Two measures of quantum correlations and some applications

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Abstract

This paper reviews two well-studied measures of quantum correlations which exist between the subsystems that consists the most simple composite systems (bipartite systems). The first one is Entanglement of Formation (EoF) and quantifies the entanglement while the second one, the quantum discord (QD), is a measure of all quantum correlations of the bipartite system. Here the theoretical background is presented in order to give the definitions of these two measures and afterwards three cases are analyzed where we can implement these measures of quantum correlations. The three applications that we discuss here, are described by completely different equations and as a result we notice the usefulness and the universality of entanglement of formation and quantum discord.
Declaration

I declare that this dissertation is my own work. Although numerous resources have been used, the manner the results are presented is my own. Additionally, I have used some parts of my previous work as well as a part of my work which is to be published soon, especially in the last two chapters. More specifically, chapter 4 is divided into two parts. Section 4.1 is a summary of the article ”Polarization-entangled photon generation by a semiconductor quantum dot coupled to a cavity interacting with external fields”. Here only the appropriate theory is given in order to describe the corresponding system as well as two characteristic diagrams which are in my opinion the most helpful to understand entanglement of formation. In section 4.2 a synopsis of an unpublished paper is given which has the temporary title ”Two-qubit correlations via periodic plasmonic nanostructures”. Again, I present only two cases out of four that exist in the paper as the other cases are beyond the purpose of this work. Additionally, in the article, the entanglement of formation and quantum discord are given for the case that the plasmonic nanostructure is not present between the two qubits but for this dissertation these cases are redundant. Furthermore, in chapter 5 an outline of the paper ”Chemical bond and entanglement of electrons in the hydrogen molecule” is presented. After a brief summary of the theory of entanglement in the case of indistinguishable particles, the most useful results of this work are shown. Finally, in the Introduction, a historical review of the development of Quantum Information and Quantum Computation is given which have been taken by these papers. Of course whenever it is appropriate the references are given.
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Chapter 1

Introduction

Quantum mechanics was developed at the beginning of the 20th century. The foundations of this astonishing theory was given by some of the greatest physicists of this period like Max Planck, Paul Dirac, Erwin Schrödinger, Werner Heisenberg, Albert Einstein, Niels Bohr, Max Born and Luis De Broglie. Of course there were many other physicists who contributed to the development of the theory but the scientists that we mentioned were among the first who understood the necessity of a new theory for the subatomic particles.

First of all, Max Planck in 1900 introduced the idea that the energy is not transmitted in a continuous manner but it is transmitted by small packets of energy, the familiar ones to us quanta. Each Planck’s quantum of energy has a corresponding energy $E = hf$, where $h$ is the Planck’s constant and $f$ the frequency of each photon. Afterwards, De Broglie in his PhD thesis in 1924 introduced the idea of wave-particle duality. According to this, each particle, not only the photon, has dual nature and as a result we can consider it as a wave or as a particle depending on the nature of our experiment each time. The relation which connects the two images is $\lambda = h/p$, where $p$ is the momentum and $\lambda$ is the wavelength of the particle.

Continuing, Heisenberg in 1927 formulated the famous uncertainty principle and he was awarded with the Nobel prize five years later for his idea. This principle states that we cannot measure with complete accuracy the position and the momentum of a particle at the same time. More generally, the uncertainty principle is not only true for the position and the momentum, but it holds for every pair of physical properties that do not commute. Going back to the idea of De Broglie, since the particles of the matter could be considered to be waves too, they should obey a wave equation. But which is this
this equation? The answer to this question was given by Erwin Schrödinger in 1925 with his famous equation which is given below

\[ i\hbar \Psi(r, t) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(r, t) + V(r, t)\Psi(r, t) \] (1.1)

and \( \Psi(r, t) \) is the wavefunction of the particle and contains the information of how it moves in the space.

The physical interpretation of the wavefunction was introduced by Max Born in 1926. According to Born, the wavefunction itself has no physical meaning but only its norm squared has and expresses the possibility that the particle is found in a certain situation. For this essential contribution to quantum theory Born was awarded with the Nobel prize in 1954.

After the establishment of the theory, quantum mechanics was divided in several sections as scientists started to specialize in a certain area of this new theory. One relatively new scientific field of quantum mechanics is Quantum Information and Quantum Computation. In this new field of physics quantum entanglement plays a key role in the transportation and the storage of the information. Quantum entanglement firstly was demonstrated by Einstein, Podolsky and Rosen (1935)[1] in one of the most famous paradoxes in physics, the EPR paradox (from the initial letters of Einstein, Podolsky and Rosen), and as a result it was the first type among quantum correlations which was studied intensively. The initial aim of the EPR was to demonstrate that quantum mechanics was an incomplete theory. Instead, they were among the first that stimulated a large number of scientists to study the strange and at the same time intrinsic property of quantum mechanics, the quantum entanglement.

As we have mentioned before, the field of Quantum Information and Quantum Computation was established recently. More specifically, this field thrived especially over the last two decades. During this period scientists tried to give a measure of quantum entanglement. As a result of this effort, a lot of measures have been adopted over the past years and among them the most familiar is the entanglement of formation [2]. The advantage of this measure is that it can be computed easily for both pure and mixed states. However, entanglement is not the only type of quantum correlations and as a result we want a more general measure which encloses all types of correlations of subatomic particles. For this purpose quantum discord [3, 4], as a measure of all quantum correlations, was introduced about a decade ago. As someone can see from these original papers (see Refs. [3, 4]) quantum discord is
defined as the difference between the total and classical correlations. Thus, by computing the quantum correlations of a system we additionally compute the classical ones. Although quantum discord is a more general measure of quantum correlations and gives us more information regarding a system of our choice, it contains much more complicated calculations compared to entanglement of formation. This is the reason why in some cases we prefer to "sacrifice" this additional information for easier calculations.

As we see in the first part of chapter 4 we prefer to compute entanglement of formation for the quantum dot-cavity system [5]. Using a system of this type someone can produce and control entangled-photon pairs. Recently, the cascade-emission process from a biexciton state in a semiconductor quantum dot (SQD, usually called artificial atoms), was proposed and demonstrated. In this more efficient entangled-photon generation scheme, the entangled photons are generated from the cascade emission through the degenerate intermediate states having different polarizations. A much better control of this process is achieved by placing the SQD in a microcavity, where the material excitations and the photons of the cavity are strongly coupled. Then the SQD-cavity system is described in terms of the coupled states of material excitations and cavity photons, which are usually called dressed states (properly treated using cavity quantum electrodynamics, i.e. describing matter and light on quantum mechanical grounds). Recently the entangled-photon generation from a SQD-cavity system, where the biexciton is efficiently excited under resonant conditions, was studied. The resonant excitations of biexciton occur through the dressed biexciton states. Two of the four Bell states can be generating by selecting the frequencies of applied fields with certain polarizations (cross-circularly polarized fields). The other two Bell states can be generated by changing the combination of polarizations or by properly adjusting only the frequencies of the input fields. Here, we give a brief summary of the theoretical investigation of the entangled-photon generation from an SQD-cavity system by calculating the thermal entanglement of formation. The calculations for this system are complicated even for entanglement of formation, let alone quantum discord and for this reason we prefer to compute only the first one.

However, in the second part of chapter 4, we have a completely different system (see also Ref.[6]). More specifically, we use qubits, namely single molecules or quantum dots, which can be strongly coupled by interacting with surface plasmons of plasmonic nanostructures. A lot of work has been already done for the computation of entanglement of two qubits which are
mediated by a one-dimensional plasmonic waveguide using concurrence. Additionally to entanglement, the behaviour of quantum discord in two qubits coupled by an one-dimensional plasmonic waveguide has also been recently studied. Thus, here we have a two-dimensional lattice of metal-coated dielectric nanoparticles which is mediated between the two qubits and enhance quantum correlations between these qubits. Therefore, we calculate both the entanglement of formation and quantum discord associated with this system, for two different initial states of the two qubit system and consequently we can make comparisons among these diagrams.

Finally, in chapter 5 we present a resume of the study for the entanglement between the electrons in the hydrogen molecule [6]. More analytically, we investigate the simplest (prototype) realistic two-electrons molecular system, the hydrogen molecule which has been extensively studied for almost a century. Due to the well-known principle of minimum energy the chemical bond is traditionally described and specified in energy terms. Hence, we concentrate in the study of the ground state of the molecular system which is the most stable state, especially in the low temperature case where the thermal energy is not enough to excite the molecule. Here, we would like to indicate the quantum entanglement of the two indistinguishable electrons of the $H_2$ molecule using the entanglement of formation. In order to do that, we should generalise this measure of entanglement in the case of non-separable particles and afterwards we present the most interesting results.
Chapter 2

Quantum measurements and quantum entanglement

2.1 EPR paradox

As we stated in the introduction the EPR paradox [1] plays a crucial role in the understanding of entanglement. These three scientists tried to formulate a thought experiment where the uncertainty principle will be violated which of course would be a paradox in quantum mechanics. The initial idea of Einstein, Podolsky and Rosen was to ”prove” that quantum mechanics is an incomplete theory and there are some hidden variables that had not been considered yet. In their initial paper they attempted to do a thought experiment in which the uncertainty principle is violated for position and momentum. Nevertheless, David Bohm ([7],[8]) implemented their idea in the components of the spin of a system of two particles in order the initial thought experiment of the EPR to be more comprehensible. In Fig.(2.1) we see the experimental configuration of the EPR paradox.

Since the $\pi^0$ particle has spin equals to zero we initially know that the electron and the positron have antiparallel spins. We also have, from the uncertainty principle, that it is impossible to know two different components of the spin of a particle at the same time. However, we can imagine that in the left corner of our experimental setup we have an apparatus which measures the spin of the electron in $x$ direction and we assume without loss of generality that it is measured in the positive direction. Similarly, we assume that there is another apparatus in the right corner which measures the spin of the positron.
Figure 2.1: EPR paradox: A $\pi^0$ particle, in the centre of the figure, which as we know has spin $S = 0$, decays into one electron ($e^-$) and one positron ($e^+$) (grey spheres) and they move in diametrically opposite directions due to the principle of conservation of angular momentum. The electron (left) and the positron (right) have opposite spin because the spin is conserved in such a process.

in the $z$ direction and now assume that it is found in the negative direction. Additionally, we consider that the two measurements take place at the same time. Since the two particles have opposite spins we can deduce that the $x$ component of the positron spin will be in the negative direction and similarly the $z$ component of the electron spin will be in the positive direction. As a result, we are aware of both $x$ and $z$ component of the spin of each particle at the same time which of course violates the Heisenberg’s uncertainty principle.

This is the renowned EPR paradox which indicates non-locality in quantum mechanics. For more information about this paradox and the flaw in the initial argument of Einstein, Podolsky and Rosen someone could also see Refs. [1, 7, 8].

Now we assume that we have the same experimental setup and as before the aparatus in the left corner carries out measurements for the $x$ component and the other one in the right for the $z$ component of the spin of the particles. From now on we focus only on the $x$ component of the spin. We assume that we carry out a measurement in the $x$ component of the electronic spin and we find it in the positive direction. As before we can simultaneously conclude that the $x$ component of the positron spin is in the negative direction. Similarly if the $x$ component of the electron spin lies in the negative
direction then the corresponding component of the positron spin is in the positive one. As a result, we can write for the state of the \( x \) components of the two particles before the measurement that

\[
|\Psi_{\text{before}}(e, p)\rangle = \frac{1}{\sqrt{2}}[|\psi_+(e)|\psi_-(p)\rangle - |\psi_-(e)|\psi_+(p)\rangle]
\] (2.1)

Assuming that a measurement in the electronic spin gives us that the \( x \) component is the positive direction then the \( x \) component of the positron spin lies in the negative direction and the state of the particles after the measurement is written as

\[
|\Psi_{\text{after}}(e, p)\rangle = |\psi_+(e)|\psi_-(p)\rangle
\] (2.2)

As we can see from the Eq.(2.2) the state after the measurement is given as a product of two wavefunctions; the first one is referred to the \( x \) component of the electron spin and the other one to the corresponding component of the positron spin. This means that if we carry out a measurement in the \( x \) component of the electron spin then this will not have any influence on the corresponding spin state of the positron. Nevertheless, if our initial state is not a product state but a linear combination of such product states (e.g. Eq.(2.2)) then a measurement in the \( x \) component of the electron spin can affect the corresponding component of the positron spin. Thus, we observe that there is correlation between the \( x \) component of the electron and the positron spin if the state of the system is given by Eq.(2.2). We will call this kind of states, i.e. states which are linear combination of product states, as entangled states. We would refer to such correlations which are observed among the particles with the term quantum entanglement. As we shall see later, quantum entanglement plays a key role in the development of Quantum Information theory.

### 2.2 Quantum measurements

In the EPR paradox above, we referred to the concept of "measurement" without giving the appropriate attention. The quantum measurement which is carried out in subatomic particles has completely different meaning compared to the classical measurement which we perform in our daily lives.

As we know from Refs.[9], [10] a general quantum measurement is characterised by an ensemble \( M_m \) of measurement operators and \( m \) are the possible
results of the measurement. We act with these operators on the state $|\psi\rangle$ which describes our system. The probability after such a measurement to take the outcome $m$ is given by

$$p(m) = \langle \psi | M_m \dagger M_m | \psi \rangle$$

and as a result the state of our system after this general measurement is

$$|\psi'\rangle = \frac{M_m | \psi \rangle}{\sqrt{\langle \psi | M_m \dagger M_m | \psi \rangle}}$$

Another characteristic feature of these operators is that they satisfy every time the completeness relation

$$\sum_m M_m \dagger M_m = I$$

As a result the completeness relation along with the Eq.(2.3) imply the fact that the probabilities must sum to one.

Now suppose we define the operators

$$E_m = M_m \dagger M_m$$

By using the completeness relation (2.5) we take

$$\sum_m M_m \dagger M_m = \sum_m E_m = I$$

Using now the Eqs. (2.3) and (2.6) we find that

$$p(m) = \langle \psi | E_m | \psi \rangle$$

As someone can see the ensemble of the positive operators $E_m$ specifies the probabilities of the possible outcomes of the measurement. Thus, this type of operators completely characterises the measurement and the complete set $E_m$ is known as POVM (Positive Operator-Valued Measure) measurement. It is obvious that POVM is a quite general type of measurement as its operators obey in relatively few rules and for this reason we can use it for more general problems.

Nevertheless, in this report, we focus only on a special case of POVM measurements, the projective ones. A projective measurement is characterised by the operators $P_m$ and they obey to the additional restriction
\[ P_m P_{m'} = \delta_{mm'} P_m \]  

(2.9)

Of course the completeness relation still holds and takes the form \( \sum_m P_m^\dagger P_m = \mathbb{I} \). Another interesting fact is that only in this special case of POVM measurements each POVM element \( E_m \) is equal to operator measurement, i.e.

\[ E_m = P_m^\dagger P_m = P_m \]  

(2.10)

A very interesting remark concerning projective measurements is that if we repeat it many times then it gives us the same result. In other words, if our system is prepared in the initial state \( |\Psi\rangle \) and we apply a projective operator \( P_m \) then it gives the outcome \( |\psi_1\rangle \) which is an eigenstate of our system. Applying the same projective operator into \( |\psi_1\rangle \) then the outcome remains the same as we have collapse of the initial wavefunction \( |\Psi\rangle \) into only one eigenstate of our system. The fact that the repetition of a measurement gives the same result seems pretty logical for our classical minds but it is not in the quantum world as the repetition of a POVM measurement does not give the same outcome.

In conclusion, the projective measurement is the most common and probably the most well-studied type of measurement in quantum mechanics. It is of great importance in Quantum Information theory as almost all of the measurements that we want to carry out are projectives. Finally, as we shall see in the next chapter taking advantage of this special kind of quantum measurements we can define a very useful and quite general measure of quantum correlations, the quantum discord.
Chapter 3

Entanglement of Formation and Quantum discord

As we said above, in this chapter we want to describe two measures of quantum correlations. The first of them, the Entanglement of Formation, is a measure of entanglement. However, entanglement is not the only type of quantum correlations and for this reason the need for a more general measure of quantum correlations, the quantum discord, arises. In order to give the definitions of these measures we should start with some necessary preliminary knowledge.

3.1 The Schmidt decomposition

The Schmidt decomposition [10] is a very useful tool which is used to write a particular pure state of a bipartite system (a composite system with only two subsystems) in an appropriate form. The Schmidt decomposition cannot generalised for composite systems with three or more subsystems and there is not an analogue for mixtures too. We start our analysis considering the Hilbert space of our composite system $H^{AB} = H^A \otimes H^B$, where $H^A$ and $H^B$ is the Hilbert space of the subsystem $S^A$ and $S^B$ correspondingly. Additionally, our density matrix of the system is given by $\rho^{AB} = |\psi^{AB}\rangle\langle\psi^{AB}|$ and using the properties of the partial trace we can find the reduced density matrices $\rho^A = tr_B[\rho^{AB}]$ and $\rho^B = tr_A[\rho^{AB}]$ of the subsystems $S^A$ and $S^B$ accordingly. By considering an orthonormalised eigenvectors for each subsystem, i.e. $\{|i^A\rangle\}$ for the subsystem $S^A$ and $\{|j^B\rangle\}$ for the subsystem $S^B$, then we can write
the vector $|\psi^{AB}\rangle$ as

$$|\psi^{AB}\rangle = \sum_{n=1}^{k} \sqrt{p_n} |i_n^A, j_n^B\rangle$$

(3.1)

where $p_n$ are positive numbers and are called Schmidt coefficients. The number $k$ is the Schmidt number (or Schmidt rank) and it always holds $k \leq \min(a, b)$ with $\dim H^A = a$ and $\dim H^B = b$. Essentially, all the information regarding the state $|\psi^{AB}\rangle$ is contained in the Schmidt coefficients. According to this decomposition (see Refs. [9],[10] for more information) we can write the reduced density operators of each subsystem in the diagonal form

$$\rho^A = \sum_{n=1}^{k} p_n |i_n^A\rangle\langle i_n^A|$$

(3.2a)

$$\rho^B = \sum_{n=1}^{k} p_n |j_n^B\rangle\langle j_n^B|$$

(3.2b)

So, we see that in this decomposition the two reduced density operators have the same spectrum.

The Schmidt decomposition is of great importance as we can extract very useful information about the state of the composite system. More specifically, if the Schmidt number $k$ is equal to one then the state of the composite system $|\psi^{AB}\rangle$ which is given by Eq.(3.1) is not entangled as it can be written as a product of two separable states. Additionally, for $k = 1$ the reduced density matrices have only one element and as an immediate result from Eqs.(3.2a),(3.2b) we have $tr[(\rho^A)^2] = tr[(\rho^B)^2] = 1$. On the other hand, if the Schmidt number is different than one then our state of the composite system is entangled as it is expressed as a linear combination of products of separable states. As a result, we see that taking advantage of the Schmidt number we can understand if the state of our composite system is entangled or not.

### 3.2 Entropy and entanglement

In order to see the significance of the Schmidt decomposition more clearly we assume again that we have a composite system $S^{AB}$ with two subsystems
and \( S^A \) and \( S^B \) and the corresponding density matrices \( \rho^{AB}, \rho^A \) and \( \rho^B \). We also define the von Neumann entropy as \([10],[9]\)

\[
S(\rho) = -\text{tr}[\rho \log_2 \rho] \quad (3.3)
\]

and is always non-negative. If we diagonalize the density matrix \( \rho \) then the Eq.(3.3) takes the form

\[
S(\rho) = -\sum_{i=1}^{l} \lambda_i \log_2 \lambda_i \quad (3.4)
\]

where \( \lambda_i \) are the eigenvalues of the density matrix and \( l \) is the dimension of the Hilbert space of our system. From now on we will omit the base 2 in the logarithm as it will implicitly given.

Here we must emphasize the physical interpretation of the von Neumann entropy as it plays a significant role in the definition of the quantum discord too. The von Neumann entropy is a measure of uncertainty that someone has before performing a measurement. For instance, if the entropy of a composite system is zero then we can conclude that this system is described by a pure state as we have the maximum information about it-no uncertainty even before the measurement. On the other hand, if the same composite system is described for example by a Bell state then the entropy takes its maximum value as the uncertainty that we have prior the measurement is also maximum. From this example we can understand that the entropy takes its maximum value when we have a uniform distribution, i.e. \( \rho = \frac{1}{d} \mathbb{1} \) where \( \rho \) is the density matrix of the composite system and \( d \) is the number of non-vanishing eigenvalues of this operator. From Eq.(3.3) the maximum values of the entropy is \( S(\rho) = \log d \). As a result the entropy of a binary (or bipartite) system takes values in the range \( 0 \leq S(\rho) \leq 1 \).

Returning to our example with the binary composite system \( S^{AB} \), we know that if this system is described by a pure state then the entropy is given by \( S(AB) = 0 \). If more specifically this pure state is also a product state then as a consequence of this we can extract the maximum information for the state of each subsystem. Because we have no uncertainty regarding the state of each subsystem the von Neumann entropy becomes \( S(A) = S(B) = 0 \), where \( S(A) \) and \( S(B) \) is the entropy of the subsystem \( S^A \) and \( S^B \) correspondingly.

For the same binary system, we assume now that the state which describes the system is not a product state but instead a Bell state, i.e. a maximally
entangled state. This is the case of the uniform distribution for a binary system and as a result the density matrices of the two subsystems are given by $\rho^A = \rho^B = \frac{1}{2} \mathbb{I}$. From all these that we have already stated above, we can write that the entropy of the two systems is given by $S(A) = S(B) = 1$.

Furthermore, as we know from Ref.[10], only classically correlated states can be produced by local operations and classical communication (LOCC). Entangled states have also non-classical correlations which are non-locally accessible. Thus, for a binary system (and more generally for every composite system) $S^{AB}$ it always holds

$$S(AB) \leq S(A) + S(B)$$ (3.5)

and the equality is true only for classically correlated states (in the more general cases the only difference is that we have more terms in the right hand side of the inequality such as $S(C)$, $S(D)$ etc). Thus, we conclude that if the composite system is described by an entangled state then there is additional information in the correlations between the subsystems of it which are non-locally accessible. In other words if we consider only the subsystems then we lose all the more information which is contained in the correlations between the states of each subsystem. So, we can consider the entropy of the subsystems as a measure of the missing information that we have comparing with the pure state of the system $S^{AB}$. As someone can see, entropy is a really convenient measure of the entanglement as for bigger entropy of the subsystems the state of the composite system becomes more entangled. Hence we can consider the entropy of the subsystems as a measure of the entanglement of the pure state of the binary system and mathematically we write

$$0 \leq E(\psi) \leq 1$$ (3.6)

where $|\psi^{AB}\rangle$ is the pure state of the composite system and $E(\psi) = S(A) = S(B)$. Of course if $E(\psi)$ is equal to one then $|\psi^{AB}\rangle$ is maximally entangled but if it is equal to zero then $|\psi^{AB}\rangle$ is separable. Using the definition of the von Neumann entropy as well as the expansion of the density matrix $\rho^A$ (or $\rho^B$) [10] we can write

$$E(\psi) = \sum_{n=1}^{k} p_n \log p_n$$ (3.7)
with $p_n$ the Schmidt coefficients. This quantitative measure $E(\psi)$ is also called the entropy of entanglement. As we can see from Eq. (3.7) and from the Schmidt decomposition analysis in section 3.1 the entropy of entanglement is independent of the basis of each subsystem as well as it does not affect by local unitary transformations on these subsystems. Generally, it only depends on the Schmidt coefficients and this is the significance of the Schmidt decomposition in our analysis.

### 3.3 Entanglement of Formation

In section 3.2 we dealt with only pure states of the composite system and we defined a measure of the entanglement. Now we want to generalise this measure and for this reason we work as follows.

Continuing our analysis of the pure state of the composite system $S^{AB}$ we can write for the entropy of entanglement

$$E(\psi^{AB}) = S(A) = -\text{tr}[\rho^A \log \rho^A]$$

$$= S(B) = -\text{tr}[\rho^B \log \rho^B]$$

(3.8)

where as before $\rho^A$ and $\rho^B$ are the density matrices of the subsystems $S^A$ and $S^B$ respectively. Considering the orthonormal base $\{|0^A, 0^B\}, \{|0^A, 1^B\}, \{|1^A, 0^B\}, \{|1^A, 1^B\}\}$ of the subsystem $S^A$ and $\{|0^B, 1^B\}$ of the subsystem $S^B$ we can expand the density matrix of the composite system as

$$\rho^{AB} = |\psi^{AB}\rangle\langle\psi^{AB}| = \begin{bmatrix}
|a|^2 & ab^* & ac^* & ad^* \\
ba^* & |b|^2 & bc^* & bd^* \\
ca^* & cb^* & |c|^2 & cd^* \\
\db^* & dc^* & |d|^2 & \\
\end{bmatrix}$$

(3.9)

with $|\psi^{AB}\rangle = a|0^A, 0^B\rangle + b|0^A, 1^B\rangle + c|1^A, 0^B\rangle + d|1^A, 1^B\rangle$ and $a, b, c, d \in \mathbb{C}$.

Taking the partial trace $\text{tr}_A[\rho^{AB}]$ (or $\text{tr}_B[\rho^{AB}]$) we find the reduced density matrix $\rho^A$ (or $\rho^B$) and diagonalising it we find that it has the eigenvalues

$$\lambda_{1,2} = 1 \pm \sqrt{1 - C(\psi^{AB})^2}$$

(3.10)

where $C(\psi^{AB}) = 2|ad - bc|$ and is called the concurrence of $|\psi^{AB}\rangle$. As we can see from Eq.(3.10) the concurrence must always be smaller than one, $C \leq 1$, and...
in order to have real eigenvalues. Using the Eq.(3.4) for the entropy $S(A)$ (or $S(B)$) and after a little algebra we find that

$$E(\psi^{AB}) = h \left( 1 + \frac{1 - C(\psi^{AB})^2}{2} \right) \quad (3.11)$$

and $h(x) = -[x \log x + (1 - x) \log(1 - x)]$ is the binary entropy function. As we can see from Eq.(3.11) the entanglement measure $E$ is a monotonic function of the concurrence $C$ and as a result both taking values in the range 0 (no entanglement for the system) to 1 (maximum entanglement). Thus, we can consider that the concurrence is also a measure of entanglement. Although concurrence is a very convinient measure of entanglement as it is easy to be computed, in some applications has a weird behaviour as in the case of the plasmonic correlations that we will see in chapter 4. This may have a simple explanation as the original measure of entanglement is $E$ and not the concurrence $C$, and as a result the physical meaning of concurrence is smaller in comparison to the entanglement measure $E$. Actually, as we also see below, concurrence is a really useful mathematical object but it gives us only a "general idea" of entanglement that is contained in a composite system. If we would like to fully consider entanglement then we have to compute the measure that is given in Eq.(3.11).

The next step in order to generalise $E(\psi)$ for mixtures is to write the concurrence in the form (first introduced by W. K. Wootters [2])

$$C(\psi^{AB}) = |\langle \psi^{AB} | \tilde{\psi}^{AB} \rangle| \quad (3.12)$$

which is the standard definition of concurrence. Here, $|\tilde{\psi}^{AB}\rangle = \sigma_y^A \otimes \sigma_y^B |\psi^{AB}\rangle^*$ and $|\psi^{AB}\rangle^*$ is obtained by taking the complex conjugate coefficients of the state $|\psi^{AB}\rangle$ which is given under the Eq.(3.9), (i.e. $a \rightarrow a^*, b \rightarrow b^*$ etc.). Additionally, $\sigma^i$ with $i = A, B$ are the Pauli matrices of the two subsystems $S^A$ and $S^B$ respectively which exchange the states of each basis and insert a relative phase $\pm i$. Also, $|\tilde{\psi}^{AB}\rangle$ is known as dual state. Thus, when we apply the operator $\sigma_y^A \otimes \sigma_y^B$ in a pure state of a composite system $|\psi^{AB}\rangle$, then we take the dual state $|\tilde{\psi}^{AB}\rangle$, which is orthogonal to our initial one, i.e. the two states are diametrically opposite if we depict them into a Bloch sphere. This results in a zero inner product and from Eq.(3.12) to zero concurrence. On the other side, if the state of our composite system is completely entangled then the operator $\sigma_y^A \otimes \sigma_y^B$ does not affect our initial
state and as a result the two states remains collinear on the Bloch sphere (|ψ\textsuperscript{AB}\rangle and |ψ\textsuperscript{AB}\rangle may differ only on a phase factor). Now the inner product of these states equals to one and from Eq.(3.12) this results in concurrence equals to unity.

Since we have already defined the state |ψ\textsuperscript{AB}\rangle we can write the matrix

\[ \bar{\rho}^{AB} = |\bar{\psi}^{AB}\rangle\langle \bar{\psi}^{AB} | = (\sigma^A_y \otimes \sigma^B_y)\rho^{AB} (\sigma^A_y \otimes \sigma^B_y) \]  \hspace{1cm} (3.13)

and using this we can write the matrix operator

\[ R^{AB} = \rho^{AB}\bar{\rho}^{AB} = \rho^{AB}(\sigma^A_y \otimes \sigma^B_y)\rho^{AB}(\sigma^A_y \otimes \sigma^B_y) \]  \hspace{1cm} (3.14)

and diagonalising the matrix \( R^{AB} \) we compute its eigenvalues \( \lambda_j \), with \( j = 1, 2, 3, 4 \). Using them we can calculate the concurrence for a mixture \( \rho^{AB} \) as with matrix representation we can generalise our formula from pure states to general mixtures. So, the concurrence for this more general case is given by

\[ C(\rho^{AB}) = \max \{ 0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4} \} \]  \hspace{1cm} (3.15)

and for the eigenvalues holds \( \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \). Now from Eq.(3.11) we can finally compute the entanglement of formation (EoF) which is given by

\[ E(\rho^{AB}) = \hbar \left( 1 + \sqrt{1 - C(\rho^{AB})^2} \right) \]  \hspace{1cm} (3.16)

Nevertheless, we can write a general mixture \( \rho \) as

\[ \rho^{AB} = \sum_n p_n |\psi_n^{AB}\rangle\langle \psi_n^{AB}| \]  \hspace{1cm} (3.17)

and \( |\psi_n^{AB}\rangle \) are an ensemble of \( n \) pure states. In order to find the entanglement \( E(\psi_n^{AB}) \) of each separate state \( |\psi_n^{AB}\rangle \) we must use the Eq.(3.11). According to Wootters [2] we find the entanglement of formation of the statistical mixture \( \rho \) taking the mean entanglement \( E(\psi_n^{AB}) \) of the pure states of the decomposition minimised over all ensemble decompositions of \( \rho^{AB} \), i.e

\[ E'(\rho^{AB}) = \min_n \sum_n p_n E(\psi_n^{AB}) \]  \hspace{1cm} (3.18)
Using the theorem of Wootters we conclude that the two definitions (see Eqs.(3.16) and (3.18)) are equivalent; \( E'(\rho^{AB}) = E(\rho^{AB}) \). Thus, the measure \( E(\rho^{AB}) \) is not only a mathematical but also a physical generalization of the entropy of entanglement in the mixed states.

To sum up, we gave the definition of a measure of entanglement for pure states (entropy of entanglement) and we generalised it for mixed states (entanglement of formation or EoF) too. During the computation of EoF we also found a quantity, the concurrence \( C \), which is a monotonic function of EoF and as a result we can also use it as a measure of entanglement. It is also more convenient than EoF as we can compute it more easily but in some cases it is observed to have some peculiarities. However, as we stated above entanglement is not the only kind of quantum correlations. So, it is necessary to introduce a more general measure which includes all types of quantum correlations. This measure is the quantum discord.

### 3.4 Mutual information

In order to go further in the definition of quantum discord, we must first introduce the definition of the mutual information. We begin with the classical case and afterwards we will generalise to the quantum mechanical one. It is also useful to introduce the classical entropy (or Shannon’s entropy) which is given by

\[
H(p) = - \sum p(x_n) \log_2 p(x_n),
\]

with \( x_n \) being the possible outcomes and \( p(x_n) \) the probabilities of each outcome (cf with the quantum mechanical analogue of Eq.(3.4) and also see [9],[10]). In Fig.(3.1) we give the Venn diagram of two classical subsystems.

Each circle in the Venn diagram of Fig.(3.1) denotes the entropy of the respective classical subsystem. If the subsystems \( H(X) \) and \( H(Y) \) are completely independent of one another then the two circles are not intersect. Then the equality holds in Eq.(3.5), but for the classical case, i.e. \( H(XY) = H(X) + H(Y) \).

Now we turn our attention in the more interesting case where the subsystems are not independent. Then from Eq.(3.5), again for the classical case, we have that \( H(XY) < H(X) + H(Y) \). Moreover, we can see in the Venn diagram above the conditional entropy \( H(X|Y) \) which is represented by the red crescent shape. This type of entropy is defined as the uncertainty that we still have about \( X \) when we had already performed a measurement on \( Y \). Similar definition holds for \( H(Y|X) \), the blue miniscus in Fig.(3.1).
Figure 3.1: The Venn diagram for the classical subsystems $H(X)$ and $H(Y)$. We also denote as $I(X : Y)$ the mutual information. The generalization to quantum mechanics is not straightforward for the conditional entropy $H(X|Y)$ (or $H(Y|X)$) and consequently for the mutual information.

Finally, we have the mutual information $I(X : Y)$ which is the most important feature in our Venn diagram. In the classical case mutual information has two equivalent expressions. We write the first definition of the mutual information $I(X : Y)$ in classical theory as

$$I(X : Y) = I(Y : X) = H(X) + H(Y) - H(XY) \quad (3.19)$$

Considering the Venn diagram of Fig. (3.1) we have that $H(XY)$ is the entropy of the composite system and we subtract it from the sum of the entropies of the subsystems. As a result we find the intersection which is illustrated in Fig. (3.1). So, we can view the mutual information as a measure of the correlations between the subsystems. In other words, mutual information is the quantity of the information that $X$ and $Y$ have in common.

An alternative way to define this quantity is through the classical conditional entropy $H(X|Y)$

$$I(X : Y) = H(X) - H(X|Y) \quad (3.20)$$

The physical interpretation of this equation is that $I(X : Y)$ is the information that one obtains about $X$ when $Y$ it is already known. Of course the opposite is also true since $I(X : Y) = I(Y : X)$ as we stated above.
As we can see again from the Venn diagram of Fig.(3.1) the two expressions of Eqs.(3.19) and (3.20) are also equivalent diagrammatically. Now we want to generalise the concept of the mutual information in the quantum mechanical case.

The generalization of the first expression of the mutual information in the quantum mechanical case, Eq.(3.19), is straightforward and we can write it as

$$ I(A : B) = S(A) + S(B) - S(AB) \quad (3.21) $$

However, the generalisation of the second expression is not straightforward. This happens due to the conditional entropy $H(X|Y)$ as in order to compute it in quantum mechanics we have to perform a measurement on subsystem $S^B$, the quantum mechanical analogue of $H(Y)$. But, as we analysed in chapter 2, any measurement in quantum mechanics perturbs the initial state of our system. Here we assume only projective measurements as it has been proven that this type of measurement is the most adequate in order to define the quantum discord [11]. Next we give the generalization of the second expression of mutual information in quantum mechanics and we also define the quantum discord [3], [4].

### 3.5 Quantum discord

We assume that we have a set of orthogonal projectors \( \{ \Pi_j^B \} \) with \( j \) possible outcomes. We act with this ensemble of operators on the subsystem \( S^B \) and the density matrix of our composite system \( S^{AB} \) becomes

$$ \rho^{AB|\Pi_j^B} = \frac{\Pi_j^B \rho^{AB} \Pi_j^B}{tr_{A,B}(\Pi_j^B \rho^{AB} \Pi_j^B)} \quad (3.22) $$

where we have divided with the probability of the occurrence of the \( j \)-th outcome \( p_j = tr_{A,B}(\Pi_j^B \rho^{AB} \Pi_j^B) = tr_{A,B}(\Pi_j^B \rho^{AB}) \). According to H. Ollivier and W. H. Zurek [3] the quantum mechanical generalisation of the conditional entropy is

$$ S(AB|\Pi_j^B) = \sum_j p_j S(\rho^{AB|\Pi_j^B}) \quad (3.23) $$

where we have taken into consideration all the possible \( j \)-measurements and \( p_j \) is the probability of the \( j \)-th outcome. The quantity \( S(\rho^{AB|\Pi_j^B}) \) is a
measure of the information that we lose about the subsystem $S^A$ when we perform a projective measurement $\Pi_j^B$ on subsystem $S^B$. Since Eq.(3.23) is the quantum mechanical analogue of the conditional entropy then using Eq.(3.20) we can write the second expression of the mutual information in quantum mechanics as

$$J(A : B) = S(A) - S(AB|\{\Pi_j^B\}) \quad (3.24)$$

The Eq.(3.24) represents the information that is gained by the subsystem $S^A$ as a result of the measurement $\{\Pi_j^B\}$ in the subsystem $S^B$. It is obvious that the value of $J(A : B)$ depends on the ensemble of the projective operators $\{\Pi_j^B\}$. According to L. Henderson and V. Vedral [4] the maximum value of $J(A : B)$ with respect to the set $\{\Pi_j^B\}$ can be defined as a measure of classical correlations (CC). Thus the CC of our composite system $S^{AB}$ is given by

$$CC(AB) = \max_{\{\Pi_j^B\}} J(A : B) = S(A) - \min_{\{\Pi_j^B\}} S(AB|\{\Pi_j^B\}) \quad (3.25)$$

Now the difference between the first expression of the mutual information, Eq.(3.21), and the second one, Eq.(3.24), which as we stated above represent the total of the classical correlations of our system, defines the quantum discord (QD)

$$Q(A : B) = I(A : B) - CC(AB)$$

$$= S(B) - S(AB) + \min_{\{\Pi_i^A\}} S(AB|\{\Pi_i^A\}) \quad (3.26)$$

Since $I(A : B)$ gives the total correlations of our system and $CC(AB)$ the total of the classical correlations then we conclude that $Q(A : B)$ gives the total of quantum correlations.

It is worth noting that QD is not symmetric under the interchange of the two subsystems $S^A$ and $S^B$. In other words if we use a set of projective operators $\{\Pi_i^A\}$ on the subsystem $S^A$ then the QD becomes

$$Q(B : A) = S(A) - S(AB) + \min_{\{\Pi_i^A\}} S(AB|\{\Pi_i^A\}) \quad (3.27)$$

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i.e. \( Q(A : B) \neq Q(B : A) \) in general. The equality \( Q(A : B) = Q(B : A) \) holds iff we have only classical correlations in our system. In conclusion, QD generally depends on the subsystem on which we perform the projective measurement.

Furthermore, QD must always be positive. From Eq.(3.26) that means

\[
S(AB) - S(B) \leq \min_{\{\Pi_j^B\}} S(AB|\{\Pi_j^B\}) \quad (3.28)
\]

Comparing with the conditional entropy in the classical case from Fig.(3.1) we have that \( H(X|Y) = H(XY) - H(X) \). In the quantum mechanical case the inequality is justified by the fact that there is additional uncertainty regarding the set of the projective operators \( \{\Pi_j^B\} \) that we use. This is an excellent example in order to demonstrate the peculiar nature of quantum measurements. As we can see, even the most simple and the most well-studied, the projective measurement, is completely different in comparison with the classical measurement.

Another interesting feature of QD is that for pure states of the composite system \( S^{AB} \) it reduces to EoF, the measure of entanglement that we mentioned above. As a result, for pure states there are no quantum correlations except entanglement.

From the definition of QD in Eq.(3.26) it is obvious that we use the appropriate projective measurement on subsystem \( S^B \) in order to minimize the conditional entropy \( S(AB|\{\Pi_j^B\}) \). This fact corresponds to find the appropriate projective measurement which causes the minimum perturbation in the quantum state of the composite system and in the same time allows the maximum information regarding the subsystem \( S^A \) to be extracted. Thus, if the QD of our system is large then there is missing and destruction of the information regarding the subsystem on which we perform the projective measurement (\( S^B \) in our case). On the other hand, if QD is small then almost all the information of the subsystem \( S^B \) (again the subsystem on which we apply the projective operators \( \{\Pi_j^B\} \) which is contained between the correlations of the subsystems \( S^A \) and \( S^B \) is locally accessible from the state of \( S^A \). Finally, if \( Q(A : B) = 0 \) then all the correlations of our system are classical and as a result the whole information can be extracted by local measurement on the subsystem \( S^B \). In other words for zero QD there are no quantum correlations.

An instructive example exists in the original paper of H. Ollivier and W. H. Zurek [3] and has to do with the Werner state, \( \rho_W = \frac{1-z}{4}I + z|\psi\rangle\langle\psi| \)
where $|\psi\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$. From this example, someone could notice that separability and zero discord have not the same physical interpretation, i.e. they are not equivalent concepts. Another very interesting application of QD is given by S. Luo [15]. In his paper an analytical expression of quantum discord is given for the family of two-qubit states which has the form $\rho_{Luo} = \frac{1}{4} \left( I + \sum_{i=1}^{3} c_i \sigma_i \otimes \sigma_i \right)$ and $c_i$ are real coefficients (see also Ref.[15] for the $c_i$'s constraints). In other words, we can write the matrix $\rho_{Luo}$ as

$$
\rho_{Luo} = \frac{1}{4} \begin{bmatrix}
1 + c_3 & 0 & 0 & c_1 - c_2 \\
0 & 1 - c_3 & c_1 + c_2 & 0 \\
0 & c_1 + c_2 & 1 - c_3 & 0 \\
c_1 - c_2 & 0 & 0 & 1 + c_3
\end{bmatrix}
$$

(3.29)

We conclude that for this family of two-qubit states besides the analytical expression for quantum discord, we also have an analytical expression for classical correlations which is really useful as we can make direct comparisons between these two expressions for different values of $c_i$s. The complete analysis contains rather long computations which are beyond the scope of this work (see Ref.[15]). For more information regarding QD and some applications of it in two qubit states someone can also see Refs.[3], [4], [11]-[16].

In the next chapter we will analyse two more applications of these measures; the first one is for a quantum dot-cavity system and the second one is about a two-qubit system mediated by plasmons.
Chapter 4

Two interesting applications

4.1 Entangled-photon generation by a quantum dot-cavity system

We begin here assuming that our composite system is composed by a semiconductor quantum dot and a cavity [5], [17]-[22]. In this system the entangled photon-pairs are generated by the cascade emission through the intermediate states.

More analytically, we describe the semiconductor quantum dot by a four level system; \( |G\rangle \) is the ground state, \( |X_R\rangle \) and \( |X_L\rangle \) is the right and left polarized degenerate exciton states and \( |B\rangle \) the biexciton state. All these states are orthogonal to each other and they are also normalized. Now we assume that this quantum dot is embedded in a microcavity where there are circularly left- and right- polarized photons of the same energy as the energy difference between the exciton and the ground state. However, we should be careful if we have to include other (excited) exciton states and biexciton states. The present model is valid once the level separation of excitons and biexcitons are greater than the vacuum Rabi splitting. As a result, the Hilbert space of this composite system is the direct product of states of the semiconductor quantum dot and the cavity-mode photons. We write this type of product states following Refs.[5], [17]-[22] as \( |Y; n_R, n_L\rangle \) where \( Y \) represent the energy states of the quantum dot and \( n_R(n_L) \) is the number of the right- (left-) circularly polarized photons in the cavity. The Hamiltonian of our quantum dot-cavity system is given by
\[ H_0 = \epsilon_0 \sum_k (|X_k\rangle\langle X_k| + \alpha_k^\dagger \alpha_k) + (2\epsilon_0 - \Delta_B)|B\rangle\langle B| \]
\[ + g \sum_k (i|G\rangle\langle X_k| \alpha_k^\dagger + H.c.) + g_B (i|X_R\rangle\langle B| \alpha_R^\dagger + i|X_L\rangle\langle B| \alpha_L^\dagger + H.c.) \]
\]

where the index \( k \) runs over \( R \) (right-polarized) and \( L \) (left-polarized) quantum dot states or cavity-mode photons. \( g(g_B) \) is the coupling constants between the exciton(biexciton) transition and one cavity-mode photon. Also, \( \epsilon_0 \) is the energy difference between the exciton and the ground state and \( \Delta_B \) is the binding energy of the biexciton state.

We usually call the eigenstates of the Hamiltonian \( H_0 \) dressed states and they are superposition of the product states. A schematic interpretation of the dressed states is given by K. Shibata and H. Ajiki [21]. Here we want only to mention that the dressed states are divided into one state of zero energy (\( |G; 0, 0\rangle \)), four states of \( \epsilon_0 \) energy (\( |G; 1, 0\rangle, |G; 0, 1\rangle, |X_R; 0, 0\rangle \) and \( |X_L; 0, 0\rangle \)), seven states of \( 2\epsilon_0 \) energy (\( |G; 1, 1\rangle, |G; 2, 0\rangle, |G; 0, 2\rangle, |X_R; 1, 0\rangle, |X_R; 0, 1\rangle, |X_L; 1, 0\rangle \) and \( |X_L; 0, 1\rangle \)) and one state of \( 2\epsilon_0 - \Delta_B \) energy (\( |B; 0, 0\rangle \)). Thus, the dressed states are categorized into three groups. The group with the lowest (zero) energy which is actually the \( |G; 0, 0\rangle \) product state. The second group with states of higher energy, all in the region of \( \epsilon_0 \). Actually we have only two energy values with a \( 2g \) energy splitting known as the vacuum Rabi splitting. These dressed states are a superposition of singly excited quantum dot of specific polarization and absence of photons and ground state quantum dot in the presence of one photon with the same polarization and hence can be characterized by their polarization (namely, \( |R_+\rangle, |R_-\rangle, |L_+\rangle \) and \( |L_-\rangle \)). Finally, we have eight dressed states of energy around \( 2\epsilon_0 \). We can separate these states into two categories, the co-polarized dressed states (linear superposition of \( |G; 2, 0\rangle, |G; 0, 2\rangle, |X_R; 1, 0\rangle \) and \( |X_L; 0, 1\rangle \) denoted as \( |RR_+\rangle, |RR_-\rangle, |LL_+\rangle \) and \( |LL_-\rangle \) and the cross-polarized dressed states (linear superposition of \( |G; 1, 1\rangle, |B; 0, 0\rangle, |X_R; 0, 1\rangle, |X_L; 1, 0\rangle \)) corresponding to a singlet state
\[ |S\rangle = \frac{1}{\sqrt{2}}(|X_R; 0, 1\rangle - |X_L; 1, 0\rangle) \]

of energy \( 2\epsilon_0 \) and three triplet states
\begin{align}
    |RR_\pm\rangle &= \frac{1}{\sqrt{2}} (|G; 2, 0\rangle \mp i|X_R; 1, 0\rangle) \tag{4.3} \\
    |LL_\pm\rangle &= \frac{1}{\sqrt{2}} (|G; 0, 2\rangle \mp i|X_L; 0, 1\rangle) \tag{4.4} \\
    |T_j\rangle &= c_j \left[ |G; 1, 1\rangle - \frac{a_j^2 - 2g^2}{2g g_B} |B; 0, 0\rangle + i \frac{a_j}{2g} (|X_R; 0, 1\rangle + |X_L; 1, 0\rangle) \right] \tag{4.5}
\end{align}

where \(c_j\) is a normalization coefficient and \(j = 1, 2, 3\). Additionally, \(\lambda_\pm^{(2)} = 2\epsilon_0 - \sqrt{2} g\), \(\lambda_S = 2\epsilon_0\) and \(\lambda_j = 2\epsilon_0 - a_j\) are the eigenergies of the corresponding dressed states and the physical interpretation of \(a_j\) is the differences of \(2\epsilon_0\) from each \(\lambda_j\) and they are the real solutions, multiplied by \(\Delta_B\), of the equation \[21\]

\[f(x) = x^3 - x^2 - (p + q)x + p = 0 \tag{4.6}\]

with \(p = 2\left(\frac{g}{\Delta_B}\right)^2\) and \(q = 2\left(\frac{g^2}{\Delta_B}\right)^2\).

Generally, the cavity is coupled to the environment by cavity-mode photons leaking out of the cavity. In order to have a control of these leaking photons we apply external electromagnetic fields interacting with the cavity. We consider CW laser fields with electric fields \(E_R e^{-i\Omega_R t}\) and \(E_L e^{-i\Omega_L t}\), with \(E_R(E_L)\) being the amplitudes and \(\Omega_R(\Omega_L)\) being the frequencies of the right-(left-) polarised laser fields all assumed real. Then the Hamiltonian which describes the interaction between the laser fields and the cavity photons is given by [21],[22]

\[H_{\text{int}} = \sqrt{\Gamma} \sum_{k=R,L} E_k (ie^{-i\Omega_k t}\alpha_k^\dagger - ie^{i\Omega_k t}\alpha_k) \tag{4.7}\]

and \(\Gamma\) is a phenomenological parameter describing the cavity photon leakage. The dynamics of the density matrix operator of the whole quantum system \((H = H_0 + H_{\text{int}})\) in which the damping of the excited states is taken into account is described by means of the following standard master equation

\[
\frac{d}{dt} \rho(t) = -i[H, \rho(t)] + \gamma_X \left( \frac{1}{2} \{ |G\rangle, |X_R\rangle \} \rho(t) + \frac{1}{2} \{ |G\rangle, |X_L\rangle \} \rho(t) \right) + \gamma_B \left( \frac{1}{2} \{ |X_R\rangle, |B\rangle \} \rho(t) + \frac{1}{2} \{ |X_L\rangle, |B\rangle \} \rho(t) \right) + \Gamma \{ \mathbb{1}, \alpha_k^\dagger \} \rho(t)
\tag{4.8}
\]
with the operator \( \{u, v\}_f = 2uu^\dagger fv - fvv^\dagger - vv^\dagger f \) and \( \gamma_X, \gamma_B \) are the damping constants from the exciton and biexciton, respectively. The last term in Eq.(4.8) gives the photon leakage from the cavity to the environment. Here we consider the steady state solution of the master equation achieved, at sufficiently large \( t \) by vanishing the time derivative, of the coupled non-linear differential equations of the master equation and practically solving an algebraic system of non-linear equations.

For more information about the mechanism that the photon-pairs being entangled someone should see Ref.[21]. Here we present only the contour plots of EoF for the quantum dot-cavity system. All the contour plots shows EoF as a function of \( g \) and \( \Omega_R' = \Omega_R - \epsilon_0 \) for fixed values of \( g_B \) and the input field frequency at \( \Omega_L = \epsilon_0 - g \). More specifically, the contour plot of Fig.(4.1) shows EoF as a function of \( g/\Gamma \) for \( \Delta_B = 15\Gamma, \ g_B = 15\Gamma, \ \gamma_X = \gamma_B = 0.1\Gamma \) and \( E_R = E_L = 0.02\sqrt{\Gamma} \).  

![Contour plot](image)

**Figure 4.1:** The entanglement of formation (EoF) for the quantum dot-cavity system for \( \Delta_B = 15\Gamma, \ g_B = 15\Gamma, \ \gamma_X = \gamma_B = 0.1\Gamma \) and \( E_R = E_L = 0.02\sqrt{\Gamma} \). The red colour corresponds to maximum entanglement whereas the black colour corresponds to completely disentangled states of the photon-pairs.

This figure for the same parameters there is also in Ref.[21] but for smaller range of \( g \) and \( \Omega_R' \).

In the figure above, the regions of maximum entanglement denote resonant excitations for the dressed states. More analytically, the top curve line with positive slope indicates resonant excitation with the dressed state \( |T_1\rangle \), the second one with \( |S\rangle \), the third one with \( |T_2\rangle \) (it seems better for \( g/\Gamma < 30 \))
and the bottom curve with positive slope with $|T_3\rangle$. In this diagram we also observe some additional features but their physical interpretation is beyond this analysis (see also Ref.[5]).

The point here is to see how useful tool is the EoF in order to depict entanglement. For this reason we give another contour plot for different parameters.

![Contour plot](image)

**Figure 4.2:** The entanglement of formation (EoF) for $\Delta_B = 150\Gamma$ and $g_B = 15\Gamma$. We see that the four major lines of resonant excitation which correspond to maximum entanglement are observed again.

Thus, we see how convenient and useful tool is the EoF. By changing any parameter we take a new contour plot and as a result we can extract all the information that we want about the quantum dot-cavity system. We can also depict and compare the entanglement for quantum dots which consist by different materials (e.g. InAs, GaAs, CuCl etc [5]). Generally, we can investigate the EoF for various values of the important parameters of the quantum dot system and depict it as a countor plot.

This was an application of the first measure of quantum correlations that we defined in chapter 3. Now we continue to the second one where we can also make a direct comparison of the two measures that we demonstrated above.
4.2 Quantum correlations via plasmonic nanostructures

Recently, it has been shown that qubits, namely single molecules or quantum dots, can be strongly coupled by interacting with surface plasmons of plasmonic nanostructures [23]-[49]. Entanglement of two qubits, mediated by a one-dimensional plasmonic waveguide has recently been studied [29, 30, 35], and quantified via the concurrence. Nevertheless, as we mentioned above concurrence is only a variable in the definition of EoF and as a result it is more appropriate to use entanglement of formation rather than concurrence in order to properly quantify the entanglement [36]. Additionally to entanglement, the behavior of QD in two qubits coupled by an one-dimensional plasmonic waveguide has also been recently studied [36, 41, 43]. Besides one-dimensional plasmonic waveguides, entanglement of two qubits separated by a metal or metamaterial slab [31], a metallic nanoparticle [34], and a hybrid photonic-plasmonic resonant structure which consists of two metal nanoparticles and a high-Q whispering-gallery-mode microcavity [42] has also been discussed.

Here we use a plasmonic nanostructure which is a two-dimensional lattice of metal-coated dielectric nanoparticles. A schematic interpretation of this plasmonic nanostructure is given in Fig.(4.3). Thus, our system consists of this nanostructure and two identical qubits which are putted on diametrically opposed distances. The presence of this nanostructure leads to enhanced dipole-dipole interaction between two quantum systems (the two qubits in our case) [26].

The combination of strong dipole-dipole interaction between two quantum systems [26] and the reduced spontaneous emission rates of an individual quantum system [23, 27, 32, 33] could lead to strong quantum correlations between the two qubits. Thus, here we present the interaction of two qubits, e.g. atoms, molecules or quantum dots, with a two-dimensional lattice of metal-coated dielectric nanoparticles. We make calculations for both EoF and QD for two different initial states, in order to indicate the difference between entanglement, which is measured by the EoF, and the total quantum correlations, which are measured by the QD (these results that we will show below together with some others are to be published).

As we said above, our system consists by two qubits (two identical two level systems) which indirectly interact through the two-dimensional lattice of
Figure 4.3: The plasmonic nanostructure which is mediated between the two qubits of our system. The two qubits are placed in identical distances from the nanostructure. (a) The structure of the metal-coated dielectric nanosphere and (b) a square lattice (monolayer) of metal-coated dielectric nanospheres.

metal-coated dielectric nanoparticles of Fig(4.3). The dipole moments of the two qubits is perpendicular to the surface of the plasmonic nanostructure and so the weak coupling approximation is valid. Therefore, we can safely perform the Born-Markov approximation in order to trace out the degrees of freedom of the hybrid nanostructure. Using this approximation the master equation which describes the dynamics of the density matrix \( \rho \) of the composite system is given by

\[
\frac{\partial}{\partial t} \rho = -\frac{i}{\hbar} [H, \rho] + \sum_{i,j=A,B} \gamma_{ij} (2\sigma_i \rho \sigma_j^\dagger - \sigma_i^\dagger \sigma_j \rho - \rho \sigma_i^\dagger \sigma_j) \tag{4.9}
\]

with \( \sigma_i \) and \( \sigma_i^\dagger \) the lowering and raising operators for each qubit. The Hamiltonian of the above master equation is

\[
H = \hbar \omega_0 \sum_{i,j=A,B} \sigma_i^\dagger \sigma_i + \hbar g_{AB}(\sigma_A^\dagger \sigma_B + \sigma_B^\dagger \sigma_A) \tag{4.10}
\]

where we have considered that the characteristic frequencies of each qubit are equal, i.e. \( \omega_A = \omega_B = \omega_0 \). The quantities \( \gamma_{AB}(= \gamma_{BA}) \) and \( g_{AB}(= g_{BA}) \) in the above equations describe the collective spontaneous decay rates and the energy shift (responsible for the coherent coupling between the two qubits),
respectively \[29, 30, 31, 35, 50\]. These parameters are calculated via the electromagnetic Green’s tensor \( \mathbf{G}(\mathbf{r}, \mathbf{r}'; \omega_0) \)

\[
\gamma_{AB} = \frac{2\omega_0^2}{\epsilon_0 c^2 \hbar} \mathbf{p} \cdot \Im \mathbf{G}(\mathbf{r}_A, \mathbf{r}_B; \omega_0) \cdot \mathbf{p} \tag{4.11}
\]

\[
g_{AB} = \frac{\omega_0^2}{\epsilon_0 c^2 \hbar} \mathbf{p} \cdot \Re \mathbf{G}(\mathbf{r}_A, \mathbf{r}_B; \omega_0) \cdot \mathbf{p} \tag{4.12}
\]

\[
\gamma_{ii} = \frac{2\omega_0^2}{\epsilon_0 c^2 \hbar} \mathbf{p} \cdot \Im \mathbf{G}(\mathbf{r}_i, \mathbf{r}_i; \omega_0) \cdot \mathbf{p} \tag{4.13}
\]

with \( i = A, B \) and \( \mathbf{p} \) being the dipole matrix element of each qubit assumed to be real. Next we consider that the two qubits are placed at two diametrically opposed positions from the plasmonic nanostructure, thus we have \( \gamma_{AA} = \gamma_{BB} = \gamma \). The distance of each qubit from the surface of the plasmonic nanostructure is denoted with \( d \). More information regarding how the Green tensor \( \mathbf{G}(\mathbf{r}, \mathbf{r}'; \omega_0) \) provides the values of \( \gamma_{AB}, g \) and \( \gamma \) as well as some more technical details of the plasmonic nanostructure that is mediated between the two qubits are given in the article that will be published.

Next we consider a convenient basis in order to solve the set of differential equations obeyed by the density matrix elements which are derived by the master equation of Eq.(4.9). One possible basis would be \( \{ |0\rangle = |g_A, g_B\rangle, |1\rangle = |e_A, g_B\rangle, |2\rangle = |g_A, e_B\rangle, |3\rangle = |e_A, e_B\rangle \} \), where \( g_i \) and \( e_i \) label the ground and excited state of the \( i \)-qubit respectively. Nevertheless, the most appropriate basis for our case is \( \{ |0\rangle = |g_A, g_B\rangle, |\pm\rangle = (1/\sqrt{2})(|e_A, g_B\rangle \pm |g_A, e_B\rangle), |3\rangle = |e_A, e_B\rangle \} \) as it provides a clearer understanding of the quantum correlations of the two-qubit system, as the states \( |\pm\rangle \) are two maximally entangled states (Bell states).

Here we consider two different initial states; the first one is \( |\Psi\rangle = \sqrt{q} |1\rangle + \sqrt{1-q} |2\rangle \) and the second is \( |\Phi\rangle = \sqrt{q} |0\rangle + \sqrt{1-q} |3\rangle \)

For the first case, i.e. for initial state \( |\Psi\rangle = \sqrt{q} |1\rangle + \sqrt{1-q} |2\rangle \) the only non-zero elements of the density matrix \( \rho(t) \) are \( \rho_{++}(t), \rho_{--}(t), \rho_{+-}(t), \rho_{-+}(t) \) and \( \rho_{00}(t) \). For this initial state and taking into consideration the expressions of the non-zero elements of \( \rho(t) \) we can derive an analytical expression for the concurrence which is
\[ C(t) = e^{-\gamma t} \left\{ \frac{1 + 2\sqrt{q(1-q)}}{2} e^{-\gamma_{AB}t} - \frac{1 - 2\sqrt{q(1-q)}}{2} e^{\gamma_{AB}t} \right\}^2 + (2q - 1)^2 \sin^2(2g_{AB}t) \right\}^{1/2} \] (4.14)

The Eq.(4.14) is a generalization of the corresponding analytical expression of Refs. [29, 30, 35], which is derived if we set \( q = 0 \) or \( q = 1 \). Using Eq.(3.16) we can also derive an analytical expression for EoF too, but it is rather lengthy and cumbersome.

Now for the second initial state, \( |\Phi\rangle = \sqrt{q}|0\rangle + \sqrt{1-q}|3\rangle \), by solving again the master equation Eq.(4.9) we find that the non-zero elements of the density matrix are \( \rho_{33}(t) \), \( \rho_{03}(t) \), \( \rho_{++}(t) \), \( \rho_{--}(t) \) and \( \rho_{00}(t) \). An analytical expression for the concurrence has already derived (see Refs.[29, 30, 35])

\[ C_1(t) = 2|\rho_{03}(t)| - |\rho_{++}(t) + \rho_{--}(t)|, \] (4.15)

\[ C_2(t) = -2\sqrt{\rho_{00}(t) \rho_{33}(t)} + |\rho_{++}(t) - \rho_{--}(t)| \] (4.16)

We find the concurrence by taking the maximum value of these expressions at each time instant, i.e. \( \max[0, C_1(t), C_2(t)] \). As before we can use Eq.(3.16) in order to find an analytical expression for EoF. Additionally, as first mentioned by Gonzalez-Tudela et al. [35] due to the double criterion of concurrence we observe the so-called revival of entanglement [51].

We start by assuming the initial state \( |\Psi\rangle \) for \( q = 1/2 \), which is the Bell maximally entangled state \( |\Psi\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) = |+\rangle \). In Fig(4.4) we see the EoF as a function of time. The axis of time has been multiplied by \( \Gamma_0 \) which is the spontaneous decay rate in free space. The different colours in the Fig.(4.4) indicate the different distances of qubits from the plasmonic nanostructure. In all figures of EoF we use blue (solid), red (dashed), yellow (dotted) and green (dot-dashed) curves to represent results for distances \( d = 0.4c/\omega_p \), \( d = 0.5c/\omega_p \), \( d = 0.6c/\omega_p \) and \( d = 0.7c/\omega_p \), respectively. The length scale is \( c/\omega_p \approx 22nm \) and \( \omega_p \) is the bulk plasma frequency.

Concerning Fig.(4.4) we observe that all curves for \( t = 0 \) have EoF equals to one since our initial state is maximally entangled state and decay with time. However, someone can easily conclude that larger the distance between the two qubits the bigger the EoF. The observed behaviour can be
easily explained by means of Eq.(4.14): for $q = 1/2$, $C(t)$ becomes a simple exponentially decaying function $(e^{-(\gamma + \gamma_{AB})t})$. As a result, we find that, in this case, the behaviour of the system is independent of the coherent coupling $g_{AB}$ and depends only on the total spontaneous decay rates, i.e. $\gamma + \gamma_{AB}$.

Now we give the corresponding figure for QD and CC for this maximally entangled initial state. In Fig.(4.5) we see the curves of QD (solid and dashed curves) and CC (dotted and dot-dashed curves) for two different values of distance $d$, $d = 0.4c/\omega_p$ (solid and dotted curves) and $d = 0.7c/\omega_p$ (dashed and dot-dashed curves). We observe that both QD and CC show a strong dependence on distance $d$ with the same trends found in the EoF behaviour (compare with Fig.(4.4)) but now the reported correlations are more sensitive to changes in distance $d$ (see Fig.(4.5)). We should also mention here that in all cases QD is higher than EoF, as expected, as QD includes all quantum correlations and not just entanglement.

Next, we turn our attention to the second initial state, $|\Phi\rangle = \sqrt{q}|0\rangle + \sqrt{1-q}|3\rangle$. As in the previous case we generally have $0 < q < 1$, but here we consider only the case for $q = 1/2$. Again as in the previous case, the value of EoF for each distance begins from one. Fig.(4.6) shows only a limited range of the values of EoF as it would be impossible to observe it if we had plotted EoF from zero to one. As we mentioned above, due to the double criterion of concurrence the revival of entanglement is observed (see Fig.(4.6)). However, it does not occur for all distances but only for the distances $d = 0.5c/\omega_p$ (red dashed curve), $d = 0.6c/\omega_p$ (yellow dotted curve) and $d = 0.7c/\omega_p$ (green dot-dashed curve). Taking the expressions of non-zero elements of the density matrix $\rho$, $\rho_{33}(t)$, $\rho_{03}(t)$, $\rho_{++}(t)$, $\rho_{--}(t)$ and $\rho_{00}(t)$ as we mentioned above, then someone could notice that the crucial elements again are the collective decay rate $\gamma_{AB}$ and the individual decay rate $\gamma$, as in the case of the state $|\Psi\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) = |+\rangle$.

Finally, Fig.(4.7) shows QD and CC as a function of time for the initial state $|\Phi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |3\rangle)$. The curves have the same punctuation and colours as in Fig.(4.5). Again, we do not plot QD and CC for all possible values from zero to one for the same reasons explained in the discussion of Fig.(4.6). From Fig.(4.7) it seems that, at least for long distances, there is a strong dependence with distance for both QD and CC. Namely, the larger the distance between the qubits the bigger the values of QD and CC. It is worth noting that for $d = 0.4c/\omega_p$, QD and CC assume practically the same values and decay with similar rates. This it is not the case for $d = 0.7c/\omega_p$, 36
where CC is larger than QD until $\Gamma_0 t \approx 3$ and smaller than QD after $\Gamma_0 t \approx 3$.

In conclusion, we reported both EoF and QD for a system that consists of two distant qubits mediated by a two-dimensional lattice of metal-coated dielectric nanoparticles. By changing the initial state of this system or by changing the distance of qubits from the plasmonic nanostructure we can produce quantum correlations taking significant values for a relatively large time interval so that it can be useful to quantum information and computation processes. These results with some additional cases (e.g. initial state $|\Psi\rangle$ with $q \neq 1/2$) and its corresponding figures will be published soon.

To sum up, in this chapter we gave two examples of how we can use, compute and depict entanglement of formation and quantum discord. The two systems that we considered above (semiconductor quantum dot-cavity system and two qubits mediated by the plasmonic nanostructure) are described by completely different equations. However, we can use both EoF and QD in order to describe the correlations of each system despite the different nature of them (for the quantum dot-cavity system we used only EoF but it is possible to implement QD too in order to have a better description of the quantum correlations). Of course, we can implement these measures to a wide variety of systems, complicated or not, and as a result we can quantify quantum correlations and compare them.

Figure 4.4: Plot of EoF as a function of time for the initial maximally entangled state $|\Psi\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) = |+\rangle$. All curves start from unity EoF and decay with time.
Figure 4.5: Plot of quantum discord (QD) and classical correlations (CC) as a function of time for the initial state $|\Psi\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) = |+\rangle$. As in the case of EoF, QD and CC start from the unity and decay with time. Here we plot the case only two different distances ($d = 0.4c/\omega_p$ (solid and dotted curves) and $d = 0.7c/\omega_p$ (dashed and dot-dashed curves)) while in the corresponding figure of EoF above we had four ($d = 0.4c/\omega_p$, $d = 0.5c/\omega_p$, $d = 0.6c/\omega_p$ and $d = 0.7c/\omega_p$).

Figure 4.6: Plots of EoF as in Fig. (4.4) but for the other maximally entangled state $|\Phi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |3\rangle)$. The longer the distance $d$ the greater the time that the revival of entanglement is observed (for the distance $d = 0.4c/\omega_p$ (blue curve) the revival is not observed).
Figure 4.7: The same figure as in Fig.(4.5) but for the initial state $|\Phi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |3\rangle)$.
Chapter 5

Quantum correlations for indistinguishable particles

Entanglement of formation and quantum discord are well-studied measures for distinguishable particles. However, they are not so widely used in indistinguishable particles. Especially for fermions (indistinguishable particles having half-integer spin obeying the Pauli exclusion principle), there are many difficulties in order to implement the measures used for distinguishable particles. Here we give a brief summary of how we can generalise the concurrence for non-separable particles. First, Schliemann et al. [52, 53] presented a corresponding measure of concurrence of fermionic pure states, taking into account the constraints due to the Pauli exclusion principle. After that, we generalise also the von Neumann entropy for indistinguishable particles [56] and in the last part of this chapter we implement all of these in the simplest molecule of the nature, the hydrogen molecule [6].

5.1 Generalization of concurrence and von Neumann entropy in fermions

To begin with, we report some basic properties of indistinguishable particles, which are necessary in order to develop the concepts of concurrence and von Neumann entropy in fermions. First of all, a general pure state of two fermions is given by [52, 53]
\[ |w\rangle = \sum_{i,j=1}^{n} w_{ij} f_i^{\dagger} f_j^{\dagger} |0\rangle \]  
(5.1)

where \( f_i^{\dagger} \) and \( f_j^{\dagger} \) are the single particle creation operators for two corresponding subsystems acting on the vacuum state and \( n \) is the dimensionality of the single-particle (one-electron) Hilbert space. Additionally, \( w \) is an antisymmetric complex square matrix \((n \times n)\) with \( w_{ij} = -w_{ji} \). The normalization condition for this antisymmetric matrix is

\[ \text{tr}(w^* w) = -1/2 \]  
(5.2)

According to Ref.[52], an equivalent to Schmidt decomposition can be constructed in the case of fermions. Under a unitary transformation of \( f_i = \sum_j U_{ij} f_j' \), we take new fermionic operators as well as new coefficient matrix \( w' \). Thus, the pure fermionic state of Eq.(5.1) becomes

\[ |w\rangle = \sum_{i,j=1}^{n} w_{ij}' f_i'^{\dagger} f_j'^{\dagger} |0\rangle \]  
(5.3)

with \( w_{ij}' = (U^\dagger w U)_{ij} \). This new matrix have a block diagonal form [55], containing \( 2 \times 2 \) blocks of the type

\[
\begin{bmatrix}
0 & z_k \\
-z_k & 0
\end{bmatrix}
\]  
(5.4)

Each block has eigenvalue \( z_k \) and as a result the state of Eq.(5.1) takes the diagonal form

\[ |w\rangle = 2 \sum_{k=1}^{\frac{n}{2}} z_k f_{2k-1}^{\dagger} f_{2k}^{\dagger} |0\rangle \]  
(5.5)

This is the equivalent of Schmidt decomposition, that we introduced in chapter 3, for distinguishable particles. Instead, now we have a sum of \( 2 \times 2 \) blocks (Slater determinants) instead of sum of product states. We know in the case of distinguishable particles that if the Schmidt number is one then our state is a product state. Respectively, in order to have a pure state in indistinguishable particles the Slater number, the equivalent of Schmidt number for non-separable particles, should be one too, i.e. our state of Eq.(5.5) must contain only one Slater determinant. Otherwise it is an entangled state.
Next, we give the definition of the von Neumann entropy and the concurrence for the case of indistinguishable particles.

According to Schliemann et al. \[55\], we define the dual state $|\bar{w}\rangle = \sum_{i,j=1}^{n} \bar{w}_{ij} f_i \dagger f_j \dagger |0\rangle$ with $\bar{w}_{ij} = \frac{1}{2} \sum_{i,j,k,l} \epsilon_{i,j,k,l} w_{kl}^*$ where the star denotes complex conjugation. The state $|\bar{w}\rangle$ is the analogue of the state $|\bar{\psi}^{AB}\rangle$ (see under the Eq.(3.12)) in the case of fermions. Using this as well as the definition of the state $|w\rangle$ from the Eq.(5.1) with $n = 4$ (bipartite system) the concurrence is given by

$$C(|w\rangle) = \langle \bar{w}|w\rangle = 8|w_{12}w_{34} + w_{13}w_{42} + w_{14}w_{23}|$$  \hspace{1cm} (5.6)

where $w_{ij}$ are elements of the antisymmetric matrix $w$. As in the case of distinguishable particles, concurrence takes values from zero to one. If concurrence is zero then the fermionic state has no entanglement, it has fermionic slater rank one and could be represented by only one Slater determinant.

Now, we turn our attention to the generalization of the entropy in the case of fermions. As in the case of distinguishable particles in order to find an equation for the entropy of each subsystem we have to trace out the other. As we have already mentioned, fermions are indistinguishable particles and as a result the two parties have the same entropy. Additionally, the two fermion density matrix is given by $\rho_F = |w\rangle\langle w|$. According to Paskauskas and You \[56\] the single particle density matrix is

$$\rho_{\nu\mu}^{f} = \frac{tr(\rho_F f_{\mu}^{\dagger} f_{\nu})}{tr(\rho_F \sum_{\mu} f_{\mu}^{\dagger} f_{\mu})} = 2(\omega^{\dagger} \omega)_{\mu\nu}$$  \hspace{1cm} (5.7)

The normalization condition becomes $\sum_{k=1}^{\leq n} |z_k|^2 = 1/4$. Finally, the von Neumann entropy is given by the equation

$$S_f = -tr[\rho^f \log(\rho^f)] = -1 - 4 \sum_{k=1}^{\leq n} |z_k|^2 \log(|z_k|^2)$$  \hspace{1cm} (5.8)

and as in the case of distinguishable particles the base of the logarithm is 2. This single particle entropy ranges from unit to $\log(n_E)$ with $n_E$ the largest even number not larger than $n$.

Both concurrence and von Neumann entropy are measures of the entanglement of our system. However, concurrence ranges from zero to unit, as in
the case of separable particles, but entropy takes values \(1 \leq S_f \leq 2\) in contrast to the case of distinguishable particles which ranges from zero to unity. This incompatibility in the range of values of entropy between the cases of distinguishable and indistinguishable particles may have a simple physical interpretation. In the case of non-separable particles, we cannot separate them, and as a result there is extra uncertainty since we are unaware about the particle that we perform the measurement. However, this extra uncertainty does not affect the range of values of concurrence (see also [6]).

Furthermore, we should mention here that quantum discord has not an analogue in the case of indistinguishable particles. The difficulty lies in the projective measurement that we should perform in order to compute this measure of quantum correlation as well as in the optimization procedure (see Eq.(3.26)). As a result, the generalization of quantum discord is much more complicated and time consuming compared to the corresponding computation of the concurrence.

As a final part of this chapter, we try to implement concurrence in a prototype molecular system (hydrogen molecule) in order to quantify the entanglement of the electrons.

### 5.2 Concurrence of electrons in the hydrogen molecule

In the hydrogen molecule there are two nuclei (protons) A and B, as well as two electrons occupying the region outside the protons. As a result, each electron could be in nucleus A or B and has spin \(|\uparrow\rangle (+1/2)\) or \(|\downarrow\rangle (-1/2)\). Consequently, in our case the single-particle (one-electron) Hilbert space is four-dimensional \((|A\rangle|\uparrow\rangle = |1\rangle, |A\rangle|\downarrow\rangle = |2\rangle, |B\rangle|\uparrow\rangle = |3\rangle, |B\rangle|\downarrow\rangle = |4\rangle\) and this resulting in a six-dimensional two-particle (two-electrons) Hilbert space. For this reason, from now on, we will deal with the pure state of Eq.(5.1) for \(n = 4\).

The Hamiltonian of our system is given by the equation (see for example, the classic book by P. Atkins and R. Friedman [54])

\[
H = H_1 + H_2 + \frac{e^2}{4\pi\varepsilon_0 R} + \frac{e^2}{4\pi\varepsilon_0 r_{12}}
\]

and \(H_i = -\frac{\hbar^2}{2m_e} \nabla_i - \frac{e^2}{4\pi\varepsilon_0 r_{iA}} - \frac{e^2}{4\pi\varepsilon_0 r_{iB}}, \) with \(i = 1, 2\).
Here, $R$ is the distance between the nuclei and $r_{12}$ the corresponding distance between the electrons. In addition, the two final terms represent the repulsive interaction between the nuclei and electrons respectively.

Since electrons are fermions, their wavefunction must be antisymmetric in order to obey in the Pauli exclusion principle. Using the linear combination of atomic orbitals (LCAO) method \[54\] we conclude that the wavefunctions of electrons are

$$
\Psi_1 = \psi_+ \sigma_-(1, 2) \\
\Psi_2 = \psi_- \sigma_-(1, 2)
$$

(5.10a)

(5.10b)

where $\sigma_-(1, 2) = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2)$, $\psi_+ = c_+(\phi_A + \phi_B)$ and $\psi_- = c_-(\phi_A - \phi_B)$. Here, $\phi_A$ and $\phi_B$ are the atomic orbitals of the hydrogen atom on ground state and $c_\pm$ are normalization factors which are $c_\pm = \frac{1}{\sqrt{2(1 \pm S)}}$, where $S$ is the overlap integral $S(s) = (1 + s + \frac{1}{3}s^2)e^{-s}$ with $s = R/\alpha_0$ and $\alpha_0$ the Bohr radius (see also Ref.[54]).

The wavefunction $\Psi_1$ gives the least energy for the hydrogen molecule but if we take into consideration also the wavefunction $\Psi_2$ we can find a better approximation for the minimum energy of the hydrogen molecule. Taking advantage of the well-known CI-method \[54\] we describe the molecule with the assistance of a wavefunction which is a linear combination of the two previously mentioned wavefunctions (Eqs.(5.10a) and (5.10b)). Hence, in the CI method the wavefunctions is described by the following expression

$$
\Psi = c_1 \Psi_1 + c_2 \Psi_2
$$

(5.11)

with $|c_1|^2 + |c_2|^2 = 1$. Thus, with the CI-method we find that the minimum energy of $H_2$ is approximately -0.237 Hartree($\approx$ -6.457 eV) for $R \approx 1.67\alpha_0$.

For an estimation of the coefficients $c_1$ and $c_2$ someone could see Ref.[6].

Now, we turn our attention to the quantum entanglement that the two electrons may have in the ground state. As we stated above, the wavefunction of two electrons (fermions) is given by Eq.(5.1) and the single-particle space is four-dimensional; \{1, 2, 3, 4\}. Nevertheless, in our case we have to set the elements $w_{13}$ and $w_{24}$ of antisymmetric matrix equal to zero because in the ground state the total spin of electrons must be zero. Hence, the antisymmetric coefficient matrix $w$ has the form \[6\]
\[
\begin{pmatrix}
0 & w_{12} & 0 & w_{14} \\
-w_{12} & 0 & w_{23} & 0 \\
0 & -w_{23} & 0 & w_{34} \\
-w_{14} & 0 & -w_{34} & 0
\end{pmatrix}
\] (5.12)

As a result the concurrence from Eq.(5.6) becomes

\[C(|w\rangle) = 8|w_{12}w_{34} + w_{14}w_{23}|\] (5.13)

Next, by writing again the wavefunction for the ground state of \(H_2\) from Eq.(5.11) and using the expressions of the coefficients \(c_1\) and \(c_2\) (see Ref.[6]) we can find the expressions of \(w_{12}, w_{34}, w_{14}\) and \(w_{23}\). Substituting these expressions in Eq.(5.13) we take

\[C(|w\rangle) = 2|c_1c_2|\] (5.14)

Figure (5.1) shows how concurrence varies for different values of \(c_1\). As we can see concurrence is zero for \(c_1 = 0\) or \(c_1 = 1\) (we have the state \(\Psi_2\) or \(\Psi_1\) respectively from Eq.(5.11)) but becomes maximum for \(c_1 = \frac{1}{\sqrt{2}}\) (Eq.(5.11) becomes a maximal entangled state).

Finally, Fig.(5.2) shows concurrence and energy as a function of the internuclear distance. It is obvious from Fig.(5.2) that concurrence takes small values for small internuclear distances and becomes bigger as the distance \(R\) is rising. Furthermore, this value of the coefficient \(c_1\) corresponds to internuclear distances \(R >\) larger than \(8\alpha_0\) (i.e. rather large distances). However, the internuclear distance for which the molecule has its minimum energy, i.e. has its most stable form, is \(R \approx 1.67\alpha_0\). For this distance concurrence takes the value 0.2378.

The above analysis demonstrates that quantum entanglement is uncorrelated concerning the construction of a chemical bond. More specifically, the fact that concurrence does not become maximum at the most stable state of the molecule \(H_2\) probably indicates that it is not the proper measure of the quantum correlations. As we mentioned in chapter 3 concurrence is only a measure of entanglement but a more general measure for quantum correlations is the quantum discord. However, the generalization of quantum discord in indistinguishable particles is rather complicated but it could be one of the future plans.
Figure 5.1: Plot of concurrence as a function of the coefficient $c_1$ for the ground state of $H_2$ in the CI method.

Figure 5.2: Concurrence (dashed curve) and energy calculated by CI-method (solid curve) as a function of $s = R/\alpha_0$. 
Chapter 6
Conclusions

To sum up, we began from the EPR paradox, one of the most famous paradoxes in physics, in order to demonstrate one of the most interesting aspects of quantum mechanics, the entanglement. After that, we introduced the concept of measurement in quantum mechanics and we concluded that it is completely different in comparison with the meaning of measurement in classical physics. Additionally, we paid special attention to projective measurement, which is one of the simplest and most well-studied types of measurements in quantum mechanics.

Afterwards, we gave some supplementary definitions such as the definition of the Schmidt decomposition, von Neumann entropy and mutual information, in order to establish the entanglement of formation or EoF. This is a measure only of quantum entanglement as it does not take into consideration all possible quantum correlations of the composite system. However, by using the two different definitions of mutual information as well as the concept of projective measurement, we can introduce a more general measure which encloses all possible quantum correlations, the quantum discord (or QD). Although quantum discord is quite general measure, it is difficult to be computed in comparison with EoF and for this reason we choose to use EoF more often than QD in complicated bipartite systems.

Furthermore, EoF and quantum discord have numerous applications and as a result we can quantify entanglement and generally the quantum correlations of the bipartite system of our interest. One bipartite system that we choose to analyse was a quantum dot embedded in a microcavity, radiated by two laser fields of left- and right- polarization. We investigated the EoF for some values of of the important parameters of the quantum dot system, such
as the biexciton binding energy, and we saw that there is a strong dependence of EoF on them.

We also gave an outline of the generation of quantum correlations by using two distant qubits mediated by a two-dimensional lattice of metal-coated dielectric nanoparticles. We reported both EoF and QD for two different initial states. Thus, we could compare EoF or QD for these two different initial states or even EoF and QD for the same initial state. As we stated above, there more results in the paper exist which will be published.

Finally, we generalized Schmidt decomposition in the case of indistinguishable particles and this has enabled us to give the definition of concurrence for this type of particles. Moreover, we generalized von Neumann entropy and we gave a physical interpretation of the range of values that it takes in the case of non-separable particles. After that, we focused on one of the simplest composite system of the nature, the hydrogen molecule. Using the standard approximations of the linear combination of atomic orbitals and the configuration interaction methods we described the electronic wavefunction of $H_2$. This fact enabled us to theoretically investigate the quantum correlations in terms of concurrence of indistinguishable electrons and we concluded in a rather simple analytic expression for the concurrence. The most interesting outcome of this analysis was that concurrence does not really show any relation to the construction of the chemical bond. Also, someone could apply the same methodology in much more complicated molecular systems in order to describe the quantum correlations of electrons in them.
Bibliography


