), parity \( (-)^n \) and having \( n \) nodes.

A good approximation to the \( \psi_0^{(1)}(p) \) obtained with our procedure is

\[ \psi_0^{(1)}(p) = e^{-p^2/2}(0.81395 - 0.14764 p^2 + 0.00821 p^4) \tag{19} \]
This expression has a deviation (squared distance) of $10^{-5}$ from the whole mode obtained including terms until $\beta^{35}$, which is the greatest power appearing for $m_0 = n_0 = 25$. On the other hand, $d_{14,25}^1 - d_{25,25}^1 = 0.213 \gg 10^{-5}$. From (19) it can be seen that in this mode the even components are greater than the odd ones (these are negligible), so it is an even state, as shown in Fig. 4

Another example is the approximation to $\psi_n^{(2)}(q)$

$$
\psi_n^{(2)}(q) = e^{-q^2/2}(2.91088q - 3.54070q^3 + 1.29062q^5 - 0.20402q^7 + 0.01598q^9 - 0.00063q^{11} + 0.00001q^{13})
$$

(20)

This has a deviation (squared distance) of $10^{-4}$ from the whole mode obtained including terms until $q^{25}$. On the other hand, $d_{14,13}^0 - d_{25,25}^0 = 0.020 \gg 10^{-4}$. More terms are needed in (20), because they go to zero more slowly with increasing powers of $q$. Here the most important components are the odd ones (the even ones are negligible), leading to an odd parity state, as shown in Fig. 4

To show how the convergence of the method depends on the specific family pairs of orthogonal functions $\{O_n^{(1)}(p)\}$, $\{O_n^{(2)}(q)\}$ chosen, we consider the cases of Hermite orthogonal functions depending on a parameter $\beta$ related to the width of the gaussian, fixed for each family pair:

![FIG. 4: Modes $\psi_n^{(1)}(p)$, $\psi_n^{(2)}(q)$ as a function of $p = \frac{2m_0}{\sigma}$ and $q = \frac{2m_0}{\sigma}$, for $n = 0, 1, 2, 3$.](image)

TABLE I: $d_{m_0,n_0}^2$ for $\beta = 1.0, 0.5, 2.0$ and $m_0 = n_0 = 25, 20, 15, 10$.

| $m_0 = n_0$ | $\beta = 1.0$ | $\beta = 0.5$ | $\beta = 2.0$ |
|------------|---------------|---------------|---------------|
| 25         | 0.020         | 0.13          | 0.037         |
| 20         | 0.024         | 0.19          | 0.041         |
| 15         | 0.032         | 0.27          | 0.050         |
| 10         | 0.062         | 0.38          | 0.064         |

(21)

We applied our method to the amplitude (18) with these sets of orthogonal functions, for $\beta = 1.0, 0.5, 2.0$, and cut-offs $m_0 = n_0 = 25, 20, 15, 10$. We show in Table I the values of $d_{m_0,n_0}^2$ for these specific parameters.

Clearly, the convergence is better for the case $\beta = 1$, which we used in the preceding calculations. In case we chose another type of orthogonal function for (18) (Legendre, Chebyshev,...), the convergence would have been much worse because of the specific shape of that amplitude.

IV. MAXIMUM ENTANGLEMENT: THE DIRAC DELTA

Another interesting case is the Dirac delta. Here we have $f(p, q) = \delta(p - q)$ and we take the same interval $(a, b)$ for $p$ and $q$. We consider complete sets of orthonormal functions satisfying $O_n^{(1)}(k) = O_n^{(2)\ast}(k)$. A particular case is when they are real functions, as for example the typical orthogonal polynomials (Legendre, Hermite, Laguerre, Chebyshev,...) are. We must take into account that the Dirac delta is not a function but a distribution, and indeed is outside $L^2$. However, we can calculate the $C_{mn}$ and study how much entanglement does this state have. We obtain straightforwardly $C_{mn} = \delta_{mn}$. This gives

$$
\delta(p - q) = \sum_{n=0}^{\infty} O_n^{(\alpha)\ast}(p)O_n^{(\alpha)}(q)
$$

(22)

which is just the resolution of the identity as given in (19). The Schmidt decomposition of the Dirac delta is not unique, because all the weights $\sqrt{\lambda_n}$ are equal to one (they are degenerate). In fact, the decomposition can be done with any complete, denumerable set of orthonormal functions, in the form (19). This expression can be seen as an infinite entanglement case, in the sense explained below. The fact that all the weights are equal to one, makes sense only because we are considering a distribution, not an $L^2$ state. The sum of the squares of the
weights, which must be equal to the square of the norm of the function \( f(p, q) \), diverges because the Dirac delta is not square-integrable.

A possible measure of the entanglement of a state \( f(p, q) \) in its Schmidt decomposition is given by the von Neumann entropy

\[
S = - \sum_{n=0}^{\infty} \lambda_n \log_2 \lambda_n
\]

(23)

This is usually called the entropy of entanglement.

The state of \( L^2 \) closer to the decomposition produced sets of points as approximation to the modes. Our method gives linear combinations of the well known orthogonal functions as approximation to them. When these functions are chosen properly, a handful of them is enough to reach the desired accuracy. We introduce some criteria for the control of convergence and truncation error. The result of our method for the decomposition of a biphoton state produced by parametric down-conversion agrees with the numeric results in the literature. We also touch on the last stage of evolution of entanglement for determined systems, analyzing the Dirac delta case.

\[
S = - \lim_{N \to \infty} \sum_{n=0}^{N-1} \frac{1}{N} \log_2 \frac{1}{N} = - \lim_{N \to \infty} \log_2 \frac{1}{N} = \infty
\]

(24)

This is the maximum entanglement case. This provides an estimate of the entropy of the Dirac delta (were it in \( L^2 \)).

The origin of our interest in the \( \delta \) comes from the fact that \( f(p, q) \) may evolve in time towards a Dirac delta, as it happens in time dependent perturbation theory of quantum mechanics. The entanglement in these cases would increase with time towards its maximum, corresponding to the Dirac delta.

V. CONCLUSIONS

In this paper we have introduced a method for computing the Schmidt decomposition of a bipartite state with continuous degrees of freedom. In the existing literature the decomposition produced sets of points as approximation to the modes. Our method gives linear combinations of the well known orthogonal functions as approximation to them. When these functions are chosen properly, a handful of them is enough to reach the desired accuracy. We introduce some criteria for the control of convergence and truncation error. The result of our method for the decomposition of a biphoton state produced by parametric down-conversion agrees with the numeric results in the literature. We also touch on the last stage of evolution of entanglement for determined systems, analyzing the Dirac delta case.

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